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APROXIMACIONES DE BORN-OPPENHEIMER Y HARTREE-FOCK APLICADAS A CAMPOS CUÁNTICOS RELATIVISTAS. VOLUMEN II

BORN-OPPENHEIMER AND HARTREE-FOCK APPROXIMATIONS APPLIED TO RELATIVISTIC QUANTUM FIELDS. VOLUME II

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Aproximaciones De Born-Oppenheimer Y Hartree-Fock Aplicadas A Campos Cuánticos Relativistas. Volumen II

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RESUMEN

En trabajos anteriores, este autor ha procurado formalizar matemáticamente y proponer las leyes relativas a la Teoría Cuántica de Campos Relativistas o Curvos, cuya finalidad, es reconciliar la relatividad general y la mecánica cuántica. Para abonar aún más a la consecución del objetivo antes referido, es indispensable acudir a la química cuántica, y muy concretamente a las métricas de Born-Oppenheimer y Hartree-Fock, en la medida en que, la primera desarrolla un escenario relativista a escala atómica y molecular en tanto que la segunda explica perfectamente las trayectorias orbitales moleculares, las cuales, en términos generales, son conceptos de muchísima utilidad para la TCCR toda vez que coadyuvan, por extrapolación, a configurar desde la química cuántica, el modelo de deformación del espacio – tiempo cuántico, por acción gravitacional de las partículas subatómicas estrella u oscuras, o por interacción de éstas, con los campos supergravitónico o gravitónico, según sea el caso, esto es, por interacción con el gravitón o el gravitino o supergravitón, según corresponda.

Palabras Clave: química cuántica, aproximación de Born-Oppenheimer, aproximación de Hartree-Fock, teoría cuántica de campos relativistas o curvos

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Born-Oppenheimer and Hartree-Fock Approximations Applied to Relativistic Quantum Fields. Volume II

ABSTRACT

In previous works, this author has tried to mathematically formalize and propose the laws related to the Quantum Theory of Relativistic or Curved Fields, whose purpose is to reconcile general relativity and quantum mechanics. To further contribute to the achievement of the aforementioned objective, it is essential to resort to quantum chemistry, and very specifically to the Born-Oppenheimer and Hartree-Fock metrics, insofar as the former develops a relativistic scenario at the atomic and molecular scale while the latter perfectly explains the molecular orbital trajectories, which, in general terms, they are very useful concepts for TCCR since they contribute, by extrapolation, to configure from quantum chemistry, the model of deformation of quantum space-time, by gravitational action of star or dark subatomic particles, or by interaction of these, with supergravitonic or gravitonic fields, as the case may be. that is, by interaction with the graviton or the gravitino or supergraviton, as appropriate.

Keywords: quantum chemistry, Born-Oppenheimer approximation, Hartree-Fock approximation, quantum theory of relativistic or curved fields

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INTRODUCCIÓN

En sentido estricto, la aproximación de Born-Oppenheimer, propone un factor que viene a ser determinante para la TCCR, y es, la incidencia del núcleo respecto del electrón, esto es, que el primero, al ser más denso que el segundo, es decir, que al tener mayor masa, repercute en el movimiento y por ende, en la velocidad del electrón, razón por la cual, el núcleo se acopla al electrón y viceversa, comportándose el núcleo, de forma estática en tanto que el electrón, actúa como una nube de carga, leyendo la posición estática del núcleo en el campo. Es en este contexto, a propósito del diferencial de masas, que la TCCR cobra mayor rigor matemático en razón a la interacción de la partícula estrella u oscura con las partículas orbitales o repercutidas.

Ahora bien, la aproximación de Hartree-Fock, también resulta vinculante a la TCCR, en la medida en que, en química cuántica, determina los orbitales moleculares, premisa superior que a escala subatómica, aplica, a propósito de la existencia de campos cuánticos curvos o deformados por la gravedad, en los que, los orbitales de las partículas subatómicas se ven metamorfoseados, para lo cual, extrapolaremos las ecuaciones multideterminantales de Slater.

Entiéndase que las partículas oscuras o estrella, muestran estados fundamentales pues accionan gravedad, en tanto que, las partículas orbitales o repercutidas, muestran estados excitados por influjo gravitacional, a propósito de las bases formales de la TCCR propuestas por este autor en trabajos previos. La gravedad y supergravedad a escala cuántica son en sí, interacciones normales o extremas, según sea el caso, entre uno y varios cuerpos subatómicos a razón de sus centros de masa – energía.

RESULTADOS Y DISCUSIÓN

Aproximación de Born-Oppenheimer para campos cuánticos relativistas o curvos. Modelo Matemático.

$$\hat{H} = \sum_{I=1}^{N} \frac{\hat{\mathbf{P}}_I^2}{2M_I} + \hat{V}(\mathbf{R}),$$

$$Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \lim_{n\to\infty} \frac{1}{(2\pi\hbar)^f} \int d^f\mathbf{R} \int d^f\mathbf{P} e^{-\beta_n H_n(\mathbf{R},\mathbf{P})}$$

$$H_n(\mathbf{R},\mathbf{P}) = \sum_{I=1}^{N}\sum_{j=1}^{n}\left[\frac{P_{I,j}^2}{2M_I}+\frac{1}{2}M_I\omega_n^2\left(R_{I,j}-R_{I,j-1}\right)^2\right] + \sum_{j=1}^{n} V\left(R_{1,j},\dots,R_{N,j}\right)$$

$$i\hbar\dot{c}_\alpha(t) = \left[\frac{1}{n}\sum_{j=1}^{n} V_\alpha\left(\mathbf{R}_j\right)\right]c_\alpha - i\hbar\sum_\beta\left[\frac{1}{n}\sum_{j=1}^{n}\dot{\mathbf{R}}_j\cdot\mathbf{d}_{\alpha\beta}\left(\mathbf{R}_j\right)\right]c_\beta(t)$$

$$\mathbf{d}_{\alpha\beta}\left(\mathbf{R}_j\right) = \langle\alpha;\mathbf{R}_j|\nabla_{\mathbf{R}_j}|\beta;\mathbf{R}_j\rangle$$

$$\overline{\mathbf{R}} = \frac{1}{n}\sum_{j=1}^{n}\mathbf{R}_j \; \overline{\mathbf{P}} = \frac{1}{n}\sum_{j=1}^{n}\mathbf{P}_j$$

$$i\hbar\dot{c}_\alpha(t) = V_\alpha(\overline{\mathbf{R}})c_\alpha(t) - i\hbar\sum_\beta\dot{\overline{\mathbf{R}}}\cdot\mathbf{d}_{\alpha\beta}(\overline{\mathbf{R}})c_\beta(t)$$

$$\mathbf{d}_{\alpha\beta}(\overline{\mathbf{R}}) = \langle\alpha;\overline{\mathbf{R}}|\nabla_{\overline{\mathbf{R}}}|\beta;\overline{\mathbf{R}}\rangle$$

$$\hat{T}_{\mathrm{n}} = -\sum_I\frac{\hbar^2}{2M_I}\nabla_{\mathbf{R}_I}^2$$

$$\tilde{V}_\alpha(\mathbf{R}) = V_\alpha(\mathbf{R}) + V_{\mathrm{DBOC}}^{(\alpha)}(\mathbf{R})$$

$$V_{\mathrm{DBOC}}^{(\alpha)}(\mathbf{R}) = \sum_{I=1}^{N}\frac{\hbar^2}{2M_I}\sum_{j=1}^{n}\sum_{\beta\neq\alpha}\left|\mathbf{d}_{I,j}^{(\alpha\beta)}\left(\mathbf{R}_j\right)\right|^2.$$

$$\mathbf{F}_{I,j} = -\nabla\tilde{V}_\alpha\left(\mathbf{R}_j\right) = -\nabla V_\alpha\left(\mathbf{R}_j\right) - \nabla V_{\mathrm{DBOC}}^{(\alpha)}\left(\mathbf{R}_j\right) = \mathbf{F}_{I,j}^{(0)} + \Delta\mathbf{F}_{I,j},$$

$$\Delta\mathbf{F}_{I,j} = \sum_{\alpha\neq\beta}\frac{1}{M_I}\mathbf{d}_{I,j}^{(\alpha\beta)}\left(\mathbf{R}_j\right)\cdot\nabla\mathbf{d}_{I,j}^{(\alpha\beta)}\left(\mathbf{R}_j\right).$$

$$\mathbf{d}_{I,j}^{(\alpha\beta)} = \frac{\langle\psi_{j,\alpha}|\nabla_{R_{I,j}}H\left(\mathbf{R}_j\right)|\psi_{j,\beta}\rangle}{V_\beta\left(\mathbf{R}_j\right)-V_\alpha\left(\mathbf{R}_j\right)}.$$

$$\nabla\mathbf{d}_{I,j}^{(\alpha\beta)} = \frac{\mathbf{d}_{I,j}^{(\alpha\beta)}\left(\mathbf{R}_j+\delta\right)-\mathbf{d}_{I,j}^{(\alpha\beta)}\left(\mathbf{R}_j-\delta\right)}{2\delta}.$$

$$\rho(\mathbf{R},\mathbf{P}) = \prod_{I=1}^{N}\prod_{j=1}^{n}\exp\left[-\beta_n\left(\frac{P_{I,j}^2}{2M_I}+\frac{1}{2}M_I\omega_I^2R_{I,j}^2\right)\right],$$

$$\rho_{\mathrm{RP}}(\tilde{\mathbf{R}},\tilde{\mathbf{P}}) = \prod_{I=1}^{N}\prod_{k=1}^{n}\exp\left[-\beta_n\left(\frac{\tilde{P}_{I,k}^2}{2M_I}+\frac{1}{2}M_I\omega_{I,k}^2\tilde{R}_{I,k}^2\right)\right],$$

$$P_\alpha = \left\langle \sum_i \left| U_{\alpha i} \right|^2 \delta_{i,\lambda} + \sum_{i<j} 2\mathrm{Re}\left[U_{\alpha i}, \rho_{ij}, U_{\alpha j}^* \right] \right\rangle,$$

$$\mathrm{d}s^2 = -N^2(T)\mathrm{d}T^2 + \underbrace{a^2(T)\delta_{ij}}_{h_{ij}(T)} \mathrm{d}x^i\, \mathrm{d}x^j$$

$$\mathcal{S}_{\mathrm{EH}} = \frac{1}{2\kappa} \int \sqrt{-g} R\, \mathrm{d}^4 x$$

$$\mathcal{S}_{\mathrm{fluid}} = \int \mathrm{d}^4 x \sqrt{-g} P(\mu)$$

$$\mu^2 = -g^{\alpha\beta} \partial_\alpha \phi \partial_\beta \phi$$

$$\mu = (\rho + P)/n$$

$$P = K\mu^{1+1/w}$$

$$\mathrm{d}P = \mu \mathrm{d}n$$

$$\mathcal{H}_{\mathrm{fluid}} = \gamma \frac{N}{(\sqrt{h})^w} p_\phi^{1+w}$$

$$\sqrt{h} = a^3, p_\phi = \left(1 + \frac{1}{w}\right) \sqrt{h} K N^{-1/w} \dot{\phi}^{1/w}$$

$$\gamma = \frac{w^w}{K^w (1+w)^{1+w}}$$

$$N = -a^{3w}$$

$$^1 N/(\sqrt{h})^w = -1$$

$$(\phi, p_\phi) \to (\tau, p_\tau)$$

$$p_\tau = -\gamma p_\phi^{1+w} \text{ and } \tau = -\frac{\phi}{\gamma(1+w) p_\phi^w}$$

$$\mathcal{H}_{\mathrm{grav}} = -\frac{\kappa N}{12 \mathcal{V}_0 a} p_a^2$$

$$p_a = -6\mathcal{V}_0 a \dot{a}/(N\kappa)$$

$$\dot{a} \equiv \mathrm{d}a/\mathrm{d}\tau$$

$$\mathcal{V}_0 = \int \sqrt{h}\, \mathrm{d}^3 x$$

$$\mathcal{H}_{\mathrm{T}} = \mathcal{H}_{\mathrm{grav}} + \mathcal{H}_{\mathrm{fluid}} = \frac{\kappa a^{3w-1}}{12\mathcal{V}_0} p_a^2 + p_\tau$$

$$q = \sqrt{\frac{12\mathcal{V}_0}{\kappa}} \frac{2a^{\frac{3}{2}(1-w)}}{3(1-w)}$$

$$p = \sqrt{\frac{\kappa}{12\mathcal{V}_0}} a^{\frac{1}{2}(3w-1)} p_a \propto a^{\frac{3}{2}(1+w)} H$$

$$H \equiv \dot{a}/(Na)$$

$$\mathcal{H}_{\text{grav}} = p^2.$$

$$|q,p\rangle_{\psi_0} = \underbrace{\exp\left(\mathrm{i}\frac{p}{2q}\hat{X}^2\right) e^{-\frac{1}{2}\mathrm{i}\ln q(\hat{X}\hat{P}+\hat{P}\hat{X})}}_{\hat{U}(q,p)} |\psi_0\rangle$$

$$\hat{A}_f(\psi_0) = \mathcal{N}_{\psi_0} \int_{\mathbb{R}_{\times\mathbb{R}^+}} |q,p\rangle_{\psi_0} f(q,p)_{\psi_0}\langle q,p| \mathrm{d}q\, \mathrm{d}p$$

$$\hat{A}_1(\psi_0) = \mathbb{1}$$

$$|\psi_0\rangle \hat{A}_q(\psi_0) = \hat{X} \text{ (with } \hat{X}\psi = x\psi \text{) and } \hat{A}_p(\psi_0) = \hat{P} \text{ (with } p \to \hat{P}\psi = -\mathrm{i}\partial_x\psi \text{)}$$

$$\left[\hat{A}_q(\psi_0), \hat{A}_p(\psi_0)\right] = [\hat{X}, \hat{P}] = |\psi_0\rangle$$

$$\hat{\mathcal{H}}_{\text{grav}} = \hat{A}_{p^2}(\psi_0) = \hat{\mathcal{H}}_\nu$$

$$\hat{\mathcal{H}}_{\text{grav}} = \hat{A}_{p^2} = \hat{\mathcal{H}}_\nu \equiv \hat{P}^2 + \left(\nu^2 - \frac{1}{4}\right)\hat{X}^{-2},$$

$$\mathcal{H}_{\text{SC}} = \mathcal{H}_{\text{SC}}(q,p) = \langle q,p|\hat{\mathcal{H}}_{\text{grav}}|q,p\rangle \propto p^2 + \frac{\xi_\nu^2}{q^2}$$

$$q_\tau = q_{\text{B}}\sqrt{1 + \omega^2(\tau - \tau_{\text{B}})^2}$$

$$p_\tau = \frac{1}{2}\dot{q}(\tau) = \frac{q_{\text{B}}\omega^2(\tau - \tau_{\text{B}})}{2\sqrt{1 + \omega^2(\tau - \tau_{\text{B}})^2}}$$

$$E = p_\tau^2 + \xi_\nu^2/q_\tau^2$$

$$q_{\text{B}} = \xi_\nu/\sqrt{E}$$

$$\omega = 2E/\xi_\nu$$

$$(p_\tau \to \hat{p}_\tau\psi = -\mathrm{i}\partial_\tau\psi)\mathcal{H}_{\text{T}} = \mathcal{H}_{\text{fluid}} + \mathcal{H}_{\text{grav}} \simeq 0$$

$$\mathrm{i}\partial_\tau\psi(x,\tau) = \underbrace{\left(-\partial_x^2 + \frac{\nu^2 - \frac{1}{4}}{x^2}\right)}_{\hat{\mathcal{H}}_\nu}\psi(x,\tau)$$

$$\psi(x,\tau) = e^{-\mathrm{i}\phi_\tau}\langle x \mid q_\tau, p_\tau\rangle_n$$

$$e^{-\mathrm{i}\phi(\tau)} = \left(\frac{\xi_\nu - \mathrm{i}p_\tau q_\tau}{\xi_\nu + \mathrm{i}p_\tau q_\tau}\right)^{\beta_n/(4\xi_\nu)}$$

$$|q_\tau, p_\tau\rangle_n = \exp\left(\mathrm{i}\frac{p_\tau}{2q_\tau}\hat{x}^2\right) e^{-\frac{1}{2}\mathrm{i}\ln\, q_\tau(\hat{x}\hat{p}+\hat{p}\hat{x})}|\Phi_n\rangle$$

$$|\Phi_n\rangle, n \in \mathbb{N}$$

$$\hat{\mathcal{H}}_{\mathrm{aux}} = \hat{\mathcal{H}}_\nu + \xi_\nu^2 \hat{X}^2$$

$$\langle x \mid q_\tau, p_\tau\rangle_n = \frac{1}{\sqrt{q_\tau}} \exp\left(\mathrm{i}\frac{p_\tau}{2q_\tau}x^2\right) \Phi_n\left(\frac{x}{q_\tau}\right).$$

$$\beta_n = 2\xi_\nu(2n + \nu + 1)$$

$$\Phi_n(x) = \langle x \mid \Phi_n\rangle$$

$$\Phi_n(x) = \sqrt{\frac{2n!}{\Gamma(n+\nu+1)}} \xi^{\frac{\nu+1}{2}} x^{\nu+\frac{1}{2}} L_n^{(\nu)}(\xi_\nu x^2) e^{-\frac{1}{2}\xi_\nu x^2}$$

$$_n\langle q_\tau, p_\tau|\hat{X}|q_\tau, p_\tau\rangle_n = q_\tau$$

$$\xi_\nu \to \xi_{\nu,n} = \left\{\frac{n!}{\Gamma(n+\nu+1)} \int_0^\infty y^{\nu+\frac{1}{2}} \left[L_n^{(\nu)}(y)\right]^2 e^{-y}\, \mathrm{d}y\right\}^2$$

$$_n\langle q_\tau, p_\tau|\hat{P}|q_\tau, p_\tau\rangle_n = p_\tau$$

$$\xi_{\nu,n} = \frac{\Gamma^2\left(\nu + \frac{3}{2}\right)}{\Gamma^2(\nu+n+1)} (\nu^{2n} + \cdots)$$

$$\xi_\nu = \Gamma^2\left(\nu + \frac{3}{2}\right)/\Gamma^2(\nu+1)$$

$$|q_\tau, p_\tau\rangle_n \equiv |E, \tau_{\mathrm{B}}\rangle_n$$

$$|\Psi_{\mathrm{U}}\rangle = |\Psi_{\mathrm{B}}\rangle \otimes |\Psi_{\mathrm{P}}\rangle$$

$$|\Psi_{\mathrm{B}}\rangle = \mathcal{N}(\tau) \sum_{n\in\mathbb{N}} \int \mathrm{d}E \int \mathrm{d}\tau_{\mathrm{B}} W_n(E, \tau_{\mathrm{B}}) |E, \tau_{\mathrm{B}}\rangle_n$$

$$W_n(E, \tau_{\mathrm{B}}) = \delta_{n,n_0} \delta(E - E_0) \delta(\tau_{\mathrm{B}} - \tau_0)$$

$$\mathcal{N}(\tau) W_n(E, \tau_{\mathrm{B}}) \to \mathcal{N}_N(\tau) \sum_{a=1}^{N} \mathfrak{w}_a \delta_{n,n_a} \delta(E - E_a) \delta\left(\tau_{\mathrm{B}} - \tau_{\mathrm{B},a}\right)$$

$$\mathcal{N}_N(\tau) = \left(\sum_{a,b=1}^{N} \mathfrak{w}_a^\star \mathfrak{w}_{bn_a} \left\langle E_a, \tau_{\mathrm{B},a} \mid E_b, \tau_{\mathrm{B},b}\right\rangle_{n_b}\right)^{-1/2}$$

$$\langle \Psi_{\mathrm{B}} \mid \Psi_{\mathrm{B}}\rangle = 1$$

$$_{na}\left\langle E_a, \tau_{\mathrm{B},a} \mid E_a, \tau_{\mathrm{B},a}\right\rangle_{n_a} = 1$$

$$_{n_a}\left\langle E_a, \tau_{\mathrm{B},a} \mid E_b, \tau_{\mathrm{B},b}\right\rangle_{n_b} \neq 0$$

$$a \equiv \{n_a, E_a, \tau_{B,a}\} \left| E_a, \tau_{B,a} \right\rangle_{n_a} \to |a\rangle$$

$$\psi_a(x) = \langle x \mid a \rangle = \langle x \mid E_a, \tau_{B,a} \rangle_{n_a}$$

$$\psi_a(x) = \sqrt{\frac{2n_a!}{\Gamma(\nu+n_a+1)}} \left(\frac{\xi_{\nu,n_a} - \mathrm{i}q_a p_a}{\xi_{\nu,n_a} + \mathrm{i}q_a p_a}\right)^{\frac{1}{2}(2n_a+\nu+1)} \xi_{\nu,n_a}^{\frac{\nu+1}{2}} \frac{x^{\nu+1/2}}{q_a^{\nu+1}} L_{n_a}^{\nu}\left(\xi_{\nu,n_a}\frac{x^2}{q_a^2}\right) \exp\left(-\frac{1}{2}(\xi_{\nu,n_a} - \mathrm{i}q_a p_a)\frac{x^2}{q_a^2}\right)$$

$$q_B \to q_{B,a} = \xi_{\nu,n_a}/\sqrt{E_a}, \omega \to \omega_a = 2E_a/\xi_{\nu,n_a}$$

$$\langle a \mid b \rangle = {}_{n_a}\langle E_a, \tau_{B,a} \mid E_b, \tau_{B,b} \rangle_{n_b} = \int_0^\infty {}_{n_a}\langle E_a, \tau_{B,a} \mid x \rangle \langle x \mid E_b, \tau_{B,b} \rangle_{n_b}\, \mathrm{d}x = \int_0^\infty \psi_a^\star(x)\psi_b(x)\mathrm{d}x$$

$$\langle a \mid b \rangle = 2\sqrt{\frac{n_a!}{\Gamma(\nu+n_a+1)}\frac{n_b!}{\Gamma(\nu+n_b+1)}} \left(\frac{\xi_{\nu,n_a} + \mathrm{i}q_a p_a}{\xi_{\nu,n_a} - \mathrm{i}q_a p_a}\right)^{\frac{1}{2}(2n_a+\nu+1)} \left(\frac{\xi_{\nu,n_b} - \mathrm{i}q_b p_b}{\xi_{\nu,n_b} + \mathrm{i}q_b p_b}\right)^{\frac{1}{2}(2n_b+\nu+1)} \left(\frac{\sqrt{\xi_{\nu,n_a}\xi_{\nu,n_b}}}{q_a q_b}\right)^{\nu+1} I_{ab}$$

$$I_{ab} \equiv \int_0^\infty L_{n_a}^{\nu}\left(\xi_{\nu,n_a}\frac{x^2}{q_a^2}\right) L_{n_b}^{\nu}\left(\xi_{\nu,n_b}\frac{x^2}{q_b^2}\right) e^{-z_{ab}x^2} x^{2\nu+1}\, \mathrm{d}x$$

$$z_{ab} \equiv \frac{1}{2}\left[\frac{\xi_{\nu,n_a}}{q_a^2} + \frac{\xi_{\nu,n_b}}{q_b^2} + \mathrm{i}\left(\frac{p_a}{q_a} - \frac{p_b}{q_b}\right)\right]$$

$$I_{ab} = \frac{1}{2}\sum_{\ell=0}^{n_a}\sum_{m=0}^{n_b} \frac{(\nu+\ell+1)_{n_a-\ell}}{(n_a-\ell)!\,\ell!} \frac{(\nu+m+1)_{n_b-m}}{(n_b-m)!\,m!} \times \left(\frac{\xi_{\nu,n_a}}{q_a^2}\right)^{\ell} \left(\frac{\xi_{\nu,n_b}}{q_b^2}\right)^{m} \frac{\Gamma(\nu+\ell+m+1)}{z_{ab}^{\nu+\ell+m+1}}$$

$$(\alpha)_n = \alpha(\alpha+1)\cdots(\alpha+n-1)$$

$$\langle a \mid b \rangle = 2^{1+\nu}\left[\left(\frac{q_a}{q_b} + \frac{q_b}{q_a}\right)^2 + \frac{\mathrm{i}}{\xi_\nu}(p_a q_b - p_b q_a)\right]^{-(1+\nu)} \times \left(\frac{\xi_\nu + \mathrm{i}q_a p_a}{\xi_\nu - \mathrm{i}q_a p_a}\right)^{\frac{1}{2}(1+\nu)} \left(\frac{\xi_\nu - \mathrm{i}q_b p_b}{\xi_\nu + \mathrm{i}q_b p_b}\right)^{\frac{1}{2}(1+\nu)}$$

$$\xi_\nu \equiv \xi_{\nu,0}$$

$$\xi_\nu = \Gamma^2\left(\nu + \frac{3}{2}\right)/\Gamma^2(\nu+1)$$

$$\langle a \mid b \rangle = \left(\frac{2\sqrt{r_{ab}}}{1 + r_{ab} + \mathrm{i}r_{ab}\omega_a\Delta\tau}\right)^{1+\nu}$$

$$r_{ab} \equiv E_a/E_b, \Delta\tau = \tau_{B,a} - \tau_{B,b}$$

$$\Re\mathrm{e}\langle a \mid b \rangle = 4r_{ab}\frac{(1+r_{ab})^2 - r_{ab}^2\omega_a^2\Delta\tau^2}{[(1+r_{ab})^2 + r_{ab}^2\omega_a^2\Delta\tau^2]^2},$$

$$\Im\mathrm{m}\langle a \mid b \rangle = -\frac{8r_{ab}^2(1+r_{ab})\omega_a\Delta\tau}{[(1+r_{ab})^2 + r_{ab}^2\omega_a^2\Delta\tau^2]^2},$$

$$|\Psi_{\mathrm{B}}\rangle = \mathcal{N}_2\big(|0\rangle + \rho e^{-\mathrm{i}\delta}|1\rangle\big),$$

$$\mathcal{N}_2 = [1 + \rho^2 + 2\rho(\cos\ \delta\Re\mathrm{e}\langle 0 \mid 1\rangle + \sin\ \delta\Im\mathrm{m}\langle 0 \mid 1\rangle)]^{-1/2}$$

$$|\Psi_{\mathrm{B}}(x,\tau)|^2$$

$$\frac{\partial}{\partial\tau}|\Psi_{\mathrm{B}}(x,\tau)|^2 + \frac{\partial}{\partial x}\left[2|\Psi_{\mathrm{B}}(x,\tau)|^2\frac{\partial S(x,\tau)}{\partial x}\right] = 0$$

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = 2\partial_x S = \frac{\Psi_{\mathrm{B}}^{\star}\partial_x\Psi_{\mathrm{B}} - \Psi_{\mathrm{B}}\partial\Psi_{\mathrm{B}}^{\star}}{\mathrm{i}|\Psi_{\mathrm{B}}|^2} = -\mathrm{i}\partial_x \ln\frac{\Psi_{\mathrm{B}}}{\Psi_{\mathrm{B}}^{\star}},$$

$$\hat{q}\Psi(x) = x\Psi(x)$$

$$x(\tau) = \sqrt{\frac{12\mathcal{V}_0}{\kappa}}\frac{2a^{\frac{3}{2}(1-w)}}{3(1-w)} \equiv \lambda a^{\frac{3}{2}(1-w)}$$

$$\ddot{x} = -2\partial_x[V(x) + Q(x,t)],$$

$$\hat{H} = -\partial_x^2 + V(x)$$

$$Q(x,\tau) \equiv -\frac{1}{|\Psi_{\mathrm{B}}|}\frac{\partial^2|\Psi_{\mathrm{B}}|}{\partial x^2}$$

$$H_{cl} = p^2 + V(q)$$

$$S_a = -\phi_a + p_a x^2/(2q_a) = -\phi_a + \frac{\omega_a^2 x^2(\tau - \tau_{\mathrm{B},a})}{2\left[1 + \omega_a^2(\tau - \tau_{\mathrm{B},a})^2\right]}$$

$$x(\tau) = x(0)\sqrt{1 + \omega_a^2(\tau - \tau_{\mathrm{B},a})^2} \equiv x_0\frac{q_a(\tau)}{q_{\mathrm{B}}}$$

$$Q(x,\tau) = \frac{2\xi_\nu(\nu+1)}{q^2} - \frac{\xi_\nu^2 x^2}{q^4} - \frac{\nu^2 - \frac{1}{4}}{x^2}$$

$$\ddot{x} = -2\frac{\partial}{\partial x}\left[\frac{\nu^2 - \frac{1}{4}}{x^2} + Q(x,\tau)\right] = \frac{4\xi_\nu^2}{q(\tau)^4}x$$

$$H = a^{-1}\,\mathrm{d}a/\mathrm{d}t = \dot{a}/(Na)$$

$$\mathrm{d}\tau = \mathrm{d}tH = \frac{2}{3(1-w)}\frac{\dot{x}}{Nx}$$

$$H^2 = \frac{\kappa}{3}\rho = \frac{4}{9(1-w)^2}\frac{\dot{x}^2}{N^2x^2} \propto \frac{(\partial_x S)^2}{a^{3(1+w)}} \propto \frac{(\partial_a S)^2}{a^4}$$

$$S(a) \sim a^{\frac{3}{2}(1-w)}$$

$$\dot{H} = -\frac{1}{2}\kappa N(\rho + P) = -\frac{3}{2}(1+w)NH^2$$

$$\dot{H} = \frac{2}{3(1-w)}\frac{\ddot{x}}{Nx} - \frac{3}{2}(1+w)NH^2$$

$$R(\tau) = 4\left(\frac{x}{\lambda}\right)^{-\frac{4}{1-w}}\left[\frac{\ddot{x}}{(1-w)x} + \frac{(1-3w)\dot{x}^2}{3(w-1)^2x^2}\right]$$

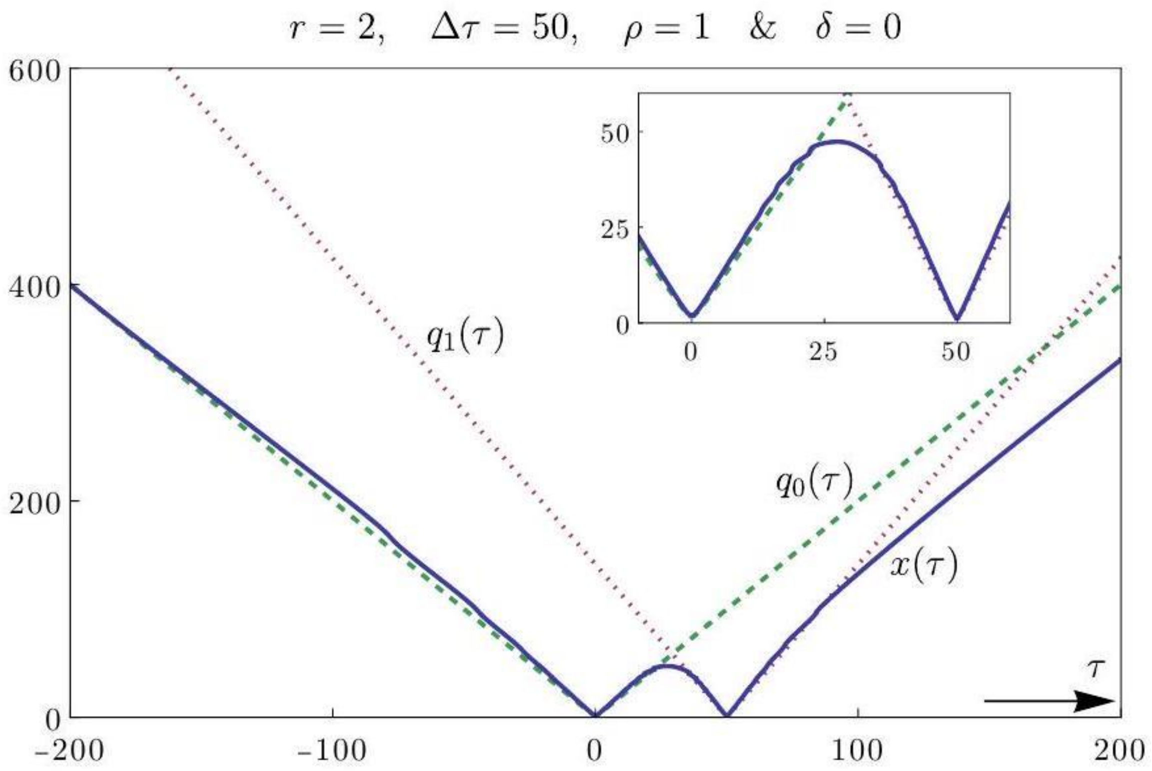
$$R_{\mathrm{B}} = \frac{4\omega^2}{1-w}\left(\frac{x_0}{\lambda}\right)^{-\frac{4}{1-w}} \propto \omega^2(1-w)^{-\frac{3w+1}{(1-w)}}x_0^{-\frac{4w}{1-w}}$$

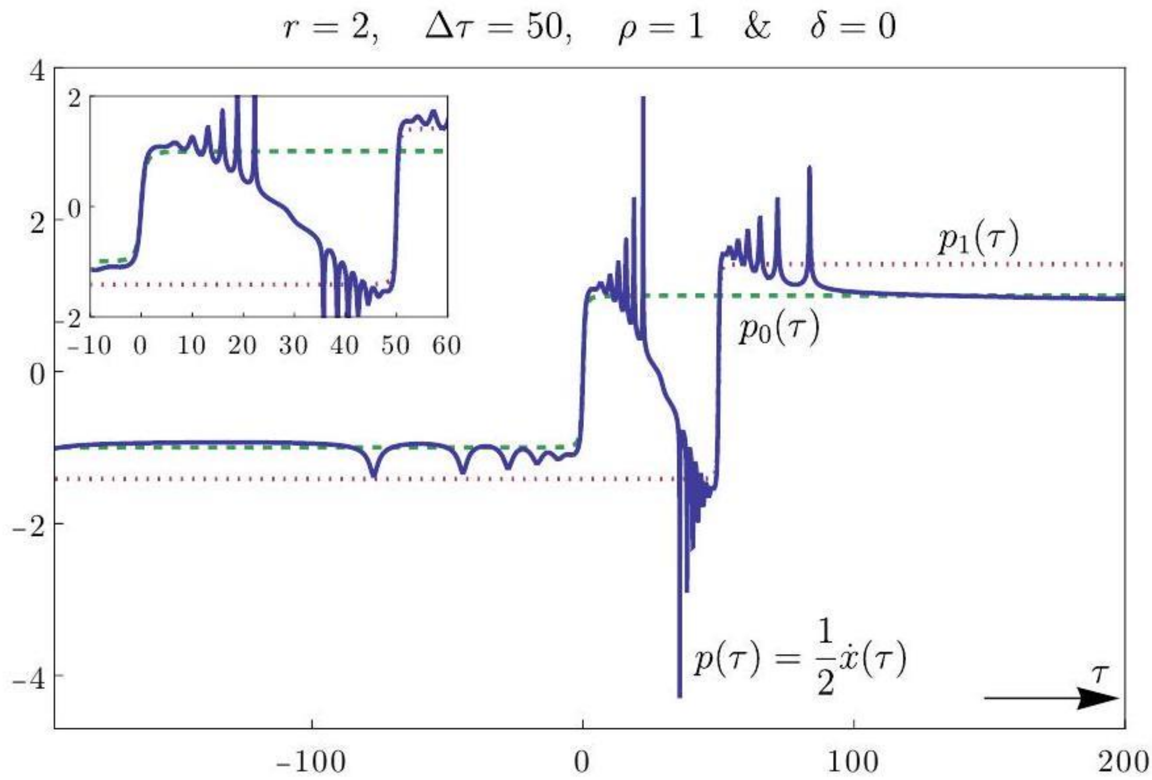
$$\tilde{x} = \sqrt{E_0}x, \tilde{q} = \sqrt{E_0}q, \text{ and } \tilde{\tau} = E_0\tau,$$

$$\tilde{\Psi}_{\mathrm{B}}(\tilde{x}) = E_0^{-1/4}\Psi_{\mathrm{B}}(x)$$

$$\int \left|\tilde{\Psi}_{\mathrm{B}}(\tilde{x})\right|^2 \mathrm{d}\tilde{x} = \int |\Psi_{\mathrm{B}}(x)|^2 \,\mathrm{d}x = 1$$

$$\frac{\partial S}{\partial \tau} + \left(\frac{\partial S}{\partial x}\right)^2 + Q + \frac{\nu^2 - \frac{1}{4}}{x^2} = 0$$





$$|\psi_a(x,\tau)| \propto \exp\left(-\frac{\xi x^2}{2q_a^2}\right)$$

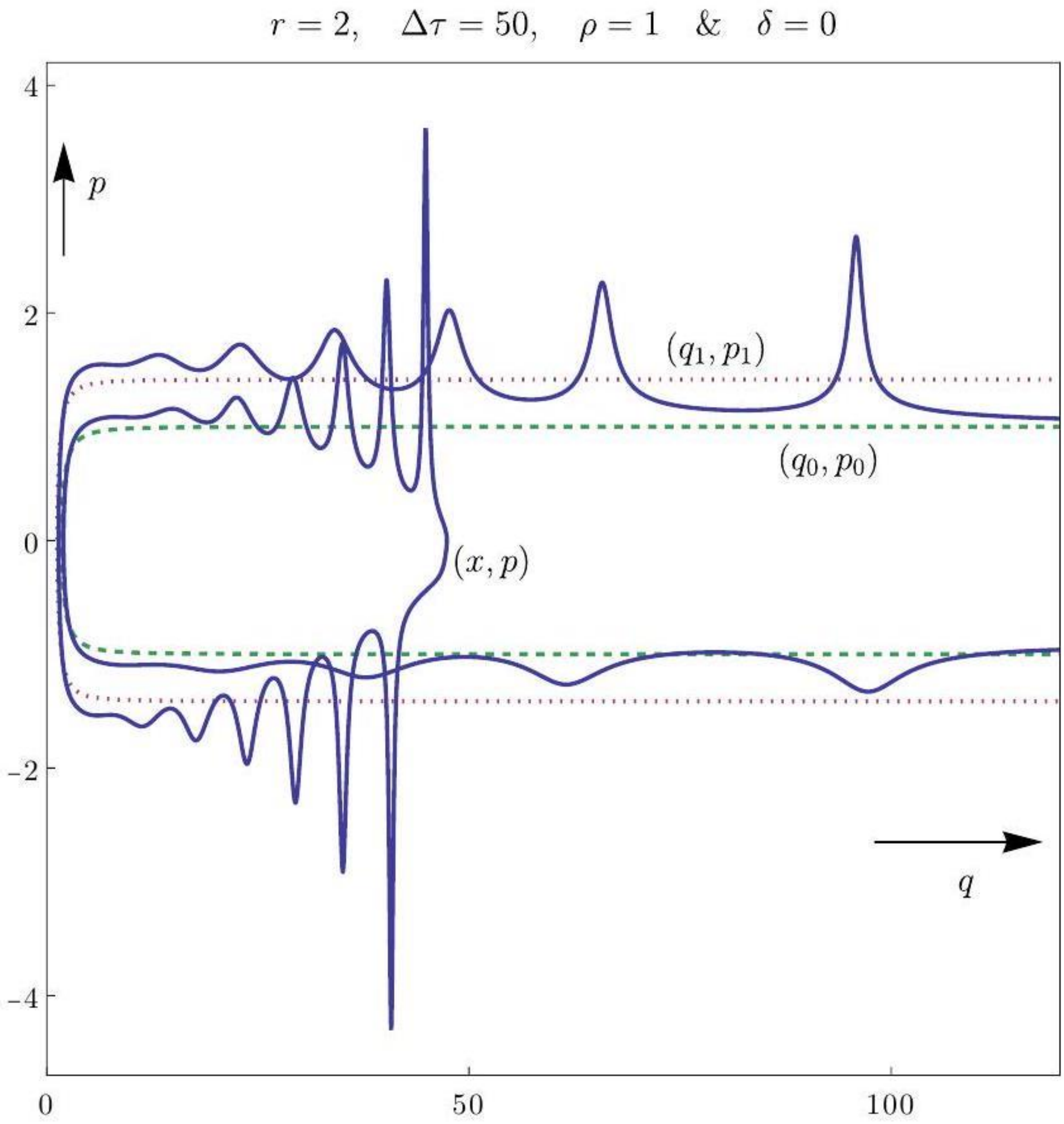
$$q_a(\tau) \to q_{\mathrm{B}}\omega_a \tau = 2\sqrt{E_a}\tau$$

$$x \propto a^{\frac{3}{2}(1-w)}$$

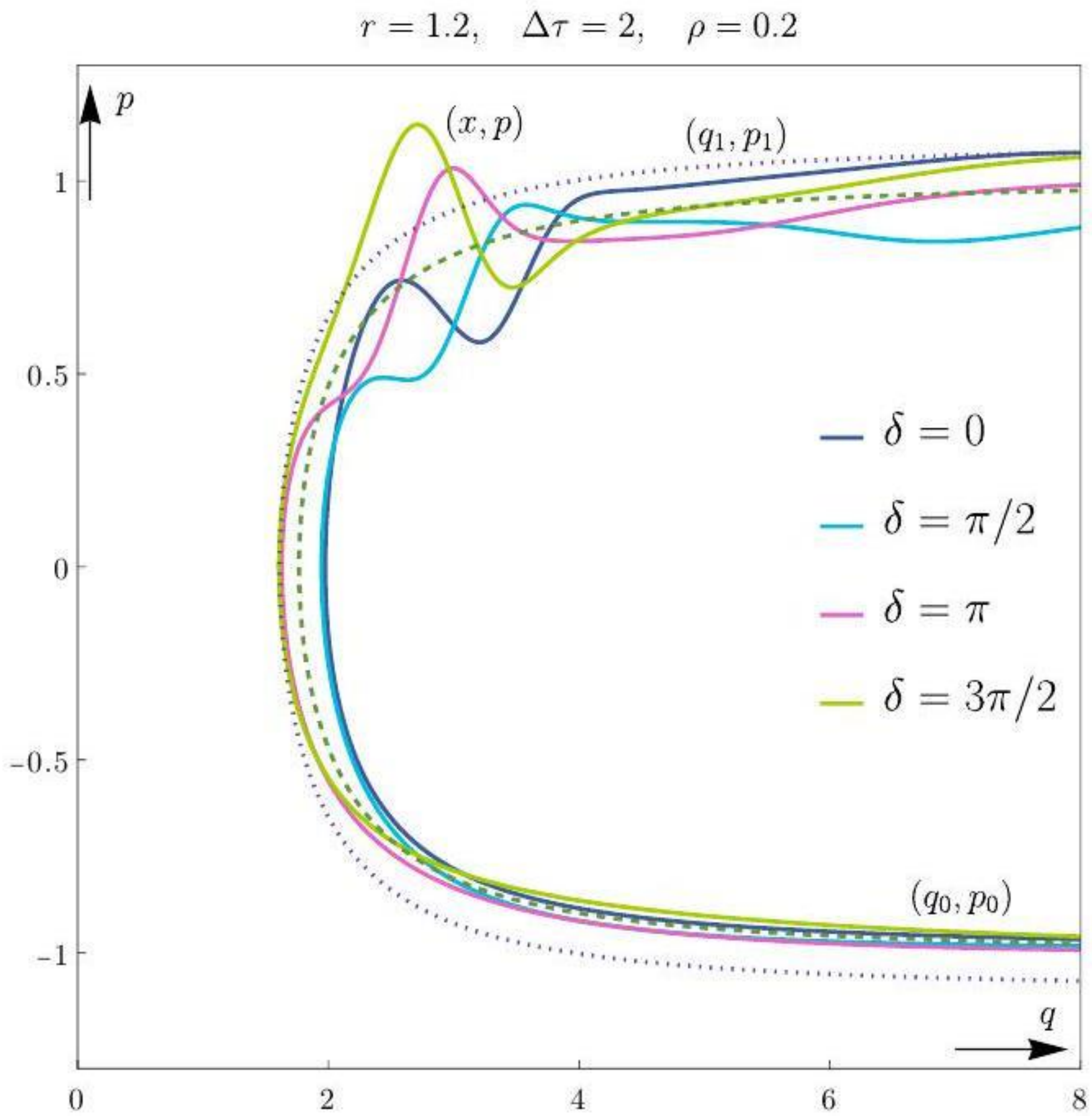
$$N \propto a^{3w}$$

$$a \underset{t\to\infty}{\propto} t^{2/[3(1+w)]} - (x^2/\tau^2) + \dot{x}^2$$

$$\dot{x}(\tau)|_{|\tau|\to\infty} = \pm p_0 x(\tau_{\mathrm{ini}})$$



$x(\tau_{\text{ini}}) = q_0(\tau_{\text{ini}})$

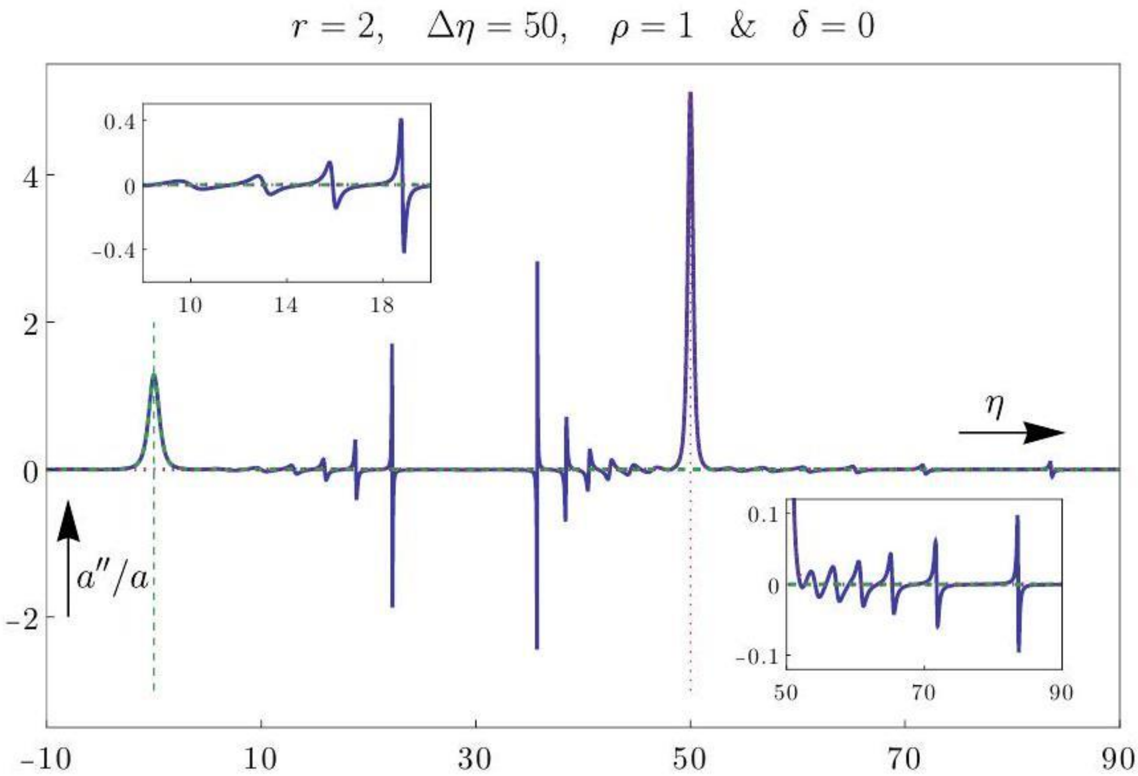


$$ds^2 = a^2(\eta)\{-d\eta^2 + [\delta_{ij} + h_{ij}(\boldsymbol{x},\eta)]\}dx^i\, dx^j,$$

$$(\partial^i h_{ij} = 0)\ (\delta^{ij} h_{ij} = 0)$$

$$H^{(2)} = \sum_{\boldsymbol{k}} \left[H^{(2)}_{\boldsymbol{k},+} + H^{(2)}_{\boldsymbol{k},\times}\right],$$

$$H^{(2)}_{\boldsymbol{k},\lambda} = \pi^{(\lambda)}_{\boldsymbol{k}} \pi^{(\lambda)}_{-\boldsymbol{k}} + \left(k^2 - \frac{a''}{a}\right) \mu^{(\lambda)}_{\boldsymbol{k}} \mu^{(\lambda)}_{-\boldsymbol{k}},$$



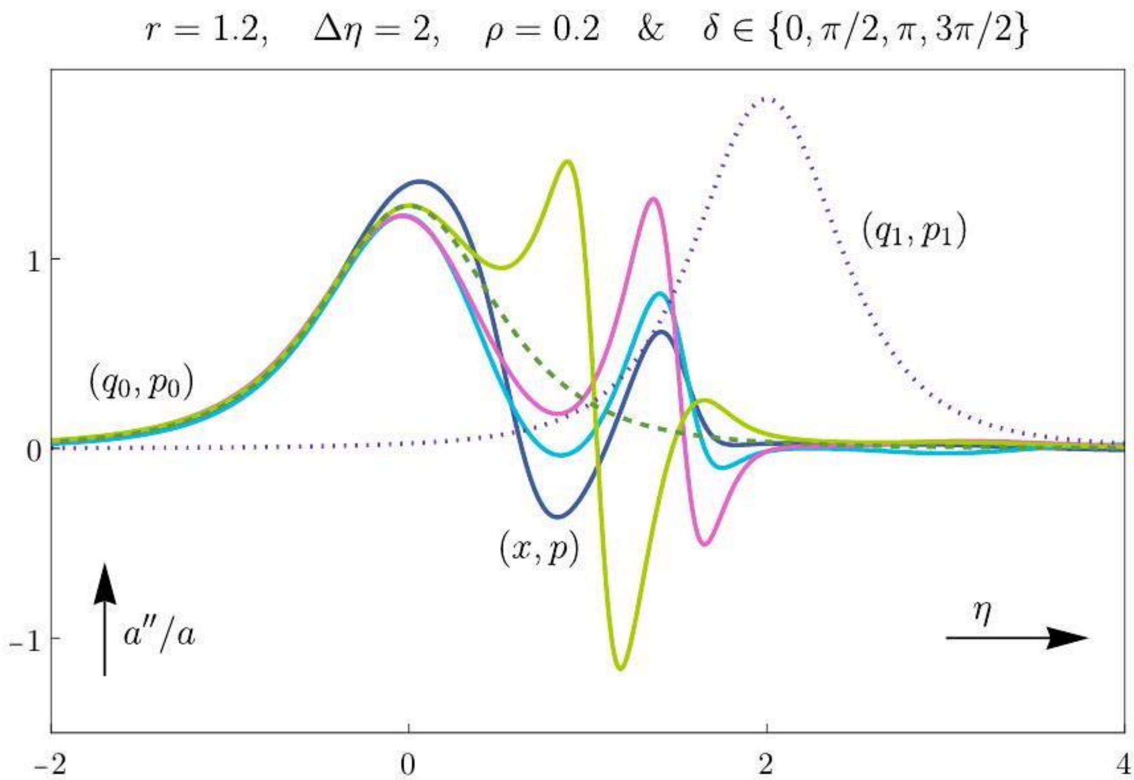
$$h_{ij}(\boldsymbol{x},\eta) = \sum_{\lambda} \mu^{(\lambda)}(\boldsymbol{x},\eta)\varepsilon_{ij(\lambda)}/a(\eta)\varepsilon_{ij(+)}\varepsilon_{ij(\times)}\mu_{\boldsymbol{k}}^{(\lambda)}$$

$$\pi_k^{(\lambda)}a' = \mathrm{d}a/\mathrm{d}\eta$$

$$\mu_{\boldsymbol{k}}(\eta)k = \sqrt{\boldsymbol{k}^2}$$

$$\mu_{\boldsymbol{k}}'' + [k^2 - V_{\text{eff}}(\eta)]\mu_{\boldsymbol{k}} = 0$$

$$V_{\text{eff}}(\eta) \equiv \frac{a''}{a}$$



$$V_{\text{eff}}(\eta) \underset{\eta\sim 0}{\simeq} q_0''/q_0$$

$$V_{\text{eff}}(\eta) \underset{\eta\sim \Delta\eta}{\simeq} q_1''/q_1$$

$$V_{\text{eff}}(\eta) = a''/aq_0''/q_0q_1''/q_1$$

$$p = \sqrt{\kappa/(12\mathcal{V}_0)}ap_a$$

$$q = \sqrt{12\mathcal{V}_0/\kappa}\log(a)$$

$$\forall\alpha \in \mathbb{N}, p^2 = x^\alpha p x^{-2\alpha} p x^\alpha$$

$$\rho^\sigma(\mathbf{r}) = \sum_i f_i^\sigma |\psi_i^\sigma(\mathbf{r})|^2.$$

$$\int d\mathbf{r}|\psi_i^\sigma(\mathbf{r})|^2 = 1, \forall i$$

$$U_{\text{BO}}(\mathbf{R}) = \min_{\rho^\sigma, f^\sigma}\left\{F_{\text{KS}}[\rho^\sigma] + \sum_\sigma \int d\mathbf{r} V_{\text{ext}}^\sigma(\mathbf{R},\mathbf{r})\rho^\sigma(\mathbf{r}) \mid \sum_{i,\sigma} f_i^\sigma = N_e\right\} + V(\mathbf{R}).$$

$$\mathbf{R} = \{\mathbf{R}_I\}. V_{\text{ext}}^\sigma(\mathbf{R},\mathbf{r})$$

$$L_{\text{BO}}(\mathbf{R},\dot{\mathbf{R}}) = \frac{1}{2}\sum_I m_I|\dot{\mathbf{R}}_I|^2 - U_{\text{BO}}(\mathbf{R}),$$

$$m_I\ddot{\mathbf{R}}_I = -\nabla_I U_{\text{BO}}(\mathbf{R}).$$

$$U_{\Delta \mathrm{SCF}}(\mathbf{R}) = \min_{\rho^\sigma}\left\{F_{\mathrm{KS}}[\rho^\sigma] + \sum_\sigma \int d\mathbf{r} V_{\mathrm{ext}}^\sigma \rho^\sigma(\mathbf{r}) \mid \mathbf{f}^\sigma \in \Omega_\sigma\right\} + V(\mathbf{R}),$$

$$O = \left(C^{\mathrm{old}}\right)^\dagger S C^{\mathrm{new}}.$$

$$p_j = \sum_i \left(O_{ij}^2\right)^{\frac{1}{2}}$$

$$L_{\Delta \mathrm{SCF}}(\mathbf{R}, \dot{\mathbf{R}}) = \frac{1}{2}\sum_I m_I \left|\dot{\mathbf{R}}_I\right|^2 - U_{\Delta \mathrm{SCF}}(\mathbf{R}),$$

$$m_I \ddot{\mathbf{R}}_I = -\nabla_I U_{\Delta \mathrm{SCF}}(\mathbf{R}).$$

$$\mathcal{F}_{\mathrm{KS}}[\rho^\sigma, n^\sigma] = F_{\mathrm{KS}}[n^\sigma] + \sum_\sigma \int d\mathbf{r}(\rho^\sigma(\mathbf{r}) - n^\sigma(\mathbf{r})) \frac{\delta F_{KS}[\{\rho^\alpha, \rho^\beta\}]}{\delta \rho^\sigma(\mathbf{r})}\Bigg|_{\rho^\sigma = n^\sigma}$$

$$\mathcal{U}_{\Delta \mathrm{SCF}}(\mathbf{R}, n^\sigma) = \min_{\rho^\sigma}\left\{\mathcal{F}_{\mathrm{KS}}[\rho^\sigma, n^\sigma] + \sum_\sigma \int d\mathbf{r} V_{ext}^\sigma(\mathbf{R}, \mathbf{r})\rho^\sigma(\mathbf{r}) \mid \mathbf{f}^\sigma \in \Omega_\sigma\right\} + V(\mathbf{R})$$

$$\mathcal{L}_{\Delta \mathrm{SCF}}(\mathbf{R}, \dot{\mathbf{R}}, n^\sigma, \dot{n}^\sigma) = \frac{1}{2}\sum_I m_I \left|\dot{\mathbf{R}}_I\right|^2 - \mathcal{U}_{\Delta \mathrm{SCF}}(\mathbf{R}, n^\sigma) + \frac{1}{2}\mu \sum_\sigma \int d\mathbf{r}(\dot{n}^\sigma(\mathbf{r}))^2$$
$$-\frac{1}{2}\mu\omega^2 \sum_{\sigma,\sigma'} \iint d\mathbf{r} d\mathbf{r}'(\rho_{\min}^\sigma[n](\mathbf{r}) - n^\sigma(\mathbf{r})) T^{\sigma\sigma'}(\mathbf{r}, \mathbf{r}') \left(\rho_{\min}^{\sigma'}[n](\mathbf{r}') - n^{\sigma'}(\mathbf{r}')\right).$$

$$T^{\sigma\sigma'} = \sum_{\sigma''} \int d\mathbf{r}'' K^{\sigma''\sigma}(\mathbf{r}'', \mathbf{r}) K^{\sigma''\sigma'}(\mathbf{r}''\mathbf{r}')$$

$$J^{\sigma\sigma'}(\mathbf{r}, \mathbf{r}') = \frac{\delta(\rho_{\min}^\sigma[n](\mathbf{r}) - n^\sigma(\mathbf{r}))}{\delta n^{\sigma'}(\mathbf{r}')}$$

$$\left|q_{\min,J}^{\sigma'}[n] - n_J^{\sigma'}\right| \propto \omega^{-2}$$

$$m_I \ddot{\mathbf{R}}_I = -\nabla_I \mathcal{U}_{\Delta \mathrm{SCF}}(\mathbf{R}, n^\sigma)|_{n^\sigma}$$
$$\ddot{n}^\sigma(\mathbf{r}) = -\omega^2 \sum_{\sigma'} \int d\mathbf{r} K^{\sigma\sigma'}(\mathbf{r}, \mathbf{r}') \left(\rho_{\min}^{\sigma'}[n](\mathbf{r}) - n^{\sigma'}(\mathbf{r})\right)$$

$$U_{\mathrm{BO}}^{\mathrm{DFTB}}(\mathbf{R}) = \min_{D^\sigma, f^\sigma}\left\{\sum_\sigma \mathrm{Tr}\left[H_\sigma^{(0)}(D^\sigma - D_0^\sigma)\right] + \frac{1}{2}\sum_{I,J} q_I \gamma_{IJ} q_J + \frac{1}{2}\sum_I M_I\left(q_I^\alpha - q_I^\beta\right)^2 \middle| \sum_{i,\sigma} f_i^\sigma = N_e\right\} + V_{\mathrm{ref}}(\mathbf{R})$$

$$q_I = \sum_\sigma \mathrm{Tr}[(D^\sigma - D_0^\sigma) S_I].$$

$$S_I' = \{S_{ij}\}_{i \in I, j \in J}, S_I = \frac{1}{2}\left(S_I' + S_I'^T\right)$$

$$\gamma_{IJ} = \begin{cases} \left|R_I - R_J\right|^{-1} & \left|R_I - R_J\right| \to \infty \\ U_{IJ} & \left|R_I - R_J\right| \to 0 \end{cases}$$

$$H_\sigma = H^{(0)} + \frac{1}{2}(V^C S + S V^C) + \frac{1}{2}(W^\sigma S + S W^\sigma)$$

$$H_\sigma^\perp = Z^T H_\sigma Z$$

$$Z^T S Z = I$$

$$H_\sigma^\perp c_i^\sigma = \epsilon_i^\sigma c_i^\sigma$$

$$D^\sigma = Z\left(\sum_i f_i^\sigma c_i^\sigma c_i^{\sigma T}\right) Z^T$$

$$V_{i\in I, j\in J}^C = v_I^C \delta_{IJ}, \text{where } v_I^C = \sum_J \gamma_{IJ} q_J$$

$$W_{i\in I, j\in J}^\alpha = w_I^\alpha \delta_{IJ}, \text{where } w_I^\alpha = M_I\left(q_I^\alpha - q_I^\beta\right)$$

$$W_{i\in I, j\in J}^\beta = w_I^\beta \delta_{IJ} \text{ where } w_I^\beta = -M_I\left(q_I^\alpha - q_I^\beta\right)$$

$$\mathcal{U}_{\Delta\text{SCF}}^{\text{DFTB}}(\mathbf{R}, n^\sigma) = \min_{D^\sigma}\left\{\sum_\sigma \text{Tr}\left[H_\sigma^{(0)}(D^\sigma - D_0^\sigma)\right] + \frac{1}{2}\sum_{I,J}(2q_I - n_I)\gamma_{IJ} n_J\right.$$
$$\left. + \frac{1}{2}\left(2\left(q_I^\alpha - q_I^\beta\right) - \left(n_I^\alpha - n_I^\beta\right)\right) M_I \left(n_I^\alpha - n_I^\beta\right)\right| \mathbf{f}^\sigma \in \Omega_\sigma\Big\} + V_{\text{ref}}(\mathbf{R})$$

$$\mathcal{L}_{\Delta\text{SCF}}^{\text{DFTB}}(\mathbf{R}, \dot{\mathbf{R}}, n^\sigma, \dot{n}^\sigma) = \frac{1}{2}\sum_I m_I |\dot{\mathbf{R}}_I|^2 - \mathcal{U}_{\Delta\text{SCF}}^{\text{DFTB}}(\mathbf{R}, n^\sigma) + \frac{1}{2}\mu \sum_{I,\sigma} |\dot{n}_I^\sigma|^2$$
$$-\frac{1}{2}\mu\omega^2 \sum_{I,J,\sigma,\sigma'} (q_{\min,I}^\sigma[n] - n_I^\sigma) T_{IJ}^{\sigma\sigma'} \left(q_{\min,J}^{\sigma'}[n] - n_J^{\sigma'}\right)$$

$$J_{IJ}^{\sigma\sigma'} = \frac{\partial}{\partial n_J^{\sigma'}}(q_{\min,I}^\sigma[n] - n_I^\sigma)$$

$$\left|q_{\min,J}^{\sigma'}[n] - n_J^{\sigma'}\right| \propto \omega^{-2}, \frac{[79]}{2]}$$

$$m_I \ddot{\mathbf{R}}_I = -\nabla_I \mathcal{U}_{\Delta\text{SCF}}^{\text{DFTB}}(\mathbf{R}, n^\sigma)\Big|_{n^\sigma},$$
$$\ddot{n}_I^\sigma = -\omega^2 \sum_{J,\sigma'} K_{IJ}^{\sigma\sigma'} \left(q_{\min,J}^{\sigma'}[n] - n_J^{\sigma'}\right),$$

$$n_I^\sigma(t+\delta t) = 2n_I^\sigma(t) - n_I^\sigma(t-\delta t) + \delta t^2 \ddot{n}_I^\sigma(t) + \alpha \sum_{k=0}^{K_{\max}} C_k n_I^\sigma(t - k\delta t)$$

$$\kappa = \delta t^2 \omega^2$$

$$\ddot{\mathbf{n}} = -\omega^2 \mathbf{K}(\mathbf{q}[\mathbf{n}] - \mathbf{n}).$$

$$\mathbf{n} = \left[\{n^\alpha\}_{i=1}^N, \{n^\beta\}_{i=1}^N\right]$$

$$\ddot{\mathbf{n}} = -\omega^2 (\mathbf{K}_0 \mathbf{J})^{-1} \mathbf{K}_0 (\mathbf{q}[\mathbf{n}] - \mathbf{n}).$$

$$\mathbf{f}_{\mathbf{v}_i}(\mathbf{n}) \equiv \left.\frac{d\mathbf{f}(\mathbf{n}+\lambda\mathbf{v}_i)}{d\lambda}\right|_{\lambda=0} = \left.\frac{d\mathbf{q}[\mathbf{n}+\lambda\mathbf{v}_i]}{d\lambda}\right|_{\lambda=0} - \mathbf{v}_i = \mathbf{J}\mathbf{v}_i.$$

$$\mathbf{J} = \sum_{k,l}^{N} \mathbf{f}_{\mathbf{v}_k}(\mathbf{n}) L_{kl} \mathbf{v}_l^T$$

$$\tilde{\mathbf{f}}_{\mathbf{v}_i}(\mathbf{n}) = \mathbf{K}_0 \mathbf{f}_{\mathbf{v}_i}(\mathbf{n}),$$

$$\tilde{\mathbf{f}}(\mathbf{n}) = \mathbf{K}_0 \mathbf{f}(\mathbf{n}),$$

$$\mathbf{K}_0\mathbf{J} = \sum_{k,l}^{N} \tilde{\mathbf{f}}_{\mathbf{v}_k} L_{kl} \mathbf{v}_l^T$$

$$(\mathbf{K}_0\mathbf{J})^{-1} = \sum_{k,l}^{N} \mathbf{v}_k M_{kl} \tilde{\mathbf{f}}_{\mathbf{v}_l}^T$$

$$(\mathbf{K}_0\mathbf{J})^{-1} \approx \sum_{k,l}^{m} \mathbf{v}_k M_{kl} \tilde{\mathbf{f}}_{\mathbf{v}}^T, m < N$$

$$\{\mathbf{v}_k\} \in \text{span}^{\perp}\{\tilde{\mathbf{f}}(\mathbf{n}), (\mathbf{K}_0\mathbf{J})\tilde{\mathbf{f}}(\mathbf{n}), (\mathbf{K}_0\mathbf{J})^2\tilde{\mathbf{f}}(\mathbf{n}), \dots\}.$$

$$\ddot{\mathbf{n}} \approx -\omega^2 \sum_{k,l}^{m<N} \mathbf{v}_k M_{kl} \tilde{\mathbf{f}}_{\mathbf{v}_l}^T \mathbf{K}_0(\mathbf{q}[\mathbf{n}] - \mathbf{n}),$$

$$\mathbf{r}_m = \mathbf{K}_0(\mathbf{q}[\mathbf{n}] - \mathbf{n}) - \left(\sum_{k,l}^{m} \tilde{\mathbf{f}}_k M_{kl} \tilde{\mathbf{f}}_{\mathbf{v}_l}^T\right) \mathbf{K}_0(\mathbf{q}[\mathbf{n}] - \mathbf{n})$$

$$\tilde{r}_m = \frac{\left\|\mathbf{K}_0(\mathbf{q}[\mathbf{n}] - \mathbf{n}) - \left(\sum_{k,l}^{m} \tilde{\mathbf{f}}_k M_{kl} \tilde{\mathbf{f}}_{\mathbf{v}_l}^T\right)\mathbf{K}_0(\mathbf{q}[\mathbf{n}] - \mathbf{n})\right\|}{\|\mathbf{K}_0(\mathbf{q}[\mathbf{n}] - \mathbf{n})\|}$$

$$\mathbf{n}_{\text{new}} = \mathbf{n}_{\text{old}} - \mathbf{K}(\mathbf{q}[\mathbf{n}_{\text{old}}] - \mathbf{n}_{\text{old}}) \approx \mathbf{n}_{\text{old}} - \sum_{k,l}^{m<N} \mathbf{v}_k M_{kl} \tilde{\mathbf{f}}_{\mathbf{v}_l}^T \mathbf{K}_0(\mathbf{q}[\mathbf{n}_{\text{old}}] - \mathbf{n}_{\text{old}})$$

$$\left|\varphi_{k_j}\right|^2 d\mu \rightharpoonup \nu \text{ when } j \to +\infty$$

$$\mathcal{D} = \ker\eta$$

$$\forall X, Y \in \Gamma(\mathcal{D}), g(X, \phi Y) = d\eta(X, Y)$$

$$0 \le \delta_0 \le \delta_1 \le \cdots \le \delta_k \le \cdots \to +\infty$$

$$-\Delta_{sR}\varphi_k = \delta_k\varphi_k \text{ and } \|\varphi_k\|_{L^2(M,\nu)} = 1$$

$$(\varphi_k)_{k\in\mathbb{N}} \, -\Delta_{sR} \, (\delta_k)_{k\in\mathbb{N}} (k_j)_{j\in\mathbb{N}}$$

$$\int_M a(x) \left|\varphi_{k_j}(x)\right|^2 d\nu(x) \underset{j\to+\infty}{\longrightarrow} \int_M a(x) d\nu(x),$$

$$G_x M = \mathrm{Exp}(\mathfrak{g}_x M)$$

$$\hat{G}M := \left\{(x,\pi): x \in M, \pi \in \widehat{G_x M}\right\},$$

$$\sigma = \left\{\sigma(x,\pi): \mathcal{H}_\pi^\infty \to \mathcal{H}_\pi^\infty : (x,\pi) \in \hat{G}M\right\},$$

$$S^m(\hat{G}M), m \in \mathbb{R} \cup -\infty$$

$$\Psi_\hbar^m(M), m \in \mathbb{R} \cup -\infty$$

$$-\hbar^2 \Delta_{sR} \in \Psi_\hbar^2(M),$$

$$H \in S^2(\hat{G}M)$$

$$[-\hbar^2 \Delta_{\mathrm{sR}}, \mathrm{Op}_\hbar(\Pi_n)] \in \hbar\Psi_\hbar^1(M) \text{ and } \mathrm{Op}_\hbar(\Pi_n) \circ \mathrm{Op}_\hbar(\Pi_n) = \mathrm{Op}_\hbar(\Pi_n) + \hbar\Psi_\hbar^{-1}(M)$$

$$\hbar^2(2n+d)|R| + \mathcal{O}(\hbar^2)$$

$$\hat{\Pi}_n^\hbar A \hat{\Pi}_n^\hbar A \in \Psi_\hbar^{-\infty}(M)$$

$$\Psi_\hbar^{-\infty}(M) - \hbar^2 \Delta_{sR}$$

$$\eta \wedge (d\eta)^d \neq 0$$

$$(\ 2d + 1\ )\text{-form } \eta \wedge (d\eta)^d$$

$$\forall x \in M, \mathcal{D}_x := \{V \in T_x M : \eta(V) = 0\}.$$

$$\eta(R) = 1 \text{ and } d\eta(R,\cdot) = 0.$$

$$\eta = dr - \frac{1}{2}\sum_{i=1}^{d} (y_i dx_i - x_i dy_i)$$

$$R = \partial_r$$

$$\Sigma^{2d+2}\left(M^{2d+1}, \eta\right)\Sigma \subset T^* M \mathcal{D}^\perp \setminus o$$

$$\mathcal{D} = \ker \eta$$

$$\Sigma = \{(x, \lambda\eta_x) \in T^* M : x \in M, \lambda \in \mathbb{R} \setminus \{0\}\}$$

$$\Sigma = \bigcup_{\lambda \in \mathbb{R}\setminus\{0\}} \Sigma_\lambda$$

$$\Sigma_\lambda = \{(x, \lambda\eta_x) \in T^* M : x \in M\}$$

$$(x, \lambda\eta_x) \in \Sigma \mapsto \lambda \in \mathbb{R}$$

$$j : (x, \lambda) \in M \times \mathbb{R} \setminus \{0\} \mapsto (x, \lambda\eta_x) \in \Sigma$$

$$\omega_{|\Sigma} = j^*(\omega) = -(d\lambda \wedge \eta + \lambda d\eta)$$

$$\omega_{|\Sigma}^{d+1} = (-1)^{d+1} \lambda^d d\lambda \wedge \eta \wedge (d\eta)^d$$

$$\tilde{X}_1, \dots, \tilde{X}_d, \tilde{Y}_1, \dots, \tilde{Y}_d, R$$

$$[\tilde{X}_i, \tilde{Y}_j] = \delta_{i,j} R \text{ and } [\tilde{X}_i, \tilde{X}_j] = [\tilde{Y}_i, \tilde{Y}_j] = 0$$

$$\mathfrak{v} = \mathrm{span}(\tilde{X}_1, \dots, \tilde{X}_d, \tilde{Y}_1, \dots, \tilde{Y}_d) \text{ and } \mathfrak{r} = \mathrm{span}(R)$$

$$\mathfrak{p} = \mathrm{span}(\tilde{X}_1, \dots, \tilde{X}_d)$$

$$\mathfrak{q} = \mathrm{span}(\tilde{Y}_1, \dots, \tilde{Y}_d)$$

$$\mathfrak{h}^d = \mathfrak{v} \oplus \mathfrak{r}$$

$$\tilde{X}_i = \partial_{x_i} - \frac{y_i}{2}\partial_r, \tilde{Y}_i = \partial_{y_i} + \frac{x_i}{2}\partial_r \text{ and } R = \partial_r$$

$$\mathrm{Exp}_{\mathbb{H}^d}: \mathfrak{h}^d \to \mathbb{H}^d$$

$$h_1 = \mathrm{Exp}(V_1 + R_1)$$

$$h_2 = \mathrm{Exp}(V_2 + R_2)$$

$$h_1 * h_2 = \mathrm{Exp}_{\mathbb{H}^d}(V + R), \text{ with } V = v_1 + v_2 \in \mathfrak{v} \text{ and } R = r_1 + r_2 + \frac{1}{2}[v_1, v_2] \in \mathfrak{r}$$

$$h^{-1} = \mathrm{Exp}_{\mathbb{H}^d}(-V - R)$$

$$\mathcal{P}(M, \mathbb{S}^1) \cong H^2(M, \mathbf{Z}),$$

$$\forall p \in P, T_pP = H_p \oplus V_p, \text{ where } V = \ker \mathrm{pr}_*,$$

$$\Phi = \mathrm{pr}^*\Omega$$

$$\phi^2 = -I + \eta \otimes R \text{ and } \eta(R) = 1.$$

$$\phi(R) = 0 \text{ and } \eta \circ \phi = 0.$$

$$\forall x \in M, \forall X, Y \in T_xM, g(\phi X, \phi Y) = g(X, Y) - \eta(X)\eta(Y).$$

$$\eta(X) = g(X, R)$$

$$Y_1 = \phi(X_1)$$

$$\mathbb{X} = (X_1, \dots, X_d, Y_1, \dots, Y_d, R)$$

$$\begin{pmatrix} 0 & -I_d & 0 \\ I_d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$O(2d) \times 1 \cap Sp(2d) \times 1 = U(d) \times 1$$

$$\forall x \in M, \forall X, Y \in T_xM, g(X, \phi Y) = d\eta(X, Y).$$

$$\forall x \in M, \forall X, Y \in T_xM, g(X, \phi Y) = d\eta(X, Y),$$

$$\eta(X) = g(X, R),$$

$$\phi^2 = -I + \eta \otimes R \text{ and } d\eta(X, Y) = g(X, \phi Y).$$

$$dvol_g = \frac{(-1)^d}{2^d d!} \eta \wedge (d\eta)^d$$

$$T_\sigma(T^*M) = T_\sigma\Sigma \oplus \mathrm{orth}_\omega(T_\sigma\Sigma),$$

$$N\Sigma = \{(\sigma, w): \sigma \in \Sigma, w \in N_\sigma\Sigma\} \subset T(T^*M),$$

$$N_\sigma\Sigma = \mathrm{orth}_\omega(T_\sigma\Sigma)$$

$$T\Sigma_U = \bigcap_{1\leq i\leq d} \ker dh_{X_i} \cap \ker dh_{Y_i} = \left\{w \in T(T_U^*M): \forall i \in \{1, \dots, d\}, dh_{X_i} \cdot w = dh_{Y_i} \cdot w = 0\right\}$$

$$= \left\{w \in T(T_U^*M): \forall i \in \{1, \dots, d\}, \omega\left(\vec{h}_{X_i}, w\right) = \omega\left(\vec{h}_{Y_i}, w\right) = 0\right\}$$

$$N_\sigma\Sigma = \mathrm{span}\left(\vec{h}_{X_1}(\sigma), \dots, \vec{h}_{X_d}(\sigma), \vec{h}_{Y_1}(\sigma), \dots, \vec{h}_{Y_d}(\sigma)\right)$$

$$\Sigma, d\pi\left(\vec{h}_{X_i}\right) = X_i \circ \pi$$

$$d\pi\left(\vec{h}_{Y_i}\right) = Y_i \circ \pi$$

$$d\pi_\sigma(N_\sigma\Sigma) = \mathcal{D}_{\pi(\sigma)}$$

$$\Xi_\sigma := (d\pi_\sigma)_{|N_\sigma\Sigma}^{\mathcal{D}_{\pi(\sigma)}}: N_\sigma\Sigma \to \mathcal{D}_{\pi(\sigma)}$$

$$\omega_\sigma^{N\Sigma} = (\omega_\sigma)_{|N_\sigma\Sigma}$$

$$\omega_\sigma^{N\Sigma}\left(\vec{h}_{X_i}(\sigma), \vec{h}_{Y_j}(\sigma)\right) = \omega_\sigma\left(\vec{h}_{X_i}(\sigma), \vec{h}_{Y_j}(\sigma)\right) = \left\{h_{X_i}, h_{Y_j}\right\}(\sigma) = \delta_{i,j} h_R(\sigma) = \lambda(\sigma)$$

$$\omega_\sigma^{N\Sigma}\left(\vec{h}_{X_i}(\sigma), \vec{h}_{X_j}(\sigma)\right) = \omega_\sigma^{N\Sigma}\left(\vec{h}_{Y_i}(\sigma), \vec{h}_{Y_j}(\sigma)\right)$$

$$\omega^{N\Sigma} = \lambda\Xi^*(-d\eta_{|\mathcal{D}})$$

$$\nu = \frac{1}{\mathrm{vol}(M)}|\mathrm{vol}| - \Delta_{\mathrm{sR}}$$

$$\forall\psi \in C^\infty(M), Q(\psi) = \int_M \|d\psi\|_{g_{\mathcal{D}}^*}^2 d\nu$$

$$g_{\mathcal{D}}^* \mathrm{Dom}(-\Delta_{sR}) \subset L^2(M, \nu)$$

$$C^\infty(M)(V_1, \dots, V_{2d})\mathcal{D}$$

$$\nabla_{sR}\psi = \sum_{i=1}^{2d} (V_i\psi)V_i$$

$$Q(\psi) = \int_M \|\nabla_{sR}\psi\|_{g_{\mathcal{D}}}^2 d\nu$$

$$\Delta_{sR} = -\sum_{i=1}^{2d} V_i^* V_i = \sum_{i=1}^{2d} \left(V_i^2 + \mathrm{div}_\nu(V_i)V_i\right)$$

$$\mathrm{div}_\nu(X)\mathcal{L}_X\nu = \mathrm{div}_\nu(X)\nu$$

$$\Delta_{\mathbb{H}^d} = \sum_{i=1}^{d} \left(\tilde{X}_i^2 + \tilde{Y}_i^2\right)$$

$$T^{0,1}M \subset TM \otimes \mathbb{C}$$

$$\dim_{\mathbb{C}} T^{0,1}M = d$$

$$T^{1,0}M \cap T^{0,1}M = \emptyset$$

$$T^{1,0}M = \overline{T^{0,1}M}$$

$$\mathcal{D} \otimes \mathbb{C} = T^{1,0}M \oplus T^{0,1}M$$

$$\phi: \mathcal{D} \to \mathcal{D}\phi^2 = -\operatorname{Id}$$

$$T^{0,1}M = \{X - i\phi X : X \in \Gamma(\mathcal{D})\}$$

$$L_\eta(X,Y) := -d\eta(X,\phi Y), X, Y \in \Gamma(\mathcal{D})$$

$$\forall f \in C^\infty(M), \bar{\partial}_b f = (df)_{|T^{0,1}M} \in \Gamma(T^{0,1}M^*)$$

$$\Box_b = \bar{\partial}_b^* \bar{\partial}_b$$

$$\Box_b = -\frac{1}{4}(\Delta_b - idR) + \ g = \mathrm{pr}^* G + \eta \otimes \eta$$

$$\Omega(X,Y) = G(X, JY)$$

$$\phi^2 = -I + \eta \otimes R.$$

$$d\eta(X,Y) = g(X, \phi(Y))$$

$$B = b\mathrm{vol}_g$$

$$d\eta = \mathrm{pr}^* B$$

$$\eta = d\theta + A$$

$$\left(d\eta_g\right)_{|\mathcal{D}} = d\mathrm{vol}_{g_{\mathcal{D}}} \text{ on } \mathcal{D}$$

$$\eta_g = b^{-1}\eta$$

$$R = b\partial_\theta - \vec{b}$$

$$\left(g_{i,j}(x_1, x_2)\right)_{1 \le i,j \le 2}$$

$$\Delta_{sR} = \frac{1}{\sqrt{|g|}} \sum_{i,j} (\partial_i - A\partial_\theta)\left[\sqrt{|g|}\, g^{i,j} \left(\partial_j - A\partial_\theta\right)\right]$$

$$|g| = \det\left(g_{i,j}\right)\left(g^{i,j}\right)_{1 \le i,j \le 2}$$

$$L^2(M) := \bigoplus_{m\in\mathbf{Z}} L^2_m(X)$$

$$L^2_m(X), m \in \mathbf{Z} - \Delta_{sR}$$

$$C^\infty_m(X) \subset L^2_m(X), m \in \mathbf{Z}$$

$$\Delta_m = \frac{1}{\sqrt{|g|}} \sum_{i,j} (\partial_i - mA)\left[\sqrt{|g|}g^{i,j}(\partial_j - mA)\right]$$

$$\mathrm{gr}(T_xM) = \mathcal{D}_x \oplus T_xM/\mathcal{D}_x$$

$$[X_x, Y_x]_{\mathfrak{g}_xM} := [X,Y](x) \bmod \mathcal{D}_x$$

$$\mathfrak{g}_xM = \left(\mathrm{gr}(T_xM), [\cdot,\cdot]_{\mathfrak{g}_xM}\right)$$

$$\mathbb{X} = (V_1, \dots, V_{2d+1})U \subset M(V_1, \dots, V_{2d})\mathcal{D}_{|U}$$

$$\langle\mathbb{X}\rangle := (\langle V_1\rangle, \dots, \langle V_{2d+1}\rangle)\mathfrak{g}_{|U}M$$

$$\mathfrak{g}M = \mathfrak{v}M \oplus \mathfrak{r}M$$

$$\forall t > 0, \delta_t(V_x + R_x) = tV_x + t^2R_x, \text{ where } V_x \in \mathfrak{v}_xM, R_x \in \mathfrak{r}_xM$$

$$\mathrm{Exp}_{G_xM} : \mathfrak{g}_xM \to G_xM$$

$$GM = \bigcup_{x\in M} G_xM$$

$$\mathbb{X} = (X_1, \dots, X_d, Y_1, \dots, Y_d, R),$$

$$\forall i,j \in \{1, \dots, d\}, d\eta(X_i, Y_j) = -\delta_{i,j} \text{ and } d\eta(X_i, X_j) = d\eta(Y_i, Y_j) = 0$$

$$d\eta(X,Y) = -\eta([X,Y]),$$

$$\forall i,j \in \{1, \dots, d\}, [X_i, Y_j] = \delta_{i,j}R \bmod \mathcal{D} \text{ and } [X_i, X_j], [Y_i, Y_j] \in \mathcal{D}$$

$$\forall i \in \{1, \dots, d\}, \langle X_i\rangle_x = X_{i,x} \text{ and } \langle Y_i\rangle_x = Y_{i,x}$$

$$\langle R\rangle_x = R_x \bmod \mathcal{D}_x$$

$$\forall x \in U, \left[\langle X_i\rangle_x, \langle Y_j\rangle_x\right]_{\mathfrak{g}_xM} = \delta_{i,j}\langle R\rangle_x \text{ and } \left[\langle X_i\rangle_x, \langle X_j\rangle_x\right]_{\mathfrak{g}_xM} = \left[\langle Y_i\rangle_x, \langle Y_j\rangle_x\right]_{\mathfrak{g}_xM} = 0.$$

$$\varphi^x_U : U \times \mathfrak{h}^d \longrightarrow \mathfrak{g}M_{|U},$$

$$\varphi^{\mathbb{X}}_U(x,v) = \left(x, \sum_{i=1}^{d} (v_i\langle X_i\rangle_x + v_{d+i}\langle Y_i\rangle_x) + v_{2d+1}\langle R\rangle_x\right),$$

$$\forall v \in \mathfrak{h}^d, \mathrm{Exp}^{\rtimes}_x(v) := \mathrm{Exp}_{G_xM}(\varphi^{\rtimes}_U(x,v)),$$

$$\mathrm{Exp}^x : U \times \mathfrak{h}^d \to G_{|U}M$$

$$\forall (x,v) \in U \times \mathfrak{h}^d, \mathrm{Exp}^{\rtimes}(x,v) := \mathrm{Exp}_x^{\rtimes}(v).$$

$$\varphi_{U_1}^{\mathbb{X}_1}\ \varphi_{U_2}^{\mathbb{X}_2} \phi\text{-frames } (U_1, \mathbb{X}_1)\ (U_2, \mathbb{X}_2)$$

$$U_1 \cap U_2 (A(x))_{x \in U_1 \cap U_2} U(d) \times 1$$

$$\forall x \in U_1 \cap U_2, \mathbb{X}_1(x) = A(x)\mathbb{X}_2(x)$$

$$\langle \mathbb{X}_1 \rangle \langle \mathbb{X}_2 \rangle \mathfrak{g} M_{|U_1 \cap U_2}$$

$$\forall (x,v) \in \left(U_1 \cap U_2, \mathfrak{h}^d\right), \varphi_{U_1}^{\mathbb{X}_1,-1} \circ \varphi_{U_2}^{\mathbb{X}_2}(x,v) = (x, A(x)v)$$

$$\mu_{GM} = \{\mu_x\}_{x \in M}$$

$$x \in M \mapsto \int_M f(x,h) d\mu_x(h)$$

$$f \in C_c^{\infty}(GM)$$

$$\left\{\mathrm{Leb}_{\mathfrak{h}^d}^{\mathbb{X}}\right\}_{x \in U} \langle \mathbb{X} \rangle_x \mathfrak{g}_{|U} M \mathrm{Exp}_{G_x M}, x \in M \{\mu_x\}_{x \in M}$$

$$\mathcal{V} = \bigoplus_{1 \le j \le p} \mathcal{V}_j (\mathcal{V}_i)_{1 \le j \le p}$$

$$\delta_r(v) = r^j v, v \in \mathcal{V}_j$$

$$Q := \sum_{j=1}^{p} j \dim\left(\mathcal{V}_j\right)$$

$$f(\delta_r v) = r^m f(v)$$

$$T: \mathcal{S}(\mathcal{V}) \to \mathcal{S}'(\mathcal{V}) (\delta_t)_{t>0} f \in \mathcal{S}(\mathcal{V})$$

$$T(f \circ \delta_r) = r^m (Tf) \circ \delta_r$$

$$|\cdot| : \mathcal{V} \to \mathbb{R}$$

$$|-v| = |v|, |v| = 0 \Leftrightarrow v = 0, \text{ and } |\delta_r v| = r|v|.$$

$$\mathfrak{h}^d = \mathfrak{v} \oplus \mathfrak{r}$$

$$|(x,y,z)| = ((x^2 + y^2)^2 + z^2)^{1/4}$$

$$\exists C > 0, \forall h_1, h_2 \in \mathbb{H}, |h_1 * h_2| \le C(|h_1| + |h_2|).$$

$$\mathcal{V}_1 = \bigoplus_{1 \le j \le p_1} \mathcal{V}_{1,j}$$

$$\mathcal{V}_2 = \bigoplus_{1 \le j \le p_2} \mathcal{V}_{2,j}$$

$$\left(\delta_{1,r}\right)_{r>0} \left(\delta_{2,r}\right)_{r>0} \left(V_1, \dots, V_{\dim(\mathcal{V}_1)}\right) \left(W_1, \dots, W_{\dim(\mathcal{V}_2)}\right) \mathcal{V}_{i,j}, i \in \{1,2\}, 1 \le j \le p_i$$

$$\lim_{\varepsilon\to 0}\delta_{2,\varepsilon^{-1}}r(\delta_{1,\varepsilon}v)=0$$

$$R:\mathbb{R}_+\times\mathcal{V}_1\to\mathcal{V}_2$$

$$\delta_{2,\varepsilon^{-1}}\left(r(\delta_{1,\varepsilon}v)\right)=\varepsilon R(\varepsilon,v)$$

$$\dot\gamma(t)=X(\gamma(t))\ \text{ and }\ \gamma(0)=x$$

$$\exp_x(X):=\gamma(1)$$

$$\mathbb{X}=(V_1,\dots,V_{2d+1})x\in Uv\in\mathbb{R}^{2d+1}$$

$$\exp_x^{\mathbb{X}}(v)=\exp_x\left(\sum_{i=1}^{2d+1}v_iV_i\right),$$

$$\mathbb{R}^{2d+1}(X_1,\dots,X_d,Y_1,\dots,Y_d,R)$$

$$U_{\mathbb{X}}\times\mathfrak{h}^d$$

$$\exp^{\mathbb{X}}:U_{\mathbb{X}}\longrightarrow U\times U$$
$$(x,v)\longmapsto\exp_x^{\mathbb{X}}(v)$$

$$\ln^{\mathbb{X}}:=\left(\exp^{\mathbb{X}}\right)^{-1}\ \text{ and }\ \ln_x^{\mathbb{X}}:=\left(\exp_x^{\mathbb{X}}\right)^{-1}.$$

$$t\in(0,1),(x,tv)$$

$$\{x\}\times\{0\}\times\{0\}\text{ in }U\times\mathfrak{h}^d\times\mathfrak{h}^d$$

$$\ln_x^{\mathbb{X}}\left(\exp_{\exp_x^{\mathbb{X}}(w)}^{\mathbb{X}}(v)\right)=w*_{\mathfrak{h}^d}v+r(x;w,v),$$

$$\mathcal{J}:\mathcal{H}_{\pi_1}\to\mathcal{H}_{\pi_2}$$

$$\pi_1=\mathcal{J}^{-1}\circ\pi_2\circ\mathcal{J}$$

$$[\pi_1]=[\pi_2]$$

$$\hat G:=\{[\pi]:\pi:G\to\mathcal{L}(\mathcal{H}_\pi)\mathcal{G}\}.$$

$$\lambda\in\mathfrak{r}^*\setminus\{0\}$$

$$\mathcal{H}_{\pi^\lambda}=L^2(\mathfrak{p})$$

$$\pi^\lambda(h)f(\xi)=\exp\left(i\lambda r+\frac{i}{2}|\lambda|x\cdot y+i\sqrt{|\lambda|}\xi\cdot y\right)f(\xi+\sqrt{|\lambda|}x)$$

$$\mathfrak{r}^*\setminus\{0\}\text{ with }\mathbb{R}\setminus\{0\}$$

$$\pi^\lambda,\lambda\in\mathfrak{r}^*\setminus\{0\}\mathrm{Exp}_{\to}(\mathbb{R}R)\mathcal{H}_{\pi^\lambda}\mathrm{Exp}_{\mathfrak{H}}(rR),r\in\mathbb{R}$$

$$e^{i\lambda r}I_{\mathcal{H}_\pi}$$

$$\mathfrak{v}\sim\mathfrak{p}\oplus i\mathfrak{q}.$$

$$\int_{\mathfrak{v}} |F(z)|^2 e^{-|\lambda||z|^2} dz < \infty$$

$$\pi_{\mathcal{F}}^{\lambda}(h)F(w) = \exp\left(i\lambda r - \frac{\lambda}{4}|z|^2 - \frac{\lambda}{2} w\bar{z}\right) F(w+z), h = (z,r) \in \mathbb{H}^d.$$

$$[\pi^{\lambda}] = [\pi_{\mathcal{F}}^{\lambda}], \lambda \in \mathbb{R}^*.$$

$$\pi^{0,\gamma}(h) = e^{i\gamma(V)}, \text{ where } h = \mathrm{Exp}_{\mathbb{H}}(V + rR), \text{with } V \in \mathfrak{v}, r \in \mathbb{R}.$$

$$\widehat{\mathbb{H}} = \{[\pi^{\lambda}]: \lambda \in \mathfrak{r}^* \setminus \{0\}\} \sqcup \{[\pi^{0,\gamma}]: \gamma \in \mathfrak{v}^*\}.$$

$$\widehat{\mathbb{H}}_{\infty} = \{[\pi^{\lambda}]: \lambda \in \mathfrak{r}^* \setminus \{0\}\},$$

$$d\mu_{\widehat{\mathbb{H}}}(\pi^{\lambda}) = (2\pi)^{-(3d+1)}|\lambda|^d d\lambda, \lambda \in \mathbb{R}^*.$$

$$\pi(X) = \frac{d}{dt}\pi(\mathrm{Exp}_G(tX))_{|t=0}, X \in \mathfrak{g}$$

$$g \in G \mapsto \pi(g)f \in \mathcal{H}_{\pi}$$

$$\pi^{\lambda}(X_i) = \sqrt{|\lambda|}\partial_{\xi_i}, \pi^{\lambda}(Y_i) = i\sqrt{|\lambda|}\xi_i \text{ and } \pi^{\lambda}(R) = i\lambda$$

$$\mathcal{H}_{\pi^{\lambda}}^{\infty}\mathcal{S}(\mathbb{R}_{\xi})$$

$$\Delta_{\mathbb{H}^d} = \sum_{i=1}^{d} (X_i^2 + Y_i^2)\mathfrak{U}(\mathfrak{h}^d)$$

$$\pi^{\lambda}(-\Delta_{\mathbb{H}^d}) = |\lambda| \sum_{i=1}^{d} (-\partial_{\xi_i}^2 + \xi_i^2).$$

$$\mathcal{F}_G(\kappa)(\pi) = \hat{\kappa}(\pi) = \pi(\kappa) = \int_G \kappa(x)\pi(x)^* dx \in \mathcal{L}(\mathcal{H}_{\pi})$$

$$\mathcal{I} \circ \pi_1 = \pi_2 \circ \mathcal{I}$$

$$\mathcal{I} \circ \mathcal{F}_G(\kappa)(\pi_1) = \mathcal{F}_G(\kappa)(\pi_2) \circ \mathcal{I}$$

$$\mathcal{F}_G(\kappa) = \{\hat{\kappa}(\pi) \in \mathcal{L}(\mathcal{H}_{\pi}): \pi \in \widehat{G}\}$$

$$\mathcal{F}_G(\kappa_1) \circ \mathcal{F}_G(\kappa_2) = \mathcal{F}_G(\kappa_2 \star_G \kappa_1), \text{ where } \kappa_2 \star_G \kappa_1(x) = \int_G \kappa_2(y)\kappa_1(y^{-1}x)dy$$

$$\forall \kappa \in \mathcal{S}(G), \forall x \in G, \kappa(x) = \int_{\widehat{G}} \mathrm{Tr}_{\mathcal{H}_{\pi}}(\pi(x)\hat{\kappa}(\pi)) d\mu_{\widehat{G}}(\pi)$$

$$\forall \kappa \in L^1(G) \cap L^2(G), \int_G |\kappa(x)|^2 dx = \int_{\widehat{G}} \|\hat{\kappa}(\pi)\|_{HS(\mathcal{H}_{\pi})}^2 d\mu_{\widehat{G}}(\pi)$$

$$\|\cdot\|_{HS(\mathcal{H}_{\pi})}\mathcal{H}_{\pi}L^2(\widehat{G})$$

$$\sigma = \{\sigma(\pi) \in \mathcal{L}(\mathcal{H}_{\pi}): \|\sigma(\pi)\|_{HS(\mathcal{H}_{\pi})} < \infty, \pi \in \widehat{G}\}$$

$$\|\sigma\|_{L^2(\hat{G})}^2 := \int_{\hat{G}} \|\sigma(\pi)\|_{HS(\mathcal{H}_\pi)}^2 d\mu_{\hat{G}}(\pi)$$

$$\mathcal{F}_G: L^2(G) \to L^2(\hat{G})$$

$$\sigma = \{\sigma(\pi) \in \mathcal{L}(\mathcal{H}_\pi): \pi \in \hat{G}\}$$

$$\|\sigma\|_{L^\infty(\hat{G})} := \sup_{\pi \in \hat{G}} \|\sigma\|_{\mathcal{L}(\mathcal{H}_\pi)}$$

$$\mathcal{F}_G(L^1(G)) \subset L^\infty(\hat{G})$$

$$\mathcal{L}(L^2(G))^G$$

$$T \in \mathcal{L}(L^2(G))^G \hat{T} \in L^\infty(\hat{G})$$

$$\forall f \in L^2(G), \mathcal{F}_G(Tf) = \hat{T}\hat{f}$$

$$\|T\|_{\mathcal{L}(L^2(G))} = \|\hat{T}\|_{L^\infty(\hat{G})}$$

$$T \in \mathcal{L}(L^2(G))^G$$

$$\kappa \in \mathcal{S}'(G) Tf = f \star_G \kappa f \in \mathcal{S}(G)$$

$$\mathcal{F}_G(\kappa) := \hat{T}$$

$$\mathcal{K}(G) := \{\kappa \in \mathcal{S}'(G): (f \mapsto f \star_G \kappa) \in \mathcal{L}(L^2(G))\}$$

$$\mathcal{F}_G: \mathcal{K}(G) \to L^\infty(\hat{G}) L_s^2(\mathbb{H}^d)$$

$$\mathcal{K}_{a,b}(\mathbb{H}^d) := \left\{\kappa \in \mathcal{S}'(\mathbb{H}^d): (f \mapsto f \star \kappa) \in \mathcal{L}\left(L_a^2(\mathbb{H}^d), L_b^2(\mathbb{H}^d)\right)\right\}$$

$$\mathcal{K}_{a,b}(\mathbb{H}^d) \mathcal{L}\left(L_a^2(\mathbb{H}^d), L_b^2(\mathbb{H}^d)\right)$$

$$L_{a,b}^\infty(\widehat{\mathbb{H}}^d) \sigma = \{\sigma(\pi): \mathcal{H}_\pi^\infty \to \mathcal{H}_\pi^\infty: \pi \in \widehat{\mathbb{M}}\}$$

$$\left(1 - \pi(\Delta_{H^d})\right)^{b/2} \sigma \left(1 - \pi(\Delta_{H^d})\right)^{-a/2}$$

$$L^\infty(\widehat{\mathbb{H}}^d) L_{a,b}^\infty(\widehat{\mathbb{H}}^d)$$

$$\|\sigma\|_{L_{a,b}^\infty(\widehat{\mathbb{H}}^d)} = \left\|\left(1 - \pi(\Delta_{\mathbb{H}^d})\right)^{b/2} \sigma \left(1 - \pi(\Delta_{\mathbb{H}^d})\right)^{-a/2}\right\|_{L^\infty(\widehat{\mathbb{H}}^d)}$$

$$\mathcal{K}_{a,b}(\mathbb{H}^d) L_{a,b}^\infty(\widehat{\mathbb{H}}^d) \mathcal{F}_{\mathbb{H}^d} : \mathcal{K}_{a,b}(\mathbb{H}^d) \to L_{a,b}^\infty(\widehat{\mathbb{H}}^d) \kappa \in \mathcal{K}_{a,b}(\mathbb{H}^d)$$

$$\|\kappa\|_{\mathcal{K}_{a,b}(\mathbb{H}^d)} = \|\mathcal{F}_{\mathfrak{H}}(\kappa)\|_{L_{a,b}^\infty(\widehat{\mathbb{H}}^d)}$$

$$\sigma = \{\sigma(\pi) : \mathcal{H}_\pi^{+\infty} \to \mathcal{H}_\pi^{-\infty}: \pi \in \widehat{\mathbb{H}}^d\} \widehat{\mathbb{H}}^d \mathcal{H}_\pi^{+\infty} \mathcal{H}_\pi^{-\infty}$$

$$q \in C^\infty(\mathbb{H}^d)$$

$$\widehat{\mathbb{H}}^d \ \Delta_{q^-} \ L_{a,b}^\infty(\widehat{\mathbb{R}}^d) q \mathcal{F}_{\mathbb{H}^d}^{-1}(\sigma) L_{c,d}^\infty(\widehat{\mathbb{H}}^d) \in \mathbb{R}$$

$$\Delta_q \sigma = \mathcal{F}_{\mathbb{H}^d}\left(q\mathcal{F}_{\mathbb{H}^d}^{-1}(\sigma)\right)$$

$$\Delta_x, \Delta_y \Delta_z \alpha \in \mathbb{N}^{2d+1} x_1^{\alpha_1} \cdots x_d^{\alpha_d} y_1^{\alpha_{d+1}} \cdots y_d^{\alpha_{2d}} z^{\alpha_{2d+1}}$$

$$S^m(\widehat{\mathbb{H}}^d)\alpha \in \mathbb{N}^{2d+1}$$

$$\Delta^\alpha \sigma \in L^\infty_{0,-m+[\alpha]}(\widehat{\mathbb{H}}^d)$$

$$[\alpha] = \sum_{i=1}^{2d} \alpha_i + 2\alpha_{2d+1} S^m(\widehat{\mathbb{H}}^d)$$

$$\|\sigma\|_{S^m(\widehat{\mathbb{H}}^d),N} := \max_{[\alpha]\leq N} \|\Delta^\alpha \sigma\|_{L^\infty_{0,-m+[\alpha]}(\widehat{\mathbb{H}}^d)} = \max_{[\alpha]\leq N} \left\| \left(1 - \pi(\Delta_{\mathbb{H}^d})\right)^{\frac{m-[\alpha]}{2}} \Delta^\alpha \sigma \right\|_{L^\infty(\widehat{\mathbb{H}}^d)}.$$

$$S^{-\infty}(\widehat{\mathbb{H}}^d) = \bigcap_{m\in\mathbb{R}} S^m(\widehat{\mathbb{H}}^d).$$

$$\mathcal{S}(\mathbb{H}) S^{-\infty}(\widehat{\mathbb{H}})(\ M^{2d+1}, \eta, g\ )$$

$$\widehat{G}M = \bigcup_{x\in M} \left(x, \widehat{G_x M}\right) \sim_{\text{Kir}}$$

$$\forall (x_1, \ell_1), (x_2, \ell_2) \in \mathfrak{g}^* M, (x_1, \ell_1) \sim_{Kir} (x_2, \ell_2) \Leftrightarrow x_1 = x_2 \text{ and } \ell_1 \in \text{Ad}^*\left(G_{x_2} M\right)(\ell_2),$$

$$\text{Ad}^*\left(G_{x_2} M\right)(\ell) \text{ for } \ell \in \mathfrak{g}_x^* M$$

$$\widehat{G}M := \mathfrak{g}^* M / \sim_{Kir}.$$

$$p: \mathfrak{g}^* M \to M$$

$$\hat{p}: \widehat{G}M \to M.$$

$$\lambda \in \mathfrak{r}_x^* M \setminus o$$

$$\mathfrak{p}_x^{\rtimes} = \text{span}(\langle X_1 \rangle_x, \dots, \langle X_d \rangle_x) \subset \mathfrak{g}_x M,$$

$$\mathcal{H}_{\pi_x^\lambda} = L^2(\mathfrak{p}_x^{\chi})$$

$$\forall f \in \mathcal{H}_{\pi_x^\lambda}, \pi_x^\lambda(h) f(\xi) = \exp\left(i\lambda z + \frac{i}{2}|\lambda| x \cdot y + i\sqrt{|\lambda|}\xi \cdot y\right) f(\xi + \sqrt{|\lambda|} x),$$

$$h = \text{Exp}_{G_x M}(x \cdot \langle X \rangle_x + y \cdot \langle Y \rangle_x + z \langle R \rangle_x), \text{ with } x, y \in \mathbb{R}^d, z \in \mathbb{R}.$$

$$\pi_x^{0,\gamma}(h) = e^{i\gamma(\langle V \rangle_x)}$$

$$h = \text{Exp}_{G_x M}(\langle V \rangle_x + z\langle R \rangle_x), \text{with } \langle V \rangle_x \in \mathfrak{v}_x M, z \in \mathbb{R}$$

$$\hat{\varphi}_U^{\mathbb{X}}: U \times \widehat{\mathbb{H}} \to \widehat{G}M_{|U}$$

$$x \in U \pi \in \widehat{\mathbb{H}}\ [\pi] = [\pi^\lambda] \lambda \in \mathfrak{r}^* \setminus \{0\} \mathfrak{r}^* \mathfrak{r}_x^* M \langle R \rangle_x$$

$$\hat{\varphi}_U^{\mathbb{X}}(x, \pi^\lambda) = (x, \pi_x^\lambda)$$

$$[\pi] = [\pi^{0,\gamma}]$$

$$\gamma \in \mathfrak{v}^*(\langle X_1\rangle_x, \dots, \langle X_d\rangle_x, \langle Y_1\rangle_x, \dots, \langle Y_d\rangle_x)$$

$$\hat{\varphi}_U^{\mathbb{X}}(x, \pi^{0,\gamma}) = \left(x, \pi_x^{0,\gamma}\right)\hat{\varphi}_U^X \hat{G} M \widehat{\mathbb{H}}^d$$

$$\hat{\varphi}_{1,2}^{\times} := \hat{\varphi}_{U_1}^{\mathbb{X}_1,-1} \circ \hat{\varphi}_{U_2}^{\mathbb{X}_2} : (U_1 \cap U_2) \times \widehat{\mathbb{H}} \to (U_1 \cap U_2) \times \widehat{\mathbb{H}}$$

$$\hat{\varphi}_{1,2}^{\mathbb{X}}(x, \pi) = (x, \tilde{\pi})$$

$$\tilde{\pi}\left(\mathrm{Exp}_{\mathbb{H}}(r\langle R\rangle_x)\right) = e^{i\lambda r} I_{\mathcal{H}_{\tilde{\pi}}}$$

$$\hat{G}_\infty M := \left\{(x, [\pi]) : [\pi] \in \hat{G}_{\infty,x} M\right\}$$

$$(x, \lambda\eta_x) \in \Sigma \mapsto \left(x, \left[\pi_x^\lambda\right]\right) \in \hat{G}_\infty M$$

$$\left\{\hat{\mu}_{\hat{G}_x M}\right\}_{x \in M} \hat{G}_x M x \in M x \mapsto \int_{\hat{G}_x M} f(x, \pi) d\hat{\mu}_{\hat{G}_x M}(\pi) f \in C_c(\hat{G} M)$$

$$f \in C_c(\hat{G} M) M \times \widehat{\mathbb{A}}^d$$

$$\hat{\varphi}_U^{\times} d\nu(x) \otimes d\hat{\mu}_{\hat{\mathbb{G}}d}(\pi)$$

$$M \times \widehat{\mathbb{H}}^d$$

$$\hat{\varphi}_{1,2}^X(x, \cdot) \widehat{\mathbb{H}}_\infty^d \hat{\mu}_{\widehat{\mathbb{H}}d} \hat{\mu}_{\hat{G} M} \hat{G} M$$

$$\mu_{GM} \kappa \in \mathcal{S}(G_x M)$$

$$\int_{G_x M} |\kappa(v)|^2 d\mu_{G_x M}(v) = \int_{\hat{G}_x M} \|\hat{\kappa}(\pi)\|_{HS(\mathcal{H}_\pi)}^2 d\hat{\mu}_{\hat{G}_x M}(\pi)$$

$$d\hat{\mu}_{\hat{G} M}\left(x, \pi^\lambda\right) = \frac{1}{(2\pi)^{3d+1}} d\nu(x) \otimes |\lambda|^d d\lambda$$

$$\hat{G}_\infty M \Sigma \mathfrak{v}_x M = \mathfrak{p}_x^{\rtimes} \oplus \mathfrak{q}_x^{\rtimes}$$

$$\mathfrak{p}_x^{\chi} \oplus i\mathfrak{q}_x^{\chi} = \mathbb{C}^d$$

$$\mathcal{F}^\lambda(\mathfrak{v}_x M) F : \mathfrak{v}_x M \to \mathbb{C}$$

$$\int_{\mathfrak{v}_x M} |F(z)|^2 e^{-\frac{|\lambda|}{2}|z|^2} dz < +\infty.$$

$$F \in \mathcal{F}^\lambda(\mathfrak{v}_x M)$$

$$\pi_{x,\mathcal{F}}^\lambda(g) F(w) = \exp\left(i\lambda r - \frac{\lambda}{4}|z|^2 - \frac{\lambda}{2} w\bar{z}\right) F(w + z), w \in \mathfrak{v}_x M = \mathfrak{p}_x M \oplus i\mathfrak{q}_x M,$$

$$g = \mathrm{Exp}_{G_x M}(x \cdot \langle X\rangle_x + y \cdot \langle Y\rangle_x + r\langle R\rangle_x), \text{ with } x, y \in \mathbb{R}^d, r \in \mathbb{R}.$$

$$\mathfrak{v}_x M = \mathfrak{p}_x^{\rtimes} \oplus \mathfrak{q}_x^{\rtimes}$$

$$\sigma = (x, \lambda\eta_x) \in \Sigma \sim \hat{G}_\infty M \Xi_\sigma \phi^{N\Sigma} g^{N\Sigma}$$

$$\phi_\sigma^{N\Sigma} = \mathrm{sgn}(\lambda(\sigma))\Xi^*(\phi_x)$$

$$g_\sigma^{N\Sigma} = \lambda(\sigma)\Xi^*(g_x)$$

$$h_\sigma^{N\Sigma}(V,W) := g_\sigma^{N\Sigma}(V,W) + i\omega_\sigma^{N\Sigma}(V,W)\omega_\sigma^{N\Sigma} g^{N\Sigma} h^{N\Sigma}$$

$$V = x \cdot \langle X \rangle_x + y \cdot \langle Y \rangle_x$$

$$\lambda(\sigma)|z|^2 = h_\sigma^{N\Sigma}(V,V) \text{ and } \lambda(\sigma) w\bar{z} = h_\sigma^{N\Sigma}(W,V),$$

$$W = p \cdot \langle X \rangle_x + q \cdot \langle Y \rangle_x$$

$$\mathcal{F}(N_\sigma\Sigma) := \left\{F : N_\sigma\Sigma \to \mathbb{C} : F \text{ is } \phi_\sigma^{N\Sigma}\text{-holomorphic} \right.$$
$$\left. \text{and } \int_{N_\sigma\Sigma} |F(W)|^2 e^{-\frac{1}{2}|g_\sigma^{N\Sigma}(W,W)|} d\mathrm{Leb}_\sigma^{N\Sigma}(W) < +\infty \right\}$$

$$\pi_{\sigma,\mathcal{F}}(g)F(W) = \exp\left(i\lambda(\sigma)r - \frac{1}{2}h_\sigma^{N\Sigma}\left(W + \frac{1}{2}V, V\right)\right)F(W+V)$$

$$g = \mathrm{Exp}_{G_x M}(V + r\langle R \rangle) V \in \mathfrak{v}_x M r \in \mathbb{R}\mathcal{F}(N\Sigma)$$

$$\mathcal{F}(N\Sigma) := \bigcup_{\sigma\in\Sigma} \mathcal{F}(N_\sigma\Sigma),$$

$$\mathcal{F}(N\Sigma) \sim \int_{\hat{G}_\infty M}^{\oplus} \mathcal{H}_{\pi_x} d\mu_{\hat{G}M}(x, \pi_x)$$

$$L^\infty_{a,b}(\hat{G}_x M), x \in M, \text{for } a, b \in \mathbb{R}$$

$$\|\cdot\|_{L^\infty_{a,b}(\hat{G}_x M)}$$

$$\sigma = \{\sigma_h\}_{h>0} \text{ on } \hat{G}M$$

$$\sigma(x,\cdot) = \left\{\sigma(x,\pi) : \mathcal{H}_\pi^\infty \to \mathcal{H}_\pi^\infty : \pi \in \hat{G}_x M\right\}$$

$$x \in M, \sigma(x,\cdot) \in L^\infty_{a,b}(\hat{G}_x M) \text{ for } a, b \in \mathbb{R}$$

$$\kappa_{\sigma,x} = \mathcal{F}^{-1}_{G_x M, \mu_x}(\sigma(x,\cdot)),$$

$$\kappa_{\sigma,x} \in \mathcal{S}'(G_x M)$$

$$\hat{\mu}_{\hat{G}_x M} \; (\; \mathbb{X}, U \;) \mathrm{Exp}_{G_x M} \kappa_{\sigma,x}^{\rtimes} \; \mathfrak{h}^d$$

$$\kappa_{\sigma,x}^{\rtimes}(v) := \kappa_{\sigma,x}(\mathrm{Exp}_x^{\rtimes}(v)) \in \mathcal{S}'(\mathfrak{h}^d).$$

$$\forall x \in U, \sigma^{\rtimes}(x,\cdot) := \mathcal{F}_{\mathbb{H}^d}(\kappa_{\sigma,x}^{\rtimes}).$$

$$S^m(\hat{G}M)\sigma = \{\sigma_\hbar\}_{\hbar>0}$$

$$x \in U \mapsto \sigma^{\mathbb{X}}(x,\cdot) \in S^m(\widehat{\mathbb{H}})$$

$$\mathcal{C} \subset U\beta \in \mathbb{N}^{2d+1}$$

$$\forall N \in \mathbb{N}, \sup_{x\in\mathcal{C}} \left\| D_{\hat{X}}^{\beta} \sigma_{\hbar}^{\rtimes}(x,\cdot) \right\|_{S^m(\widehat{\mathbb{H}}),N} < +\infty$$

$$D_{\hat{X}}^{\beta} = X_1^{\beta_1} \cdots X_d^{\beta_d} Y_1^{\beta_{d+1}} \cdots Y_d^{\beta_{2d}} R^{\beta_{2d+1}}$$

$$m_1 \leq m_2 \Longrightarrow S^{m_1}(\hat{G}M) \subset S^{m_2}(\hat{G}M)$$

$$S^{-\infty}(\hat{G}M) := \bigcap_{m\in\mathbb{R}} S^m(\hat{G}M)$$

$$\sigma = \{\sigma_\hbar\}_{\hbar>0}$$

$$r^N = r_\hbar^N \ {}_{\hbar>0}\ S^{m-N}(\hat{G}M)$$

$$\sigma_\hbar = \sum_{i=0}^{N-1} \hbar^i \sigma_i + \hbar^N r_\hbar^N \mathrm{End}(\mathcal{F}(N\Sigma))$$

$$\sigma \in S^0(\hat{G}M),$$

$$\hat{G}_\infty M \sim \Sigma,$$

$$\mathcal{F}(N_\sigma\Sigma), \sigma \in \Sigma,$$

$$S^0(\hat{G}M)S^0(\widehat{\mathbb{R}})\ \sigma \in \Sigma$$
$$(\ M, \eta\ )\hat{G}_\infty M$$

$$\chi \in C^\infty(M \times M)\exp^{\mathbb{X}}(U_{\mathbb{X}}) \subset U \times U$$

$$\chi_x(y) := \chi(x,y)$$

$$\sigma \in S^m(\hat{G}M)$$

$$\kappa_\sigma \mathcal{S}'(GM)\mathrm{Op}_\hbar^{\mathbb{X},\chi}(\sigma)f \in C^\infty(M)$$

$$\forall x \in U, \mathrm{Op}_\hbar^{\times,\chi}(\sigma)f(x) := \int_{w\in G_xM} \kappa_{\sigma,x}^{\hbar}(w)(\chi_x f)\big(\exp_x^{\times}(-\mathrm{Ln}_x^{\times}(w))\big)d\mu_x(w)$$

$$\kappa_{\sigma,x}^{\hbar} \in \mathcal{S}'(G_xM)$$

$$\kappa_{\sigma,x}^{\hbar}(w) := \hbar^{-Q}\kappa_{\sigma,x}(\delta_{\hbar^{-1}}w)$$

$$\mathrm{Op}_\hbar^{\mathbb{X},\chi}(\sigma)f(x) = \hbar^{-Q}\int_{v\in\mathbb{R}^n} \kappa_{\sigma,x}^{\mathbb{X},\hbar}(v)(\chi_x f)\big(\exp_x^{\mathbb{X}}(-v)\big)dv$$

$$\kappa_{\sigma,x}^{\mathbb{X},\hbar}(v) := \hbar^{-Q}\kappa_{\sigma,x}^{\mathbb{X}}(\delta_{\hbar^{-1}}v)$$

$$y = \exp_x^{\rtimes}(-v)$$

$$v \mapsto \exp_x^{\mathbb{X}}(-v)$$

$$\mathrm{Op}_\hbar^{\mathbb{X},\chi}(\sigma)f(x) = \hbar^{-Q}\int_M \kappa_{\sigma,x}^{\rtimes}\left(-\delta_\hbar^{-1}\ln_x^{\mathbb{X}}\ y\right)(\chi_x f)(y)\mathrm{jac}_y\left(\ln_x^{\mathbb{X}}\right)d\mathrm{vol}(y)$$

$$\mathrm{jac}_y\left(\ln_x^{\mathbb{X}}\right)\frac{d\ln_x^{\times}}{dy}\left(\exp_x^{\mathbb{X}}(-v)\right)^* dv\mathrm{Op}_\hbar^{\mathbb{X},\chi}(\sigma)$$

$$(x,y)\mapsto \hbar^{-Q}\kappa_{\sigma,x}^{\rtimes}(-\hbar^{-1}\ln_x^{\rtimes}(y))\chi_x(y)\mathrm{jac}_y(\ln_x^{\rtimes}) =: K_\hbar^{\rtimes}(x,y).$$

$$\gamma := \exp_{x_0}^{\tilde{\mathbb{X}}} : V\subset \mathbb{H}^d \to U,$$

$$v\in\mathbb{H}^d \sim \mathbb{R}^{2d+1}$$

$$\exp_x^{\tilde{\mathbb{X}}}(v) = \gamma\left(v *_{\mathbb{H}^d}\gamma^{-1}(x)\right)$$

$$(x,v)\in U\times\mathbb{H}^d\{\mu_x\}_{x\in M}$$

$$\forall x\in U, d\mu_x(v) = c(x)dv$$

$$\kappa_{\sigma,x} = \mathcal{F}_{G_xM,\mu_x}^{-1}(\sigma(x,\cdot))\{\tilde{\mu}_x\}_{x\in U}$$

$$\forall v\in\mathbb{R}^{2d+1}, \kappa_{\sigma,x}^{\tilde{\mathbb{X}}}(v) = c(x)^{-1}\mathcal{F}_{G_xM,\tilde{\mu}_x}^{-1}(\sigma(x,\cdot))\left(\mathrm{Exp}_x^{\tilde{\mathbb{X}}}(v)\right)$$

$$\begin{aligned}\forall x\in V, \left(\gamma^{-1}\circ\mathrm{Op}_\hbar^{\mathbb{X},\chi}(\sigma)\circ\gamma\right)f(x) &= \int_{\mathbb{H}^d}\kappa_{\sigma,x}^{\tilde{x},\hbar}(v)(\chi_x f)\left(v^{-1} *_{\mathbb{H}^d} x\right)c(x)dv\\ &= \int_{\widehat{\mathbb{H}}^d}\mathrm{Tr}_{\mathcal{H}_\pi}\left(\sigma^{\tilde{\mathbb{X}}}(x,\hbar\cdot\pi)\mathcal{F}_{\mathbb{H}^d}(\chi_x f)(\pi)\right)d\hat{\mu}_{\hat{\mathbb{A}}d}(\pi)\end{aligned}$$

$$\sigma^{\tilde{\mathbb{X}}}\ \mathrm{Op}_{\mathrm{H}^d,\hbar}$$

$$\gamma^{-1}\circ\mathrm{Op}_\hbar^{\mathbb{X},\chi}(\sigma)\circ\gamma = \mathrm{Op}_{\mathbb{H}^d,\hbar}\left(\sigma^{\tilde{\mathbb{X}}}\right).$$

$$P = \{P_\hbar\}_{\hbar>0} : C^\infty(M)\to C^\infty(M)$$

$$\psi_1,\psi_2\in C^\infty(M)\mathrm{supp}(\psi_1)\cap\mathrm{supp}(\psi_2) = \emptyset$$

$$\|\psi_1 P_\hbar\psi_2\|_{H^{-N}(M)\to H^N(M)} = \mathcal{O}(\hbar^\infty)$$

$$\psi\in C_c^\infty(U)$$

$$\sigma\in S^m(\hat{G}M)\hat{G}_{|U}M$$

$$\psi P_\hbar(\psi f) = \mathrm{Op}_\hbar^{\mathbb{X},\chi}(\sigma)f, f\in C^\infty(M)$$

$$\Psi_\hbar^\infty(M) := \bigcup_{m\in\mathbb{R}\cup\{-\infty\}}\Psi_\hbar^m(M)$$

$$\Psi_\hbar^m(M)\subset\Psi_\hbar^{m'}(M)$$

$$P_1\in\Psi_\hbar^{m_1}(M)P_2\in\Psi_\hbar^{m_2}(M)P_1\circ P_2 \text{ is in } \Psi_\hbar^{m_1+m_2}(M)$$

$$\mathcal{L}(H^s(M), H^{s-m}(M)) \text{ for any } s\in\mathbb{R}$$

$$\mathcal{A} = (\mathbb{X}_\alpha, U_\alpha, \chi_\alpha, \psi_\alpha)_{\alpha\in A}$$

$$(\psi_\alpha)_{\alpha\in A}\sum_\alpha \psi_\alpha^2 = (x,y)\in M\times M \mapsto \psi_\alpha(x)\psi_\alpha(y)\{\chi_\alpha(x,y)=1\}$$

$$\mathcal{A} = (\mathbb{X}_\alpha, U_\alpha, \chi_\alpha, \psi_\alpha)_{\alpha\in A}$$

$$\sigma \in S^m(\widehat{G}M) m \in \mathbb{R}\cup\{-\infty\} f \in C^\infty(M)$$

$$\forall x \in M, \mathrm{Op}_\hbar^{\mathcal{A}}(\sigma)f(x) := \sum_{\alpha\in A} \mathrm{Op}_\hbar^{\chi_\alpha,\chi_\alpha}(\psi_\alpha\sigma)(\psi_\alpha f)(x)$$

$$P = \{P_\hbar\}_{\hbar>0}: C^\infty(M) \to C^\infty(M)$$

$$m \in \mathbb{R}\cup\{-\infty\}$$

$$\sigma = \{\sigma_\hbar\}_{\hbar>0} \in S^m(\widehat{G}M)$$

$$R_\hbar: C^\infty(M) \to C^\infty(M)$$

$$A_\hbar = \mathrm{Op}_\hbar^{\mathcal{A}}(\sigma) + R_\hbar$$

$$\mathrm{princ}_\hbar: \Psi_\hbar^m(M) \to S^m(\widehat{G}M)/\hbar S^{m-1}(\widehat{G}M),$$

$$\sigma \in S^m(\widehat{G}M)$$

$$\mathrm{princ}_\hbar(\mathrm{Op}_\hbar(\sigma)) = [\sigma] \in S^m(\widehat{G}M)/\hbar S^{m-1}(\widehat{G}M)$$

$$P_1 \in \Psi_\hbar^{m_1}(M) \text{ and } P_2 \in \Psi_\hbar^{m_2}(M)$$

$$\mathrm{princ}_\hbar(P_1\circ P_2) = \mathrm{princ}_\hbar(P_1)\circ \mathrm{princ}_\hbar(P_2) \text{ and } \mathrm{princ}_\hbar(P_1^*) = \mathrm{princ}_\hbar(P_1)^*.$$

$$P = \{P_\hbar\}_{\hbar>0} \in \Psi_\hbar^m(M)\Psi_\hbar^\infty(M)$$

$$f \in C_c^\infty(\mathbb{R})$$

$$Q_{f,N}(\hbar) \in \Psi_\hbar^{-\infty}(M) R_{f,N}(\hbar) L^2(M)$$

$$f(-\hbar^2\Delta_{sR}) = Q_{f,N}(\hbar) + R_{f,N}(\hbar), \text{ with } R_{f,N}(\hbar) = \mathcal{O}_{L^2(M)\to L^2(M)}(\hbar^{N+1})$$

$$Q_{f,N}(\hbar)$$

$$\mathrm{princ}_\hbar\big(Q_{f,N}(\hbar)\big) = f(H)\mathrm{princ}_\hbar(-\hbar^2\Delta_{sR})\widehat{G}_\infty M$$

$$\sigma = \{\sigma_\hbar\}_{\hbar>0}$$

$$S^{-\infty}(\widehat{G}M)$$

$$K \subset \widehat{G}_\infty M$$

$$\mathrm{supp}(\chi)\cap K = \emptyset \text{ implies } \chi\sigma_\hbar \in \hbar^\infty S^{-\infty}(\widehat{G}M)$$

$$\chi \in C_c^\infty\big(\widehat{G}_\infty M\big)$$

$$\text{ess supp}_\infty(\sigma) \subset \widehat{G}_\infty M$$

$$P = \{P_\hbar\}_{\hbar>0} \in \Psi_\hbar^{-\infty}(M)$$

$$P_\hbar = \mathrm{Op}_\hbar(\sigma_\hbar) + R_\hbar$$

$$\sigma = \{\sigma_\hbar\}_{\hbar>0} \in S^{-\infty}(\hat{G}M)$$

$$\mathrm{WF}'_\infty(P) := \text{ ess supp}(\sigma)$$

$$\hat{G}_\infty M \sim \Sigma$$

$$P_1, P_2 \in \Psi_\hbar^{-\infty}(M)$$

$$\mathrm{WF}'_\infty(P_1 + P_2) \subset \mathrm{WF}'_\infty(P_1) \cup \mathrm{WF}'_\infty(P_2), \mathrm{WF}'_\infty(P_1 \circ P_2) \subset \mathrm{WF}'_\infty(P_1) \cap \mathrm{WF}'_\infty(P_2),$$

$$\mathrm{WF}'_\infty(P_1^*) = \mathrm{WF}'_\infty(P_1)$$

$$K \subset \hat{G}_\infty M$$

$$\Psi_\hbar^{-\infty}(M)$$

$$K \cap \mathrm{WF}'_\infty(P_1 - P_2) = \emptyset(\ M^{2d+1}, \eta, g\ ) - \hbar^2\Delta_{\mathrm{sR}}$$

$$\mathbb{X} = (X_1, \dots, X_d, Y_1, \dots, Y_d, R)$$

$$-\hbar^2\Delta_{\mathrm{sR}} = \sum_{i=1}^{d} (\hbar^2 X_i^* X_i + \hbar^2 Y_i^* Y_i)$$

$$(\hbar X_i, \hbar Y_i)_{i=1,\dots,d} \Psi_\hbar^1(M) \Psi_\hbar^2(M) \hat{G}M_{|U}$$

$$\mathrm{princ}_\hbar^2(-\hbar^2\Delta_{\mathrm{sR}})(x, \pi) = -\sum_{i=1}^{d} (\pi(\langle X_i \rangle_x)^2 + \pi(\langle Y_i \rangle_x)^2).$$

$$\hat{\varphi}_U^{\mathbb{X}} \hat{G}_\infty M(x, [\pi_x^\lambda]) \in \hat{G}_\infty M$$

$$H(x, [\pi_x^\lambda]) = |\lambda| \sum_{i=1}^{d} (-\partial_{\xi_i}^2 + \xi_i^2).$$

$$\xi \in \langle \mathfrak{p} \rangle_x\ \mathbb{R}^d$$

$$H(\lambda)(e_n)_{n\in\mathbb{N}} L^2(\mathbb{R})\ \xi \in \mathbb{R}$$

$$-e_n''(\xi) + \xi^2 e_n(\xi) = (2n+1)e_n(\xi).$$

$$\alpha \in \mathbb{N}^d$$

$$e_\alpha(\xi) := \prod_{i=1}^{d} e_{\alpha_i}(\xi_i), \xi = (\xi_1, \dots, \xi_d) \in \mathbb{R}^d$$

$$|\lambda|(2|\alpha| + d)$$

$$H(\lambda)e_\alpha = |\lambda|(2|\alpha| + d)e_\alpha, \alpha \in \mathbb{N}^d (e_\alpha)_{\alpha\in\mathbb{N}^d}$$

$$L^2(\mathbb{R}^d) H(\lambda) \{|\lambda|(2n + d)\}_{n\in\mathbb{N}} (e_\alpha)_{\alpha\in\mathbb{N}^d}$$

$$\mathrm{mult}(|\lambda|(2n+d)) = \binom{n+d-1}{n}.$$

$$e_\alpha, \alpha \in \mathbb{N}^d$$

$$|\alpha| = n$$

$$\Pi_n(x,[\pi_x^\lambda])H(x,[\pi_x^\lambda])$$

$$|\lambda|(2n+d)(x,[\pi_x^\lambda]) \in \hat{G}_\infty M\dot{S}^0(\hat{G}M)$$

$$\rho \in C_c^\infty(\hat{G}_\infty M,[0,1])\Pi_n^\rho$$

$$\forall (x,[\pi_x^\lambda]) \in \hat{G}_\infty M, \Pi_n^\rho(x,[\pi_x^\lambda]) := \rho(x,\lambda)\Pi_n(x,[\pi_x^\lambda])$$

$$\rho \in C_c^\infty(\hat{G}_\infty M,[0,1])S^{-\infty}(\hat{G}M)\mathrm{Op}_\hbar(\Pi_n^\rho)$$

$$[-\hbar^2\Delta_{\mathrm{sR}}, \mathrm{Op}_\hbar(\Pi_n^\rho)]$$

$$[H,\rho\Pi_n] = 0$$

$$[-\hbar^2\Delta_{\mathrm{sR}}, \mathrm{Op}_\hbar(\Pi_n^\rho)] \in \hbar\Psi_\hbar^{-\infty}(M)$$

$$\mathrm{Op}_\hbar(\Pi_n^\rho) \circ \mathrm{Op}_\hbar(\Pi_n^\rho) = \mathrm{Op}_\hbar\left(\Pi_n^{\rho^2}\right) + \hbar\Psi_\hbar^{-\infty}(M)$$

$$\mathrm{Op}_\hbar(\Pi_n^\rho)\{\rho = 1\} \subset \hat{G}_\infty M\mathcal{O}(\hbar) - \hbar^2\Delta_{\mathrm{sR}}\Pi_n^\rho\mathcal{O}(\hbar)$$

$$\hat{\Pi}_n^{\rho,\hbar}\ \Psi_\hbar^{-\infty}(M)\{\rho = 1\}$$

$$\left[-\hbar^2\Delta_{\mathrm{sR}}, \hat{\Pi}_n^{\rho,\hbar}\right] = 0 \ \text{ and } \ \hat{\Pi}_n^{\rho,\hbar} = \left(\hat{\Pi}_n^{\rho,\hbar}\right)^* = \hat{\Pi}_n^{\rho,\hbar} \circ \hat{\Pi}_n^{\rho,\hbar}(\hat{\Pi}_n^{\rho,k})_{k\in\mathbb{N}}$$

$$\hat{\Pi}_n^{\rho,0} = \mathrm{Op}_\hbar(\hat{\Pi}_n^\rho) \ \text{ and } \ \hat{\Pi}_n^{\rho,k} \in \Psi_\hbar^{-\infty}(M), k \geq 1,$$

$$\hat{\Pi}_n^{\rho,[k]} \circ \hat{\Pi}_n^{\rho,[k]} - \hat{\Pi}_n^{\rho,[k]} = \hbar^{k+1}R_{k+1} \ \text{ microlocally on } \{\rho = 1\}$$
$$\left[-\hbar^2\Delta_{\mathrm{sR}}, \hat{\Pi}_n^{\rho,[k]}\right] = \hbar^{k+1}T_{k+1}$$

$$\Psi_\hbar^{-\infty}(M)$$

$$\hat{\Pi}_n^{\rho,[k]} = \hat{\Pi}_n^{\rho,0} + \hbar\hat{\Pi}_n^{\rho,1} + \cdots + \hbar^k\hat{\Pi}_n^{\rho,k}\hat{\Pi}_n^{\rho,\hbar}$$

$$\hat{\Pi}_n^{\rho,0}, \hat{\Pi}_n^{\rho,1}, \ldots, \hat{\Pi}_n^{\rho,k}\Pi_n^{\rho,k+1} \in S^{-\infty}(\hat{G}M)$$

$$\Pi_n^\rho\Pi_n^{\rho,k+1} - \Pi_n^{\rho,k+1}\Pi_n^{\rho,\perp} + R_{k+1,0} = 0 \ \text{ and } \ [H,\Pi_n^{\rho,k+1}] + T_{k+1,0} = 0$$

$$\mathrm{princ}_\hbar(R_{k+1})\mathrm{princ}_\hbar(T_{k+1})R_{k+1,0}T_{k+1,0}\Pi_n^{\rho,\perp} = \mathrm{Id} - \Pi_n^\rho$$

$$\Pi_n^{\rho,k+1} \text{ on } \{\rho = 1\}$$

$$\Pi_n^\rho\Pi_n^{\rho,k+1}\Pi_n^\rho = -\Pi_n^\rho R_{k+1,0}\Pi_n^\rho \ \text{ and } \ \Pi_n^{\rho,\perp}\Pi_n^{\rho,k+1}\Pi_n^{\rho,\perp} = \Pi_n^{\rho,\perp}R_{k+1,0}\Pi_n^{\rho,\perp}$$

$$[\Pi_n^\rho, R_{k+1,0}] = \Pi_n^{\rho,k+1}$$

$$[H, \Pi_n^\rho \Pi_{k+1} \Pi_n^{\rho,\perp}] = -\Pi_n^\rho T_{k+1,0} \Pi_n^{\rho,\perp} \text{ and } [H, \Pi_n^{\rho,\perp} \Pi_{k+1} \Pi_n^\rho] = -\Pi_n^{\rho,\perp} T_{k+1,0} \Pi_n^\rho.$$

$$\Pi_n^\rho [H, R_{k+1,0}] \Pi_n^\rho = \Pi_n^\rho T_{k+1,0} \Pi_n^\rho \text{ and } \Pi_n^{\rho,\perp} [H, R_{k+1,0}] \Pi_n^{\rho,\perp} = -\Pi_n^{\rho,\perp} T_{k+1,0} \Pi_n^{\rho,\perp}.$$

$$Y = -\Pi_n^\rho T_{k+1,0} \Pi_n^{\rho,\perp}$$

$$X = \Pi_n^\rho \Pi_{k+1} \Pi_n^{\rho,\perp}$$

$$(H\Pi_n^\rho) X - X (H \Pi_n^{\rho,\perp}) = Y.$$

$$(x, \lambda) \in \hat{G}_\infty M$$

$$X = -\frac{1}{2\pi i} \int_\gamma (H\Pi_n^\rho - z)^{-1} Y (H\Pi_n^{\rho,\perp} - z)^{-1} dz$$

$$\Pi_n^\rho \Pi_n^{\rho,\perp}(x,\lambda) \in \mathrm{supp}(\rho) S^{-\infty}(\hat{G}M) \Pi_n^{\rho,k+1}$$

$$\hat{\Pi}_n^{\rho,k} = \mathrm{Op}_\hbar(\Pi_n^{\rho,k}) \in \Psi_\hbar^{-\infty}(M).$$

$$\begin{aligned}\hat{\Pi}_n^{\rho,[k]} R_{k+1} \left(1 - \hat{\Pi}_n^{\rho,[k]}\right) &= \hbar^{-k-1} \hat{\Pi}_n^{\rho,[k]} \left(\hat{\Pi}_n^{\rho,[k]} \circ \hat{\Pi}_n^{\rho,[k]} - \hat{\Pi}_n^{\rho,[k]}\right) \left(1 - \hat{\Pi}_n^{\rho,[k]}\right) \\ &= -\hbar^{-k-1} \left(\hat{\Pi}_n^{\rho,[k]} \circ \hat{\Pi}_n^{\rho,[k]} - \hat{\Pi}_n^{\rho,[k]}\right)^2 = -\hbar^{k+1} R_{k+1}^2\end{aligned}$$

$$\Pi_n^\rho R_{k+1,0} (1 - \Pi_n^\rho) = (1 - \Pi_n^\rho) R_{k+1,0} \Pi_n^\rho$$

$$\begin{aligned}\hat{\Pi}_n^{\rho,[k]} T_{k+1} \hat{\Pi}_n^{\rho,[k]} &= \hbar^{-k-1} \hat{\Pi}_n^{\rho,[k]} \left[-\hbar^2 \Delta_{sR}, \hat{\Pi}_n^{\rho,[k]}\right] \hat{\Pi}_n^{\rho,[k]} \\ &= \hbar^{-k-1} \hat{\Pi}_n^{\rho,[k]} \left(\hat{\Pi}_n^{\rho,[k]} (-\hbar \Delta_{sR}) \left(\hat{\Pi}_n^{\rho,[k]}\right)^2 - \left(\hat{\Pi}_n^{\rho,[k]}\right)^2 (-\hbar^2 \Delta_{sR}) \hat{\Pi}_n^{\rho,[k]}\right) \hat{\Pi}_n^{\rho,[k]} \\ &= \hat{\Pi}_n^{\rho,[k]} (-\hbar^2 \Delta_{sR}) R_{k+1} - R_{k+1} (-\hbar^2 \Delta_{sR}) \hat{\Pi}_n^{\rho,[k]}\end{aligned}$$

$$\Pi_n^\rho H R_{k+1,0} - R_{k+1,0} H \Pi_n^\rho = \Pi_n^\rho T_{k+1,0} \Pi_n^\rho$$

$$\Pi_n^\rho [H, R_{k+1,0}] \Pi_n^\rho = \Pi_n^\rho T_{k+1,0} \Pi_n^\rho$$

$$[\Pi_n^\rho, R_{k+1,0}] = \hat{\Pi}_n^{\rho,\hbar} \in \Psi_h^{-\infty}(M)$$

$$\hat{\Pi}_n^{\rho,\hbar} \sim \sum_{k \geq 0} \hbar^k \hat{\Pi}_n^{\rho,k}$$

$$\Pi_n^{\rho,k+1} \hat{\Pi}_n^{\rho,[k]} \hat{\Pi}_n^\rho \{\rho = 1\}$$

$$\left(\hat{\Pi}_n^{\rho,\hbar}\right)^* = \hat{\Pi}_n^{\rho,\hbar}$$

$$\{\rho = 1\} \left(\hat{\Pi}_n^{\rho,\hbar}\right)^* \Pi_n^\rho - \hbar^2 \Delta_{sR}$$

$$\left[-\hbar^2 \Delta_{sR}, \left(\hat{\Pi}_n^{\rho,\hbar}\right)^*\right] = 0 \text{ microlocally on } \{\rho = 1\}$$

$$\hat{\Pi}_n^{\rho,\hbar}, n \geq 0$$

$$\hat{\Pi}_n^{\rho,\hbar} \circ \hat{\Pi}_m^{\rho,\hbar} = 0 \text{ microlocally on } \{\rho = 1\}.$$

$$f \in C_c^\infty(\mathbb{R})$$

$$\left[f(-\hbar^2\Delta_{sR}), \hat{\Pi}_n^{\rho,\hbar}\right] = 0 \text{ microlocally on } \{\rho = 1\}$$

$$\rho \in C_c^\infty(\hat{G}_\infty M, [0,1])\Psi_\hbar^{-\infty}(M)$$

$$\mathcal{T}_n^\rho(M)\Psi_\hbar^{-\infty}(M)$$

$$\mathcal{T}_n^\rho(M) := \left\{\hat{\Pi}_n^{\rho,\hbar} \circ A \circ \hat{\Pi}_n^{\rho,\hbar} : A \in \Psi_\hbar^\infty(M)\right\}.$$

$$B \in \Psi_\hbar^{-\infty}(M)\mathcal{T}_n^\rho(M)\{\rho = 1\}\hat{G}_\infty M \sim \Sigma\mathcal{L}_n(N\Sigma)\Pi_n\mathcal{F}(N\Sigma)$$

$$\mathcal{L}_n(N\Sigma) = \Pi_n\mathcal{F}(N\Sigma)\mathcal{T}_n^\rho(M)\hat{\Pi}_n^{\rho,\hbar}A\hat{\Pi}_n^{\rho,\hbar}\mathrm{End}(\mathcal{L}_n(N\Sigma))$$

$$\Theta_n \in \mathcal{T}_n^\rho(M)\{\rho = 1\}$$

$$-\hbar^2\Delta_{sR}\hat{\Pi}_n^{\rho,\hbar} = \hat{\Pi}_n^{\rho,\hbar}((2n+d)\hbar^2|R|)\hat{\Pi}_n^{\rho,\hbar} + \hbar^2\Theta_n.$$

$$\theta_n \in C^\infty\left(\hat{G}_\infty M, \mathrm{End}(\mathcal{L}_n(N\Sigma))\right)\Theta_n\mathcal{T}_n^\rho(M)$$

$$\hat{\Pi}_n^{\rho,\hbar}(-\hbar^2\Delta_{sR} - (2n+d)\hbar^2|R|)\hat{\Pi}_n^{\rho,\hbar} \in \hbar^2\Psi_\hbar^{-\infty}(M) \text{ microlocally on } \{\rho = 1\}$$

$$\Pi_n^\rho\hbar\Psi_\hbar^{-\infty}(M)$$

$$\tilde{\mathbb{X}} = (\tilde{X}_1, \dots, \tilde{X}_d, \tilde{Y}_1, \dots, \tilde{Y}_d, R)\mathrm{Op}_{\mathbb{H}^d,\hbar}\mathbb{H}^d$$

$$-\hbar^2\Delta_{sR} = \mathrm{Op}_{\mathbb{H}^d,\hbar}(\tilde{H}_0 + \hbar\tilde{H}_1) \text{ and } \hbar^2|R| = \mathrm{Op}_{\mathbb{H}^d,\hbar}(\lambda)$$

$$S^2(\mathbb{H}^d \times \hat{\mathbb{H}}^d) \text{ and } S^1(\mathbb{H}^d \times \hat{\mathbb{H}}^d)$$

$$\hat{\Pi}_n^{\rho,\hbar} = \mathrm{Op}_{\mathbb{H}^d,\hbar}(\tilde{\Pi}_n^0 + \hbar\tilde{\Pi}_n^1 + \hbar^2\tilde{\Pi}_n^{\geq 2})$$

$$\tilde{\Pi}_n^0, \tilde{\Pi}_n^1 \text{ and } \tilde{\Pi}_n^{\geq 2}$$

$$\tilde{H}_0\tilde{\Pi}_n^0 = (2n+d)\tilde{\Pi}_n^0$$

$$(\tilde{g}_{i,j}(x))_{1\leq i,j\leq 2d}, x \in \mathbb{H}^d$$

$$g_{\mathcal{D}}(x)(\tilde{V}_1, \dots, \tilde{V}_d) = (\tilde{X}_1, \dots, \tilde{X}_d, \tilde{Y}_1, \dots, \tilde{Y}_d)\tilde{H}_0$$

$$\tilde{H}_0(x, \tilde{\pi}^\lambda) = \sum_{1\leq i,j\leq 2d} \tilde{g}_{i,j}(x)\tilde{\pi}^\lambda(\tilde{V}_i)\tilde{\pi}^\lambda(\tilde{V}_j)$$

$$\mathcal{H}_{\tilde{\pi}^\lambda}^{-\infty} = L^2(\tilde{\mathfrak{p}}_x)$$

$$g_{\mathcal{D}}(x)\mathcal{D}_x \sim \tilde{\mathfrak{v}}_x$$

$$(d\eta)_{|\mathcal{D},x}\tilde{\mathfrak{v}}_x = \tilde{\mathfrak{p}}_x \oplus \tilde{\mathfrak{q}}_x$$

$$(\xi, \zeta) \in \mathbb{R}^{2d}g_{\mathcal{D}}(x)$$

$$|\lambda| \sum_{i=1}^{d} \left(\xi_i^2 + \zeta_i^2\right).$$

$$L^2(\tilde{\mathfrak{p}}_x)\tilde{H}_0\left(x, \tilde{\pi}^\lambda\right)$$

$$(-\hbar^2 \Delta_{sR} - (2n+d)\hbar^2 |R|)\hat{\Pi}_n^{\rho,\hbar} = \hbar \mathrm{O}_{\mathbb{H}^d,\hbar}(T_1) + \hbar^2 \Psi_\hbar^{-\infty}\left(\mathbb{H}^d\right)$$

$$T_1 = \left(\tilde{H}_0 - (2n+d)|\lambda|\right)\tilde{\Pi}_n^1 + \tilde{H}_1 \tilde{\Pi}_n^0 + \Delta_{\tilde{v}}\left(\tilde{H}_0 - (2n+d)\lambda\right) \cdot \tilde{V}\tilde{\Pi}_n^0$$

$$\hat{\Pi}_n^{\rho,\hbar}\{\rho = 1\}$$

$$\tilde{\Pi}_n^0 T_1 \tilde{\Pi}_n^0 = 0 \ \text{ on } \{\rho = 1\}$$

$$\tilde{\Pi}_n^0 \mathrm{Op}_{\mathbb{H}^d,h} \tilde{\mathbb{X}}$$

$$\left[\tilde{H}_0, \tilde{\Pi}_n^1\right] + \left[\tilde{H}_1, \tilde{\Pi}_n^0\right] + \Delta_{\tilde{v}}\tilde{H}_0 \cdot \tilde{V}\tilde{\Pi}_n^0 - \Delta_{\tilde{v}}\tilde{\Pi}_n^0 \cdot \tilde{V}\tilde{H}_0 = 0.$$

$$\tilde{\Pi}_n^0 T_1 \tilde{\Pi}_n^0 = \tilde{\Pi}_n^0 \tilde{H}_1 \tilde{\Pi}_n^0 + \tilde{\Pi}_n^0\left(\Delta_{\tilde{v}}\tilde{\Pi}_n^0 \cdot \tilde{V}\tilde{H}_0\right)\tilde{\Pi}_n^0$$

$$\tilde{\Pi}_n^0 \tilde{H}_1 \tilde{\Pi}_n^0 = \mathfrak{G}$$

$$\tilde{V}\tilde{H}_0\left(x, \tilde{\pi}^\lambda\right) = \sum_{1 \le i,j \le 2d} \tilde{V}\tilde{g}_{i,j}(x)\tilde{\pi}^\lambda\left(\tilde{V}_i\right)\tilde{\pi}^\lambda\left(\tilde{V}_j\right)$$

$$\tilde{\Pi}_n^0\left(\Delta_{\tilde{v}}\tilde{\Pi}_n^0 \cdot \tilde{V}\tilde{H}_0\right)\tilde{\Pi}_n^0 = -\hbar^2 \Delta_{sR}$$

$$\hbar^2 |R| + \hbar^2 \Theta_n$$

$$\mathcal{L}_n(N\Sigma)(\sigma(t), v(t))\sigma(t) \in \Sigma\, \vec{\lambda} \in \Gamma(\Sigma) v(t) \in \mathcal{L}_n\left(N_{\sigma(t)}\Sigma\right)$$

$$\frac{d}{dt} v(t) = i\theta_n(\sigma(t)) v(t) \Phi_t^n$$

$$(\Phi_t^n)^* C^\infty(\Sigma, \mathcal{L}_n(N\Sigma))\mathcal{L}_n(N\Sigma)\mathrm{Ad}(\Phi_t^n)\mathrm{End}(\mathcal{L}_n(N\Sigma))C^\infty\left(\Sigma, \mathrm{End}(\mathcal{L}_n(N\Sigma))\right)\mathrm{Ad}(\Phi_t^n)^*$$

$$\sigma \in C^\infty\left(\Sigma, \mathrm{End}(\mathcal{L}_n(N\Sigma))\right)$$

$$\frac{d}{dt}\mathrm{Ad}(\Phi_t^n)^* \sigma = \vec{\lambda}\sigma + i[\theta_n, \sigma]$$

$$A \in \mathcal{T}_n^\rho(M)$$

$$\alpha \in C^\infty\left(\hat{G}_\infty M, \mathcal{L}_n(N\Sigma)\right)$$

$$(\tilde{A}(t))_{0 \le t \le T}(\tilde{\alpha}_t)_{0 \le t \le T}$$

$$\forall 0 \le t \le T, \tilde{\alpha}_t = \mathrm{Ad}(\Phi_t^n)^* \alpha$$

$$e^{it\Delta_{sR}} A e^{-it\Delta_{sR}} = \tilde{A}(t) + \mathcal{O}(\hbar) \ \text{ uniformly for } 0 \le t \le T.$$

$$\partial_t \tilde{\alpha}_t = \vec{\lambda}\tilde{\alpha}_t + i[\theta_n, \tilde{\alpha}_t]$$

$$\frac{i}{\hbar^2}\left[-\hbar^2\Delta_{sR}, \tilde{A}(t)\right] = \frac{i}{\hbar^2}\left[-\hbar^2 iR + \hbar^2\Theta_n, \tilde{A}(t)\right]$$

$$\vec{\lambda}\tilde{\alpha}_t + i[\theta_n\tilde{\alpha}_t]$$

$$\partial_t\tilde{A}(t) = \frac{i}{\hbar^2}\left[-\hbar^2\Delta_{sR}, \tilde{A}(t)\right] + E(t), E(t) \in \hbar\Psi_{\hbar}^{-\infty}(M)$$

$$\partial_t\left(e^{-it\Delta_{sR}}\tilde{A}(t)e^{it\Delta_{sR}}\right) = e^{-it\Delta_{sR}}\left(\partial_t\tilde{A}(t) - \frac{i}{\hbar^2}\left[-\hbar^2\Delta_{sR}, \tilde{A}(t)\right]\right)e^{it\Delta_{sR}}$$
$$= e^{-it\Delta_{sR}}E(t)e^{it\Delta_{sR}} = \mathcal{O}_{L^2(M)\to L^2(M)}(\hbar)$$

$$\Psi_{\hbar}^{-\infty}(M)(\,-\Delta_{sR}, \mathrm{Dom}(-\Delta_{sR}))$$

$$0 \le \delta_0 \le \delta_1 \le \cdots \le \delta_k \le \cdots \to +\infty(\varphi_k)_{k\in\mathbb{N}}$$

$$-\Delta_{sR}\varphi_k = \delta_k\varphi_k \text{ and } \|\varphi_k\|_{L^2(M)} = 1$$

$$\forall k \in \mathbb{N}, -\hbar^2\Delta_{sR}\varphi_k = \delta_k(\hbar)\varphi_k \text{ where } \delta_k(\hbar) = \hbar^2\delta_k$$

$$B \in \Psi_{\hbar}^{-\infty}(M)$$

$$\hbar^Q \sum_{a\le\delta_k(\hbar)\le b} \langle B\varphi_k, \varphi_k\rangle \underset{\hbar\to 0}{\longrightarrow} \mathrm{vol}(M)\int_{\hat{G}M} \mathrm{Tr}\left(\mathbf{1}_{[a,b]}(H)(x,\pi)\beta(x,\pi)\right)d\mu_{\hat{G}M}(x,\pi)$$

$$\beta \in S^{-\infty}(\hat{G}M)$$

$$B = \hat{\Pi}_n^{\rho,\hbar}$$

$$2\frac{\mathrm{vol}(M)}{(d+1)(2\pi)^{3d+1}}\frac{\binom{n+d-1}{n}}{(2n+d)^{d+1}} - \Delta_{sR}$$

$$B \in \Psi_{\hbar}^{-\infty}(M)L^2(M)$$

$$\beta \in S^{-\infty}(\hat{G}M)$$

$$\mathrm{Tr}(B) = \mathrm{vol}(M)\int_{\hat{G}M} \mathrm{Tr}_{\mathcal{H}_\pi}(\beta(x,\pi))d\hat{\mu}_{\hat{G}M}(x,\pi) + \mathcal{O}(\hbar)$$

$$B = \sum_{\alpha\in A} \mathrm{Op}_{\hbar}^{\mathbb{X}_\alpha,\chi_\alpha}(\psi_\alpha\beta_\hbar)\psi_\alpha + R_\hbar$$

$$S^{-\infty}(\hat{G}M)\beta_\hbar = \beta + \hbar S^{-\infty}(\hat{G}M)\mathcal{A} = (\mathbb{X}_\alpha, U_\alpha, \chi_\alpha, \psi_\alpha)R_\hbar\colon C^\infty(M) \to C^\infty(M)$$

$$\sigma \in S^{-\infty}(\hat{G}M)$$

$$\mathrm{Op}_{\hbar}^{\chi_\alpha,\chi_\alpha}(\psi_\alpha\sigma)\psi_\alpha$$

$$K_{\hbar}^{\rtimes_\alpha}(x,y) = \hbar^{-Q}\kappa_{\sigma,x}^{\rtimes_\alpha}(-\hbar^{-1}\ln_x^{\rtimes}(y))\chi_x(y)\mathrm{jac}_y(\ln_x^{\rtimes})\psi_\alpha(x)\psi_\alpha(y),$$

$$\kappa_\sigma^{\rtimes_\alpha}M \times M\mathrm{Op}_{\hbar}^{\rtimes_\alpha,\chi_\alpha}(\psi_\alpha\sigma)\psi_\alpha\mathcal{O}(\hbar^\infty)$$

$$\mathrm{Op}_{\hbar}^{\hat{\alpha}_\alpha,\chi_\alpha}(\psi_\alpha\sigma)\psi_\alpha K_{\hbar}^{\hat{\alpha}_\alpha}$$

$$\mathrm{Tr}\big(\mathrm{Op}_\hbar^{\chi_\alpha,\chi_\alpha}(\psi_\alpha\sigma)\psi_\alpha\big)=\int_M K_\hbar^{\rtimes_\alpha}(x,x)d\mathrm{vol}(x)$$
$$=\hbar^{-Q}\int_M \kappa_{\sigma,x}^{\chi_\alpha}(0)\psi_\alpha(x)^2 d\mathrm{vol}(x)$$
$$=\hbar^{-Q}\int_M\int_{\hat{G}_xM}\mathrm{Tr}_{\mathcal{H}_\pi}(\sigma(x,\pi))\psi_\alpha(x)^2 d\hat{\mu}_{\hat{G}_xM}(\pi)d\nu(x)$$

$$\mathrm{Tr}(B)=\hbar^{-Q}\sum_{\alpha\in A}\int_M\int_{\hat{G}_xM}\mathrm{Tr}_{\mathcal{H}_\pi}(\beta(x,\pi))\psi_\alpha(x)^2 d\hat{\mu}_{\hat{G}_xM}(\pi)d\nu(x)+\mathcal{O}(\hbar)$$
$$=\hbar^{-Q}\int_{\hat{G}M}\mathrm{Tr}_{\mathcal{H}_\pi}(\beta(x,\pi))d\hat{\mu}_{\hat{G}M}(x,\pi)+\mathcal{O}(\hbar)$$

$$\underline{f}\mathbf{1}_{[a,b]}=\underline{f}\ \text{ and }\ \bar{f}\mathbf{1}_{[a,b]}=\mathbf{1}_{[a,b]},$$

$$\mathrm{supp}\left(\underline{f_\varepsilon}\right)\subset[a+\varepsilon,b-\varepsilon]\mathrm{supp}\left(\overline{f_\varepsilon}\right)\subset[a-\varepsilon,b+\varepsilon]-\hbar^2\Delta_{sR}[a,b]$$

$$\sum_{a\le\delta_k(\hbar)\le b}\langle B\varphi_k,\varphi_k\rangle=\mathrm{Tr}\big(B\Pi_{[a,b]}\big)=\mathrm{Tr}\left(\underline{f_\varepsilon}(-\hbar^2\Delta_{sR})B\right)+\mathrm{Tr}\left(\left(\overline{f_\varepsilon}\left(1-\underline{f_\varepsilon}\right)\right)(-\hbar^2\Delta_{sR})B\Pi_{[a,b]}\right).$$

$$\mathrm{Tr}\left(|\,\overline{f_\varepsilon}\left(1-\underline{f_\varepsilon}\right)\right)(-\hbar^2\Delta_{sR})\,|\Big)\le(c_1(\varepsilon)+c_2(\hbar,\varepsilon))\hbar^{-Q}$$

$$\lim_{\varepsilon\to0}c_1(\varepsilon)=\varepsilon\underline{f_\varepsilon}\,\overline{f_\varepsilon}\lim_{\hbar\to0}c_2(\hbar,\varepsilon)$$

$$\hbar^Q\mathrm{Tr}\big(B\Pi_{[a,b]}\big)=\hbar^Q\mathrm{Tr}\left(\underline{f_\varepsilon}(-\hbar^2\Delta_{sR})B\right)+\mathcal{O}\left(\|B\Pi_{[a,b]}\|_{\mathcal{L}(L^2(M))}(c_1(\varepsilon)+c_2(\hbar,\varepsilon))\right.$$
$$=\int_{\hat{G}M}\mathrm{Tr}_{\mathcal{H}_\pi}\left(\underline{f_\varepsilon}(H)(x,\pi)\beta(x,\pi)\right)d\hat{\mu}_{\hat{G}M}(x,\pi)+\mathcal{O}_\varepsilon(\hbar)+\mathcal{O}(c_1(\varepsilon)+c_2(\hbar,\varepsilon))$$

$$\limsup_{\hbar\to0}\hbar^Q\mathrm{Tr}\big(B\Pi_{[a,b]}\big)=\int_{\hat{G}M}\mathrm{Tr}_{\mathcal{H}_\pi}\underline{(f_\varepsilon}(H)(x,\pi)\beta(x,\pi)\Big)d\hat{\mu}_{\hat{G}M}(x,\pi)+\mathcal{O}(c_1(\varepsilon))$$

$$(\delta_k)_{k\in\mathbb{N}}\ -\Delta_{sR}$$

$$\frac{1}{N(\delta)}\sum_{k,\delta_k\le\delta}\left|\langle a(\cdot)\varphi_k,\varphi_k\rangle-\int_M a(x)d\nu(x)\right|^2\underset{\delta\to+\infty}{\longrightarrow}-\Delta_{sR}\text{: for } n\in\mathbb{N}^*$$

$$\hbar_n=\frac{1}{\sqrt{\delta_n}}$$

$$N_{\hbar_n}=\mathrm{Card}(\{k\in\mathbb{N}:\delta_k(\hbar_n)\in[0,1]\}),$$

$$N_{\hbar_n}=N(\delta_n)L^2(M)$$

$$\mathrm{Var}_{\hbar_n}(B)=\frac{1}{N_{\hbar_n}}\sum_{0\le\delta_k(\hbar_n)\le1}|\langle B\varphi_k,\varphi_k\rangle|^2.$$

$$A=(a(\cdot)-m_a)f(-\hbar_n^2\Delta_{sR})\in\mathcal{L}(L^2(M)),$$

$$m_a := \int_M a(x) d\nu(x)$$

$$\limsup_{\hbar_n \to 0} \mathrm{Var}_{\hbar_n}(A) = \Psi_\hbar^{-\infty}(M)$$

$$(a(\cdot) - m_a) f(H) \Psi_\hbar^{-\infty}(M)$$

$$|\langle CB\varphi_k, \varphi_k \rangle|^2 \le \|CB\varphi_k\|_{L^2(M)}^2 \le \|C\|_{\mathcal{L}(L^2(M))}^2 \langle B^* B \varphi_k, \varphi_k \rangle.$$

$$\limsup_{\hbar_n \to 0} \mathrm{Var}_{\hbar_n}(CB) \le \|C\|_{\mathcal{L}(L^2(M))}^2 \limsup_{\hbar_n \to 0} \frac{1}{N_{\hbar_n}} \sum_{0 \le \delta_k(\hbar_n) \le 1} \langle B^* B \varphi_k, \varphi_k \rangle$$
$$\lesssim \|C\|_{\mathcal{L}(L^2(M))}^2 \int_{\hat{G}M} \mathrm{Tr}_{\mathcal{H}_\pi}\big(\beta(x,\pi)^* \beta(x,\pi) \mathbf{1}_{[0,1]}(H)(x,\pi)\big) d\hat{\mu}_{\hat{G}M}(x,\pi)$$

$$\rho_m \in C_c^\infty\big(\hat{G}_\infty M\big)$$

$$\rho_m(x,\lambda) = 1 \text{ if } \lambda \text{ is in } [(2m+d)^{-1}, 1]$$

$$\hat{\Pi}_j^{\rho_m,\hbar}, j = 1, \ldots, m-1$$

$$\hat{\Pi}_{<m}^{\hbar_n} = \sum_{j=1}^{m-1} \hat{\Pi}_j^{\rho_m,\hbar_n} \in \Psi_\hbar^{-\infty}(M)$$

$$\Pi_{<m}^{\rho_m} := \rho_m \sum_{j=0}^{m-1} \Pi_j$$

$$\limsup_{\hbar_n \to 0} \mathrm{Var}_{\hbar_n}(A) \le 2\limsup_{\hbar_n \to 0} \mathrm{Var}_{\hbar_n}(B_1) + 2\limsup_{\hbar_n \to 0} \mathrm{Var}_{\hbar_n}(B_2),$$

$$B_1 = \hat{\Pi}_{<m}^{\hbar_n} A \hat{\Pi}_{<m}^{\hbar_n},$$

$$B_2 = \hat{\Pi}_{<m}^{\hbar_n} A \left(\mathrm{Id} - \hat{\Pi}_{<m}^{\hbar_n}\right) + \left(\mathrm{Id} - \hat{\Pi}_{<m}^{\hbar_n}\right) A \hat{\Pi}_{<m}^{\hbar_n} + \left(\mathrm{Id} - \hat{\Pi}_{<m}^{\hbar_n}\right) A \left(\mathrm{Id} - \hat{\Pi}_{<m}^{\hbar_n}\right).$$

$$B_2 = \left(\mathrm{Id} - \hat{\Pi}_{<m}^{\hbar_n}\right) A \left(\mathrm{Id} - \hat{\Pi}_{<m}^{\hbar_n}\right) + \mathcal{O}_{L^2(M) \to L^2(M)}(\hbar).$$

$$\limsup_{\hbar_n \to 0} \mathrm{Var}_{\hbar_n}(B_2) \le \|A\|_{\mathcal{L}(L^2(M))}^2 \int_{\hat{G}M} \mathrm{Tr}_{\mathcal{H}_\pi}\left(\left(1 - \Pi_{<m}^{\rho_m}\right)^2 \mathbf{1}_{[0,1]}(H)\right) d\hat{\mu}_{\hat{G}M}$$

$$\lambda \in [(2m+d)^{-1}, 1]$$

$$\mathrm{Tr}_{\mathcal{H}_{\pi^\lambda}}\left(\left(1 - \Pi_{<m}^{\rho_m}(x,\lambda)\right)^2 \mathbf{1}_{[0,1]}(H(\lambda)\right) = 0$$

$$\rho_m(x,\lambda) = H(\lambda)\Pi_{<m} = \sum_{j=0}^{m-1} \Pi_j \{\lambda \le (2m+d)^{-1}\}$$

$$\mathrm{Tr}_{\mathcal{H}_{\pi^\lambda}}\big(\mathbf{1}_{[0,1]}(H(\lambda))\big) \le C_d |\lambda|^{-d}$$

$$C_d \|A\|_{\mathcal{L}(L^2(M))}^2 \int_{M \times \mathbb{R}^*} \mathbf{1}_{[0,(2m+d)^{-1}]}(|\lambda|) d\lambda d\nu(x) = 2C_d \|A\|_{\mathcal{L}(L^2(M))}^2 (2m+d)^{-1}$$

$$B_1 = \sum_{j=0}^{m-1} \hat{\Pi}_j^{\rho_m,\hbar_n} A \hat{\Pi}_j^{\rho_m,\hbar_n} + \mathcal{O}_{L^2(M)\to L^2(M)}(\hbar)$$

$$\hat{\Pi}_j^{\rho_m,\hbar_n} A \hat{\Pi}_j^{\rho_m,\hbar_n} B_1^j \; \mathcal{T}_j^{\rho_m}(M)\beta_j \in C^\infty\big(\hat{G}_\infty M, \mathrm{End}(\mathcal{L}_m(N\Sigma))\big)$$

$$\mathcal{L}_j(N\Sigma)a(\cdot) - m_a$$

$$\beta_j(x,\lambda) = f_j(\lambda)(a(x) - m_a)$$

$$f_j \in C_c^\infty(\mathbb{R}^*)$$

$$\left\langle B_1^j \varphi_k, \varphi_k \right\rangle = \left\langle B_1^j e^{-it\delta_k}\varphi_k, e^{-it\delta_k}\varphi_k \right\rangle = \left\langle B_1^j e^{-it\Delta_{sR}}\varphi_k, e^{-it\Delta_{sR}}\varphi_k \right\rangle$$

$$B_1^j(t) = e^{it\Delta_{sR}} B_1^j e^{-it\Delta_{sR}}$$

$$\left\langle B_1^j \varphi_k, \varphi_k \right\rangle = \left\langle \left\langle B_1^j \right\rangle_T \varphi_k, \varphi_k \right\rangle,$$

$$\left\langle B_1^j \right\rangle_T = \frac{1}{T}\int_0^T B_1^j(t)dt$$

$$\left\langle B_1^j \right\rangle_T = \left\langle \tilde{B}_1^j \right\rangle_T + \mathcal{O}_{L^2(M)\to L^2(M)}(\hbar),$$

$$\tilde{B}_1^j(t) \; \mathcal{T}_m^\rho(M)\tilde{\beta}_j(t)$$

$$\tilde{\beta}_j(t) = \mathrm{Ad}\big(\Phi_t^j\big)^* \beta_j$$

$$\left\langle \tilde{B}_1^j \right\rangle_T = \frac{1}{T}\int_0^T \tilde{B}_1^j(t)dt$$

$$\mathrm{Ad}\big(\Phi_t^j\big)^* \tilde{\beta}_j(t)$$

$$\tilde{\beta}_j(t) = \beta_j\big(\Phi_t^j\big)\mathcal{L}_j(N\Sigma)$$

$$\langle \tilde{\beta}^j \rangle_T = \frac{1}{T}\int_0^T \tilde{\beta}_j(t)dt$$

$$\tilde{\rho}_m \in C_c^\infty\big(\hat{G}_\infty M\big) \mathrm{supp}(\tilde{\rho}_m) \subset \{\rho_m = 1\}$$

$$\tilde{\rho}_m(x,\lambda) = 1 \text{ if } \lambda \text{ is in } [(2m-1+d)^{-1}, 1]$$

$$\limsup_{\hbar_n\to 0}\mathrm{Var}_{\hbar_n}(B_1^j) = \limsup_{\hbar_n\to 0}\mathrm{Var}_{\hbar_n}\left(\left\langle B_1^j\right\rangle_T\right)$$
$$= \limsup_{\hbar_n\to 0}\mathrm{Var}_{\hbar_n}\left(\mathrm{Op}(\tilde{\rho}_m)\left\langle \tilde{B}_1^j\right\rangle_T\right) + \limsup_{\hbar_n\to 0}\mathrm{Var}_{\hbar_n}\left(\left(\mathrm{Id}-\mathrm{Op}_{\hbar_n}(\tilde{\rho}_m)\right)\left\langle B_1^j\right\rangle_T\right)$$
$$\leq \int_{\hat{G}M} |\tilde{\rho}_m|^2 \mathrm{Tr}_{\mathcal{H}}\left(\langle\tilde{\beta}_j\rangle_T^*\langle\tilde{\beta}_j\rangle_T \mathbf{1}_{[0,1]}(H)\right) d\hat{\mu}_{\hat{G}M}$$
$$+\left\|\left\langle B_1^j\right\rangle_T\right\|_{\mathcal{L}(L^2(M))}\int_{\hat{G}M}(1-\tilde{\rho}_m)^2\mathrm{Tr}_{\mathcal{H}_\pi}\left(\mathbf{1}_{[0,1]}(H)\right)d\hat{\mu}_{\hat{G}M}$$
$$\leq \int_{\hat{G}M}\left|\langle\tilde{\beta}_j\rangle_T\right|^2 \mathrm{Tr}_{\mathcal{H}_\pi}\left(\Pi_m^\rho \mathbf{1}_{[0,1]}(H)\right)d\hat{\mu}_{\hat{G}M}$$
$$+\|B_1^j\|_{\mathcal{L}(L^2(M))}\int_{\hat{G}M}(1-\tilde{\rho}_m)^2\mathrm{Tr}_{\mathcal{H}_\pi}\left(\mathbf{1}_{[0,1]}(H)\right)d\hat{\mu}_{\hat{G}M}$$

$$C_d\int_{\mathbb{R}^*}\left(\int_M \left|\langle a\rangle_T^\lambda(x)-m_a\right|^2 d\nu(x)\right)\left|f_j(\lambda)\right|^2 d\lambda$$

$$\langle a\rangle_T^\lambda := \frac{1}{T}\int_0^T a\left(\Phi_t^{\mathrm{sgn}(\lambda)}\right)dt$$

$$\int_M \left|\langle a\rangle_T^\lambda(x)-m_a\right|^2 d\nu(x) \underset{T\to+\infty}{\longrightarrow} 0$$

$$\limsup_{\hbar_n\to 0}\mathrm{Var}_{\hbar_n}(B_1^j) = +\limsup_{\hbar_n\to 0}\mathrm{Var}_{\hbar_n}(B_1)$$

$$f\in C_c^\infty(\mathbb{R})f(-\hbar^2\Delta_{sR})L^2(M)$$

$$\tilde{\mathcal{A}} = \left(\tilde{\mathbb{X}}_\alpha, U_\alpha, \chi_\alpha, \psi_\alpha\right)_{\alpha\in A}\tilde{\mathbb{X}}_\alpha, \alpha\in A\exp_{x_\alpha}^{\tilde{x}_\alpha}V_\alpha\subset\mathbb{H}^d U_\alpha\gamma_\alpha K_\alpha\subset U_\alpha\mathrm{supp}(\psi_\alpha)\subset\mathrm{Int}(K_\alpha)$$

$$\bar{\psi}_\alpha, \bar{\bar{\psi}}_\alpha\in C_c^\infty(M)\mathrm{Int}(K_\alpha)\bar{\psi}_\alpha\equiv\mathrm{supp}(\psi_\alpha)\text{ and }\bar{\bar{\psi}}_\alpha\equiv\mathrm{supp}(\bar{\psi}_\alpha)$$

$$V_\alpha\subset\mathbb{H}^d\gamma_\alpha$$

$$T_\alpha(\hbar), \hbar > \rho_\alpha\in C_c^\infty\left(\mathbb{H}^d\right)\rho_\alpha\equiv\gamma_\alpha^{-1}(K_\alpha)\subset V_\alpha$$

$$T_\alpha(\hbar) := \rho_\alpha(\gamma_\alpha^{-1})^*(-\hbar^2\Delta_{sR})\gamma_\alpha^* + (1-\rho_\alpha)\left(-\hbar^2\Delta_{\mathbb{H}^d}\right)\Delta_{\mathbb{H}^d}\mathbb{H}^d$$

$$\tau_\alpha\in S^2\left(\mathbb{H}^d\times\widehat{\mathbb{H}}^d\right)\hbar$$

$$T_\alpha(\hbar) = \mathrm{Op}_{\mathbb{H}^d,\hbar}(\tau_\alpha) + \hbar\Psi_\hbar^1\left(\mathbb{C}^d\right)$$

$$-\hbar^2\Delta_{sR}\varphi = T_\alpha(\hbar)(\varphi\circ\gamma_\alpha)\circ\gamma_\alpha^{-1}$$

$$\varphi\in C_c^\infty(M)\mathrm{supp}(\varphi)\subset K_\alpha - \hbar^2\Delta_{sR} - z\mathcal{L}(L^2(M))z\in\mathbb{C}\setminus\mathbb{R}$$

$$f(-\hbar^2\Delta_{sR}) = \frac{1}{i\pi}\int_{\mathbb{C}}\bar{\partial}_z\tilde{f}(z)(-\hbar^2\Delta_{sR}-z)^{-1}dz$$

$$\tilde{f}:\mathbb{C}\to\mathbb{C}(-\hbar^2\Delta_{sR}-z)^{-1}\,T_\alpha(\hbar)(T_\alpha(\hbar)-z)^{-1}$$

$$(T_\alpha(\hbar)-z)^{-1}: C_c^\infty\left(\mathbb{H}^d\right)\to C^\infty\left(\mathbb{C}^d\right)$$

$$P(\hbar, z): C^\infty(M) \to C^\infty(M)$$

$$P(\hbar, z) := \sum_{\alpha \in A} (\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ (T_\alpha(\hbar) - z)^{-1}) \circ \bar{\psi}_\alpha$$

$$\begin{aligned} P(\hbar, z) \circ (-\hbar^2 \Delta_{sR} - z) &= \sum_{\alpha \in A} (\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ (T_\alpha(\hbar) - z)^{-1}) \circ \bar{\psi}_\alpha \circ (-\hbar^2 \Delta_{sR} - z) \circ \bar{\bar{\psi}}_\alpha \\ &= \sum_{\alpha \in A} \Big[(\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ (T_\alpha(\hbar) - z)^{-1}) \circ (\gamma_\alpha^{-1})^* (-\hbar^2 \Delta_{sR} - z) \circ \bar{\bar{\psi}}_\alpha \\ &\quad - (\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ (T_\alpha(\hbar) - z)^{-1}) \circ (1 - \bar{\psi}_\alpha) \circ (-\hbar^2 \Delta_{sR} - z) \circ \bar{\bar{\psi}}_\alpha \Big] \\ &= 1 - \sum_{\alpha \in A} \tilde{\mathcal{R}}_\alpha(\hbar, z), \end{aligned}$$

$$\tilde{\mathcal{R}}_\alpha(\hbar, z) := (\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ (T_\alpha(\hbar) - z)^{-1}) \circ (1 - \bar{\psi}_\alpha) \circ (-\hbar^2 \Delta_{sR} - z) \circ \bar{\bar{\psi}}_\alpha.$$

$$(-\hbar^2 \Delta_{sR} - z)^{-1} = P(\hbar, z) + \sum_{\alpha \in A} \mathcal{R}_\alpha(\hbar, z),$$

$$\mathcal{R}_\alpha(\hbar, z) := \tilde{\mathcal{R}}_\alpha(\hbar, z) \circ (-\hbar^2 \Delta_{sR} - z)^{-1}.$$

$$\begin{aligned} f(-\hbar^2 \Delta_{sR}) &= \frac{1}{i\pi} \int_{\mathbb{C}} \bar{\partial}_z \tilde{f}(z) \left(\sum_{\alpha \in A} (\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ (T_\alpha(\hbar) - z)^{-1}) \circ \bar{\psi}_\alpha + \mathcal{R}_\alpha(\hbar, z) \right) dz \\ &= \sum_{\alpha \in A} \left[(\gamma_\alpha^{-1})^* \left(\psi_\alpha^2 \circ \frac{1}{i\pi} \int_{\mathbb{C}} \bar{\partial}_z \tilde{f}(z) (T_\alpha(\hbar) - z)^{-1} dz \right) \circ \bar{\psi}_\alpha + \mathcal{R}_\alpha(\hbar) \right] \\ &= \sum_{\alpha \in A} [(\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ f(T_\alpha(\hbar)) \circ \bar{\psi}_\alpha + \mathcal{R}_\alpha(\hbar)], \end{aligned}$$

$$\mathcal{R}_\alpha(\hbar) := \frac{1}{i\pi} \int_{\mathbb{C}} \bar{\partial}_z \tilde{f}(z) \mathcal{R}_\alpha(\hbar, z) dz$$

$$f(T_\alpha(\hbar)) \alpha \in A$$

$$f(T_\alpha(\hbar)) = \mathrm{O}_{\mathbb{H}^d, \hbar}(\sigma_\alpha) + \mathfrak{R}_\alpha(\hbar),$$

$$\sigma_\alpha S^{-\infty}(\mathbb{M}^d \times \widehat{\mathbb{M}}^d) \hbar f(\tau_\alpha) \mathfrak{R}_\alpha(\hbar)$$

$$\mathcal{R}_\alpha(\hbar) \mathcal{O}(\hbar^\infty) L^2(M)$$

$$\mathcal{R}_\alpha(\hbar) \psi_1, \psi_2 \in C_c^\infty(\mathbb{H}^d)$$

$$\|\psi_1 \circ (T_\alpha(\hbar) - z)^{-1} \circ \psi_2\|_{\mathcal{L}(L^2(\mathbb{H}^d))} \leq C_N \hbar^N |\mathrm{Im} z|^{-N-1}.$$

$$\|[T_\alpha(\hbar), \psi] \circ (T_\alpha(\hbar) - z)^{-1}\|_{\mathcal{L}(L^2(\mathbb{H}^d))} = \mathcal{O}(\hbar |\mathrm{Im} z|)$$

$$\psi \in C_c^\infty(\mathbb{H}^d)$$

$$\left\| (\gamma_\alpha^{-1})^* (\psi_\alpha^2 \circ (T_\alpha(\hbar) - z)^{-1}) \circ (1 - \bar{\psi}_\alpha) \right\|_{\mathcal{L}(L^2(M))} \leq C_N \hbar^N |\mathrm{Im} z|^{-N-1}$$

$$\left\|(-\hbar^2\Delta_{sr}-z)\circ\overline{\overline{\psi}}_\alpha\circ(-\hbar^2\Delta_{sR}-z)^{-1}\right\|_{\mathcal{L}(L^2(M))}$$

$$=\left\|\left[-\hbar^2\Delta_{sR},\overline{\overline{\psi}}_\alpha\right]\circ(-\hbar^2\Delta_{sR}-z)^{-1}+\overline{\overline{\psi}}_\alpha\right\|_{\mathcal{L}(L^2(M))}\leq C\hbar|\mathrm{Imz}|^{-1}+1$$

$$\left\|\tilde{\mathcal{R}}_\alpha(\hbar,z)\right\|_{\mathcal{L}(L^2(M))}\leq C'_N\hbar^N|\mathrm{Imz}|^{-N-1}$$

$$f\in C_c^\infty(\mathbb{R})$$

$$\exists C_N>0,\forall z\in\mathrm{supp}(\tilde{f}),\left|\bar{\partial}_z\tilde{f}(z)\right|\leq C_N|\mathrm{Imz}|^N$$

$$\|\mathcal{R}_\alpha(\hbar)\|_{\mathcal{L}(L^2(M))}=\mathcal{O}_{L^2(M)\to L^2(M)}(\hbar^\infty)$$

$$\hat{H}=\hat{T}_e+\hat{U}+\hat{T}_N=\hat{H}_0+\hat{T}_N$$

$$\hat{H}_0=\hat{T}_e+\hat{U}$$

$$\kappa^4=m/M_0$$

$$\hat{T}_N=\kappa^4\hat{H}_1$$

$$\hat{H}=\hat{H}_0+\kappa^4\hat{H}_1$$

$$\hat{H}=\sum_{g=1}^{A}\frac{\hat{P}_g^2}{2M_g}+\sum_{i=1}^{N}\frac{\hat{p}_i^2}{2m}+\frac{e^2}{8\pi\varepsilon_0}\sum_{\substack{g,h=1\\g\neq h}}^{A}\frac{Z_gZ_h}{\left|\hat{R}_g-\hat{R}_h\right|}+\frac{e^2}{8\pi\varepsilon_0}\sum_{\substack{i,j=1\\i\neq j}}^{N}\frac{1}{\left|\hat{r}_i-\hat{r}_j\right|}-\frac{e^2}{4\pi\varepsilon_0}\sum_{g=1}^{A}\sum_{i=1}^{N}\frac{Z_g}{\left|\hat{r}_i-\hat{R}_g\right|},$$

$$\hat{H}_0=\sum_{i=1}^{N}\frac{\hat{p}_i^2}{2m}+\frac{e^2}{8\pi\varepsilon_0}\sum_{\substack{g,h=1\\g\neq h}}^{A}\frac{Z_gZ_h}{\left|\hat{R}_g-\hat{R}_h\right|}+\frac{e^2}{8\pi\varepsilon_0}\sum_{\substack{i,j=1\\i\neq j}}^{N}\frac{1}{\left|\hat{r}_i-\hat{r}_j\right|}-\frac{e^2}{4\pi\varepsilon_0}\sum_{g=1}^{A}\sum_{i=1}^{N}\frac{Z_g}{\left|\hat{r}_i-\hat{R}_g\right|},$$

$$\hat{H}_0(\hat{r}_i,\hat{R}_g)\Psi_n(r_i,R_g)=E_n\Psi_n(r_i,R_g)$$

$$\hat{H}^{cn}=\sum_{i=1}^{N}\frac{\hat{p}_i^2}{2m}+\frac{e^2}{8\pi\varepsilon_0}\sum_{\substack{i,j=1\\i\neq j}}^{N}\frac{1}{\left|\hat{r}_i-\hat{r}_j\right|}-\frac{e^2}{4\pi\varepsilon_0}\sum_{g=1}^{A}\sum_{i=1}^{N}\frac{Z_g}{\left|\hat{r}_i-R_g\right|}$$

$$\hat{H}^{cn}(\hat{r}_i;R_g)\Psi_n^{cn}(r_i;R_g)=E_n^{cn}(R_g)\Psi_n^{cn}(r_i;R_g)$$

$$E_0^{(ec)}(\underline{R},x_\lambda)=\left\langle\Psi_0^{(ec)}(\underline{R},x_\lambda)\right|\hat{H}_{ec}\left|\Psi_0^{(ec)}(\underline{R},x_\lambda)\right\rangle,$$

$$\left|\Psi_0^{(ec)}(\underline{R},x_\lambda)\right\rangle$$

$$\hat{H}_{ec}=\sum_{pq}h_\lambda^{pq}\hat{E}_{pq}+\frac{1}{2}\sum_{pqrs}\tilde{g}_{pqrs}\hat{e}_{pqrs}+\tilde{V}_{nc}$$

$$\hat{E}_{pq} = \sum_{\sigma} \hat{a}^{\dagger}_{p\sigma}\hat{a}_{q\sigma}$$

$$\hat{e}_{pqrs} = \hat{E}_{pq}\hat{E}_{rs} - \delta_{qr}\hat{E}_{ps}$$

$$h_{\lambda}^{pq} = h_{pq} + \frac{g_0^2}{2}O_{\lambda}^{pq} - g_0\omega_c d_{\lambda}^{pq}x_{\lambda} + g_0^2 d_{\lambda}^{pq}\hat{d}_{\lambda}^{(n)}$$

$$\tilde{g}_{pqrs} = (pq \mid rs) + g_0^2 d_{\lambda}^{pq} d_{\lambda}^{rs}$$

$$d_{\lambda}^{pq} = -e\langle \chi_p | r_{i\lambda} | \chi_q \rangle$$

$$O_{\lambda}^{pq} = e^2\langle \chi_p | r_{i\lambda}^2 | \chi_q \rangle$$

$$\hat{d}_{\lambda}^{(n)} g_0 = \frac{1}{\sqrt{\epsilon_0 V_c}}$$

$$\tilde{V}_{nc} = V_{nn} + \frac{\omega_c^2}{2}x_{\lambda}^2 - g_0\omega_c\hat{d}_{\lambda}^{(n)}x_{\lambda} + \frac{g_0^2}{2}\hat{d}_{\lambda}^{(n)}\hat{d}_{\lambda}^{(n)}$$

$$E_0^{(ec)}(\underline{R}, x_{\lambda}) = \mathcal{V}_0^{(ec)}(\underline{R}) + \frac{1}{2}\underline{C}^T \underline{\underline{H}}_0^{(ec)}\underline{C}$$

$$\mathcal{V}_0^{(ec)}(\underline{R}) = E_0^{(ec)}(\underline{R}, x_{\lambda}^0)$$

$$\frac{\partial}{\partial x_{\lambda}} E_0^{(ec)}\bigg|_{x_{\lambda}^0} = 0 \Leftrightarrow \left\langle \Psi_0^{(ec)} \middle| \underline{\hat{E}_{\perp}} \middle| \Psi_0^{(ec)} \right\rangle = 0$$

$$x_{\lambda}^0 = \frac{g_0}{\omega_c}\left\langle \Psi_0^{(ec)} \middle| \hat{d}_{\lambda}^{(en)} \middle| \Psi_0^{(ec)} \right\rangle$$

$$\hat{d}_{\lambda}^{(en)} = \hat{d}_{\lambda}^{(e)} + \hat{d}_{\lambda}^{(n)}$$

$$\mathcal{V}_0^{(ec)}(\underline{R}) = \left\langle \Psi_0^{(ec)} \middle| \hat{\mathcal{H}}_e \middle| \Psi_0^{(ec)} \right\rangle - \frac{g_0^2}{2}\left\langle \Psi_0^{(ec)} \middle| \hat{d}_{\lambda}^{(e)} \middle| \Psi_0^{(ec)} \right\rangle^2 \quad (14)$$

$$\hat{\mathcal{H}}_e = \sum_{pq} \tilde{h}_{\lambda}^{pq}\hat{E}_{pq} + \frac{1}{2}\sum_{pqrs} \tilde{g}_{pqrs}\hat{e}_{pqrs} + V_{nn}$$

$$\tilde{h}_{\lambda}^{pq} = h_{pq} + \frac{g_0^2}{2}O_{\lambda}^{pq}$$

$$\mathcal{V}_0^{(ec)} = \left\langle \Psi_0^{(ec)} \middle| \hat{\mathcal{H}}_e^{\Psi_0} \middle| \Psi_0^{(ec)} \right\rangle$$

$$\hat{\mathcal{H}}_e^{\Psi_0} = \hat{\mathcal{H}}_e - \frac{g_0^2}{2}\left\langle \Psi_0^{(ec)} \middle| \hat{d}_{\lambda}^{(e)} \middle| \Psi_0^{(ec)} \right\rangle \hat{d}_{\lambda}^{(e)}$$

$$\left| \Psi_0^{(ec)} \right\rangle \approx e^{-\hat{\kappa}}\left| \Phi_0^{(ec)} \right\rangle = \left| \Phi_0^{(ec)}(\underline{\kappa}) \right\rangle,$$

$$\mathcal{V}_{\text{rhf}}^{(ec)}(\underline{\kappa}) = \left\langle \Phi_0^{(ec)}(\underline{\kappa}) \right| \hat{\mathcal{H}}_e \left| \Phi_0^{(ec)}(\underline{\kappa}) \right\rangle - \frac{g_0^2}{2} \left\langle \Phi_0^{(ec)}(\underline{\kappa}) \right| \hat{d}_\lambda^{(e)} \left| \Phi_0^{(ec)}(\underline{\kappa}) \right\rangle^2$$

$$\hat{\kappa} = \sum_{p>q} \kappa_{pq} (\hat{E}_{pq} - \hat{E}_{qp}) = \sum_{p>q} \kappa_{pq} \hat{E}_{pq}^{-}$$

$$\mathcal{V}_{pq}^{(1)} = \left\langle \Phi_0^{(ec)} \right| [\hat{E}_{pq}^{-}, \hat{\mathcal{H}}_e^{\Phi_0}] \left| \Phi_0^{(ec)} \right\rangle = 0,$$

$$\hat{\mathcal{H}}_e^{\Phi_0} = \hat{\mathcal{H}}_e - \frac{g_0^2}{2} \left\langle \Phi_0^{(ec)} \right| \hat{d}_\lambda^{(e)} \left| \Phi_0^{(ec)} \right\rangle \hat{d}_\lambda^{(e)}$$

$$\hat{f}_\lambda^{(e)} = \sum_{pq} (\tilde{h}_\lambda^{pq} + \tilde{v}_\lambda^{pq}) \hat{E}_{pq}$$

$$\tilde{v}_\lambda^{pq} = \sum_i (2 g_{pqii} - g_{piiq} - g_0^2 d_\lambda^{pi} d_\lambda^{iq})$$

$$\mathcal{V}_{\text{rhf}}^{(ec)} = E_{\text{rhf}}^{(ec)} + g_0^2 \left(\sum_i O_\lambda^{ii} - \sum_{ij} d_\lambda^{ij} d_\lambda^{ji} \right)$$

$$\left| \Psi_0^{(ec)} \right\rangle \approx \left| \Psi_{\text{CC}}^{(ec)} \right\rangle = e^{\hat{T}} \left| \Phi_0^{(ec)} \right\rangle$$

$$\left\langle \Psi_0^{(ec)} \right| \approx \left\langle \Psi_\Lambda^{(ec)} \right| = \left\langle \Phi_0^{(ec)} \right| (1 + \hat{\Lambda}) e^{-\hat{T}}$$

$$\mathcal{L}_{\text{cc}}^{(ec)} = \left\langle \Psi_\Lambda^{(ec)} \right| \hat{\mathcal{H}}_e \left| \Psi_{\text{CC}}^{(ec)} \right\rangle - \frac{g_0^2}{2} \left\langle \Psi_\Lambda^{(ec)} \right| \hat{d}_\lambda^{(e)} \left| \Psi_{\text{CC}}^{(ec)} \right\rangle^2$$

$$\hat{T} = \hat{T}_1 + \hat{T}_2, \hat{\Lambda} = \hat{\Lambda}_1 + \hat{\Lambda}_2,$$

$$\hat{T}_1 = \sum_{ai} t_i^a \hat{E}_{ai}, \hat{T}_2 = \frac{1}{4} \sum_{aibj} t_{ij}^{ab} \hat{E}_{ai} \hat{E}_{bj}$$

$$\hat{\Lambda}_1 = \sum_{ai} \lambda_a^i \hat{E}_{ai}^\dagger, \hat{\Lambda}_2 = \frac{1}{4} \sum_{aibj} \lambda_{ab}^{ij} \hat{E}_{ai}^\dagger \hat{E}_{bj}^\dagger$$

$$\{\hat{O}\} = \hat{O} - \left\langle \Phi_0^{(ec)} \right| \hat{O} \left| \Phi_0^{(ec)} \right\rangle,$$

$$\mathcal{L}_{\text{cc}}^{(ec)} = \mathcal{V}_{\text{rhf}}^{(ec)} + \left\langle \Psi_\Lambda^{(ec)} \right| \{\hat{\mathcal{H}}_e^{\text{crp}}\} \left| \Psi_{\text{CC}}^{(ec)} \right\rangle - \frac{g_0^2}{2} \left\langle \Psi_\Lambda^{(ec)} \right| \{\hat{d}_\lambda^{(e)}\} \left| \Psi_{\text{CC}}^{(ec)} \right\rangle^2$$

$$\{\hat{\mathcal{H}}_e^{\text{crp}}\} = \{\hat{f}_\lambda^{(e)}\} + \{\hat{W}_{ee}\}$$

$$\{\hat{W}_{ee}\} = \frac{1}{4} \sum_{pqrs} \bar{w}_{rs}^{pq} \{\hat{e}_{pqrs}\}$$

$$\mathcal{L}_{\text{cc}}^{(ec)} = \mathcal{V}_{\text{rhf}}^{(ec)} + \left\langle \Psi_{\Lambda}^{(ec)} \middle| \{\hat{\mathcal{H}}_e^{\Lambda}\} \middle| \Psi_{\text{CC}}^{(ec)} \right\rangle + \frac{g_0^2}{2} \left\langle \Psi_{\Lambda}^{(ec)} \middle| \left\{\hat{d}_{\lambda}^{(e)}\right\} \middle| \Psi_{\text{CC}}^{(ec)} \right\rangle^2$$

$$\{\hat{\mathcal{H}}_e^{\Lambda}\} = \{\hat{\mathcal{H}}_e^{\text{crp}}\} - g_0^2 \left\langle \Psi_{\Lambda}^{(ec)} \middle| \left\{\hat{d}_{\lambda}^{(e)}\right\} \middle| \Psi_{\text{CC}}^{(ec)} \right\rangle \left\{\hat{d}_{\lambda}^{(e)}\right\}$$

$$\frac{\partial \mathcal{L}_{\text{cc}}^{(ec)}}{\partial \lambda_{\nu}} = 0\,, \frac{\partial \mathcal{L}_{\text{cc}}^{(ec)}}{\partial t_{\nu}} = 0$$

$$\langle \Phi_{\nu} | e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\Lambda}\} e^{\hat{T}} | \Phi_0 \rangle = 0,$$
$$\langle \Phi_0 | (1 + \hat{\Lambda}) \left[e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\Lambda}\} e^{\hat{T}}, \hat{\tau}_{\nu} \right] | \Phi_0 \rangle = 0,$$

$$|\Phi_{\nu}\rangle = \hat{\tau}_{\nu} |\Phi_0\rangle \{\hat{\mathcal{H}}_e^{\Lambda}\}$$

$$\{\hat{\mathcal{H}}_e^{\Lambda}\} = \{\hat{f}_{\lambda}^{\Lambda}\} + \{\hat{W}_{ee}\}$$

$$\{\hat{f}_{\lambda}^{\lambda}\} = \left\{\hat{f}_{\lambda}^{(e)}\right\} - g_0^2 \sum_{rs} d_{\lambda}^{rs} \gamma_{rs}^{\Lambda} \sum_{pq} d_{\lambda}^{pq} \{\hat{E}_{pq}\}$$

$$\gamma_{rs}^{\Lambda} = \langle \Phi_0 | (1 + \hat{\Lambda}) e^{-\hat{T}} \{\hat{E}_{rs}\} e^{\hat{T}} | \Phi_0 \rangle,$$

$$\gamma_{ij}^{\Lambda} = -\sum_{c} \lambda_c^j t_i^c - \frac{1}{2} \sum_{kcd} \lambda_{cd}^{jk} t_{ik}^{cd}$$
$$\gamma_{ab}^{\Lambda} = \sum_{k} \lambda_b^k t_k^a + \frac{1}{2} \sum_{klc} \lambda_{bc}^{kl} t_{kl}^{ac}$$
$$\gamma_{ia}^{\Lambda} = \lambda_a^i$$
$$\gamma_{ai}^{\Lambda} = t_i^a + \sum_{jb} \lambda_b^j \left(t_{ji}^{ba} - t_i^b t_j^a \right) - \frac{1}{2} \sum_{jkcb} \lambda_{cb}^{kj} \left(t_{ki}^{cb} t_j^a - t_{kj}^{ca} t_i^b \right)$$

$$\mathcal{L}_{\text{cc}}^{(ec)} = \mathcal{V}_{\text{cc}}^{(ec)} + \sum_{\nu} \lambda_{\nu} \langle \Phi_{\nu} | e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\Lambda}\} e^{\hat{T}} | \Phi_0 \rangle$$

$$\mathcal{V}_{\text{cc}}^{(ec)} = \mathcal{V}_{\text{rhf}}^{(ec)} + \Delta \mathcal{V}_{\text{cc}}^{(ec)}$$

$$\Delta \mathcal{V}_{\text{cc}}^{(ec)} = \Delta \mathcal{V}_{\text{cc}}^{\mathcal{H}} + \Delta \mathcal{V}_{\text{cc}}^{d} + \Delta \mathcal{V}_{\text{cc}}^{\Lambda}$$

$$\Delta \mathcal{V}_{\text{cc}}^{\mathcal{H}} = \langle \Phi_0 | e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\text{crp}}\} e^{\hat{T}} | \Phi_0 \rangle$$
$$\Delta \mathcal{V}_{\text{cc}}^{d} = -\frac{g_0^2}{2} \langle \Phi_0 | e^{-\hat{T}} \left\{\hat{d}_{\lambda}^{(e)}\right\} e^{\hat{T}} | \Phi_0 \rangle^2$$
$$\Delta \mathcal{V}_{\text{cc}}^{\Lambda} = \frac{g_0^2}{2} \sum_{pq} d_{\lambda}^{pq} \tilde{\gamma}_{pq}^{\Lambda} \sum_{rs} d_{\lambda}^{rs} \tilde{\gamma}_{rs}^{\Lambda}$$

$$\Delta\mathcal{V}^{\mathcal{H}}_{\text{ccsd}} = \sum_{aibj} (t_i^a t_j^b + t_{ij}^{ab}) L_{iajb}$$
$$+2g_0^2 \sum_{aibj} (t_i^a t_j^b + t_{ij}^{ab}) d_\lambda^{ai} d_\lambda^{bj}$$
$$-g_0^2 \sum_{aibj} (t_i^a t_j^b + t_{ij}^{ab}) d_\lambda^{bi} d_\lambda^{aj}$$

$$L_{iajb} = 2g_{iajb} - g_{ibja}$$

$$\Delta\mathcal{V}^{d}_{\text{ccsd}} = -2g_0^2 \sum_{ai} d_\lambda^{ai} t_i^a \sum_{bj} d_\lambda^{bj} t_j^b$$

$$\langle \Phi_\nu | e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\text{crp}}\} e^{\hat{T}} | \Phi_0 \rangle = 0 \text{ for } \{t_\nu\}$$
$$\langle \Phi_0 | (1 + \hat{\Lambda}) [e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\text{crp}}\} e^{\hat{T}}, \hat{\tau}_\nu] | \Phi_0 \rangle = 0 \text{ for } \{\lambda_\nu\}$$

Calculate

$d_\lambda^{\Lambda} = \sum_{rs} d_\lambda^{rs} \gamma_{rs}^{\Lambda}$ via Eq.(45)

$\Delta\mathcal{V}_{\text{cc}}^{(ec)}$ via Eq.(48)

for $0 < i \leq i_{\max}$ **do**

2a) $\{\hat{\mathcal{H}}_e^{\Lambda_i}\}$ via Eq.(43)

2b) Solve Eqs.(40) and (41) for $\{t_\nu^i, \lambda_\nu^i\}$

2c) $\Delta\mathcal{V}_{\text{cc}}^{(ec)}(i)$ via Eq.(48)

if $|\Delta\mathcal{V}_{\text{cc}}^{(ec)}(i) - \Delta\mathcal{V}_{\text{cc}}^{(ec)}(i-1)| < \Delta\mathcal{V}_{\min}$ **then**

CRP-CC correlation energy $\Delta\mathcal{V}_{\text{cc}}^{(ec)}$ converged

else

$d_\lambda^{\Lambda_i} = \sum_{rs} d_\lambda^{rs} \gamma_{rs}^{\Lambda_i}$ via Eq.(45) $\Rightarrow$ 2a) $\{\hat{\mathcal{H}}_e^{\Lambda_{i+1}}\}$

end

end

Λ-Linearised CRP-CC Lagrangian	Amplitude Equations	t_ν	$\Delta\mathcal{V}_{\text{cc}}^{(ec)}$
$\mathcal{L}_{\text{cc}}^{\text{mf}} = \mathcal{V}_{\text{rhf}}^{(ec)} + \langle\Phi_0\vert(1+\hat{\Lambda})e^{-\hat{T}}\{\hat{\mathcal{H}}_e^{\text{crp}}\}e^{\hat{T}}\vert\Phi_0\rangle$	$\tilde{R}_\nu^{\text{mf}} = \langle\Phi_\nu\vert e^{-\hat{T}}\{\hat{\mathcal{H}}_e^{\text{crp}}\}e^{\hat{T}}\vert\Phi_0\rangle = 0$	✗	✗
$\mathcal{L}_{\text{cc}}^{\Lambda_0} = \mathcal{L}_{\text{cc}}^{\text{mf}} - \frac{g_0^2}{2}\langle\Phi_0\vert\{\hat{d}_\lambda^{(e)}\}_T\vert\Phi_0\rangle^2$	$\tilde{R}_\nu^{\Lambda_0} = \tilde{R}_\nu^{\text{mf}} = 0$	✗	✓
$\mathcal{L}_{\text{cc}}^{\Lambda} = \mathcal{L}_{\text{cc}}^{\Lambda_0} - g_0^2\langle\Phi_0\vert\hat{\Lambda}\{\hat{d}_\lambda^{(e)}\}_T\vert\Phi_0\rangle\langle\Phi_0\vert\{\hat{d}_\lambda^{(e)}\}_T\vert\Phi_0\rangle$	$\tilde{R}_\nu^{\Lambda} = \tilde{R}_\nu^{\Lambda_0} - g_0^2\langle\Phi_\nu\vert\{\hat{d}_\lambda^{(e)}\}_T\vert\Phi_0\rangle\langle\Phi_0\vert\{\hat{d}_\lambda^{(e)}\}_T\vert\Phi_0\rangle = 0$	✓	✓

Λ-Linearised CRP-CC Lagrangian	Amplitude Equations	t_ν	$\Delta\mathcal{V}_{\text{cc}}^{(ec)}$
$\mathcal{L}_{\text{cc}}^{\text{mf}} = \mathcal{V}_{\text{rhf}}^{(ec)} + \langle\Phi_0\vert(1 + \hat{\Lambda})e^{-\hat{T}}\{\hat{\mathcal{H}}_e^{\text{crp}}\}e^{\hat{T}}\vert\Phi_0\rangle$	$\tilde{R}_\nu^{\text{mf}} = \langle\Phi_\nu\vert e^{-\hat{T}}\{\hat{\mathcal{H}}_e^{\text{crp}}\}e^{\hat{T}}\vert\Phi_0\rangle = 0$	×	×
$\mathcal{L}_{\text{cc}}^{\Lambda_0} = \mathcal{L}_{\text{cc}}^{\text{mf}} - \frac{g_0^2}{2}\langle\Phi_0\vert\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0\rangle^2$	$\tilde{R}_\nu^{\Lambda_0} = \tilde{R}_\nu^{\text{mf}} = 0$	×	✓
$\mathcal{L}_{\text{cc}}^{\Lambda} = \mathcal{L}_{\text{cc}}^{\Lambda_0} - g_0^2\langle\Phi_0\vert\hat{\Lambda}\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0\rangle\langle\Phi_0\vert\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0$	$\tilde{R}_\nu^{\Lambda} = \tilde{R}_\nu^{\Lambda_0} - g_0^2\langle\Phi_\nu\vert\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0\rangle\langle\Phi_0\vert\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0 = 0$	✓	✓

$$\mathcal{L}_{\Lambda^2}^{(ec)} = \frac{g_0^2}{2}\langle\Phi_0\vert\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0\rangle^2 + g_0^2\langle\Phi_0\vert\hat{\Lambda}\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0\rangle\langle\Phi_0\vert\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0\rangle + \frac{g_0^2}{2}\langle\Phi_0\vert\hat{\Lambda}\left\{\hat{d}_\lambda^{(e)}\right\}_T\vert\Phi_0\rangle^2$$

$$\left\{\hat{d}_\lambda^{(e)}\right\}_T = e^{-\hat{T}}\left\{\hat{d}_\lambda^{(e)}\right\}e^{\hat{T}}$$

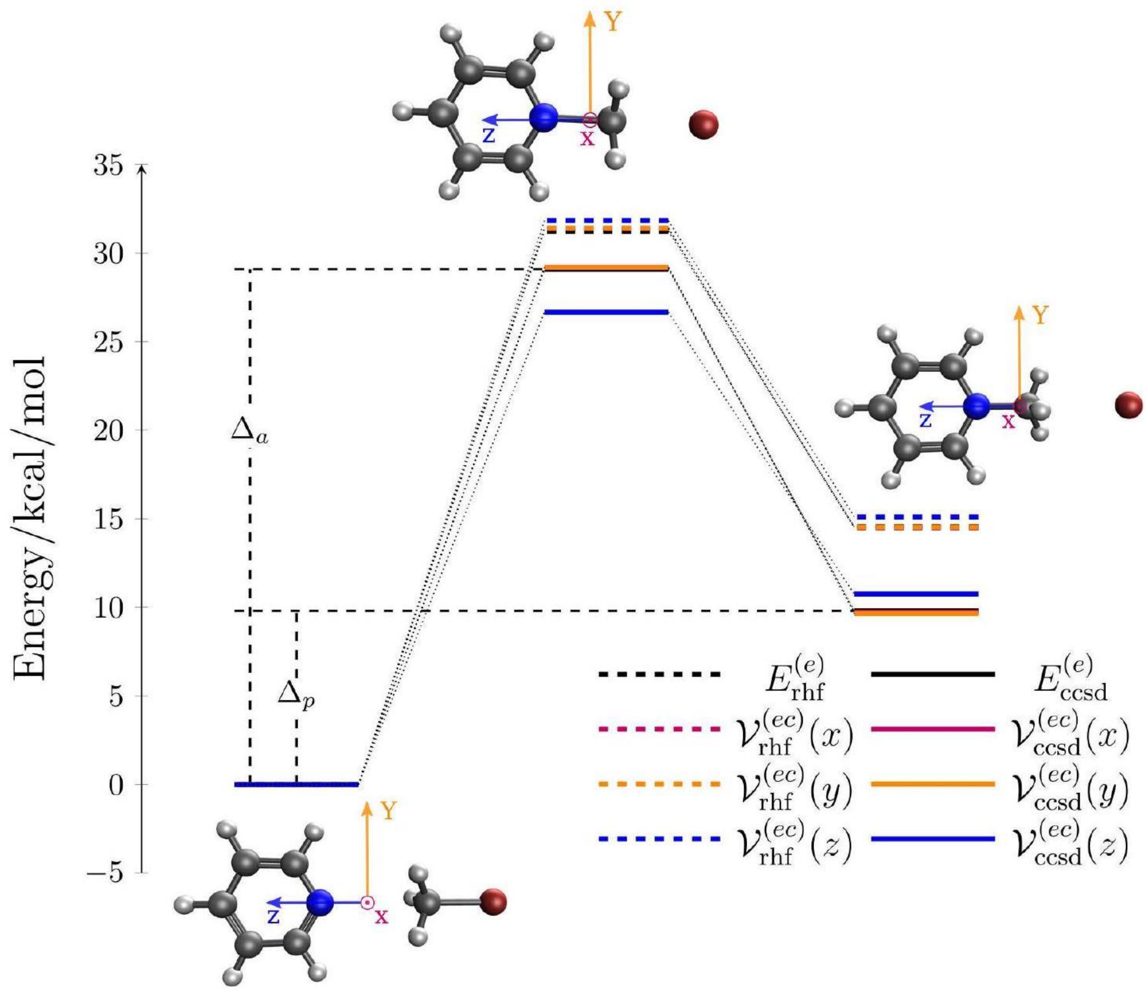
$$\mathcal{L}_{\Lambda^2}^{(ec)}\Delta\mathcal{V}_{\text{cc}}^{(ec)}\mathcal{L}_{\Lambda^2}^{(ec)}\mathcal{L}_{\text{cc}}^{\text{mf}}\tilde{R}_\nu^{\text{mf}}\{\hat{\mathcal{H}}_e^{\text{crp}}\}$$

$$\Delta\mathcal{V}_{\text{ccsd}}^{\text{mf}} = \Delta\mathcal{V}_{\text{ccsd}}^{\mathcal{H}}$$

$$\Delta\mathcal{V}_{\text{ccsd}}^{\Lambda_0} = \Delta\mathcal{V}_{\text{ccsd}}^{\mathcal{H}} + \Delta\mathcal{V}_{\text{ccsd}}^{d}$$

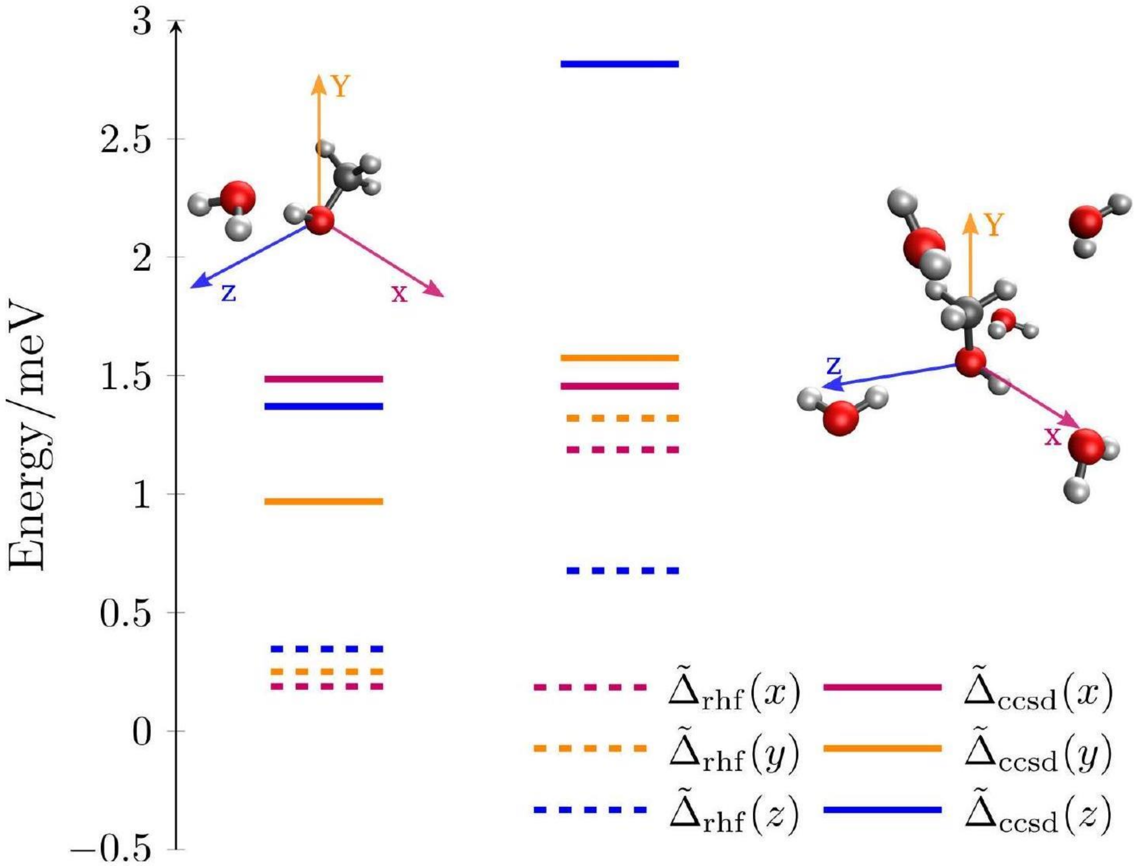
$$\mathcal{L}_{\text{cc}}^{\Lambda_0}\mathcal{L}_{\Lambda^2}^{(ec)}\mathcal{L}_{\text{cc}}^{\Lambda}$$

$$\Delta\mathcal{V}_{\text{ccsd}}^{\Lambda} = \Delta\mathcal{V}_{\text{ccsd}}^{\Lambda_0}$$



$$\tilde{E}_{AB} = \tilde{E}_A + \tilde{E}_B + \Delta\tilde{E}_{AB}$$

$$\tilde{E}_X = E_X + \tilde{\Delta}_X \,, X = A, B$$



$$\Delta\tilde{E}_{AB} = \Delta E_{AB} + \tilde{\Delta}_{AB}$$

$$E_0^{(ec)} = \left\langle \Psi_0^{(ec)} \right| \hat{H}_e + \frac{\omega_c^2}{2}\left(x_\lambda - \frac{g_0}{\omega_c}\hat{d}_\lambda^{(en)}\right)^2 \left| \Psi_0^{(ec)} \right\rangle,$$

$$\hat{d}_\lambda^{(en)} = \hat{d}_\lambda^{(e)} + \hat{d}_\lambda^{(n)}$$

$$\begin{aligned} x_\lambda^0 - \frac{g_0}{\omega_c}\hat{d}_\lambda^{(en)} &= \frac{g_0}{\omega_c}\left\langle \Psi_0^{(ec)} \right| \hat{d}_\lambda^{(en)} \left| \Psi_0^{(ec)} \right\rangle - \frac{g_0}{\omega_c}\hat{d}_\lambda^{(en)} \\ &= \frac{g_0}{\omega_c}\left\langle \Psi_0^{(ec)} \right| \hat{d}_\lambda^{(e)} \left| \Psi_0^{(ec)} \right\rangle - \frac{g_0}{\omega_c}\hat{d}_\lambda^{(e)} \end{aligned}$$

$$\begin{aligned} \mathcal{V}_0^{(ec)} &= \left\langle \Psi_0^{(ec)} \right| \mathcal{H}_e \left| \Psi_0^{(ec)} \right\rangle \\ &- g_0^2 \left\langle \Psi_0^{(ec)} \right| \left(\left\langle \Psi_0^{(ec)} \right| \hat{d}_\lambda^{(e)} \left| \Psi_0^{(ec)} \right\rangle \hat{d}_\lambda^{(e)} \right) \left| \Psi_0^{(ec)} \right\rangle \\ &+ \frac{g_0^2}{2} \left\langle \Psi_0^{(ec)} \right| \hat{d}_\lambda^{(e)} \left| \Psi_0^{(ec)} \right\rangle^2 \end{aligned}$$

$$\mathcal{H}_e = \hat{H}_e + \frac{g_0^2}{2}\hat{O}_\lambda^{(e)} + \frac{g_0^2}{2}\hat{U}_\lambda^{(ee)}$$

$$\hat{O}_\lambda^{(e)} = e^2 \sum_i r_{i\lambda}^2$$

$$\hat{U}_\lambda^{(e)} = e^2 \sum_{i \neq j} r_{i\lambda} r_{j\lambda}$$

$$\hat{d}_\lambda^{(e)} + \Delta_\lambda = -e\sum_i (r_{i\lambda} + \Delta_\lambda) = \hat{d}_\lambda^{(e)} + N_e\Delta_\lambda^{(e)}$$

$$\Delta_\lambda^{(e)} = -e\Delta_\lambda$$

$$\mathcal{V}_0^{(ec)} = \left\langle \Psi_0^{(ec)} \middle| \hat{H}_e \middle| \Psi_0^{(ec)} \right\rangle + \Delta\mathcal{V}_0^{(ec)}$$

$$\Delta\mathcal{V}_0^{(ec)} = \left\langle \hat{O}_\lambda^{(e)} \right\rangle + \left\langle \hat{U}_\lambda^{(ee)} \right\rangle - \left\langle \hat{d}_\lambda^{(e)} \right\rangle^2$$

$$\langle \dots \rangle = \left\langle \Psi_0^{(ec)} \middle| \dots \middle| \Psi_0^{(ec)} \right\rangle \Delta_\lambda$$

$$\left\langle \hat{O}_\lambda^{(e)} \right\rangle \to \left\langle \hat{O}_\lambda^{(e)} \right\rangle + 2\left\langle \hat{d}_\lambda^{(e)} \right\rangle \Delta_\lambda^{(e)} + N_e\left(\Delta_\lambda^{(e)}\right)^2$$
$$\left\langle \hat{U}_\lambda^{(ee)} \right\rangle \to \left\langle \hat{U}_\lambda^{(ee)} \right\rangle + 2(N_e - 1)\left\langle \hat{d}_\lambda^{(e)} \right\rangle \Delta_\lambda^{(e)}$$
$$+ N_e(N_e - 1)\left(\Delta_\lambda^{(e)}\right)^2$$
$$\left\langle \hat{d}_\lambda^{(e)} \right\rangle^2 \to \left\langle \hat{d}_\lambda^{(e)} \right\rangle^2 + 2N_e\left\langle \hat{d}_\lambda^{(e)} \right\rangle \Delta_\lambda^{(e)} + N_e^2\left(\Delta_\lambda^{(e)}\right)^2,$$

$$\Delta_\lambda^{(e)} \left(\Delta_\lambda^{(e)}\right)^2 \Delta\mathcal{V}_0^{(ec)}\mathcal{V}_0^{(ec)}$$

$$\mathcal{V}_{\mathrm{rhf}}^{(ec)}(\underline{\kappa}) = \mathcal{V}_{\mathrm{rhf}}^{(ec)}(\underline{0}) + \underline{\kappa}^{\mathrm{T}}\underline{\mathcal{V}}_{\mathrm{rhf}}^{(1)} + \mathcal{O}(\underline{\kappa}^2)$$

$$\mathcal{V}_{pq}^{(1)} = \left.\frac{\partial\mathcal{V}_{\mathrm{rhf}}^{(ec)}(\underline{\kappa})}{\partial\kappa_{pq}}\right|_{\underline{\kappa}=\underline{0}}$$

$$\left\langle \Phi_0^{(ec)} \middle| e^{\hat{\kappa}}\hat{\mathcal{H}}_e e^{-\hat{\kappa}} \middle| \Phi_0^{(ec)} \right\rangle = \left\langle \Phi_0^{(ec)} \middle| \hat{\mathcal{H}}_e \middle| \Phi_0^{(ec)} \right\rangle$$
$$+ \left\langle \Phi_0^{(ec)} \middle| \left[\hat{\kappa}, \hat{\mathcal{H}}_e\right] \middle| \Phi_0^{(ec)} \right\rangle$$
$$+ \mathcal{O}(\hat{\kappa}^2)$$

$$\left\langle \Phi_0^{(ec)} \middle| e^{\hat{\kappa}}\hat{d}_\lambda^{(e)} e^{-\hat{\kappa}} \middle| \Phi_0^{(ec)} \right\rangle^2 = \left\langle \Phi_0^{(ec)} \middle| \hat{d}_\lambda^{(e)} \middle| \Phi_0^{(ec)} \right\rangle^2$$
$$+ 2\left\langle \Phi_0^{(ec)} \middle| \hat{d}_\lambda^{(e)} \middle| \Phi_0^{(ec)} \right\rangle \left\langle \Phi_0^{(ec)} \middle| \left[\hat{\kappa}, \hat{d}_\lambda^{(e)}\right] \middle| \Phi_0^{(ec)} \right\rangle$$
$$+ \mathcal{O}(\hat{\kappa}^2)$$

$$\mathcal{V}_{\mathrm{rhf}}^{(ec)} = \left\langle \Phi_0^{(ec)} \middle| \hat{\mathcal{H}}_e \middle| \Phi_0^{(ec)} \right\rangle - \frac{g_0^2}{2}\left\langle \Phi_0^{(ec)} \middle| \hat{d}_\lambda^{(e)} \middle| \Phi_0^{(ec)} \right\rangle^2$$
$$= E_{\mathrm{rhf}}^{(ec)} + \frac{g_0^2}{2}\sum_{pq} O_\lambda^{pq} D_{pq}$$
$$- \frac{g_0^2}{4}\sum_{pqrs} d_\lambda^{ps} d_\lambda^{rq} D_{pq} D_{rs}$$

$$\mathcal{V}_{\text{rhf}}^{(1)} = \left\langle \Phi_0^{(ec)} \middle| \left[\hat{\kappa}, \hat{\mathcal{H}}_e\right] \middle| \Phi_0^{(ec)} \right\rangle$$
$$-g_0^2 \left\langle \Phi_0^{(ec)} \middle| \hat{d}_\lambda^{(e)} \middle| \Phi_0^{(ec)} \right\rangle \left\langle \Phi_0^{(ec)} \middle| \left[\hat{\kappa}, \hat{d}_\lambda^{(e)}\right] \middle| \Phi_0^{(ec)} \right\rangle$$
$$= \left\langle \Phi_0^{(ec)} \middle| \left[\hat{\kappa}, \hat{\mathcal{H}}_e - g_0^2 \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0 \hat{d}_\lambda^{(e)}\right] \middle| \Phi_0^{(ec)} \right\rangle,$$
$$= \left\langle \Phi_0^{(ec)} \middle| \left[\hat{\kappa}, \hat{\mathcal{H}}_e^{\Phi_0}\right] \middle| \Phi_0^{(ec)} \right\rangle,$$

$$\left\langle \hat{d}_\lambda^{(e)} \right\rangle_0 = \left\langle \Phi_0^{(ec)} \middle| \hat{d}_\lambda^{(e)} \middle| \Phi_0^{(ec)} \right\rangle$$
$$\hat{\mathcal{H}}_e^{\Phi_0} = \hat{\mathcal{H}}_e - g_0^2 \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0 \hat{d}_\lambda^{(e)}$$

$$\mathcal{V}_{\text{rhf}}^{(1)} = \sum_{p>q} \kappa_{pq} \mathcal{V}_{pq}^{(1)}$$

$$\hat{\mathcal{H}}_e = \langle \hat{\mathcal{H}}_e \rangle_0 + \{\hat{\mathcal{H}}_e\}$$
$$\hat{d}_\lambda^{(e)} = \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0 + \left\{\hat{d}_\lambda^{(e)}\right\}$$

$$\langle \dots \rangle_0 = \left\langle \Phi_0^{(ec)} \middle| \dots \middle| \Phi_0^{(ec)} \right\rangle$$

$$\mathcal{L}_{\text{cc}}^{(ec)} = \langle \hat{\mathcal{H}}_e \rangle_0 - \frac{g_0^2}{2} \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0^2$$
$$+ \left\langle \Psi_\Lambda^{(ec)} \middle| \{\hat{\mathcal{H}}_e\} \middle| \Psi_{\text{CC}}^{(ec)} \right\rangle$$
$$-g_0^2 \left\langle \Psi_\Lambda^{(ec)} \middle| \left\{\hat{d}_\lambda^{(e)}\right\} \middle| \Psi_{\text{CC}}^{(ec)} \right\rangle \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0$$
$$-\frac{g_0^2}{2} \left\langle \Psi_\Lambda^{(ec)} \middle| \left\{\hat{d}_\lambda^{(e)}\right\} \middle| \Psi_{\text{CC}}^{(ec)} \right\rangle^2$$

$$\mathcal{V}_{\text{rhf}}^{(ec)} = \langle \hat{\mathcal{H}}_e \rangle_0 - \frac{g_0^2}{2} \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0^2$$

$$\hat{\mathcal{H}}_e^{\text{crp}} = \{\hat{\mathcal{H}}_e\} - g_0^2 \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0 \left\{\hat{d}_\lambda^{(e)}\right\}.$$

$$\{\hat{\mathcal{H}}_e\} = \sum_{pq} h_\lambda^{pq} \{\hat{E}_{pq}\} + \sum_{pqi} \bar{w}_{qi}^{pi} \{\hat{E}_{pq}\}$$
$$+ \frac{1}{4} \sum_{pqrs} \bar{w}_{rs}^{pq} \{\hat{e}_{pqrs}\}$$

$$\bar{w}_{qi}^{pi} = (pi \mid qi) - (pi \mid iq) + g_0^2 \left(d_\lambda^{pq} d_\lambda^{ii} - d_\lambda^{pi} d_\lambda^{iq}\right)$$

$$-\frac{g_0^2}{2} \left\langle \hat{d}_\lambda^{(e)} \right\rangle_0 \left\{\hat{d}_\lambda^{(e)}\right\} = -g_0^2 \sum_{pqi} d_\lambda^{pq} d_\lambda^{ii} \{\hat{E}_{pq}\}$$

$$\left\langle \Psi_{\Lambda}^{(ec)} \middle| \{\hat{\mathcal{H}}_e^{\Lambda}\} \middle| \Psi_{\text{CC}}^{(ec)} \right\rangle = \left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\Lambda}\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle + \sum_{\nu} \lambda_{\nu} \left\langle \Phi_{\nu}^{(ec)} \middle| e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\Lambda}\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle$$

$$\left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\Lambda}\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle = \left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{crp}\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle - g_0^2 \left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \left\{\hat{d}_{\lambda}^{(e)}\right\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle^2 - g_0^2 \left\langle \Phi_0^{(ec)} \middle| \hat{\Lambda} \left\{\hat{d}_{\lambda}^{(e)}\right\}_T \middle| \Phi_0^{(ec)} \right\rangle \left\langle \Phi_0^{(ec)} \middle| \left\{\hat{d}_{\lambda}^{(e)}\right\}_T \middle| \Phi_0^{(ec)} \right\rangle,$$

$$\mathcal{L}_{\text{cc}}^{(ec)} = \mathcal{V}_{\text{rhf}}^{(ec)} + \left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\text{crp}}\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle - \frac{g_0^2}{2} \left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \left\{\hat{d}_{\lambda}^{(e)}\right\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle^2 + \frac{g_0^2}{2} \langle \Phi_0 | \hat{\Lambda} e^{-\hat{T}} \left\{\hat{d}_{\lambda}^{(e)}\right\} e^{\hat{T}} | \Phi_0 \rangle^2 + \sum_{\nu} \lambda_{\nu} \left\langle \Phi_{\nu}^{(ec)} \middle| e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\Lambda}\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle$$

$$\mathcal{V}_{\text{cc}}^{(ec)} = \mathcal{V}_{\text{rhf}}^{(ec)} + \left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \{\hat{\mathcal{H}}_e^{\text{crp}}\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle - \frac{g_0^2}{2} \left\langle \Phi_0^{(ec)} \middle| e^{-\hat{T}} \left\{\hat{d}_{\lambda}^{(e)}\right\} e^{\hat{T}} \middle| \Phi_0^{(ec)} \right\rangle^2 + \frac{g_0^2}{2} \langle \Phi_0 | \hat{\Lambda} e^{-\hat{T}} \left\{\hat{d}_{\lambda}^{(e)}\right\} e^{\hat{T}} | \Phi_0 \rangle^2$$

$$\tilde{\Delta}_x(\lambda) = \Delta_x(\lambda) - E_{\text{ccsd}}^{(e)}, x = a, p$$

$$E_n(\varepsilon) = -\alpha^2 + |\sigma_n| \alpha^2 \varepsilon^{2/3} + O(\varepsilon)$$

$$\left[-\frac{\alpha^2}{4 + \varepsilon^2}, +\infty \right)$$

$$L_{\text{b/f}}^2(\mathbb{R}^3) := \{\Psi \in L^2(\mathbb{R}^3) : \Psi(x_1, x_2, x_3) = (+)_{\text{b/f}} \Psi(x_2, x_1, x_3)\},$$

$$H_{2+1}^{\text{b/f}} := -\frac{\hbar^2}{2M} \partial_{x_1}^2 - \frac{\hbar^2}{2M} \partial_{x_2}^2 - \frac{\hbar^2}{2m} \partial_{x_3}^2 + \beta \delta(x_3 - x_1) + \beta \delta(x_3 - x_2).$$

$$\Pi_1 := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 = x_1\} \text{ and } \Pi_2 := \{(x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_3 = x_2\}.$$

$$x_{cm} = \frac{M(x_1 + x_2) + m x_3}{M_{tot}}, x = x_1 - x_2, y = x_3 - \frac{x_1 + x_2}{2}$$

$$M_{tot} = 2M + m, \mu = \frac{2Mm}{M_{tot}}$$

$$H_{2+1}^{\text{b/f}} \Psi(x_{cm}, x, y) = (+)_{\text{b/f}} \Psi(x_{cm}, -x, y)$$

$$H_{2+1}^{\text{b/f}} = -\frac{1}{2M_{tot}} \partial_{x_{cm}}^2 - \frac{1}{M} \partial_x^2 - \frac{1}{2\mu} \partial_y^2 + \beta \delta(y - x/2) + \beta \delta(y + x/2)$$

$$L^2_{\mathrm{b/f}}(\mathbb{R}^2) := \{\psi \in L^2(\mathbb{R}^2) : \psi(x,y) = (+)_{\mathrm{b/f}}\psi(-x,y)\}$$

$$\Pi_1 = \{(x,y) \in \mathbb{R}^2 : y = x/2\} \text{ and } \Pi_2 = \{(x,y) \in \mathbb{R}^2 : y = -x/2\}.$$

$$H^{\mathrm{b/f}}_\varepsilon = -\varepsilon^2\partial_x^2 - \partial_y^2 + \alpha\delta(y - x/2) + \alpha\delta(y + x/2)$$

$$\varepsilon^2 = \frac{2\mu}{M}$$

$$L^2_{\mathrm{b/f}}(\mathbb{R}^2) H^{\mathrm{b/f}}_\varepsilon$$

$$H^{\mathrm{b/f}}_\varepsilon = 2\mu\left(H^{\mathrm{b/f}}_{2+1} - K_{cm}\right)$$

$$K_{cm} = -\frac{1}{2M_{\mathrm{tot}}}\partial^2_{x_{cm}}\alpha = 2\mu\beta$$

$$\sigma\left(H^{\mathrm{b/f}}_\varepsilon\right) \subseteq [-\alpha^2, +\infty), \sigma_{ess}\left(H^{\mathrm{b/f}}_\varepsilon\right) = \left[-\frac{\alpha^2}{4+\varepsilon^2}, +\infty\right)$$

$$-\alpha^2 < E^{\mathrm{b/f}}_{\varepsilon,0} < E^{\mathrm{b/f}}_{\varepsilon,1} < \cdots < E^{\mathrm{b/f}}_{\varepsilon,n} < -\frac{\alpha^2}{4+\varepsilon^2}$$
$$E^{\mathrm{b/f}}_{\varepsilon,k} = -\alpha^2 + s^{\mathrm{b/f}}_k \alpha^2\varepsilon^{2/3} + O(\varepsilon)$$

$$s^{\mathrm{b}}_k = |\sigma_{2k}|, s^{\mathrm{f}}_k = |\sigma_{2k+1}|,$$

$$\cdots < \sigma_{2k+1} < \sigma_{2k} < \sigma_{2k-1} < \cdots < \sigma_2 < \sigma_1 < \sigma_0 < 0$$

$$\mathrm{Ai}'(\sigma_{2k}) = 0, \mathrm{Ai}(\sigma_{2k+1}) = 0$$

$$\left(-\frac{\varepsilon^2}{2}\partial_x\psi + \partial_y\psi\right)(x,(x/2)^+) - \left(-\frac{\varepsilon^2}{2}\partial_x\psi + \partial_y\psi\right)(x,(x/2)^-) = \alpha\psi(x,x/2) \text{ for a.e. } x \in \mathbb{R},$$

$$\mathcal{B}^{\mathrm{b/f}}_\varepsilon : H^1(\mathbb{R}^2) \cap L^2_{\mathrm{b/f}}(\mathbb{R}^2) \to \mathbb{R}$$
$$\mathcal{B}^{\mathrm{b/f}}_\varepsilon(\psi) = \int_{\mathbb{R}^2} \varepsilon^2|\partial_x\psi(x,y)|^2 + \left|\partial_y\psi(x,y)\right|^2 \mathbf{dx} + 2\alpha\int_{\mathbb{R}} |\psi(s,s/2)|^2 ds$$

$$\sigma_{ess}\left(H^{\mathrm{b/f}}_\varepsilon\right) = \begin{cases} \sigma\left(H^{\mathrm{b/f}}_\varepsilon\right) = [0,+\infty) & \alpha \geq 0 \\ \left[-\frac{\alpha^2}{4+\varepsilon^2}, +\infty\right) & \alpha < 0 \end{cases}$$

$$b_x : H^1(\mathbb{R}) \to \mathbb{R}$$
$$b_x(u) = \int_{\mathbb{R}} |u'(y)|^2 dy + \alpha|u(x/2)|^2 + \alpha|u(-x/2)|^2$$

$$u'((x/2)^+) - u'((x/2)^-) = \alpha u(x/2) \text{ and } u'((-x/2)^+) - u'((-x/2)^-) = \alpha u(-x/2).$$

$$\mathcal{B}^{\mathrm{b/f}}_\varepsilon(\phi) = \int_{\mathbb{R}^2} \varepsilon^2|\partial_x\phi(x,y)|^2 \mathbf{dx} + \int_{\mathbb{R}} b_x(\phi_x)dx$$

$$\alpha < 0, \sigma\left(H^{\mathrm{b/f}}_\varepsilon\right) \subset [-\alpha^2, +\infty)$$
$$\psi^{BO}(x,y) \equiv \psi^{BO}_x(y)$$

$$\mathcal{P}: L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2), \mathcal{P}\phi(x,y) := \psi^{BO}(x,y) f_\phi(x),$$

$$f_\phi(x) := \int_{\mathbb{R}} \psi^{BO}(x,y)\phi(x,y)dy = \int_{\mathbb{R}} \langle \psi_x^{BO}, \phi_x \rangle_{L^2(\mathbb{R},dy)} dx$$

$$\mathcal{P}^\perp := 1 - \mathcal{P} L_{\mathrm{b}}^2(\mathbb{R}^2) L_{\mathrm{f}}^2(\mathbb{R}^2)$$

$$D\left(\widehat{\mathcal{B}}_\varepsilon^{\mathrm{b/f}}\right) := H_{\mathrm{b/f}}^1(\mathbb{R}^2)\ \widehat{\mathcal{B}}_\varepsilon^{\mathrm{b/f}}(\phi) := \widehat{\mathcal{B}}_\varepsilon^{\mathrm{b/f}}(\mathcal{P}\phi) + \widehat{\mathcal{B}}_\varepsilon^{\mathrm{b/f}}(\mathcal{P}^\perp\phi) \widehat{H}_\varepsilon^{\mathrm{b/f}} H_\varepsilon^{\mathrm{b/f}}$$

$$\mathrm{d}_\varepsilon \equiv \mathrm{d}_\varepsilon(\mu) := \mathrm{dist}\left(\mu, \sigma\left(H_\varepsilon^{\mathrm{b/f}}\right)\right), \text{ and } \hat{\mathrm{d}}_\varepsilon \equiv \hat{\mathrm{d}}_\varepsilon(\mu) := \mathrm{dist}\left(\mu, \sigma\left(\widehat{H}_\varepsilon^{\mathrm{b/f}}\right)\right),$$

$$\left\{\mu \in [-\alpha^2, +\infty) \cap \rho\left(\widehat{H}_\varepsilon^{\mathrm{b/f}}\right) : \frac{4\varepsilon\delta}{\sqrt{\widehat{\mathrm{d}}_\varepsilon(\mu)}} \sqrt{1 + \frac{\mu + \alpha^2}{\widehat{\mathrm{d}}_\varepsilon(\mu)}} < \frac{1}{2}\right\} \subseteq \left\{\mu \in \rho\left(H_\varepsilon^{\mathrm{b/f}}\right) : \mathrm{d}_\varepsilon(\mu) \geq \frac{\hat{\mathrm{d}}_\varepsilon(\mu)}{32}\right\}$$

$$\mu \in \rho\left(H_\varepsilon^{\mathrm{b/f}}\right) \cap \rho\left(\widehat{H}_\varepsilon^{\mathrm{b/f}}\right), \mu > -\alpha^2$$

$$\left\| \left(H_\varepsilon^{\mathrm{b/f}} - \mu\right)^{-1} - \left(\widehat{H}_\varepsilon^{\mathrm{b/f}} - \mu\right)^{-1} \right\|_{\mathcal{B}\left(L^2(\mathbb{R}^2)\right)} \leq 2\varepsilon\delta\left(\frac{1}{\widehat{\mathrm{d}}_\varepsilon}\sqrt{\frac{1}{\mathrm{d}_\varepsilon}\left(1 + \frac{\mu + \alpha^2}{\mathrm{d}_\varepsilon}\right)} + \frac{1}{\mathrm{d}_\varepsilon}\sqrt{\frac{1}{\widehat{\mathrm{d}}_\varepsilon}\left(1 + \frac{\mu + \alpha^2}{\widehat{\mathrm{d}}_\varepsilon}\right)}\right)$$

$$\widehat{H}_\varepsilon^{\mathrm{b/f}} = \widehat{H}_{\varepsilon,\mathcal{P}}^{\mathrm{b/f}} \oplus \widehat{H}_{\varepsilon,\mathcal{P}\perp}^{\mathrm{b/f}}, \sigma\left(\widehat{H}_\varepsilon^{\mathrm{b/f}}\right) = \sigma\left(\widehat{H}_{\varepsilon,\mathcal{P}}^{\mathrm{b/f}}\right) \cup \sigma\left(\widehat{H}_{\varepsilon,\mathcal{P}\perp}^{\mathrm{b/f}}\right),$$

$$\widehat{H}_{\varepsilon,\mathcal{P}}^{\mathrm{b/f}} : D\left(\widehat{H}_{\varepsilon,\mathcal{P}}^{\mathrm{b/f}}\right) \subset \mathrm{ran}\left(\mathcal{P} \mid L_{\mathrm{b/f}}^2(\mathbb{R}^2)\right) \to \mathrm{ran}\left(\mathcal{P} \mid L_{\mathrm{b/f}}^2(\mathbb{R}^2)\right)$$
$$\widehat{H}_{\varepsilon,\mathcal{P}\perp}^{\mathrm{b/f}} : D\left(\widehat{H}_{\varepsilon,\mathcal{P}\perp}^{\mathrm{b/f}}\right) \subset \mathrm{ran}\left(\mathcal{P}^\perp \mid L_{\mathrm{b/f}}^2(\mathbb{R}^2)\right) \to \mathrm{ran}\left(\mathcal{P}^\perp \mid L_{\mathrm{b/f}}^2(\mathbb{R}^2)\right)$$

$$\sigma\left(\widehat{H}_{\varepsilon,\mathcal{P}}^{\mathrm{b/f}}\right) \subseteq [-\alpha^2, +\infty), \sigma\left(\widehat{H}_{\varepsilon,\mathcal{P}\perp}^{\mathrm{b/f}}\right) \subseteq [-\alpha^2/4, +\infty)$$

$$D\left(H_\varepsilon^{\mathrm{eff}} b/f\right) = H^2(\mathbb{R}) \cap L_{\mathrm{b/f}}^2(\mathbb{R})\ H_\varepsilon^{\mathrm{eff}} b/f = -\varepsilon^2 \frac{d^2}{dx^2} - \lambda_0 + \varepsilon^2 R$$

$$\varepsilon^2 R(x) := \varepsilon^2 \int_{\mathbb{R}} |\partial_x \psi^{BO}(x,y)|^2 dy$$

$$\mathrm{ran}\left(\mathcal{P} \mid D\left(H_\varepsilon^{\mathrm{b/f}}\right)\right) \nsubseteq D\left(H_\varepsilon^{\mathrm{b/f}}\right) \widehat{H}_{\varepsilon,\mathcal{P}}^{\mathrm{b/f}} \mathcal{P} H_\varepsilon^{\mathrm{b/f}} \mathcal{P}$$

$$-\alpha^2 < E_{\varepsilon,0}^{\mathrm{effb/f}} < E_{\varepsilon,1}^{\mathrm{eff\,b/f}} < \cdots < E_{\varepsilon,n}^{\mathrm{effb/f}} < -\frac{\alpha^2}{4 + \varepsilon^2}$$
$$E_{\varepsilon,k}^{\mathrm{effb/f}} = -\alpha^2 + s^{\mathrm{b/f}} \alpha^2 \varepsilon^{2/3} + O(\varepsilon)$$

$$-\mathbf{x} = (x,y) \in \mathbb{R}^2.$$
$$-\mathbf{k} = (k,p) \in \mathbb{R}^2.$$

$$\hat{\psi}(\mathbf{k}) := \frac{1}{2\pi} \int_{\mathbb{R}^2} e^{-i\mathbf{k}\cdot\mathbf{x}} \psi(\mathbf{x}) \mathbf{dx}$$

$$\hat{\xi}(p) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ipy} \xi(y) dy$$

$$H^{\nu}(\mathbb{R}^n), \nu \in \mathbb{R}$$

$$\nu; H_{\natural}^{\nu}(\mathbb{R}^2) := H^{\nu}(\mathbb{R}^2) \cap L_{\natural}^2(\mathbb{R}^2), \nu - \langle \cdot,\cdot \rangle_{\mp\nu,\pm\nu}$$

$$H^{\pm\nu}(\mathbb{R}^n) - H^{\mp\nu}(\mathbb{R}^n) L^2(\mathbb{R}^n)$$

$$\sigma_{ac}(L), \sigma_{sc}(L), \sigma_{ess}(L), \sigma_p(L), \sigma_d(L)$$

$$\mathcal{Q}(\psi) = \mathcal{Q}(\psi, \psi)$$

$$C_0^{\infty}(\mathbb{R}^n) \mathbb{R}^n \mathbb{C} \lambda_+ := \max\{0, \lambda\}$$

$$D(H_{\varepsilon}^0) := H^2(\mathbb{R}^2), H_{\varepsilon}^0 := -\varepsilon^2 \partial_x^2 - \partial_y^2$$

$$\Pi = \Pi_1 \cup \Pi_2$$

$$L_{\natural}^2(\mathbb{R}^2) := \{\psi \in L^2(\mathbb{R}^2) : \psi(x,y) = (+)_{\natural} \psi(-x,y)\},$$

$$H_{\natural}^1(\mathbb{R}^2) = H^1(\mathbb{R}^2) \cap L_{\natural}^2(\mathbb{R}^2)$$

$$\mathcal{B}_{\varepsilon}^{\natural}(\varphi, \psi) := \int_{\mathbb{R}^2} \varepsilon^2 \partial_x \bar{\varphi}(x,y) \partial_x \psi(x,y) + \partial_y \bar{\varphi}(x,y) \partial_y \psi(x,y) \mathbf{dx} + 2\alpha \int_{\mathbb{R}} \bar{\varphi}(s, s/2) \psi(s, s/2) ds$$

$$(\tau_1 \phi)(s) := \phi(s, s/2), (\tau_2 \phi)(s) := \phi(-s, s/2), s \in \mathbb{R}.$$

$$\tau_1 : H^{\nu}(\mathbb{R}^2) \to H^{\nu-1/2}(\mathbb{R}), \tau_2 : H^{\nu}(\mathbb{R}^2) \to H^{\nu-1/2}(\mathbb{R})$$

$$C_0^{\infty}(\mathbb{R}) \subset \operatorname{ran}(\tau_j) C_0^{\infty}(\mathbb{R}^2 \setminus \Pi_j) \subset \ker(\tau_j)$$

$$L^2(\mathbb{R}^2), j = 1,2$$

$$\mathcal{T} : H^{\nu}(\mathbb{R}^2) \to H^{\nu-\frac{1}{2}}(\mathbb{R}) \oplus H^{\nu-\frac{1}{2}}(\mathbb{R}), \mathcal{T}\phi := \tau_1 \phi \oplus \tau_2 \phi, \nu > 1/2.$$

$$C_0^{\infty}(\mathbb{R} \setminus \{0\}) \times C_0^{\infty}(\mathbb{R} \setminus \{0\}) \subset \operatorname{ran}(\mathcal{T})$$

$$L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$$

$$C_0^{\infty}(\mathbb{R}^2 \setminus \Pi) \subset \ker(\mathcal{T}) L^2(\mathbb{R}^2)$$

$$\operatorname{ran}(\mathcal{T}) \subseteq \{\xi_1 \oplus \xi_2 \in H^{\nu-1/2}(\mathbb{R}) \oplus H^{\nu-1/2}(\mathbb{R}) : \xi_1(0) = \xi_2(0)\} \subsetneq H^{\nu-1/2}(\mathbb{R}) \oplus H^{\nu-1/2}(\mathbb{R})$$

$$R_{\varepsilon}^0(z) := (H_{\varepsilon}^0 - z)^{-1}$$

$$R_{\varepsilon}^0(z) : H^{\nu}(\mathbb{R}^2) \to H^{\nu+2}(\mathbb{R}^2), \nu \geq 0$$

$$R_{\varepsilon}^0(z) : H^{\nu}(\mathbb{R}^2) \to H^{\nu+2}(\mathbb{R}^2), \nu < 0$$

$$\breve{\mathbb{G}}_{\varepsilon}(z) : H^{\nu}(\mathbb{R}^2) \to H^{\nu+3/2}(\mathbb{R}) \oplus H^{\nu+3/2}(\mathbb{R}), \breve{\mathbb{G}}_{\varepsilon}(z) := \mathcal{T} R_{\varepsilon}^0(z), \nu > -3/2$$

$$\breve{\mathbb{G}}_{\varepsilon}(z)\psi = \breve{G}_{1,\varepsilon}(z)\psi \oplus \breve{G}_{2,\varepsilon}(z)\psi;\ \breve{G}_{j,\varepsilon}(z) : H^{\nu}(\mathbb{R}^2) \to H^{\nu+3/2}(\mathbb{R}), \breve{G}_{j,\varepsilon}(z) = \tau_j R_{\varepsilon}^0(z), j = 1,2.$$

$$\operatorname{ran}(\breve{G}_{j,\varepsilon}(z)) = H^{\nu+3/2}(\mathbb{R})$$

$$\operatorname{ran}(\breve{\mathbb{G}}_{\varepsilon}(z)) \subsetneq H^{\nu+3/2}(\mathbb{R}) \oplus H^{\nu+3/2}(\mathbb{R})$$

$$\mathbb{G}_\varepsilon(z) := \breve{\mathbb{G}}_\varepsilon(\bar{z})^*: H^\nu(\mathbb{R}) \oplus H^\nu(\mathbb{R}) \to H^{\nu+3/2}(\mathbb{R}^2), \nu < 0$$

$$H^{-\nu}(\mathbb{R}^d) - H^\nu(\mathbb{R}^d) L^2(\mathbb{R}^d)$$

$$\mathbb{G}_\varepsilon(z)(\xi_1 \oplus \xi_2) = G_{1,\varepsilon}(z)\xi_1 + G_{2,\varepsilon}(z)\xi_2;\ G_{j,\varepsilon}(z): H^\nu(\mathbb{R}) \to H^{\nu+3/2}(\mathbb{R}^2), G_{j,\varepsilon}(z) = \breve{G}_{j,\varepsilon}(\bar{z})^*$$

$$G_{j,\varepsilon}(z) \in \mathcal{B}\big(L^2(\mathbb{R}), H^\nu(\mathbb{R}^2)\big), \mathbb{G}_\varepsilon(z) \in \mathcal{B}\big(L^2(\mathbb{R}) \oplus L^2(\mathbb{R}), H^\nu(\mathbb{R}^2)\big)$$

$$\operatorname{ran}\big(G_{j,\varepsilon}(z) \mid L^2(\mathbb{R})\big) \subseteq H^{3/2-}(\mathbb{R}^2), \operatorname{ran}(\mathbb{G}_\varepsilon(z) \mid L^2(\mathbb{R}) \oplus L^2(\mathbb{R})) \subseteq H^{3/2-}(\mathbb{R}^2)$$

$$H^{3/2-}(\mathbb{R}^2) := \cap_{\nu<3/2} H^\nu(\mathbb{R}^2)$$

$$\operatorname{ran}(\mathbb{G}_\varepsilon(z) \mid L^2(\mathbb{R}) \oplus L^2(\mathbb{R})) \cap D(H_\varepsilon^0) = \{0\}$$

$$Q \in (L^2(\mathbb{R}) \setminus \{0\}) \oplus (L^2(\mathbb{R}) \setminus \{0\})$$

$$\phi \in L^2(\mathbb{R}^2) \setminus \{0\}$$

$$R_\varepsilon^0(z)\phi = \mathbb{G}_\varepsilon(z) Q$$

$$\psi \in L^2(\mathbb{R}^2)$$

$$\langle \phi, R_\varepsilon^0(\bar{z})\psi \rangle_{L^2(\mathbb{R}^2)} = \langle Q, \mathcal{T} R_\varepsilon^0(\bar{z})\psi \rangle_{L^2(\mathbb{R}) \oplus L^2(\mathbb{R})}.$$

$$R_\varepsilon^0(\mathbf{x}, \mathbf{x}'; z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}}{\varepsilon^2 k^2 + p^2 - z} \mathbf{dk}$$

$$\breve{G}_{1,\varepsilon}(s, \mathbf{x}'; z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{e^{i\left(k+\frac{p}{2}\right)s} e^{-i\mathbf{k}\mathbf{x}'}}{\varepsilon^2 k^2 + p^2 - z} \mathbf{dk};\ \breve{G}_{2,\varepsilon}(s, \mathbf{x}'; z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{e^{i\left(-k+\frac{p}{2}\right)s} e^{-i\mathbf{k}\mathbf{x}'}}{\varepsilon^2 k^2 + p^2 - z} \mathbf{dk}$$

$$G_{1,\varepsilon}(\mathbf{x}, s'; z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{e^{i\mathbf{k}\mathbf{x}} e^{-i\left(k+\frac{p}{2}\right)s'}}{\varepsilon^2 k^2 + p^2 - z} \mathbf{dk};\ G_{2,\varepsilon}(\mathbf{x}, s'; z) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{e^{i\mathbf{k}\mathbf{x}} e^{-i\left(-k+\frac{p}{2}\right)s'}}{\varepsilon^2 k^2 + p^2 - z} \mathbf{dk}$$

$$M_{\ell j,\varepsilon}(z): H^\nu(\mathbb{R}) \to H^{\nu+1}(\mathbb{R}), M_{\ell j,\varepsilon}(z) := \tau_\ell G_{j,\varepsilon}(z)\ \ell, j = 1,2;\ \nu > -1$$

$$\mathbb{M}_\varepsilon(z): H^\nu(\mathbb{R}) \oplus H^\nu(\mathbb{R}) \to H^{\nu+1}(\mathbb{R}) \oplus H^{\nu+1}(\mathbb{R}), \mathbb{M}_\varepsilon(z) := \mathcal{T}\mathbb{G}_\varepsilon(z), \nu > -1$$

$M_{\ell j,\varepsilon}(z) \in \mathcal{B}(L^2(\mathbb{R}))$ and $\mathbb{M}_\varepsilon(z) \in \mathcal{B}(L^2(\mathbb{R}) \oplus L^2(\mathbb{R}))$

$$\mathbb{M}_\varepsilon(z) = \begin{bmatrix} M_{11,\varepsilon}(z) & M_{12,\varepsilon}(z) \\ M_{21,\varepsilon}(z) & M_{22,\varepsilon}(z) \end{bmatrix}$$

$$\breve{\mathbb{G}}_\varepsilon(z) - \breve{\mathbb{G}}_\varepsilon(w) = (z-w)\breve{\mathbb{G}}_\varepsilon(z) R_\varepsilon^0(w) = (z-w)\breve{\mathbb{G}}_\varepsilon(w) R_\varepsilon^0(z)$$
$$\mathbb{G}_\varepsilon(z) - \mathbb{G}_\varepsilon(w) = (z-w) R_\varepsilon^0(w)\mathbb{G}_\varepsilon(z) = (z-w) R_\varepsilon^0(z)\mathbb{G}_\varepsilon(w)$$
$$\mathbb{M}_\varepsilon(z) - \mathbb{M}_\varepsilon(w) = (z-w)\breve{\mathbb{G}}_\varepsilon(w)\mathbb{G}_\varepsilon(z) = (z-w)\breve{\mathbb{G}}_\varepsilon(z)\mathbb{G}_\varepsilon(w)$$

$$R_\varepsilon^0(z) - R_\varepsilon^0(w) = (z-w) R_\varepsilon^0(z) R_\varepsilon^0(w) = (z-w) R_\varepsilon^0(w) R_\varepsilon^0(z)$$

$$\mathbb{G}_\varepsilon(z), \breve{\mathbb{G}}_\varepsilon(z) \mathbb{M}_\varepsilon(z) M_{\ell j,\varepsilon}(z)$$

$$M_{11,\varepsilon}(s,s';z) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \frac{e^{i\left(k+\frac{p}{2}\right)(s-s')}}{\varepsilon^2k^2+p^2-z}\mathbf{dk};\ M_{12,\varepsilon}(s,s';z) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \frac{e^{i\left(k+\frac{p}{2}\right)s}e^{-i\left(-k+\frac{p}{2}\right)s'}}{\varepsilon^2k^2+p^2-z}\mathbf{dk}$$

$$M_{21,\varepsilon}(s,s';z) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \frac{e^{i\left(-k+\frac{p}{2}\right)s}e^{-i\left(k+\frac{p}{2}\right)s'}}{\varepsilon^2k^2+p^2-z}\mathbf{dk};\ M_{22,\varepsilon}(s,s';z) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \frac{e^{i\left(-k+\frac{p}{2}\right)(s-s')}}{\varepsilon^2k^2+p^2-z}\mathbf{dk}$$

$$M_{11,\varepsilon}(s,s';z) = M_{22,\varepsilon}(s,s';z) \text{ and } M_{12,\varepsilon}(s,s';z) = M_{21,\varepsilon}(s,s';z)$$

$$M_{d,\varepsilon}(s,s';z) := M_{11,\varepsilon}(s,s';z) = M_{22,\varepsilon}(s,s';z) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \frac{e^{i\left(k+\frac{p}{2}\right)(s-s')}}{\varepsilon^2k^2+p^2-z}\mathbf{dk}$$

$$M_{od,\varepsilon}(s,s';z) := M_{12,\varepsilon}(s,s';z) = M_{21,\varepsilon}(s,s';z) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \frac{e^{i\left(k+\frac{p}{2}\right)s}e^{-i\left(-k+\frac{p}{2}\right)s'}}{\varepsilon^2k^2+p^2-z}\mathbf{dk}$$

$$\mathbb{M}_\varepsilon(z) = \begin{bmatrix} M_{d,\varepsilon}(z) & M_{od,\varepsilon}(z) \\ M_{od,\varepsilon}(z) & M_{d,\varepsilon}(z) \end{bmatrix}$$

$$\left\langle \xi, M_{d,\varepsilon}(z)\xi \right\rangle = \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{|\hat{\xi}(k+p/2)|^2}{\varepsilon^2k^2+p^2-z}\mathbf{dk} = \left\langle M_{d,\varepsilon}(\bar{z})\xi, \xi \right\rangle$$

$$\left\langle \eta, M_{od,\varepsilon}(z)\xi \right\rangle = \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{\overline{\hat{\eta}(k+p/2)}\hat{\xi}(-k+p/2)}{\varepsilon^2k^2+p^2-z}\mathbf{dk} = \left\langle M_{od,\varepsilon}(\bar{z})\eta, \xi \right\rangle$$

$$\Xi, \tilde{\Xi} \in L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$$

$$\left\langle \tilde{\Xi}, \mathbb{M}_\varepsilon(z)\Xi \right\rangle_{L^2(\mathbb{R}^2)\oplus L^2(\mathbb{R})} = \left\langle \tilde{\xi}_1, M_{d,\varepsilon}(z)\xi_1 \right\rangle + \left\langle \tilde{\xi}_2, M_{d,\varepsilon}(z)\xi_2 \right\rangle + \left\langle \tilde{\xi}_2, M_{od,\varepsilon}(z)\xi_1 \right\rangle + \left\langle \tilde{\xi}_1, M_{od,\varepsilon}(z)\xi_2 \right\rangle$$

$$\mathbb{M}_\varepsilon(z) = \mathbb{M}_\varepsilon(\bar{z})^*\ z \in \mathbb{C} \setminus [0,+\infty)$$

$$\mathbb{M}_\varepsilon(z) = \mathcal{T}\left(\mathcal{T}R_\varepsilon^0(\bar{z})\right)^* = \mathcal{T}R_\varepsilon^0(z)\mathcal{T}^*$$

$$\frac{1}{\alpha} + \mathbb{M}_\varepsilon(z): L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \to L^2(\mathbb{R}) \oplus L^2(\mathbb{R}), \alpha \in \mathbb{R} \setminus \{0\}, z \in \mathbb{C} \setminus [0,+\infty)$$

$$\frac{1}{\alpha} + \mathbb{M}_\varepsilon(-\lambda)$$

$$T: D(T) \subset \mathcal{H} \to \mathcal{H}$$

$$|\langle u, Tu \rangle_{\mathcal{H}}| \geq c\|u\|_{\mathcal{H}}^2\ \forall u \in D(T)$$

$$\|Tu\|_{\mathcal{H}} \geq c\|u\|_{\mathcal{H}}\ \forall u \in D(T).$$

$$\overline{\operatorname{ran}(T)} = \mathcal{H}$$

$$\{u_n\} \in D(T)$$

$$\|Tu_n - v\|_{\mathcal{H}} \to 0$$

$$\frac{1}{\alpha} + \mathbb{M}_\varepsilon(-\lambda)$$

$$\left|\left\langle \Xi, \left(\frac{1}{\alpha} + \mathbb{M}_\varepsilon(-\lambda)\right)\Xi \right\rangle\right| \geq c_\lambda\|\Xi\|^2\ \forall \Xi \in L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}),$$

$$\langle \xi, M_{d,\varepsilon}(-\lambda)\xi \rangle = \int_{\mathbb{R}} |\hat{\xi}(\nu)|^2 \int_{\mathbb{R}} \frac{1}{\pi} \frac{1}{\varepsilon^2 k^2 + 4(\nu-k)^2 + \lambda} dk d\nu = \int_{\mathbb{R}} \frac{|\hat{\xi}(\nu)|^2}{\sqrt{4\varepsilon^2\nu^2 + (4+\varepsilon^2)\lambda}} d\nu$$

$$\langle \eta, M_{od,\varepsilon}(-\lambda)\xi \rangle = \frac{2}{\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{\overline{\hat{\eta}(\nu)}\hat{\xi}(\nu')}{(4+\varepsilon^2)(\nu^2+\nu'^2) + 2(4-\varepsilon^2)\nu\nu' + 4\lambda} d\nu d\nu'$$

$$\hat{M}_{d,\varepsilon}(\nu; -\lambda) = \frac{1}{\sqrt{4\varepsilon^2\nu^2 + (4+\varepsilon^2)\lambda}}$$

$$\hat{M}_{od,\varepsilon}(\nu,\nu'; -\lambda) = \frac{2}{\pi} \frac{1}{(4+\varepsilon^2)(\nu^2+\nu'^2) + 2(4-\varepsilon^2)\nu\nu' + 4\lambda}$$

$$\left\| M_{d,\varepsilon}(-\lambda) \right\|_{\mathcal{B}(L^2(\mathbb{R}))} \leq \frac{1}{\sqrt{(4+\varepsilon^2)\lambda}}$$

$$M_{od,\varepsilon}(-\lambda)(4+\varepsilon^2)(\nu^2+\nu'^2) + 2(4-\varepsilon^2)\nu\nu' \geq 2\min(\varepsilon^2, 4)(\nu^2+\nu'^2)$$

$$\int_{\mathbb{R}^2} \left| \hat{M}_{od,\varepsilon}(\nu,\nu'; -\lambda) \right|^2 d\nu d\nu' \leq \frac{4}{\pi^2} \left(\int_{\mathbb{R}} \frac{1}{2\min(\varepsilon^2,4)\nu^2 + 4\lambda} d\nu \right)^2 = \frac{1}{2\min(\varepsilon^2,4)\lambda}$$

$$\left\| M_{od,\varepsilon}(-\lambda) \right\|_{\mathcal{B}(L^2(\mathbb{R}))} \leq \left\| M_{od,\varepsilon}(-\lambda) \right\|_{HS} \leq \sqrt{\frac{1}{2\min(\varepsilon^2,4)\lambda}}$$

$$\left| (\Xi, \mathbb{M}_\varepsilon(-\lambda)\Xi)_{L^2(\mathbb{R}^2)\oplus L^2(\mathbb{R})} \right| \leq C_\varepsilon \|\Xi\|^2 / \sqrt{\lambda}$$

$$\left| \left\langle \Xi, \left(\frac{1}{\alpha} + \mathbb{M}_\varepsilon(-\lambda) \right) \Xi \right\rangle \right| \geq \left(\frac{1}{|\alpha|} - \frac{C_\varepsilon}{\sqrt{\lambda}} \right) \|\Xi\|^2 \geq c_\lambda \|\Xi\|^2$$

$$D(\widetilde{H}_\varepsilon) := \{\phi \in H^{3/2-}(\mathbb{R}^2) : \phi + \alpha \mathbb{G}_\varepsilon(z)\mathcal{T}\phi \in H^2(\mathbb{R}^2)\}$$
$$(\widetilde{H}_\varepsilon - z)\phi := (H_\varepsilon^0 - z)(\phi + \alpha \mathbb{G}_\varepsilon(z)\mathcal{T}\phi)$$

$$H_\varepsilon^0 \restriction \ker(\mathcal{T}) 1 + \alpha \mathbb{M}_\varepsilon(z) : L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \to L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) z \in \rho(\widetilde{H}_\varepsilon) \cap \mathbb{C} \setminus [0, +\infty) \widetilde{H}_\varepsilon$$

$$\tilde{R}_\varepsilon(z) = R_\varepsilon^0(z) - \alpha \mathbb{G}_\varepsilon(z)(1 + \alpha \mathbb{M}_\varepsilon(z))^{-1} \breve{\mathbb{G}}_\varepsilon(z) \; z \in \rho(\widetilde{H}_\varepsilon) \cap \mathbb{C} \setminus [0, +\infty)$$

$$\tilde{R}_\varepsilon(-\lambda) : L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2) \; \lambda > \lambda_{\alpha,\varepsilon}$$
$$\tilde{R}_\varepsilon(-\lambda) := R_\varepsilon^0(-\lambda) - \mathbb{G}_\varepsilon(-\lambda) \left(\frac{1}{\alpha} + \mathbb{M}_\varepsilon(-\lambda) \right)^{-1} \breve{\mathbb{G}}_\varepsilon(-\lambda)$$

$$\widetilde{H}_\varepsilon \geq -\lambda_{\alpha,\varepsilon} \text{ of } H_\varepsilon^0 \restriction \ker(\mathcal{T})$$

$$\widetilde{D} := \left\{ \phi \in L^2(\mathbb{R}^2) : \phi = \phi_{-\lambda} - \mathbb{G}_\varepsilon(-\lambda) \left(\frac{1}{\alpha} + \mathbb{M}_\varepsilon(-\lambda) \right)^{-1} \mathcal{T}\phi_{-\lambda}, \phi_{-\lambda} \in D(H_\varepsilon^0) \right\}$$
$$\widetilde{H}_\varepsilon : \widetilde{D} \subseteq L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2), (\widetilde{H}_\varepsilon + \lambda)\phi := (H_\varepsilon^0 + \lambda)\phi_{-\lambda}$$

$$\tilde{R}_\varepsilon(-\lambda) - \tilde{R}_\varepsilon(-\mu) = (\mu - \lambda)\tilde{R}_\varepsilon(-\lambda)\tilde{R}_\varepsilon(-\mu) \; \lambda, \mu > \lambda_{\alpha,\varepsilon}$$

$$\tilde{R}_\varepsilon(-\lambda)\psi = 0$$

$$R_\varepsilon^0(-\lambda)\psi = \mathbb{G}_\varepsilon(-\lambda)Q$$

$$Q = \left(\frac{1}{\alpha} + \mathbb{M}_\varepsilon(-\lambda)\right)^{-1} \breve{\mathbb{G}}_\varepsilon(-\lambda)\psi$$

$$\tilde{R}_\varepsilon(-\lambda)\tilde{D} := \mathrm{ran}\big(\tilde{R}_\varepsilon(-\lambda)\big)$$

$$\widetilde{H}_\varepsilon = \tilde{R}_\varepsilon(-\lambda)^{-1} - \lambda$$

$$\tilde{R}_\varepsilon(-\lambda)^* = \tilde{R}_\varepsilon(-\lambda)$$

$$\phi \in D(H_\varepsilon^0) \cap \ker(\mathcal{T})$$

$$\phi = \phi_{-\lambda}\widetilde{H}_\varepsilon\phi = H_{0,\varepsilon}\phi$$

$$z \in \rho\big(\widetilde{H}_\varepsilon\big) \cap \mathbb{C} \setminus [0, +\infty)$$

$$\widetilde{D} = \left\{\phi \in L^2(\mathbb{R}^2) : \phi = \phi_z - \mathbb{G}_\varepsilon(z)\left(\frac{1}{\alpha} + \mathbb{M}_\varepsilon(z)\right)^{-1} \mathcal{T}\phi_z, \phi_z \in D(H_\varepsilon^0)\right\}$$

$$\big(\widetilde{H}_\varepsilon - z\big)\phi = (H_\varepsilon^0 - z)\phi_z$$

$$\widetilde{H}_\varepsilon\widetilde{D} \subseteq H^{3/2-}(\mathbb{R}^2)\mathbb{G}_\varepsilon(z)$$

$$\widetilde{D} = D\big(\widetilde{H}_\varepsilon\big)$$

$$\mathrm{ran}(\mathbb{G}_\varepsilon(z) - \mathbb{G}_\varepsilon(w)) \subseteq D(H_\varepsilon^0) = H^2(\mathbb{R}^2)$$

$$\widetilde{D} = D\big(\widetilde{H}_\varepsilon\big)$$

$$\rho\big(\widetilde{H}_\varepsilon\big) \cap \mathbb{C} \setminus [0, +\infty)$$

$$\mathcal{T}\phi = \mathcal{T}\phi_z - \alpha\mathbb{M}_\varepsilon(z)(1 + \alpha\mathbb{M}_\varepsilon(z))^{-1}\mathcal{T}\phi_z$$

$$\mathcal{T}\phi = (1 + \alpha\mathbb{M}_\varepsilon(z))^{-1}\mathcal{T}\phi_z$$

$$\phi_z = \phi + \alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi$$

$$\widetilde{D} \subseteq D\big(\widetilde{H}_\varepsilon\big)\phi \in D\big(\widetilde{H}_\varepsilon\big)\phi_z \in H^2(\mathbb{R}^2)$$

$$\phi_z := \phi + \alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi$$

$$\mathcal{T}\phi + \alpha\mathbb{M}_\varepsilon(z)\mathcal{T}\phi = \mathcal{T}\phi_z$$

$$\mathcal{T}\phi = (1 + \alpha\mathbb{M}_\varepsilon(z))^{-1}\mathcal{T}\phi_z$$

$$\phi = \phi_z - \alpha\mathbb{G}_\varepsilon(z)(1 + \alpha\mathbb{M}_\varepsilon(z))^{-1}\mathcal{T}\phi_z$$

$$D\big(\widetilde{H}_\varepsilon\big) \subseteq \widetilde{D}$$

$$\widetilde{D} = D\big(\widetilde{H}_\varepsilon\big)$$

$$\big(\widetilde{H}_\varepsilon - z\big)\phi = (H_\varepsilon^0 - z)(\phi + \alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi), z \in \rho\big(\widetilde{H}_\varepsilon\big) \cap \mathbb{C} \setminus [0, +\infty)$$

$$w \in \rho\big(\widetilde{H}_\varepsilon\big) \cap \mathbb{C} \setminus [0, +\infty)$$

$$(\widetilde{H}_\varepsilon - z)\phi = (\widetilde{H}_\varepsilon - w)\phi + (w-z)\phi = (H_\varepsilon^0 - w)(\phi + \alpha\mathbb{G}_\varepsilon(w)\mathcal{T}\phi) + (w-z)\phi$$
$$=(H_\varepsilon^0 - w)(\phi + \alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi) + \alpha(H_\varepsilon^0 - w)(\mathbb{G}_\varepsilon(w) - \mathbb{G}_\varepsilon(z))\mathcal{T}\phi + (w-z)\phi$$
$$=(H_\varepsilon^0 - w)(\phi + \alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi) + (w-z)\alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi + (w-z)\phi$$
$$=(H_\varepsilon^0 - z)(\phi + \alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi)$$

$$\mathcal{T}^*: H^{-\nu+1/2}(\mathbb{R}) \oplus H^{-\nu+1/2}(\mathbb{R}) \to H^{-\nu}(\mathbb{R}^2), \nu > 1/2$$

$$\xi_1 \oplus \xi_2 \in L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$$

$$\mathcal{T}^*\xi_1 \oplus \xi_2 \in \mathcal{S}'(\mathbb{R}^2) f \in \mathcal{S}(\mathbb{R}^2)$$

$$(\mathcal{T}^*\xi_1 \oplus \xi_2)f = \int_{\mathbb{R}} \xi_1(s) f(s, s/2) ds + \int_{\mathbb{R}} \xi_2(s) f(-s, s/2) ds$$

$$\mathbb{G}_\varepsilon(z) = R_\varepsilon^0(z)\mathcal{T}^*$$

$$(-\varepsilon^2\partial_x^2 - \partial_y^2 - z)\mathbb{G}_\varepsilon(z)\xi_1 \oplus \xi_2 = \mathcal{T}^*\xi_1 \oplus \xi_2$$

$$\phi \in D(\widetilde{H}_\varepsilon)$$

$$\widetilde{H}_\varepsilon\phi = (-\varepsilon^2\partial_x^2 - \partial_y^2)\phi + \alpha\mathcal{T}^*\mathcal{T}\phi$$

$$\phi \in \ker(\mathcal{T}) L^2(\mathbb{R}^2)$$

$$\operatorname{supp}(\mathcal{T}^*\xi_1 \oplus \xi_2) = \Pi$$

$$\widetilde{H}_\varepsilon\phi(\mathbf{x}) = (-\varepsilon^2\partial_x^2 - \partial_y^2)\phi(\mathbf{x}) \text{ for a.e. } \mathbf{x} \text{ in } \mathbb{R}^2 \setminus \Pi.$$

$$\widetilde{\mathcal{B}}_\varepsilon: H^1(\mathbb{R}^2) \times H^1(\mathbb{R}^2) \subseteq L^2(\mathbb{R}^2) \times L^2(\mathbb{R}^2) \to \mathbb{C}$$

$$\widetilde{\mathcal{B}}_\varepsilon(\varphi, \phi) := \varepsilon^2\langle\partial_x\varphi, \partial_x\phi\rangle + \langle\partial_y\varphi, \partial_y\phi\rangle + \alpha(\langle\tau_1\varphi, \tau_1\phi\rangle + \langle\tau_2\varphi, \tau_2\phi\rangle).$$

$$\widetilde{\mathcal{B}}_\varepsilon(\varphi, \phi) = \langle\varphi, \widetilde{H}_\varepsilon\phi\rangle \; \forall\varphi \in H^1(\mathbb{R}^2), \forall\phi \in D(\widetilde{H}_\varepsilon)$$

$$\mathcal{B}_\varepsilon^0(\varphi, \phi) = \langle\varphi, H_\varepsilon^0\phi\rangle \; \forall\varphi \in H^1(\mathbb{R}^2), \forall\phi \in H^2(\mathbb{R}^2)$$

$$\mathcal{B}_\varepsilon^0(\varphi, \phi) = \langle(-\varepsilon^2\partial_x^2 - \partial_y^2)\varphi, \phi\rangle_{-1,+1} = \langle\varphi, (-\varepsilon^2\partial_x^2 - \partial_y^2)\phi\rangle_{+1,-1} \; \forall\psi, \phi \in H^1(\mathbb{R}^2)$$

$$H^{\pm\nu}(\mathbb{R}^2) - H^{\mp\nu}(\mathbb{R}^2) L^2(\mathbb{R}^2) \langle\cdot,\cdot\rangle_{\mp\nu,\pm\nu}$$

$$\phi_z := \phi + \alpha\mathbb{G}_\varepsilon(z)\mathcal{T}\phi$$

$$\mathbb{G}_\varepsilon(z)\mathcal{T}\phi H^{3/2-}(\mathbb{R}^2) \subset H^1(\mathbb{R}^2)$$

$$\langle\varphi, \widetilde{H}_\varepsilon\phi\rangle = \langle\varphi, (\widetilde{H}_\varepsilon - z)\phi\rangle + z\langle\varphi, \phi\rangle = (\varphi, (H_\varepsilon^0 - z)\phi_z\rangle + z\langle\varphi, \phi\rangle$$
$$= (\mathcal{B}_\varepsilon^0 - z)(\varphi, \phi_z) + z\langle\varphi, \phi\rangle = \mathcal{B}_\varepsilon^0(\varphi, \phi) + \alpha(\mathcal{B}_\varepsilon^0 - z)(\varphi, \mathbb{G}_\varepsilon(z)\mathcal{T}\phi)$$
$$= \mathcal{B}_\varepsilon^0(\varphi, \phi) + \alpha\langle\varphi, (-\varepsilon^2\partial_x^2 - \partial_y^2 - z)\mathbb{G}_\varepsilon(z)\mathcal{T}\phi\rangle_{+1,-1}$$
$$= \mathcal{B}_\varepsilon^0(\varphi, \phi) + \alpha\langle\varphi, \mathcal{T}^*\mathcal{T}\phi\rangle_{+1,-1} = \mathcal{B}_\varepsilon^0(\varphi, \phi) + \alpha(\langle\tau_1\varphi, \tau_1\phi\rangle + \langle\tau_2\varphi, \tau_2\phi\rangle)$$
$$= \widetilde{\mathcal{B}}_\varepsilon(\varphi, \phi)$$

$$\varepsilon^2\partial_x^2 + \partial_y^2 + z$$

$$D(\widetilde{H}_\varepsilon) = \{\phi \in H^{3/2-}(\mathbb{R}^2): \phi = \phi_1 + \phi_2, \phi_j \in H^2(\mathbb{R}^2 \setminus \Pi_j), [\tau'_{j,\varepsilon}]\phi_j = \alpha\tau_j\phi, j = 1,2\}$$

$$[\tau'_{j,\varepsilon}]\phi_j \varepsilon^2 \partial_x^2 + \partial_y^2$$

$$\widetilde{H}_{\varepsilon,\alpha} \text{ onto } L^2_{\natural}(\mathbb{R}^2)$$

$$R^0_\varepsilon(z): L^2_{\natural}(\mathbb{R}^2) \to H^2_{\natural}(\mathbb{R}^2)\ \forall z \in \mathbb{C} \setminus [0, +\infty).$$

$$S: H^\nu(\mathbb{R}^2) \to H^\nu(\mathbb{R}^2), \nu \geq 0, (S\psi)(x,y) := \psi(-x,y),$$

$$\frac{1(+)_\natural S}{2}: L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2), \operatorname{ran}\left(\frac{1(+)_\natural S}{2}\right) = L^2_\natural(\mathbb{R}^2).$$

$$S\psi = (+)_\natural \psi\ \forall \psi \in L^2_\natural(\mathbb{R}^2).$$

$$\tau_1 S = \tau_2, \tau_2 S = \tau_1$$
$$\breve{G}_{2,\varepsilon}(z) = \breve{G}_{1,\varepsilon}(z)S, G_{2,\varepsilon}(z) = SG_{1,\varepsilon}(z)$$

$$\tau_1\psi = (+)_\natural \tau_2 \psi\ \forall \psi \in H^2_\natural(\mathbb{R}^2),$$

$$\tau \equiv \tau_1$$

$$\breve{G}_\varepsilon(z): L^2_\natural(\mathbb{R}^2) \to L^2(\mathbb{R}), \breve{G}_\varepsilon(z) := \tau R^0_\varepsilon(z) \equiv \breve{G}_{1,\varepsilon}(z) \mid L^2_\natural(\mathbb{R}^2),$$
$$G_\varepsilon(z): L^2(\mathbb{R}) \to L^2_\natural(\mathbb{R}^2), G_\varepsilon(z) := \breve{G}_\varepsilon(\bar{z})^* \equiv \frac{1(+)_\natural S}{2} G_{1,\varepsilon}(z),$$
$$M_\varepsilon(z): L^2(\mathbb{R}) \to L^2(\mathbb{R}), M_\varepsilon(z) := \tau G_\varepsilon(z).$$

$$M_\varepsilon(z) = \tau_1 \frac{1(+)_\natural S}{2} G_{1,\varepsilon}(z) = \frac{1}{2}\big(\tau_1 G_{1,\varepsilon}(z)(+)_\natural \tau_1 S G_{1,\varepsilon}(z)\big) = \frac{1}{2}\big(\tau_1 G_{1,\varepsilon}(z)(+)_\natural \tau_1 G_{2,\varepsilon}(z)\big)$$
$$= \frac{1}{2}\big(M_{d,\varepsilon}(z)(+)_\natural M_{od,\varepsilon}(z)\big)$$

$$\breve{\mathbb{G}}_\varepsilon(z)\psi = \breve{G}_\varepsilon(z)\psi \oplus \big((+)_\natural \breve{G}_\varepsilon(z)\psi\big), \forall \psi \in L^2_\natural(\mathbb{R}^2)$$
$$\mathbb{G}_\varepsilon(z)\xi \oplus ((+)_\natural \xi) = G_{1,\varepsilon}(z)\xi(+)_\natural G_{2,\varepsilon}(z)\xi = (1(+)_\natural S)G_{1,\varepsilon}(z)\xi = 2G_\varepsilon(z)\xi$$
$$\mathbb{M}_\varepsilon(z)\xi \oplus ((+)_\natural \xi) = 2\big(M_\varepsilon(z)\xi \oplus ((+)_\natural M_\varepsilon(z)\xi)\big)$$
$$(1 + \alpha\mathbb{M}_\varepsilon(z))^{-1}\xi \oplus ((+)_\natural \xi) = (1 + 2\alpha M_\varepsilon(z))^{-1}\xi \oplus ((+)_\natural (1 + 2\alpha M_\varepsilon(z))^{-1}\xi).$$

$$\psi \in L^2_\natural(\mathbb{R}^2) z \in \rho\big(\widetilde{H}_\varepsilon\big) \cap \mathbb{C} \setminus [0, +\infty)$$

$$\tilde{R}_\varepsilon(z)\psi = R^0_\varepsilon(z)\psi - \alpha\mathbb{G}_\varepsilon(z)(1 + \alpha\mathbb{M}_\varepsilon(z))^{-1}\breve{\mathbb{G}}_\varepsilon(z)\psi$$
$$= R^0_\varepsilon(z)\psi - 2\alpha G_\varepsilon(z)(1 + 2\alpha M_\varepsilon(z))^{-1}\breve{G}_\varepsilon(z)\psi.$$

$$R^\natural_\varepsilon(z) := \tilde{R}_\varepsilon(z) \mid L^2_\natural(\mathbb{R}^2)$$

$$\big(R^\natural_\varepsilon(z)\big)^* = R^\natural_\varepsilon(\bar{z})$$

$$R^\natural_\varepsilon(z)\widehat{H}^\natural_\varepsilon \text{ in } L^2_\natural(\mathbb{R}^2)\widetilde{H}_\varepsilon \text{ onto } L^2_\natural(\mathbb{R}^2)$$

$$\widehat{H}^\natural_\varepsilon = \frac{1(+)_\natural S}{2}\widetilde{H}_\varepsilon\frac{1(+)_\natural S}{2} \equiv \widetilde{H}_\varepsilon\Big|\ D\big(\widetilde{H}_\varepsilon\big) \cap L^2_\natural(\mathbb{R}^2).$$

$$z \in \mathbb{C} \setminus [0, +\infty) \cap \rho\big(\widehat{H}^\natural_\varepsilon\big)$$

$$D\big(H^\natural_\varepsilon\big) := \Big\{\psi \in H^{3/2-}_\natural(\mathbb{R}^2): \psi + 2\alpha G_\varepsilon(z)\tau\psi \in H^2_\natural(\mathbb{R}^2)\Big\},$$
$$\big(H^\natural_\varepsilon - z\big)\psi := (H^0_\varepsilon - z)(\psi + 2\alpha G_\varepsilon(z)\tau\psi)$$

$$H_\varepsilon^0 \upharpoonright \ker\left(\tau \upharpoonright H_\natural^2(\mathbb{R}^2)\right)$$

$$1 + 2\alpha M_\varepsilon(z) \colon L^2(\mathbb{R}) \to L^2(\mathbb{R})$$

$$z \in \rho\left(H_\varepsilon^\natural\right) \cap \mathbb{C} \setminus [0, +\infty)$$

$$R_\varepsilon^\natural(z) = R_\varepsilon^0(z) - 2\alpha G_\varepsilon(z)(1 + 2\alpha M_\varepsilon(z))^{-1}\breve{G}_\varepsilon(z)\ z \in \rho\left(H_\varepsilon^\natural\right) \cap \mathbb{C} \setminus [0, +\infty)$$

$$\tau^* \colon H^{-\nu+1/2}(\mathbb{R}) \to H^{-\nu}(\mathbb{R}^2), \nu > 1/2$$

$$\xi \in L^2(\mathbb{R})$$

$$\tau^*\xi \in \mathcal{S}'(\mathbb{R}^2)$$

$$f \in \mathcal{S}(\mathbb{R}^2)$$

$$(\tau^*\xi)f = \int_{\mathbb{R}} \xi(s) f(s, s/2) ds$$

$$G_\varepsilon(z) = R_\varepsilon^0(z)\tau^*$$

$$\left(-\varepsilon^2\partial_x^2 - \partial_y^2 - z\right)G_\varepsilon(z)\xi = \tau^*\xi$$

$$\mathcal{T}^*\xi \oplus \xi = 2\tau^*\xi$$

$$H_\varepsilon^\natural\psi = \left(-\varepsilon^2\partial_x^2 - \partial_y^2\right)\psi + 2\alpha\tau^*\tau\psi.$$

$$\mathcal{B}_\varepsilon^\natural \colon H_\natural^1(\mathbb{R}^2) \times H_\natural^1(\mathbb{R}^2) \subseteq L_\natural^2(\mathbb{R}^2) \times L_\natural^2(\mathbb{R}^2) \to \mathbb{C}$$

$$\mathcal{B}_\varepsilon^\natural(\varphi, \psi) := \varepsilon^2\langle\partial_x\varphi, \partial_x\psi\rangle + \left\langle\partial_y\varphi, \partial_y\psi\right\rangle + 2\alpha\langle\tau\psi, \tau\phi\rangle.$$

$$\mathcal{B}_\varepsilon^\natural(\psi, \phi) = \left\langle\psi, H_\varepsilon^\natural\phi\right\rangle\ \forall\psi \in H_\natural^1(\mathbb{R}^2), \forall\phi \in D\left(H_\varepsilon^\natural\right).$$

$$D\left(H_\varepsilon^\natural\right)\xi \in L^2(\mathbb{R})$$

$$H_\varepsilon^\natural\breve{G}_\varepsilon(z) = \tau R_\varepsilon^0(z), G_\varepsilon(z) = (\tau R_\varepsilon^0(\bar{z}))^* M_\varepsilon(z) = \tau G_\varepsilon(z)$$

$$\breve{G}_\varepsilon(z) - \breve{G}_\varepsilon(w) = (z - w)\breve{G}_\varepsilon(z)R_\varepsilon^0(w) = (z - w)\breve{G}_\varepsilon(w)R_\varepsilon^0(z)$$
$$G_\varepsilon(z) - G_\varepsilon(w) = (z - w)R_\varepsilon^0(w)G_\varepsilon(z) = (z - w)R_\varepsilon^0(z)G_\varepsilon(w)$$
$$M_\varepsilon(z) - M_\varepsilon(w) = (z - w)\breve{G}_\varepsilon(w)G_\varepsilon(z) = (z - w)\breve{G}_\varepsilon(z)G_\varepsilon(w)$$

$$w, z \in \mathbb{C} \setminus [0, +\infty) \text{ and } \psi \in D\left(H_\varepsilon^\natural\right)$$

$$\psi_z := \psi + 2\alpha G_\varepsilon(z)\tau\psi$$

$$\left(H_\varepsilon^\natural - w\right)\psi = (H_\varepsilon^0 - w)\psi_z - (z - w)2\alpha G_\varepsilon(z)\tau\psi.$$

$$w \in \mathbb{C} \setminus [0, +\infty), z \in \rho\left(H_\varepsilon^\natural\right) \cap \mathbb{C} \setminus [0, +\infty) \text{ and } \xi \in L^2(\mathbb{R})$$

$$\phi_{w,\xi} := R_\varepsilon^\natural(z)G_\varepsilon(w)\xi$$

$$\left(H_\varepsilon^\natural - w\right)\phi_{w,\xi} = G_\varepsilon(z)(1 + 2\alpha M_\varepsilon(z))^{-1}(1 + 2\alpha M_\varepsilon(w))\xi.$$

$$\begin{aligned}(H_\varepsilon^\natural - w)\psi &= (H_\varepsilon^0 - z)(\psi + 2\alpha G_\varepsilon(z)\tau\psi) + (z-w)\psi\\ &= (H_\varepsilon^0 - z)\psi_z + (z-w)(\psi_z - 2\alpha G_\varepsilon(z)\tau\psi)\\ &= (H_\varepsilon^0 - w)\psi_z - (z-w)2\alpha G_\varepsilon(z)\tau\psi\end{aligned}$$

$$\begin{aligned}&(H_\varepsilon^\natural - w)\phi_{w,\xi} = (H_\varepsilon^\natural - z)\phi_{w,\xi} + (z-w)\phi_{w,\xi} = G_\varepsilon(w)\xi + (z-w)\phi_{w,\xi}\\ &= G_\varepsilon(w)\xi + (z-w)R_\varepsilon^0(z)G_\varepsilon(w)\xi - (z-w)2\alpha G_\varepsilon(z)(1+2\alpha M_\varepsilon(z))^{-1}\breve{G}_\varepsilon(z)G_\varepsilon(w)\xi\\ &= G_\varepsilon(z)\xi - G_\varepsilon(z)(1+2\alpha M_\varepsilon(z))^{-1}(1+2\alpha M_\varepsilon(z) - 1 - 2\alpha M_\varepsilon(w))\xi\\ &= G_\varepsilon(z)(1+2\alpha M_\varepsilon(z))^{-1}(1+2\alpha M_\varepsilon(w))\xi\end{aligned}$$

(i) $-\lambda \in \sigma_p(H_\varepsilon^\natural)$ if and only if $0 \in \sigma_p(1+2\alpha M_\varepsilon(-\lambda))$;
(ii) $-\lambda \in \sigma_{\text{ess}}(H_\varepsilon^\natural)$ if and only if $0 \in \sigma_{\text{ess}}(1+2\alpha M_\varepsilon(-\lambda))$.

$$-\lambda \in \rho(H_\varepsilon^0)$$

$$\psi \in D(H_\varepsilon^\natural)$$

$$0 = (H_\varepsilon^\natural + \lambda)\psi = (H_\varepsilon^0 + \lambda)(\psi + 2\alpha G_\varepsilon(z)\tau\psi) - (z+\lambda)2\alpha G_\varepsilon(z)\tau\psi, \forall z \in \mathbb{C}\setminus[0,+\infty)$$

$$\psi + 2\alpha G_\varepsilon(-\lambda)\tau\psi = 2\alpha(G_\varepsilon(-\lambda) - G_\varepsilon(z))\tau\psi - 2\alpha(z+\lambda)R_\varepsilon^0(-\lambda)G_\varepsilon(z)\tau\psi$$

$$(1+2\alpha M_\varepsilon(-\lambda))\tau\psi = 2\alpha(M_\varepsilon(-\lambda) - M_\varepsilon(z))\tau\psi - 2\alpha(z+\lambda)\breve{G}_\varepsilon(-\lambda)G_\varepsilon(z)\tau\psi = 0.$$

$$\xi \in L^2(\mathbb{R})(1+2\alpha M_\varepsilon(-\lambda))\xi = 0$$

$$\phi_{-\lambda,\xi} = R_\varepsilon^\natural(z)G_\varepsilon(-\lambda)\xi, z \in \rho(H_\varepsilon^\natural) \cap \mathbb{C}\setminus[0,+\infty)$$

$$\psi_n \in D(H_\varepsilon^\natural), \|\psi_n\| = 1, \psi_n \rightharpoonup 0, \text{ and } \|(H_\varepsilon^\natural + \lambda)\psi_n\| \to 0$$

$$\begin{aligned}&\breve{G}_\varepsilon(-\lambda)(H_\varepsilon^\natural + \lambda)\psi_n = \tau R_\varepsilon^0(-\lambda)\big((H_\varepsilon^0 + \lambda)(\psi_n + 2\alpha G_\varepsilon(z)\tau\psi_n) + (z+\lambda)2\alpha G_\varepsilon(z)\tau\psi_n\big)\\ &= \tau(\psi_n + 2\alpha G_\varepsilon(z)\tau\psi_n) + (z+\lambda)2\alpha\breve{G}_\varepsilon(-\lambda)G_\varepsilon(z)\tau\psi_n\\ &= (1+2\alpha M_\varepsilon(-\lambda))\tau\psi_n - 2\alpha(M_\varepsilon(-\lambda) - M_\varepsilon(z))\tau\psi_n + 2\alpha(z+\lambda)\breve{G}_\varepsilon(-\lambda)G_\varepsilon(z)\tau\psi_n\\ &= (1+2\alpha M_\varepsilon(-\lambda))\tau\psi_n\end{aligned}$$

$$(1+2\alpha M_\varepsilon(-\lambda))\tau\psi_n \to 0$$

$$\tau\psi_n \rightharpoonup 0$$

$$\psi_{n,z} := \psi_n + 2\alpha G_\varepsilon(z)\tau\psi_n \in H_\natural^2(\mathbb{R}^2)$$

$$f \in H^{-2}(\mathbb{R}^2) z \in \mathbb{C}\setminus[0,+\infty)$$

$$\begin{aligned}\langle (H_\varepsilon^\natural + \lambda)\psi_n, R_\varepsilon^0(\bar{z})f\rangle &= \langle (H_\varepsilon^0 - z)\psi_{n,z}, R_\varepsilon^0(\bar{z})f\rangle + (\lambda - z)\langle \psi_n, R_\varepsilon^0(\bar{z})f\rangle\\ &= \langle \psi_{n,z}, f\rangle_{+2,-2} + (\lambda - z)\langle \psi_n, R_\varepsilon^0(\bar{z})f\rangle\end{aligned}$$

$$\psi_{n,z} \rightharpoonup H^2(\mathbb{R}^2)$$

$$\tau \in \mathcal{B}(H^2(\mathbb{R}^2) L^2(\mathbb{R}))$$

$$\tau\psi_n = (1+2\alpha M_\varepsilon(z))^{-1}\tau\psi_{n,z}$$

$$\tau\psi_n \rightharpoonup 0 \text{ in } L^2(\mathbb{R})$$

$$\left\|(H_\varepsilon^0+\lambda)\psi_{n,z}\right\| \to \|\psi_n\| = \left\|\psi_{n,z}\right\| \to \psi_{n,z}/\left\|\psi_{n,z}\right\| - \lambda \in \sigma_{ess}(H_\varepsilon^0)$$

$$\{\xi_n\}, \|\xi_n\| = 1, \xi_n \rightharpoonup 0$$

$$\|(1+2\alpha M_\varepsilon(-\lambda))\xi_n\| \to 0$$

$$\{\phi_n\}, \phi_n := R_\varepsilon^\natural(z)G_\varepsilon(-\lambda)\xi_n, z \in \rho\left(H_\varepsilon^\natural\right) \cap \mathbb{C} \setminus [0,+\infty)$$

$$\left\|\left(H_\varepsilon^\natural+\lambda\right)\phi_n\right\| \to 0$$

$$R_\varepsilon^0(z) = R_\varepsilon^\natural(z) + 2\alpha G_\varepsilon(z)\tau R_\varepsilon^0(z)$$

$$\phi_n + 2\alpha G_\varepsilon(z)\tau\phi_n = R_\varepsilon^0(z)G_\varepsilon(-\lambda)\xi_n$$

$$\left(H_\varepsilon^\natural+\lambda\right)\phi_n = (H_\varepsilon^0 - z)(\phi_n + 2\alpha G_\varepsilon(z)\tau\phi_n) + (z+\lambda)\phi_n = G_\varepsilon(-\lambda)\xi_n + (z+\lambda)\phi_n,$$

$$G_\varepsilon(-\lambda)\xi_n \to 1 + 2\alpha M_\varepsilon(z)$$

$$\|(1+2\alpha M_\varepsilon(z))\xi_n\| \geq c_z\|\xi_n\| = c_z$$

$$\begin{aligned} 0 < \|(1+2\alpha M_\varepsilon(z))\xi_n\| &\leq \|(1+2\alpha M_\varepsilon(-\lambda))\xi_n\| + 2|\alpha|\|(M_\varepsilon(z) - M_\varepsilon(-\lambda))\xi_n\| \\ &= \|(1+2\alpha M_\varepsilon(-\lambda))\xi_n\| + 2|\alpha||z+\lambda|\left\|\breve{G}_\varepsilon(z)G_\varepsilon(-\lambda)\xi_n\right\| \end{aligned}$$

$$\alpha \in \mathbb{R}, [0,+\infty) \subseteq \sigma_{\text{ess}}\left(H_\varepsilon^\natural\right)$$

$$\chi_n(\mathbf{x}) := \frac{\sqrt{2}}{n}\chi\left(\frac{\mathbf{x}-\mathbf{x}_n}{n}\right), \mathbf{x}_n = (3n, 0)$$

$$\psi_n(\mathbf{x}) := e^{-i\mathbf{k}\cdot\mathbf{x}}\chi_n(\mathbf{x})\ \mathbf{k} = \left(\varepsilon^{-1}\sqrt{\lambda/2}, \sqrt{\lambda/2}\right)$$

$$\psi_n^\natural := \frac{1(+)_\natural S}{2}\psi_n,$$

$$\frac{1(+)_\natural S}{2}\left\|\psi_n^\natural\right\| = 1$$

$$\psi_n^\natural \in D\left(H_\varepsilon^\natural\right) \cap D(H_\varepsilon^0) H_\varepsilon^\natural\psi_n^\natural = H_\varepsilon^0\psi_n^\natural$$

$$\nabla_\varepsilon\phi = \left(\varepsilon\partial_x\phi, \partial_y\phi\right)$$

$$\begin{aligned} \left\|\left(H_\varepsilon^\natural - \lambda\right)\psi_n^\natural\right\| &= \left\|(H_\varepsilon^0 - \lambda)\psi_n^\natural\right\| \\ &\leq \|(H_\varepsilon^0 - \lambda)\psi_n\| = \left\|2(\nabla_\varepsilon\chi_n)\cdot\left(\nabla_\varepsilon e^{-i\mathbf{k}\cdot\mathbf{x}}\right) + (H_\varepsilon^0\chi_n)e^{-i\mathbf{k}\cdot\mathbf{x}}\right\| \\ &\leq 2\sqrt{\lambda}\|\nabla_\varepsilon\chi_n\| + \|H_\varepsilon^0\chi_n\| \\ &\leq c_\varepsilon\left(\frac{\sqrt{\lambda}}{n} + \frac{1}{n^2}\right) \end{aligned}$$

$$\chi \in C_0^\infty(\mathbb{R}^2)$$

$$\lim_{n\to\infty}\left\|\left(H_\varepsilon^\natural - \lambda\right)\psi_n^\natural\right\| = 0.$$

$$\phi \in L_{\mathrm{t}}^2(\mathbb{R}^2)$$

$$\left|\langle\phi,\psi_n^{\natural}\rangle\right|^2 = |\langle\phi,\psi_n\rangle|^2 \le \frac{2}{n^2}\text{Area}(D_n)\int_{\mathbb{R}^2}\left|\phi(\mathbf{x})\chi\left(\frac{\mathbf{x}-\mathbf{x}_n}{n}\right)\right|^2 \mathbf{dx} \to 0.$$

$$[0,+\infty) \subseteq \sigma_{ess}(H_\varepsilon^{\natural}) \text{ for any } \alpha \in \mathbb{R}$$

$$\sigma(H_\varepsilon^{\natural}) \subseteq [0,+\infty) \subseteq \sigma_{ess}(H_\varepsilon^{\natural}) \subseteq \sigma(H_\varepsilon^{\natural})M_{od,\varepsilon}(-\lambda)$$

$$\sigma_{ess}(1+2\alpha M_\varepsilon(-\lambda)) = \sigma_{ess}\left(1+\alpha\left(M_{d,\varepsilon}(-\lambda)(+)_{\natural}M_{od,\varepsilon}(-\lambda)\right)\right) = \sigma_{ess}(1+\alpha M_{d,\varepsilon}(-\lambda)).$$

$$f_{\lambda,\varepsilon}(s) = 1 + \frac{\alpha}{\sqrt{4\varepsilon^2 s^2 + (4+\varepsilon^2)\lambda}}$$

$$\sigma_{ess}(1+2\alpha M_\varepsilon(-\lambda)) = \sigma_{ess}(\widehat{M}_{\lambda,\varepsilon}) = \sigma(\widehat{M}_{\lambda,\varepsilon}) = \text{range}(f_{\lambda,\varepsilon}) = \left[1 - \frac{|\alpha|}{\sqrt{(4+\varepsilon^2)\lambda}}, 1\right]$$

$$\lambda > 0, -\lambda \in \sigma_{ess}(H_\varepsilon^{\natural})$$

$$0 \in \left[1 - \frac{|\alpha|}{\sqrt{(4+\varepsilon^2)\lambda}}, 1\right] \sigma_{ess}(H_\varepsilon^{\natural}) = \left[-\frac{\alpha^2}{4+\varepsilon^2}, 0\right) \cup [0,+\infty)$$

$$D(h_x) := \{u \in H^2(\mathbb{R}\setminus\{\pm x/2\}) \cap H^1(\mathbb{R}) : [u'](\pm x/2) = \alpha u(\pm x/2)\}$$
$$h_x u(y) = -u''(y) \text{ for a.e. } y \in \mathbb{R}\setminus\{\pm x/2\}$$

$$b_x : H^1(\mathbb{R}) \times H^1(\mathbb{R}) \subset L^2(\mathbb{R}) \times L^2(\mathbb{R}) \to \mathbb{C}$$
$$b_x(u,v) := \langle u', v'\rangle + \alpha\bar{u}(x/2)v(x/2) + \alpha\bar{u}(-x/2)v(-x/2).$$

$$r^0(y-y';z) = i\frac{e^{i\sqrt{z}|y-y'|}}{2\sqrt{z}} \quad z \in \mathbb{C}\setminus[0,+\infty), \text{Im}\sqrt{z} > 0$$

$$\breve{\mathbf{g}}_x(z) : L^2(\mathbb{R}) \to \mathbb{C}^2, \breve{\mathbf{g}}_x(z)u := \left((r^0(z)u)(x/2), (r^0(z)u)(-x/2)\right);$$
$$\mathbf{g}_x(z) : \mathbb{C}^2 \to L^2(\mathbb{R}), \mathbf{g}_x(z) := \breve{\mathbf{g}}_x(\bar{z})^*$$
$$\left(\mathbf{g}_x(z)(\zeta_1,\zeta_2)\right)(y) = r^0(y-x/2;z)\zeta_1 + r^0(y+x/2;z)\zeta_2$$

$$\mathbf{m}_x(z) : \mathbb{C}^2 \to \mathbb{C}^2 \ \mathbf{m}_x(z) := \frac{i}{2\sqrt{z}}\begin{bmatrix} 1 & e^{i\sqrt{z}|x|} \\ e^{i\sqrt{z}|x|} & 1 \end{bmatrix}$$

$$(h_x - z)^{-1} = r^0(z) - \alpha\mathbf{g}_x(z)(1+\alpha\mathbf{m}_x(z))^{-1}\breve{\mathbf{g}}_x(z)$$

$$(\alpha + 2\sqrt{\lambda})^2 = \alpha^2 e^{-2\sqrt{\lambda}|x|}$$

(i) $\sigma_{ac}(h_x) = \sigma_{ess}(h_x) = [0,+\infty)$;
(ii) $\sigma_{sc}(h_x) = \emptyset$;
(iii)

$$\sigma_p(h_x) = \sigma_d(h_x) = \begin{cases} \emptyset & \alpha \ge 0 \\ \{-\lambda_0(x)\} & \alpha < 0, |x| \le 2/|\alpha| \\ \{-\lambda_0(x), -\lambda_1(x)\} & \alpha < 0, |x| > 2/|\alpha| \end{cases}$$

$$W(x)e^{W(x)} = x$$

$$\lambda_0:\mathbb{R}\to(0,+\infty),\lambda_0(x)=\left(\frac{W\left(\frac{|\alpha||x|}{2}e^{-\frac{|\alpha||x|}{2}}\right)}{|x|}+\frac{|\alpha|}{2}\right)^2$$

$$\lambda_1:\mathbb{R}\setminus[-2/|\alpha|,2/|\alpha|]\to(0,+\infty),\lambda_1(x)=\left(\frac{W\left(-\frac{|\alpha||x|}{2}e^{-\frac{|\alpha||x|}{2}}\right)}{|x|}+\frac{|\alpha|}{2}\right)^2$$

(i) $\alpha^2/4<\lambda_0(x)\le\alpha^2, 0<\lambda_1(x)<\alpha^2/4$;
(iii) $\lambda_0(0)=\alpha^2, \lim_{x\to(\pm2/|\alpha|)_\pm}\lambda_1(x)=0, \lim_{x\to\pm\infty}\lambda_0(x)=\lim_{x\to\pm\infty}\lambda_1(x)=\alpha^2/4$;
(iv) $\lambda_0\in C^\infty(\mathbb{R}\setminus\{0\}),\lambda_1\in C^\infty(\mathbb{R}\setminus[-2/|\alpha|,2/|\alpha|])$.

$$h_xu_0=\mathbb{R}\setminus\left\{\pm\frac{x}{2}\right\}-u_0''=\left(-\infty,\frac{x}{2}\right]\text{ and }\left[\frac{x}{2},+\infty\right)$$

$$\min_{x\in\mathbb{R}}-\lambda_0(x)=-\lambda_0(0)=-\alpha^2,$$

$$\lim_{|x|\to+\infty}-\lambda_1(x)=-\alpha^2/4.$$

$$\psi_x^{BO}(y):=N(x)\left(e^{-\sqrt{\lambda_0(x)}|x/2-y|}+e^{-\sqrt{\lambda_0(x)}|x/2+y|}\right),$$

$$N(x):=\left(\frac{\sqrt{\lambda_0(x)}}{2\left(1+e^{-\sqrt{\lambda_0(x)}|x|}\left(1+\sqrt{\lambda_0(x)}|x|\right)\right)}\right)^{1/2}.$$

$$P_x\phi:=\langle\psi_x^{BO},\phi\rangle\psi_x^{BO}$$

$$\phi_x(y):=\phi(x,y)$$

$$x\mapsto\|\phi_x\|_{L^2(\mathbb{R})}$$

$$\|\phi\|_{L^2(\mathbb{R}^2)}^2=\int_{\mathbb{R}}\|\phi_x\|_{L^2(\mathbb{R})}^2dx$$

$$\phi\in H^1(\mathbb{R}^2)$$

$$x\mapsto\|\phi_x\|_{H^1(\mathbb{R})}$$

$$\|\phi\|_{H^1(\mathbb{R}^2)}^2=\int_{\mathbb{R}^2}|\partial_x\phi(x,y)|^2\mathbf{dx}+\int_{\mathbb{R}}\|\phi_x\|_{H^1(\mathbb{R})}^2dx$$

$$(\varphi,\psi)\in H_\natural^1(\mathbb{R}^2)\times H_\natural^1(\mathbb{R}^2)$$

$$\mathcal{B}_\varepsilon^\natural(\varphi,\psi)=\int_{\mathbb{R}^2}\varepsilon^2\partial_x\bar{\varphi}(x,y)\partial_x\psi(x,y)\mathbf{dx}+\int_{\mathbb{R}}b_x(\varphi_x,\psi_x)dx$$

$$-\alpha^2H_\varepsilon^\natural q_x(u,v):=b_x(u,v)+\alpha^2h_x+\alpha^2Q_\varepsilon^\natural D\left(Q_\varepsilon^\natural\right)=H_\natural^1(\mathbb{R}^2)$$

$$Q_\varepsilon^\natural(\varphi,\psi):=\mathcal{B}_\varepsilon^\natural(\varphi,\psi)+\alpha^2(\varphi,\psi)_{L^2(\mathbb{R}^2)}=\int_{\mathbb{R}^2}\varepsilon^2\partial_x\bar{\varphi}(x,y)\partial_x\psi(x,y)\mathbf{dx}+\int_{\mathbb{R}}q_x(\varphi_x,\psi_x)dx\quad(4.2)$$

$$\mathcal{L}_\varepsilon^\natural:=H_\varepsilon^\natural+\alpha^2.$$

$$\mathcal{P}: L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)\ (\mathcal{P}\phi)_x := P_x\phi_x$$

$$\mathcal{P}^{\perp} := 1 - \mathcal{P}.$$

$$\psi^{BO}(x,y) \equiv \psi_x^{BO}(y)$$

$$\mathcal{P}: L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2), \mathcal{P}\phi(x,y) := \psi^{BO}(x,y) f_\phi(x)$$

$$f_\phi(x) := \int_{\mathbb{R}} \psi^{BO}(x,y)\phi(x,y)dy = \int_{\mathbb{R}} \langle \psi_x^{BO}, \phi_x \rangle dx$$

$$\|f_\phi\|_{L^2(\mathbb{R})}^2 \le \int_{\mathbb{R}} \left(\int_{\mathbb{R}} |\psi^{BO}(x,y)||\phi(x,y)|dy \right)^2 dx \le \int_{\mathbb{R}} \|\psi_x^{BO}\|_{L^2(\mathbb{R})}^2 \|\phi_x\|_{L^2(\mathbb{R})}^2 dx = \|\phi\|_{L^2(\mathbb{R}^2)}^2$$

$$\phi \in L_{\mathrm{b}}^2(\mathbb{R}^2)\phi \in L_{\mathrm{f}}^2(\mathbb{R}^2)$$

$$L_{\natural}^2(\mathbb{R}^2) H^1(\mathbb{R}^2) [\partial_x, \mathcal{P}]: H^1(\mathbb{R}^2) \subset L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2) L^2(\mathbb{R}^2)$$

$$\|[\partial_x, \mathcal{P}]\|_{\mathcal{B}\left(L^2(\mathbb{R}^2)\right)} \le \delta$$

$$\delta := 2\left(\sup_{x\in\mathbb{R}} \int |\partial_x \psi^{BO}(x,y)|^2 dy \right)^{1/2}$$

$$\partial_y \psi^{BO}(x,y) = N\sqrt{\lambda_0}\left(\operatorname{sgn}(x/2 - y) e^{-\sqrt{\lambda_0}|x/2-y|} - \operatorname{sgn}(x/2+y) e^{-\sqrt{\lambda_0}|x/2+y|} \right)$$

$$\begin{aligned} \int_{\mathbb{R}} \left|\partial_y \psi^{BO}(x,y)\right|^2 dy &= 2N^2\sqrt{\lambda_0}\left(1 + e^{-\sqrt{\lambda_0}}|x| - \sqrt{\lambda_0}|x| e^{-\sqrt{\lambda_0}|x|}\right) \\ &= \lambda_0 \frac{1 + e^{-\sqrt{\lambda_0}}|x|}{1 + \sqrt{\lambda_0}|x| e^{-\sqrt{\lambda_0}}|x|} \\ &\le \lambda_0 \le \alpha^2 \end{aligned}$$

$$\begin{aligned} \int_{\mathbb{R}^2} \left|\partial_y \mathcal{P}\phi(x,y)\right|^2 \mathbf{dx} &= \int_{\mathbb{R}^2} \left|\partial_y \psi^{BO}(x,y)\right|^2 \left|f_\phi(x)\right|^2 dxdy \\ &\le \left(\sup_{x\in\mathbb{R}} \int_{\mathbb{R}} \left|\partial_y \psi^{BO}(x,y)\right|^2 dy \right) \|f_\phi\|_{L^2(\mathbb{R})}^2 \\ &\le \alpha^2 \|\phi\|_{L^2(\mathbb{R}^2)}^2 \end{aligned}$$

$$\tilde{f}_\phi(x) := \int_{\mathbb{R}} (\partial_x \psi^{BO}(x,y))\phi(x,y)dy$$

$$\|\tilde{f}_\phi\| \le \frac{\delta}{2}\|\phi\|$$

$$\partial_x \mathcal{P}\phi = (\partial_x \psi^{BO}) f_\phi + \psi^{BO}\tilde{f}_\phi + \psi^{BO} f_{\partial_x\phi}$$

$$\begin{aligned} \|\partial_x \mathcal{P}\phi\| &\le \left\|(\partial_x \psi^{BO}) f_\phi\right\|_{L^2(\mathbb{R}^2)} + \left\|\psi^{BO}\tilde{f}_\phi\right\| + \left\|\psi^{BO} f_{\partial_x\phi}\right\| \\ &\le \frac{\delta}{2}\|f_\phi\| + \|\tilde{f}_\phi\| + \|\partial_x\phi\| \le (1+\delta)\|\phi\|_{H^1(\mathbb{R}^2)} \end{aligned}$$

$$[\partial_x, \mathcal{P}]\phi = (\partial_x \psi^{BO}) f_\phi + \psi^{BO}\tilde{f}_\phi$$

$$\|[\partial_x, \mathcal{P}]\phi\|_{L^2(\mathbb{R}^2)} \leq \delta \|\phi\|_{L^2(\mathbb{R}^2)} \partial_x \psi^{BO}$$

$$\partial_x \psi^{BO}(x,y) = \underbrace{\frac{N'}{N}\psi^{BO}}_{\varphi_1^{BO}} - \underbrace{\frac{N\lambda_0'}{2\sqrt{\lambda_0}}\left(|x/2-y|e^{-\sqrt{\lambda_0}|x/2-y|} + |x/2+y|e^{-\sqrt{\lambda_0}|x/2+y|}\right)}_{\varphi_2^{BO}}$$

$$\underbrace{-\frac{N\sqrt{\lambda_0}}{2}\left(\operatorname{sgn}(x/2-y)e^{-\sqrt{\lambda_0}|x/2-y|} + \operatorname{sgn}(x/2+y)e^{-\sqrt{\lambda_0}|x/2+y|}\right)}_{\varphi_3^{BO}}$$

$$\|\varphi_1^{BO}\|^2 = \left(\frac{N'}{N}\right)^2$$

$$\frac{N'}{N} = \frac{\left(\sqrt{\lambda_0}\right)'}{2\sqrt{\lambda_0}} + \frac{\frac{\left(\sqrt{\lambda_0}\right)'}{\sqrt{\lambda_0}}\left(\lambda_0 x^2 + \frac{\lambda_0^{3/2}}{\left(\sqrt{\lambda_0}\right)'}x\right)}{2\left(\sqrt{\lambda_0}|x| + e^{\sqrt{\lambda_0}|x|} + 1\right)}$$

$$\lambda_0(x) = \frac{\alpha^2}{4}\nu^2(|\alpha|x/2)\ x \geq 0$$

$$\nu(x) = \frac{W(xe^{-x})}{x} + 1$$

$$\left|\frac{\left(\sqrt{\lambda_0}\right)'}{2\sqrt{\lambda_0}}\right| = \frac{|\alpha|}{4}\left|\frac{\nu'(ax/2)}{\nu(ax/2)}\right|$$

$$W(x)e^{W(x)} = x, x \geq 0$$

$$\nu(x) = e^{-x\nu(x)} + 1$$

$$\frac{\nu'(x)}{\nu(x)} = -\frac{1}{e^{x\nu(x)} + x}$$

$$|\nu'(x)/\nu(x)| \leq \frac{1}{e^x + x} \leq 1$$

$$\left|\frac{\left(\sqrt{\lambda_0}\right)'}{2\sqrt{\lambda_0}}\right| \leq \frac{|\alpha|}{4}$$

$$\sqrt{\lambda_0} \leq |\alpha|$$

$$\left|\frac{\frac{\left(\sqrt{\lambda_0}\right)'}{\sqrt{\lambda_0}}\left(\lambda_0 x^2 + \frac{\lambda_0^{3/2}}{\left(\sqrt{\lambda_0}\right)'}x\right)}{2\left(\sqrt{\lambda_0}|x| + e^{\sqrt{\lambda_0}|x|} + 1\right)}\right| \leq \frac{\frac{|\alpha|}{2}\lambda_0 x^2 + |\alpha|\sqrt{\lambda_0}|x|}{2\left(\sqrt{\lambda_0}|x| + e^{\sqrt{\lambda_0}|x|} + 1\right)} \leq \frac{|\alpha|}{4}$$

$$\frac{\frac{1}{2}s^2 + s}{2(s + e^s + 1)} \leq \frac{1}{4}, s \geq 0$$

$$\left|\frac{N'}{N}\right| \leq \frac{|\alpha|}{2} \text{ and } \|\varphi_1^{BO}\|_{L^2(\mathbb{R},dy)}^2 = \left(\frac{N'}{N}\right)^2 \leq \frac{\alpha^2}{4}$$

$$\|\varphi_2^{BO}\|^2 = \frac{(N\lambda_0')^2}{4(\lambda_0)^{5/2}}\left(1 + \frac{\left(\sqrt{\lambda_0}|x|\right)^3}{3} e^{-\sqrt{\lambda_0}|x|} + \left(1 + \sqrt{\lambda_0}|x|\right)e^{-\sqrt{\lambda_0}|x|}\right)$$

$$= \frac{(\lambda_0')^2}{2(\lambda_0)^2}\frac{1 + \frac{\left(\sqrt{\lambda_0}|x|\right)^3}{3} e^{-\sqrt{\lambda_0}|x|} + \left(1 + \sqrt{\lambda_0}|x|\right)e^{-\sqrt{\lambda_0}|x|}}{1 + e^{-\sqrt{\lambda_0}|x|} + \sqrt{\lambda_0}|x|e^{-\sqrt{\lambda_0}|x|}} \leq \frac{(\lambda_0')^2}{(\lambda_0)^2} \leq \alpha^2$$

$$|\lambda_0'/\lambda_0| \leq |\alpha|\|\varphi_3^{BO}\|$$

$$\|\varphi_3^{BO}\|^2 = \frac{N^2\sqrt{\lambda_0}}{2}\left(1 - e^{-\sqrt{\lambda_0}|x|} + \sqrt{\lambda_0}|x|e^{-\sqrt{\lambda_0}|x|}\right)$$

$$= \frac{\lambda_0}{4}\frac{1 - e^{-\sqrt{\lambda_0}|x|} + \sqrt{\lambda_0}|x|e^{-\sqrt{\lambda_0}|x|}}{1 + e^{-\sqrt{\lambda_0}|x|} + \sqrt{\lambda_0}|x|e^{-\sqrt{\lambda_0}|x|}} \leq \frac{\lambda_0}{4} \leq \frac{\alpha^2}{4}$$

$$\|\partial_x\psi^{BO}\| \leq \sum_{j=1}^{3} \|\varphi_j^{BO}\| \leq 2|\alpha|\delta \leq 4|\alpha|$$

$$H_\natural^1(\mathbb{R}^2) L_\natural^2(\mathbb{R}^2)$$

$$D\left(\hat{Q}_\varepsilon^\natural\right) = H_\natural^1(\mathbb{R}^2)\ \hat{Q}_\varepsilon^\natural(\phi,\psi) := Q_\varepsilon^\natural(\mathcal{P}\phi,\mathcal{P}\psi) + Q_\varepsilon^\natural(\mathcal{P}^\perp\phi,\mathcal{P}^\perp\psi).$$

$$\phi,\psi \in H_\natural^1(\mathbb{R}^2)$$

$$\left|Q_\varepsilon^\natural(\phi,\psi) - \hat{Q}_\varepsilon^\natural(\phi,\psi)\right| \leq 2\varepsilon\delta\left(\sqrt{Q_\varepsilon^\natural(\phi)}\|\psi\| + \|\phi\|\sqrt{\hat{Q}_\varepsilon^\natural(\psi)}\right)\hat{Q}_\varepsilon^\natural$$

$$Q_\varepsilon^\natural(\phi,\psi) - \hat{Q}_\varepsilon^\natural(\phi,\psi) = Q_\varepsilon^\natural(\mathcal{P}\phi,\mathcal{P}^\perp\psi) + Q_\varepsilon^\natural(\mathcal{P}^\perp\phi,\mathcal{P}\psi)$$

$$S_\varepsilon\phi := -i\varepsilon\partial_x q_x(\mathcal{P}_x u, \mathcal{P}_x^\perp u) = q_x(\mathcal{P}_x^\perp u, \mathcal{P}_x u) = 0$$

$$\begin{aligned}
Q_\varepsilon^\natural(\phi,\psi) - \hat{Q}_\varepsilon^\natural(\phi,\psi) =& \langle S_\varepsilon\mathcal{P}\phi, S_\varepsilon\mathcal{P}^\perp\psi\rangle + \langle S_\varepsilon\mathcal{P}^\perp\phi, S_\varepsilon\mathcal{P}\psi\rangle \\
=& \langle S_\varepsilon\mathcal{P}\phi, S_\varepsilon(1-\mathcal{P})\psi\rangle + \langle S_\varepsilon(1-\mathcal{P})\phi, S_\varepsilon\mathcal{P}\psi\rangle \\
=& \langle S_\varepsilon\mathcal{P}\phi, S_\varepsilon\psi\rangle + \langle S_\varepsilon\phi, S_\varepsilon\mathcal{P}\psi\rangle - 2\langle S_\varepsilon\mathcal{P}\phi, S_\varepsilon\mathcal{P}\psi\rangle \\
=& \langle [S_\varepsilon,\mathcal{P}]\phi, S_\varepsilon\psi\rangle + \langle \mathcal{P}S_\varepsilon\phi, S_\varepsilon\psi\rangle \\
&+ \langle S_\varepsilon\phi, S_\varepsilon\mathcal{P}\psi\rangle - 2\langle [S_\varepsilon,\mathcal{P}]\phi, S_\varepsilon\mathcal{P}\psi\rangle - 2\langle \mathcal{P}S_\varepsilon\phi, S_\varepsilon\mathcal{P}\psi\rangle
\end{aligned}$$

$$\begin{aligned}
-2\langle \mathcal{P}S_\varepsilon\phi, S_\varepsilon\mathcal{P}\psi\rangle &= -2\langle S_\varepsilon\phi, \mathcal{P}S_\varepsilon\mathcal{P}\psi\rangle \\
&= -2\langle S_\varepsilon\phi, [\mathcal{P}, S_\varepsilon]\mathcal{P}\psi\rangle - 2\langle S_\varepsilon\phi, S_\varepsilon\mathcal{P}^2\psi\rangle \\
&= 2\langle S_\varepsilon\phi, [S_\varepsilon, \mathcal{P}]\mathcal{P}\psi\rangle - 2\langle S_\varepsilon\phi, S_\varepsilon\mathcal{P}\psi\rangle
\end{aligned}$$

$$\langle \mathcal{P}S_\varepsilon\phi, S_\varepsilon\psi\rangle = \langle S_\varepsilon\phi, \mathcal{P}S_\varepsilon\psi\rangle = -\langle S_\varepsilon\phi, [S_\varepsilon,\mathcal{P}]\psi\rangle + \langle S_\varepsilon\phi, S_\varepsilon\mathcal{P}\psi\rangle$$

$$\begin{aligned}\mathcal{Q}_\varepsilon^\natural(\phi,\psi)-\hat{\mathcal{Q}}_\varepsilon^\natural(\phi,\psi)=&\langle[S_\varepsilon,\mathcal{P}]\phi,S_\varepsilon\psi\rangle+(-\langle S_\varepsilon\phi,[S_\varepsilon,\mathcal{P}]\psi\rangle+\langle S_\varepsilon\phi,S_\varepsilon\mathcal{P}\psi\rangle)\\&+\langle S_\varepsilon\phi,S_\varepsilon\mathcal{P}\psi\rangle-2\langle[S_\varepsilon,\mathcal{P}]\phi,S_\varepsilon\mathcal{P}\psi\rangle+(2\langle S_\varepsilon\phi,[S_\varepsilon,\mathcal{P}]\mathcal{P}\psi\rangle-2\langle S_\varepsilon\phi,S_\varepsilon\mathcal{P}\psi\rangle)\\=&\langle[S_\varepsilon,\mathcal{P}]\phi,S_\varepsilon\psi\rangle-\langle S_\varepsilon\phi,[S_\varepsilon,\mathcal{P}]\psi\rangle-2\langle[S_\varepsilon,\mathcal{P}]\phi,S_\varepsilon\mathcal{P}\psi\rangle+2\langle S_\varepsilon\phi,[S_\varepsilon,\mathcal{P}]\mathcal{P}\psi\rangle\\=&\langle[S_\varepsilon,\mathcal{P}]\phi,S_\varepsilon\mathcal{P}^\perp\psi\rangle-\langle S_\varepsilon\phi,[S_\varepsilon,\mathcal{P}]\mathcal{P}^\perp\psi\rangle-\langle[S_\varepsilon,\mathcal{P}]\phi,S_\varepsilon\mathcal{P}\psi\rangle+\langle S_\varepsilon\phi,[S_\varepsilon,\mathcal{P}]\mathcal{P}\psi\rangle\end{aligned}$$

$$\begin{aligned}&\left|\mathcal{Q}_\varepsilon^\natural(\phi,\psi)-\hat{\mathcal{Q}}_\varepsilon^\natural(\phi,\psi)\right|\\&\le\varepsilon\delta\big(\|\varepsilon\partial_x\phi\|(\|\mathcal{P}\psi\|+\|\mathcal{P}^\perp\psi\|)+\|\phi\|(\|\varepsilon\partial_x\mathcal{P}\psi\|+\|\varepsilon\partial_x\mathcal{P}^\perp\psi\|)\big).\end{aligned}$$

$$a+b\le 2\sqrt{a^2+b^2}$$

$$\begin{aligned}&\left|\mathcal{Q}_\varepsilon^\natural(\phi,\psi)-\hat{\mathcal{Q}}_\varepsilon^\natural(\phi,\psi)\right|\\&\le 2\varepsilon\delta\left(\|\varepsilon\partial_x\phi\|\sqrt{\|\mathcal{P}\psi\|^2+\|\mathcal{P}^\perp\psi\|^2}+\|\phi\|\sqrt{\|\varepsilon\partial_x\mathcal{P}\psi\|^2+\|\varepsilon\partial_x\mathcal{P}^\perp\psi\|^2}\right)\\&\le 2\varepsilon\delta\left(\sqrt{\mathcal{Q}_\varepsilon^\natural(\phi)}\|\psi\|+\|\phi\|\sqrt{\hat{\mathcal{Q}}_\varepsilon^\natural(\psi)}\right)\end{aligned}$$

$$\hat{\mathcal{Q}}_\varepsilon^\natural\ \widehat{\mathcal{L}_\varepsilon^\natural}\text{ in }L_\natural^2(\mathbb{R}^2)$$

$$\widehat{\mathcal{L}_\varepsilon^\natural}=\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}}^\natural\oplus\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}^\perp}^\natural,\sigma\left(\widehat{\mathcal{L}_\varepsilon^\natural}\right)=\sigma\left(\widehat{\mathcal{L}_{\varepsilon,\mathcal{P}}^\natural}\right)\cup\sigma\left(\widehat{\mathcal{L}_{\varepsilon,\mathcal{P}^\perp}^\natural}\right),$$

$$\begin{aligned}\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}}^\natural&:D\big(\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}}^\natural\big)\subset\operatorname{ran}\left(\mathcal{P}\mid L_\natural^2(\mathbb{R}^2)\right)\to\operatorname{ran}\left(\mathcal{P}\mid L_\natural^2(\mathbb{R}^2)\right),\\\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}^\perp}^\natural&:D\big(\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}\perp}^\natural\big)\subset\operatorname{ran}\left(\mathcal{P}^\perp\mid L_\natural^2(\mathbb{R}^2)\right)\to\operatorname{ran}\left(\mathcal{P}^\perp\mid L_\natural^2(\mathbb{R}^2)\right);\end{aligned}$$

$$\begin{aligned}\big\langle\psi,\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}}^\natural\psi\big\rangle&=\mathcal{Q}_\varepsilon^\natural(\mathcal{P}\psi,\mathcal{P}\psi)\ge 0,\forall\psi\in D\big(\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}}^\natural\big),\\\big\langle\psi,\hat{\mathcal{L}}_{\varepsilon,\mathcal{P}\perp}^\natural\psi\big\rangle&=\mathcal{Q}_\varepsilon^\natural(\mathcal{P}^\perp\psi,\mathcal{P}^\perp\psi)\ge\inf_{x\in\mathbb{R}}(-\lambda_1(x))+\alpha^2=\frac{3}{4}\alpha^2,\forall\psi\in D\left(\widehat{\mathcal{L}_{\varepsilon,\mathcal{P}}^\natural}\right).\end{aligned}$$

$$\lambda\in\mathbb{R},\phi\in D\big(\mathcal{L}_\varepsilon^\natural\big)\ \psi\in D\left(\widehat{\mathcal{L}_\varepsilon^\natural}\right)$$

$$\begin{aligned}&\left|\left\langle\phi,\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)\psi\right\rangle-\langle(\mathcal{L}_\varepsilon^\natural-\lambda)\phi,\psi\rangle\right|\\&\le 2\varepsilon\delta\left(\|\psi\|\sqrt{\left(\big\|(\mathcal{L}_\varepsilon^\natural-\lambda)\phi\big\|+\lambda_+\|\phi\|\right)\|\phi\|}+\|\phi\|\sqrt{\left(\left\|\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)\psi\right\|+\lambda_+\|\psi\|\right)\|\psi\|}\right).\end{aligned}$$

$$\phi\in D\big(\mathcal{L}_\varepsilon^\natural\big)$$

$$\mathcal{Q}_\varepsilon^\natural(\phi)=\langle\phi,(\mathcal{L}_\varepsilon^\natural-\lambda)\phi\rangle+\lambda\|\phi\|^2.$$

$$\mathcal{Q}_\varepsilon^\natural(\phi)\le\left(\big\|(\mathcal{L}_\varepsilon^\natural-\lambda)\phi\big\|+\lambda_+\|\phi\|\right)\|\phi\|.$$

$$\psi\in D\left(\widehat{\mathcal{L}_\varepsilon^\natural}\right)$$

$$\hat{\mathcal{Q}}_\varepsilon^\natural(\psi)\le\left(\left\|\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)\psi\right\|+\lambda_+\|\psi\|\right)\|\psi\|.$$

$$\phi\in D\big(\mathcal{L}_\varepsilon^\natural\big)\text{ and }\psi\in D\left(\widehat{\mathcal{L}_\varepsilon^\natural}\right)$$

$$\left\langle\phi,\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)\psi\right\rangle-\left\langle\mathcal{L}_\varepsilon^\natural-\lambda)\phi,\psi\right\rangle=\langle\phi,\hat{\mathcal{L}}_\varepsilon^\natural\psi\rangle-\langle\mathcal{L}_\varepsilon^\natural\phi,\psi\rangle=\hat{\mathcal{Q}}_\varepsilon^\natural(\phi,\psi)-\mathcal{Q}_\varepsilon^\natural(\phi,\psi).$$

$$\left|\left\langle \phi, \left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)\psi\right\rangle - \langle (\mathcal{L}_\varepsilon^\natural - \lambda)\phi, \psi\rangle\right|$$
$$\leq 2\varepsilon\delta\left(\|\psi\|\sqrt{(\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\| + \lambda_+\|\phi\|)\|\phi\|} + \|\phi\|\sqrt{\left(\left\|\left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)\psi\right\| + \lambda_+\|\psi\|\right)\|\psi\|}\right).$$

$$d_\varepsilon \equiv d_\varepsilon(\lambda) := \operatorname{dist}\left(\lambda, \sigma(\mathcal{L}_\varepsilon^\natural)\right), \text{ and } \hat{d}_\varepsilon \equiv \hat{d}_\varepsilon(\lambda) := \operatorname{dist}\left(\lambda, \sigma(\hat{\mathcal{L}}_\varepsilon^\natural)\right)$$

$$\left\{\lambda \in [0, +\infty) \cap \rho\left(\widehat{\mathcal{L}_\varepsilon^\natural}\right) : \frac{4\varepsilon\delta}{\sqrt{\hat{d}_\varepsilon(\lambda)}}\sqrt{1 + \frac{\lambda}{\hat{d}_\varepsilon(\lambda)}} < \frac{1}{2}\right\} \subseteq \left\{\lambda \in \rho(\mathcal{L}_\varepsilon^\natural) : d_\varepsilon(\lambda) \geq \frac{\hat{d}_\varepsilon(\lambda)}{32}\right\}.$$

$$\lambda \in \rho(\mathcal{L}_\varepsilon^\natural) \cap \rho\left(\widehat{\mathcal{L}_\varepsilon^\natural}\right)$$

$$\left\|(\mathcal{L}_\varepsilon^\natural - \lambda)^{-1} - \left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)^{-1}\right\|_{\mathcal{B}(L^2(\mathbb{R}^2))} \leq 2\varepsilon\delta\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{\frac{1}{d_\varepsilon}\left(1 + \frac{\lambda_+}{d_\varepsilon}\right)} + \frac{1}{d_\varepsilon}\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1 + \frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right).$$

$$\psi = \left(\widehat{\mathcal{L}_\varepsilon^\star} - \lambda\right)^{-1}\phi$$

$$\text{I } \|\phi\|^2 - \left\langle (\mathcal{L}_\varepsilon^\natural - \lambda)\phi, \left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)^{-1}\phi\right\rangle$$
$$\leq 2\varepsilon\delta\left(\left\|\left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)^{-1}\phi\right\|\sqrt{(\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\| + \lambda_+\|\phi\|)\|\phi\|}\right.$$
$$\left.+\|\phi\|\sqrt{\left(\|\phi\| + \lambda_+\left\|\left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)^{-1}\phi\right\|\right)\left\|\left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)^{-1}\phi\right\|}\right)$$
$$\leq 2\varepsilon\delta\|\phi\|\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{(\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\| + \lambda_+\|\phi\|)\|\phi\|} + \|\phi\|\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1 + \frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right)$$
$$\leq 2\varepsilon\delta\|\phi\|\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\|\|\phi\|} + \frac{\|\phi\|}{\hat{d}_\varepsilon}\sqrt{\lambda_+} + \|\phi\|\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1 + \frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right)$$
$$\leq 2\varepsilon\delta\|\phi\|\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\|\|\phi\|} + 2\|\phi\|\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1 + \frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right)$$

$$\|\phi\|^2 \leq \left|\left\langle (\mathcal{L}_\varepsilon^\natural - \lambda)\phi, \left(\widehat{\mathcal{L}_\varepsilon^\natural} - \lambda\right)^{-1}\phi\right\rangle\right| + 2\varepsilon\delta\|\phi\|\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\|\|\phi\|} + 2\|\phi\|\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1 + \frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right).$$

$$\|\phi\| \leq \frac{1}{\hat{d}_\varepsilon}\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\| + 2\varepsilon\delta\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\|\|\phi\|} + 2\|\phi\|\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1 + \frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right)$$

$$s := \sqrt{\frac{\|(\mathcal{L}_\varepsilon^\natural - \lambda)\phi\|}{\hat{d}_\varepsilon\|\phi\|}},$$

$$\left(s+\frac{\varepsilon\delta}{\sqrt{\hat{d}_\varepsilon}}\right)^2-\frac{\varepsilon^2\delta^2}{\hat{d}_\varepsilon}\geq 1-\frac{4\varepsilon\delta}{\sqrt{\hat{d}_\varepsilon}}\sqrt{1+\frac{\lambda_+}{\hat{d}_\varepsilon}}$$

$$\frac{4\varepsilon\delta}{\sqrt{\hat{d}_\varepsilon}}\sqrt{1+\frac{\lambda_+}{\hat{d}_\varepsilon}}<\frac{1}{2}$$

$$s\geq-\frac{\varepsilon\delta}{\sqrt{\hat{d}_\varepsilon}}+\sqrt{\frac{\varepsilon^2\delta^2}{\hat{d}_\varepsilon}+\frac{1}{2}}\geq\frac{1}{4}\frac{1}{\sqrt{1+\frac{\varepsilon^2\delta^2}{\hat{d}_\varepsilon}}}$$

$$\left\|\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)\phi\right\|\geq\frac{\widehat{d_\varepsilon}}{16}\frac{1}{1+\frac{\varepsilon^2\delta^2}{\hat{d}_\varepsilon}}\|\phi\|\geq\frac{\hat{d}_\varepsilon}{32}\|\phi\|>0$$

$$\lambda\in\rho\left(\mathcal{L}_\varepsilon^\natural\right)$$

$$(-\infty,0)\subset\rho\left(\mathcal{L}_\varepsilon^\natural\right)$$

$$\tilde{\chi},\chi\in L_\natural^2(\mathbb{R}^2)$$

$$\phi=\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)^{-1}\tilde{\chi}\text{ and }\psi=\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)^{-1}\chi$$

$$\begin{aligned}&\left|\left\langle\tilde{\chi},\left(\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)^{-1}-\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)^{-1}\right)\chi\right\rangle\right|\\ &\leq 2\varepsilon\delta\left(\left\|\left(\hat{\mathcal{L}}_\varepsilon^\natural-\lambda\right)^{-1}\chi\right\|\sqrt{\left(\|\tilde{\chi}\|+\lambda_+\left\|\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)^{-1}\tilde{\chi}\right\|\right)\left\|\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)^{-1}\tilde{\chi}\right\|}\right.\\ &\qquad\left.+\left\|\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)^{-1}\tilde{\chi}\right\|\sqrt{\left(\|\chi\|+\lambda_+\left\|\left(\hat{\mathcal{L}}_\varepsilon^\natural-\lambda\right)^{-1}\chi\right\|\right)\left\|\left(\hat{\mathcal{L}}_\varepsilon^\natural-\lambda\right)^{-1}\chi\right\|}\right)\\ &\leq 2\varepsilon\delta\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{\frac{1}{d_\varepsilon}\left(1+\frac{\lambda_+}{d_\varepsilon}\right)}+\frac{1}{d_\varepsilon}\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1+\frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right)\|\chi\|\|\tilde{\chi}\|.\end{aligned}$$

$$\tilde{\chi}=\left(\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)^{-1}-\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)^{-1}\right)\chi$$

$$\left\|\left(\left(\mathcal{L}_\varepsilon^\natural-\lambda\right)^{-1}-\left(\widehat{\mathcal{L}_\varepsilon^\natural}-\lambda\right)^{-1}\right)\chi\right\|\leq 2\varepsilon\delta\left(\frac{1}{\hat{d}_\varepsilon}\sqrt{\frac{1}{d_\varepsilon}\left(1+\frac{\lambda_+}{d_\varepsilon}\right)}+\frac{1}{d_\varepsilon}\sqrt{\frac{1}{\hat{d}_\varepsilon}\left(1+\frac{\lambda_+}{\hat{d}_\varepsilon}\right)}\right)\|\chi\|.$$

$$\mathcal{Q}_\varepsilon^\natural(\mathcal{P}\varphi,\mathcal{P}\psi)$$

$$\mathcal{Q}_\varepsilon^\natural(\mathcal{P}\varphi,\mathcal{P}\psi)=\int_{\mathbb{R}^2}\varepsilon^2\partial_x\left(\overline{\psi^{BO}f_\varphi}\right)\partial_x\left(\psi^{BO}f_\psi\right)\mathbf{dx}+\int_{\mathbb{R}}q_x(\psi_x^{BO},\psi_x^{BO})\overline{f_\varphi}f_\psi dx$$

$$\int_{\mathbb{R}^2}\partial_x\left(\overline{\psi^{BO}f_\varphi}\right)\partial_x\left(\psi^{BO}f_\psi\right)\mathbf{dx}=\int_{\mathbb{R}}\overline{f_\varphi'}f_\psi'dx+\int_{\mathbb{R}}\left(\int_{\mathbb{R}}|\partial_x\psi^{BO}|^2dy\right)\overline{f_\varphi}f_\psi dx$$

$$\int_{\mathbb{R}} \psi^{BO} \partial_x \psi^{BO} dy = \|\psi_x^{BO}\| = 1$$

$$q_x(\psi_x^{BO}, \psi_x^{BO}) = -\lambda_0(x) + \alpha^2$$

$$Q_\varepsilon^\natural(\mathcal{P}\varphi, \mathcal{P}\psi) = \int_{\mathbb{R}} \left(\varepsilon^2 \overline{f_\varphi'} f_\psi' + (V + \varepsilon^2 R) \overline{f_\varphi} f_\psi \right) dx$$

$$V(x) := -\lambda_0(x) + \alpha^2 = -\left(\frac{W\left(\frac{|\alpha||x|}{2} e^{\frac{-|\alpha||x|}{2}}\right)}{|x|} + \frac{|\alpha|}{2} \right)^2 + \alpha^2$$

$$R(x) := \int_{\mathbb{R}} |\partial_x \psi^{BO}(x,y)|^2 dy$$

$$L_\natural^2(\mathbb{R}) := \{f \in L^2(\mathbb{R}) : f(x) = (+)_\natural f(-x)\}, H_\natural^1(\mathbb{R}) := H^1(\mathbb{R}) \cap L_\natural^2(\mathbb{R})$$

$$U_{BO} : \operatorname{ran}\left(\mathcal{P} \mid L_\natural^2(\mathbb{R}^2)\right) \to L_\natural^2(\mathbb{R}), U_{BO}\left(\psi^{BO} f_\phi\right) := f_\phi.$$

$$\|\psi_x^{BO}\| = 1$$

$$\left\langle \psi^{BO} f_\phi, \psi^{BO} f_\psi \right\rangle = \int_{\mathbb{R}} \langle \psi_x^{BO}, \psi_x^{BO} \rangle \bar{f}_\phi(x) f_\psi(x) dx = \left\langle f_\phi, f_\psi \right\rangle,$$

$$U_{BO}^{-1} f = \psi^{BO} f$$

$$\operatorname{ran}\left(\mathcal{P} \mid L_\natural^2(\mathbb{R}^2)\right) \simeq L_\natural^2(\mathbb{R}).$$

$$Q_\varepsilon^\natural(\mathcal{P} \times \mathcal{P}) L_\natural^2(\mathbb{R})$$

$$D\left(\mathrm{Q}_\varepsilon^{\mathrm{eff}\,\natural}\right) := H_\natural^1(\mathbb{R}) \times H_\natural^1(\mathbb{R}), \mathrm{Q}_\varepsilon^{\mathrm{eff}\,\natural}(f, g) := \int_{\mathbb{R}} \varepsilon^2 \overline{f'} g' + (V + \varepsilon^2 R) \bar{\mathrm{f}} g dx.$$

$$V + \varepsilon^2 R L_\natural^2(\mathbb{R})$$

$$D\left(\mathcal{L}_\varepsilon^{\mathrm{eff}}\right) = H_\natural^2(\mathbb{R}) := H^2(\mathbb{R}) \cap L_\natural^2(\mathbb{R}) \; \mathcal{L}_\varepsilon^{\mathrm{eff}} = -\varepsilon^2 \frac{d^2}{dx^2} + V + \varepsilon^2 R.$$

$$\mathcal{L}_\varepsilon^{\mathrm{eff}\natural} - \varepsilon^2 R = -\varepsilon^2 \frac{d^2}{dx^2} + V$$

(i) $0 \leq V(x) < \frac{3}{4}\alpha^2$
(ii) $V(0) = \lim_{x \to \pm\infty} V(x) = \frac{3}{4}\alpha^2$

$$(W(ye^{-y}) + y)^2 - 4y^2 = -8y^3 + O(y^4), y \ll 1,$$

$$V(x) = |\alpha|^3 |x| + O(x^2), |x| \ll 1$$

$$\Lambda := \varepsilon^{-1}$$

$$\mathrm{L}_\Lambda^\natural := \Lambda^2 \mathcal{L}_{1/\Lambda}^{\mathrm{eff}\natural} - R \equiv -\frac{d^2}{dx^2} + \Lambda^2 V$$

$$\sigma_{ess}(\mathrm{L}_\Lambda^\natural) \subseteq \sigma_{ess}(\mathrm{L}_\Lambda) = \sigma_{ess}\left(-\frac{d^2}{dx^2} + \frac{3}{4}\alpha^2\Lambda^2\right) = \left[\frac{3}{4}\alpha^2\Lambda^2, +\infty\right)$$

$$0 < \ell_{\Lambda,0}^\natural < \ell_{\Lambda,1}^\natural < \cdots < \ell_{\Lambda,n}^\natural < \cdots.$$

$$\ell_{\Lambda,n}^\natural = e_n^\natural \Lambda^{4/3} + O(\Lambda), e_n^{\mathrm{b}} := e_{2n}, e_n^{\mathrm{f}} := e_{2n+1},$$

$$D(\dot{\mathrm{K}}^1) = C_0^\infty(\mathbb{R}), \dot{\mathrm{K}}^1 := -\frac{d^2}{dx^2} + |\alpha|^3|x|.$$

$$\sigma_{2n} = \bar{\bar{\sigma}}_{n+1} \text{ and } \sigma_{2n+1} = \bar{\sigma}_{n+1}$$

$$\phi_k \in L^2(\mathbb{R})$$

$$\mathrm{K}^1\phi_k = e_k\phi_k, k = 0,1,2, \ldots$$

$$\phi_{2n}(x) = C_{2n}\mathrm{Ai}(|\alpha||x| + \sigma_{2k}), n = 0,1,2, \ldots,$$
$$\phi_{2n+1}(x) = C_{2n+1}\mathrm{sgn}(x)\mathrm{Ai}(|\alpha||x| + \sigma_{2n+1}), n = 0,1,2, \ldots,$$

$$\cdots < \sigma_{2n+1} < \sigma_{2n} < \cdots < \sigma_1 < \sigma_0 < 0$$

$$\mathrm{Ai}'(\sigma_{2n}) = 0$$

$$\mathrm{Ai}(\sigma_{2n+1}) = 0$$

$$0 < e_0 < e_1 < e_2 < \cdots < e_k < \cdots$$

$$e_k = |\sigma_k|\alpha^2$$

$$L^2(\mathbb{R}) = L^2_{\mathrm{b}}(\mathbb{R}) \oplus L^2_{\mathrm{f}}(\mathbb{R})$$

$$\mathrm{K}^1 = \mathrm{K}^{1\,\mathrm{b}} \oplus \mathrm{K}^{1\mathrm{f}}$$

$$\{e_n^{\mathrm{b}}, \phi_n^{\mathrm{b}}\} := \{e_{2n}, \phi_{2n}\}\{e_n^{\mathrm{f}}, \phi_n^{\mathrm{f}}\} := \{e_{2n+1}, \phi_{2n+1}\}$$

$$\mathrm{Ai}(x) = \frac{1}{2\sqrt{\pi}x^{1/4}} e^{-\frac{2}{3}x^{3/2}}\left(1 + O\left(x^{-3/2}\right)\right)$$

$$-\left(\frac{3\pi}{8}(4n+3) + \frac{3}{2}\arctan\frac{5}{18\pi(4n+3)}\right)^{2/3} \leq \sigma_{2n+1} \leq -\left(\frac{3\pi}{8}(4n+3)\right)^{2/3}$$

$$\sigma_{2n+1} < \sigma_{2n} < \sigma_{2(n-1)+1}$$

$$-\left(\frac{3\pi}{8}(4n+3) + \frac{3}{2}\arctan\frac{5}{18\pi(4n+3)}\right)^{2/3} \leq \sigma_{2n} \leq -\left(\frac{3\pi}{8}(4n-1)\right)^{2/3}$$

$$\mathrm{L}_\Lambda^{1\natural} := \Lambda^{4/3}U_\Lambda \mathrm{K}^{1\natural}U_\Lambda^{-1}$$

$$U_\Lambda\ L^2_\natural(\mathbb{R})(U_\Lambda f)(x) := \Lambda^{1/3}f\left(\Lambda^{2/3}x\right)$$

$$\psi \in C_0^\infty(\mathbb{R}) \cap L^2_\natural(\mathbb{R})$$

$$\mathrm{L}_\Lambda^{1\natural}\psi(x) = -\psi''(x) + \Lambda^2|\alpha|^3|x|\psi(x)$$

$$\Lambda^{-4/3}\ \mathrm{L}_\Lambda^{1\natural}\{\Lambda^{4/3}e_n^\natural, U_\Lambda\phi_n^\natural\}$$

$$j\in C_0^\infty(\mathbb{R})\cap L^2(\mathbb{R})$$

$$\mathrm{J}_1(x):=j\left(\Lambda^{1/2}x\right)$$

$$\mathrm{J}_0(x):=\sqrt{1-\mathrm{J}_1^2(x)}\ (\mathrm{J}_0^2+\mathrm{J}_1^2=1)$$

$$|x|\leq 2/\Lambda^{1/2}\ \mathrm{J}_1(\ \mathrm{L}_\Lambda^\natural-\mathrm{L}_\Lambda^{1\natural})\mathrm{J}_1=\mathrm{J}_1\left(\Lambda^2(V-|\alpha|^3|x|)\right)\mathrm{J}_1$$

$$\left\|\mathrm{J}_1(\ \mathrm{L}_\Lambda^\natural-\mathrm{L}_\Lambda^{1\natural})\mathrm{J}_1\right\|=\left\|\mathrm{J}_1\left(\Lambda^2(V-|\alpha|^3|x|)\right)\mathrm{J}_1\right\|\leq C\|\ \mathrm{J}_1(\Lambda^2x^2)\mathrm{J}_1\|=O(\Lambda)\ell_{\Lambda,n}^\natural$$

$$\ell_{\Lambda,n}^\natural\geq\Lambda^{4/3}e_n^\natural+O(\Lambda)\ \Lambda\gg 1.$$

$$\mathrm{L}_\Lambda^\natural\geq e_n^\natural\Lambda^{4/3}+\mathrm{F}_1^\natural+O(\Lambda),$$

$$\mathrm{F}_1^\natural:=\mathrm{J}_1(\ \mathrm{L}_\Lambda^{1\natural}-e_n\Lambda^{4/3})\mathrm{P}_\Lambda^{1\natural}\ \mathrm{J}_1.$$

$$\left(\psi,\mathrm{L}_\Lambda^\natural\psi\right)\geq e_n^\natural\Lambda^{4/3}\|\psi\|^2+\left(\psi,\mathrm{F}_1^\natural\psi\right)+O(\Lambda)\psi\in D(\ \mathrm{L}_\Lambda^\natural)$$

$$\ell_{\Lambda,n}^\natural\geq\langle\psi,\mathrm{L}_\Lambda^\natural\psi\rangle\geq e_n^\natural\Lambda^{4/3}+O(\Lambda)$$

$$\mathrm{L}_\Lambda^\natural=\sum_{i=0}^{1}\ \mathrm{J_i}\ \mathrm{L}_\Lambda^\natural\mathrm{J_i}-\sum_{i=0}^{1}\ (\ \mathrm{J}_\mathrm{i}')^2.$$

$$\mathrm{L}_\Lambda^\natural=\mathrm{J}_0\ \mathrm{L}_\Lambda^\natural\mathrm{J}_0+\mathrm{J}_1\ \mathrm{L}_\Lambda^{1\natural}\ \mathrm{J}_1+\mathrm{J}_1(\ \mathrm{L}_\Lambda^\natural-\mathrm{L}_\Lambda^{1\natural})\mathrm{J}_1-\sum_{i=0}^{1}\ (\ \mathrm{J}_\mathrm{i}')^2.$$

$$\left\|\sum_{i=0}^{1}\ (\ \mathrm{J}_\mathrm{i}')^2\right\|=O(\Lambda)$$

$$\mathrm{L}_\Lambda^{1\natural}=\mathrm{L}_\Lambda^{1\natural}\mathrm{P}_\Lambda^{1\natural}+\mathrm{L}_\Lambda^{1\natural}\left(\mathrm{I}-\mathrm{P}_\Lambda^{1\natural}\right)=\mathrm{F}^\natural+e_n^\natural\Lambda^{4/3}\mathrm{P}_\Lambda^{1\natural}+\mathrm{L}_\Lambda^{1\natural}\left(\mathrm{I}-\mathrm{P}_\Lambda^{1\natural}\right)\geq\mathrm{F}^\natural+e_n^\natural\Lambda^{4/3},$$

$$\mathrm{F}^\natural:=\left(\mathrm{L}_\Lambda^{1\natural}-e_n^\natural\Lambda^{4/3}\right)\mathrm{P}_\Lambda^{1\natural}.$$

$$\mathrm{J}_1\ \mathrm{L}_\Lambda^{1\natural}\ \mathrm{J}_1\geq\mathrm{F}_1^\natural+e_n^\natural\Lambda^{4/3}\ \mathrm{J}_1\ ^2.$$

$$\langle\psi,\mathrm{J}_1\ \mathrm{L}_\Lambda^{1\natural}\ \mathrm{J}_1\psi\rangle\psi\in D(\ \mathrm{L}_\Lambda^\natural)$$

$$\psi\in D(\ \mathrm{L}_\Lambda^\natural)\mathrm{J}_1\psi\in D(\ \mathrm{L}_\Lambda^{1\natural})$$

$$V(x)\geq V\left(1/\Lambda^{1/2}\right)\geq\frac{c}{\Lambda^{1/2}}\ \mathrm{supp}(\mathrm{J}_0)-\frac{d^2}{dx^2}$$

$$\mathrm{J}_0\ \mathrm{L}_\Lambda^\natural\mathrm{J}_0\geq c\Lambda^{3/2}(\ \mathrm{J}_0)^2\geq e_n^\natural\Lambda^{4/3}(\ \mathrm{J}_0)^2,$$

$$\ell_{\Lambda,n}^\natural\leq\Lambda^{4/3}e_n^\natural+O(\Lambda).$$

$$\mathrm{L}_\Lambda^{1\natural}\left(U_\Lambda\phi_n^\natural\right)=\Lambda^{4/3}e_n^\natural\left(U_\Lambda\phi_n^\natural\right).$$

$$\psi_n^\natural:=\mathrm{J}_1U_\Lambda\phi_n^\natural$$

$$\langle \psi_n^\natural, \psi_m^\natural \rangle = \delta_{mn} + O\left(e^{-c\Lambda^{1/4}}\right),$$

$$\mathrm{J}_1\, \mathrm{L}_\Lambda^{1\natural}\, \mathrm{J}_1 = \frac{1}{2}\left(\mathrm{J}_1^2\, \mathrm{L}_\Lambda^{1\natural} + \mathrm{L}_\Lambda^{1\natural}\, \mathrm{J}_1^2\right) + (\mathrm{J}_1')^2$$

$$\begin{aligned}\langle \psi_n^\natural, \mathrm{L}_\Lambda^{1\natural}\psi_m^\natural \rangle &= \Lambda^{4/3}\left(\frac{e_n^\natural + e_m^\natural}{2}\right)\langle \psi_n^\natural, \psi_m^\natural \rangle + \left(U_\Lambda \phi_n^\natural, (J_1')^2 U_\Lambda \phi_m^\natural\right) \\ &= \Lambda^{4/3} e_n^\natural \delta_{nm} + O(\Lambda)\end{aligned}$$

$$\langle \psi_n^\natural, \mathrm{L}_\Lambda^\natural \psi_m^\natural \rangle = \langle \psi_n^\natural, \mathrm{L}_\Lambda^{1\natural}\psi_m^\natural \rangle + O(\Lambda) = \Lambda^{4/3} e_n^\natural \delta_{mn} + O(\Lambda)\{\psi_i^\natural\}_{i=0}^n$$

$$\langle \tilde{\psi}_n^\natural, \mathrm{L}_\Lambda^{1\natural}\tilde{\psi}_m^\natural \rangle = \Lambda^{4/3} e_n^\natural \delta_{nm} + O(\Lambda)\{\tilde{\psi}_i^\natural\}_{i=1}^n$$

$$\ell_{\Lambda,n}^\natural \le \Lambda^{4/3} e_n^\natural + O(\Lambda)$$

$$\sigma_{\mathrm{ess}}\left(\mathrm{L}_\Lambda^\natural\right) \subseteq \left[\frac{3}{4}\alpha^2\Lambda^2, +\infty\right)$$

$$\mathcal{E}_{\varepsilon,n}\mathrm{eff}\natural = s_n^\natural \alpha^2 \varepsilon^{2/3} + O(\varepsilon),$$

$$\widetilde{\mathrm{L}}_\Lambda^\natural := \Lambda^2 \mathcal{L}_{1/\Lambda}^{\mathrm{eff}\,\natural} = \mathrm{L}_\Lambda^\natural + R.$$

$$\mathcal{L}_\varepsilon^{\mathrm{eff}} = \varepsilon^2\, \widetilde{\mathrm{L}}_{1/\varepsilon}^\natural$$

$$\mathcal{E}_{\varepsilon,n-1}^{eff} < \mu_{\varepsilon,n}^\natural < \mathcal{E}_{\varepsilon,n}^{\mathrm{efft}}\, \hat{d}_\varepsilon\left(\mu_{\varepsilon,n}^\natural\right) > c_n \varepsilon^{2/3}$$

$$\mu_{\varepsilon,n}^\natural := \mathcal{E}_{\varepsilon,n}\mathrm{eff}^\natural - c_n \varepsilon^{2/3}$$

$$\left(\mu_{\varepsilon,n}^\natural - \mathcal{E}_{\varepsilon,n}\,\mathrm{eff}^\natural\right)^{-1}\left(\mu_{\varepsilon,n}^\natural - \widehat{\mathcal{L}_\varepsilon^\natural}\right)^{-1}$$

$$\left(\mu_{\varepsilon,n}^\natural - \mathcal{E}_{\varepsilon,n}^{\mathrm{eff}}\right)^{-1} = \min_{\psi \in L_\natural^2(\mathbb{R}^2), \|\psi\|=1} \left\langle \psi, \left(\mu_{\varepsilon,n}^\natural - \hat{\mathcal{L}}_\varepsilon^\natural\right)^{-1}\psi \right\rangle.$$

$$\mu_{\varepsilon,n}^\natural \in \rho\left(\mathcal{L}_\varepsilon^\natural\right) d_\varepsilon\left(\mu_{\varepsilon,n}^\natural\right) > c_n' \varepsilon^{2/3} \mathcal{E}_{\varepsilon,n}^\natural$$

$$\left(\mu_{\varepsilon,n}^\natural - \mathcal{E}_{\varepsilon,n}^\natural\right)^{-1} = \inf_{\psi \in L_\natural^2(\mathbb{R}^2), \|\psi\|=1} \left\langle \psi, \left(\mu_{\varepsilon,n}^\natural - \mathcal{L}_\varepsilon^\natural\right)^{-1}\psi \right\rangle.$$

$$\mathcal{E}_{\varepsilon,n}^\natural = \inf \sigma_{ess}\left(\mathcal{L}_\varepsilon^\natural\right) \inf \sigma_{\mathrm{ess}}\left(\mathcal{L}_\varepsilon^\natural\right) = \frac{3+\varepsilon^2}{4+\varepsilon^2}\alpha^2$$

$$\left|\left(\mathcal{E}_{\varepsilon,n}^\natural - \mu_{\varepsilon,n}^\natural\right)^{-1} - \left(\mathcal{E}_{\varepsilon,n}^{\mathrm{eff}\natural} - \mu_{\varepsilon,n}^\natural\right)^{-1}\right| \le c_n''.$$

$$\begin{aligned}\left|\mathcal{E}_{\varepsilon,n}^\natural - \mathcal{E}_{\varepsilon,n}\mathrm{eff}\right| &\le c_n''\left|\mathcal{E}_{\varepsilon,n}^\natural - \mu_{\varepsilon,n}^\natural\right|\left|\mathcal{E}_{\varepsilon,n}\mathrm{effb} - \mu_{\varepsilon,n}^\natural\right| \le c_n'' c_n \varepsilon^{2/3}\left|\mathcal{E}_{\varepsilon,n}^\natural - \mathcal{E}_{\varepsilon,n}\mathrm{effb} + c_n\varepsilon^{2/3}\right| \\ &\le c_n'' c_n \varepsilon^{2/3}\left|\mathcal{E}_{\varepsilon,n}^\natural - \mathcal{E}_{\varepsilon,n}\mathrm{eff}\right| + c_n'' c_n^2 \varepsilon^{4/3}\end{aligned}$$

$$\mathcal{E}_{\varepsilon,n}^\natural = \mathcal{E}_{\varepsilon,n}^{\mathrm{eff}\natural} + O\left(\varepsilon^{4/3}\right) = s_n^\natural \alpha^2 \varepsilon^{2/3} + O(\varepsilon).$$

$$\mathcal{E}_{\varepsilon,n}^\natural < \inf \sigma_{ess}\left(\mathcal{L}_\varepsilon^\natural\right)$$

$$\mathcal{E}^{\mathrm{efft}}_{\varepsilon,k} - \tilde{c}_k \varepsilon^{4/3} \leq \mathcal{E}^{\natural}_{\varepsilon,k} \leq \mathcal{E}^{\mathrm{eff}\natural}_{\varepsilon,k} + \tilde{c}_k \varepsilon^{4/3} \; k = 0, \dots, n$$
$$\mathcal{E}^{\mathrm{eff}\natural}_{\varepsilon,k-1} + \tilde{c}_{k-1} \varepsilon^{4/3} \leq \mathcal{E}^{\mathrm{eff}\natural}_{\varepsilon,k} - \tilde{c}_k \varepsilon^{4/3} \; k = 1, \dots, n$$

$$\sigma_d(H^{\natural}_{\varepsilon}) = \sigma_d(\mathcal{L}^{\natural}_{\varepsilon}) - \alpha^2$$

$$\hat{\mathbf{H}}_{\mathrm{tot}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) = \hat{\mathbf{H}}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) + T_{N_c}(\mathbf{P}^{\mathrm{N_c}}) + W_{N_c}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}),$$

$$\hat{\mathbf{H}}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) = \hat{T}_{\mathrm{N}} + \mathcal{W}^{\mathrm{MM}}_{\mathrm{N}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) + \hat{\mathbf{H}}_{\mathrm{BO}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{R}^{\mathrm{N_N}}),$$

$$\hat{\mathbf{H}}_{\mathrm{BO}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{R}^{\mathrm{N_N}}) = \hat{T}_{\mathrm{e}} + \hat{W}_{\mathrm{ee}} + \hat{W}_{\mathrm{Ne}}(\mathbf{R}^{\mathrm{N_N}}) + \hat{W}_{\mathrm{NN}}(\mathbf{R}^{\mathrm{N_N}}) + \mathcal{W}^{\mathrm{MM}}_{\mathrm{e}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})$$

$$\mathcal{W}^{\mathrm{MM}}_{\mathrm{N}} = \sum_{i=1}^{\mathrm{N_c}} \sum_{j=1}^{\mathrm{N_N}} w^{\mathrm{MM}}_{\mathrm{N}}(\mathbf{R}_j, \tilde{\mathbf{Q}}_i),$$
$$\mathcal{W}^{\mathrm{MM}}_{\mathrm{e}} = \sum_{i=1}^{\mathrm{N_c}} \sum_{j=1}^{\mathrm{N_e}} w^{\mathrm{MM}}_{\mathrm{e}}(\mathbf{r}_j, \tilde{\mathbf{Q}}_i),$$

$$\hat{\mathcal{P}}^{\mathrm{N_c}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{P}^{\mathrm{N_c}}) = \frac{e^{-\beta\left(\hat{\mathbf{H}}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) + W_{N_c}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})\right)} \mathrm{e}^{-\beta T_{N_c}(\mathbf{P}^{\mathrm{N_c}})}}{\mathcal{Z}_{\mathrm{N_c}}},$$

$$\mathcal{Z}_{\mathrm{N_c}} = \iint \mathrm{Tr}_{\mathrm{QM}}\left[e^{-\beta \hat{\mathbf{H}}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})}\right] \mathrm{e}^{-\beta(W_{N_c}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) + T_{N_c})} d\mathbf{P}^{\mathrm{N_c}} d\tilde{\mathbf{Q}}^{\mathrm{N_c}}$$

$$\hat{\mathcal{P}}^{\mathrm{GC}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{P}^{\mathrm{N_c}}) = \frac{e^{-\beta(\hat{\mathbf{H}}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) + W_{N_c}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) - \mu \mathrm{N_c})} \mathrm{e}^{-\beta T_{N_c}(\mathbf{P}^{\mathrm{N_c}})}}{\Xi},$$

$$\Xi = \sum_{\mathrm{N_c}=0}^{\infty} \frac{1}{\mathrm{N_c}!} \mathcal{Z}_{\mathrm{N_c}} e^{\beta \mu \mathrm{N_c}}$$
$$\equiv \mathrm{Tr}_{\mathrm{GC}}[\hat{\mathcal{P}}^{\mathrm{GC}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{P}^{\mathrm{N_c}})],$$

$$\Omega = -\frac{1}{\beta} \log(\Xi).$$

$$\hat{\mathcal{P}}^{\mathrm{GC}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{P}^{\mathrm{N_c}}) = p^{\mathrm{GC}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{P}^{\mathrm{N_c}}) \hat{\boldsymbol{\rho}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}),$$

$$p^{\mathrm{GC}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{P}^{\mathrm{N_c}}) = \mathcal{Z}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) \frac{\mathrm{e}^{-\beta\left(W_{N_c}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) + T_{N_c}(\mathbf{P}^{\mathrm{N_c}}) - \mu \mathrm{N_c}\right)}}{\Xi},$$

$$\hat{\boldsymbol{\rho}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) = \frac{\mathrm{e}^{-\beta \hat{\mathbf{H}}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})}}{\mathcal{Z}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})} \text{ and}$$

$$\mathcal{Z}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) = \mathrm{Tr}_{\mathrm{QM}}\left\{\mathrm{e}^{-\beta \hat{\mathbf{H}}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})}\right\}.$$

$$\hat{\boldsymbol{\rho}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) = \sum_{\alpha,n} \frac{e^{-\beta \mathcal{E}^{\alpha}_{n}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})}}{\mathcal{Z}_{\mathrm{QM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})} |\Phi^{\alpha}_{n}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})\rangle\langle\Phi^{\alpha}_{n}(\tilde{\mathbf{Q}}^{\mathrm{N_c}})|.$$

$$\hat{\boldsymbol{\rho}}_{\mathrm{eq}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) = \hat{\boldsymbol{\rho}}^{0}_{\mathrm{N}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}) \hat{\boldsymbol{\rho}}^{0}_{\mathrm{el}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}}, \mathbf{R}^{\mathrm{N_N}}),$$

$$\hat{\boldsymbol{\rho}}_{\text{el}}^{0}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{R}^{\text{N}_\text{N}}) = |\Psi^{0}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{R}^{\text{N}_\text{N}})\rangle\langle\Psi^{0}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{R}^{\text{N}_\text{N}})|$$

$$\hat{\boldsymbol{\rho}}_{\text{N}}^{0}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}}) = \sum_{n} \frac{e^{-\beta\mathcal{E}_{n}^{0}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}})}}{\mathcal{Z}_{\mathbf{QM}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}})} |\chi_{\text{N}}^{0,n}(\mathbf{R}^{\text{N}_\text{N}};\tilde{\mathbf{Q}}^{\text{N}_\text{c}})\rangle\langle\chi_{\text{N}}^{0,n}(\mathbf{R}^{\text{N}_\text{N}};\tilde{\mathbf{Q}}^{\text{N}_\text{c}})|,$$

$$\mathcal{Z}_{\text{QM}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}}) = \sum_{n} e^{-\beta\mathcal{E}_{n}^{0}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}})}$$

$$\hat{\mathcal{P}}^{\text{GC}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{P}^{\text{N}_\text{c}}) = p^{\text{GC}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{P}^{\text{N}_\text{c}})\hat{\boldsymbol{\rho}}_{\text{QM}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}}).$$

$$\omega[\hat{\mathcal{P}}^{\text{GC}}] = \mathcal{U}_{\text{int}}[\hat{\mathcal{P}}^{\text{GC}}] - \frac{1}{\beta}\mathcal{S}_{\text{int}}[\hat{\mathcal{P}}^{\text{GC}}]$$

$$\mathcal{U}_{\text{int}}[\hat{\mathcal{P}}^{\text{N}_\text{c}}] = \text{Tr}_{\text{GC}}\{p^{\text{GC}}\hat{\boldsymbol{\rho}}_{\text{QM}}[\hat{\mathbf{H}}_{\text{QM}} + W_{N_\text{c}} + T_{N_\text{c}} - \mu\text{N}_\text{c}]\}$$

$$\mathcal{S}_{\text{int}}[\hat{\mathcal{P}}^{\text{GC}}] = -\text{Tr}_{\text{GC}}\{p^{\text{GC}}\hat{\boldsymbol{\rho}}_{\text{QM}}\log(p^{\text{GC}}\hat{\boldsymbol{\rho}}_{\text{QM}})\}$$

$$\Omega = \min_{\hat{\mathcal{P}}^{\text{GC}}}\omega[\hat{\mathcal{P}}^{\text{GC}}], \hat{\mathcal{P}}_{\text{eq}}^{\text{GC}} = \text{argmin}\,\omega[\hat{\mathcal{P}}^{\text{GC}}]$$

$$\hat{\mathcal{P}}_{\text{MF}}^{\text{GC}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{P}^{\text{N}_\text{c}}) = p^{\text{GC}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{P}^{\text{N}_\text{c}})\hat{\boldsymbol{\rho}}_{\text{N}}\hat{\boldsymbol{\rho}}_{\text{el}}(\mathbf{R}^{\text{N}_\text{N}}).$$

$$\Omega_{\text{MF}} = \min_{\hat{\mathcal{P}}_{\text{MF}}^{\text{GC}}}\omega[\hat{\mathcal{P}}_{\text{MF}}^{\text{GC}}], \Omega \leq \Omega_{\text{MF}}.$$

$$\Omega_{\text{MF}} = \min_{\hat{\boldsymbol{\rho}}_{\text{N}}}\left(\mathcal{U}_{\text{N}}[\hat{\boldsymbol{\rho}}_{\text{N}}] - \frac{1}{\beta}\mathcal{S}_{\text{QM}}[\hat{\boldsymbol{\rho}}_{\text{N}}]\right),$$

$$\mathcal{S}_{\text{QM}}[\hat{\boldsymbol{\rho}}_{\text{N}}] = -\text{Tr}\{\hat{\boldsymbol{\rho}}_{\text{N}}\log(\hat{\boldsymbol{\rho}}_{\text{N}})\},$$

$$\mathcal{U}_{\text{N}}[\hat{\boldsymbol{\rho}}_{\text{N}}] = \text{Tr}\{\hat{\boldsymbol{\rho}}_{\text{N}}[\hat{T}_{\text{N}} + \hat{\mathcal{W}}_{\text{NN}}^{\text{tot}}(\mathbf{R}^{\text{N}_\text{N}})]\}.$$

$$\hat{\mathcal{W}}_{\text{NN}}^{\text{tot}}(\mathbf{R}^{\text{N}_\text{N}}) = \hat{W}_{\text{NN}}(\mathbf{R}^{\text{N}_\text{N}}) + \mathcal{W}_{\text{N}}^{\text{eff}}(\mathbf{R}^{\text{N}_\text{N}}),$$

$$\mathcal{W}_{\text{N}}^{\text{eff}}(\mathbf{R}^{\text{N}_\text{N}}) = \min_{\hat{\boldsymbol{\rho}}_{\text{el}},p^{\text{GC}}}\left(f_{\text{el}}[\hat{\boldsymbol{\rho}}_{\text{el}}] + f_{\text{MM}}[p^{\text{GC}}] + f_{\text{QM}}^{\text{MM}}[\hat{\boldsymbol{\rho}}_{\text{el}},p^{\text{GC}}] + V_{\text{el}}^{\text{N}}[\hat{\boldsymbol{\rho}}_{\text{el}};\mathbf{R}^{\text{N}_\text{N}}] + V_{\text{MM}}^{\text{N}}[p^{\text{GC}};\mathbf{R}^{\text{N}_\text{N}}]\right)$$

$$f_{\text{el}}[\hat{\boldsymbol{\rho}}_{\text{el}}] = \text{Tr}_{\text{QM}}\{\hat{\boldsymbol{\rho}}_{\text{el}}(\hat{T}_{\text{e}} + \hat{W}_{\text{ee}})\},$$

$$f_{\text{MM}}^{\text{GC}}[p^{\text{GC}}] = \sum_{\text{N}_\text{c}=0}^{\infty}\iint\left(W_{N_\text{c}} + T_{N_\text{c}} - \mu\text{N}_\text{c} + \frac{1}{\beta}\log(p^{\text{GC}})\right)d\tilde{\mathbf{Q}}^{\text{N}_\text{c}}d\mathbf{P}^{\text{N}_\text{c}}.$$

$$E_{\text{QM}}^{\text{MM}}[\hat{\boldsymbol{\rho}}_{\text{el}},p^{\text{GC}}] = \sum_{\text{N}_\text{c}=0}^{\infty}\iint p^{\text{GC}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}},\mathbf{P}^{\text{N}_\text{c}})\text{Tr}_{\text{QM}}[\hat{\boldsymbol{\rho}}_{\text{el}}(\tilde{\mathbf{Q}}^{\text{N}_\text{c}})\mathcal{W}_{\text{e}}^{\text{MM}}]d\tilde{\mathbf{Q}}^{\text{N}_\text{c}}d\mathbf{P}^{\text{N}_\text{c}}$$

$$V_{\text{el}}^{\text{N}}[\hat{\boldsymbol{\rho}}_{\text{el}};\mathbf{R}^{\text{N}_\text{N}}] = \text{Tr}_{\text{QM}}[\hat{\boldsymbol{\rho}}_{\text{el}}\hat{W}_{\text{Ne}}(\mathbf{R}^{\text{N}_\text{N}})],$$

$$V_{\mathrm{MM}}^{\mathrm{N}}[p^{\mathrm{GC}};\mathbf{R}^{\mathrm{N_N}},\mathbf{P}^{\mathrm{N_c}})] =$$
$$\sum_{\mathrm{N_c}=0}^{\infty} \iint p^{\mathrm{GC}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}},\mathbf{P}^{\mathrm{N_c}})\mathcal{W}_{\mathrm{N}}^{\mathrm{MM}}(\tilde{\mathbf{Q}}^{\mathrm{N_c}},\mathbf{R}^{\mathrm{N_N}})d\tilde{\mathbf{Q}}^{\mathrm{N_c}}d\mathbf{P}^{\mathrm{N_c}}.$$

$$\mathcal{W}_{\mathrm{N}}^{\mathrm{eff}}(\mathbf{R}^{\mathrm{N_N}}) = \min_{\rho,n} w_{\mathrm{N}}^{\mathrm{eff}}[\rho,n,\mathbf{R}^{\mathrm{N_N}}],$$

$$w_{\mathrm{N}}^{\mathrm{eff}}[\rho,n,\mathbf{R}^{\mathrm{N_N}}] = \mathcal{F}_{\mathrm{el}}[\rho] + (v_{\mathrm{Ne}}(\mathbf{R}^{\mathrm{N_N}}) \mid \rho) + \mathcal{F}_{\mathrm{MM}}[n]$$
$$+(v_{\mathrm{N}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n) + (n|v_{\mathrm{e}}^{\mathrm{MM}}|\rho).$$

$$(v_{\mathrm{N}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n) = \int d\tilde{\mathbf{Q}} v_{\mathrm{N}}^{\mathrm{MM}}(\tilde{\mathbf{Q}};\mathbf{R}^{\mathrm{N_N}})n(\tilde{\mathbf{Q}}),$$

$$v_{\mathrm{N}}^{\mathrm{MM}}(\tilde{\mathbf{Q}};\mathbf{R}^{\mathrm{N_N}}) = \sum_{i=1}^{\mathrm{N_N}} w_{\mathrm{N}}^{\mathrm{MM}}(\mathbf{R}_i,\tilde{\mathbf{Q}})(n|v_{\mathrm{e}}^{\mathrm{MM}}|\rho)$$

$$(n|v_{\mathrm{e}}^{\mathrm{MM}}|\rho) = \int d\mathbf{r}d\tilde{\mathbf{Q}}\rho(\mathbf{r})v_{\mathrm{el}}^{\mathrm{MM}}(\mathbf{r},\tilde{\mathbf{Q}})n(\tilde{\mathbf{Q}})$$

$$\Omega = \hat{\mathcal{W}}_{\mathrm{NN}}^{\mathrm{tot}}(\mathbf{R}_{\mathrm{eq}}^{\mathrm{N_N}}) + \sum_k \left(\frac{\omega_k}{2} + \frac{1}{\beta}\log\left(1 - e^{-\beta\omega_k}\right)\right).$$

$$\mathcal{F}_{\mathrm{MM}}[n] = \mathcal{F}_{\mathrm{id}}[n] + \mathcal{F}_{\mathrm{exc}}[n]$$

$$\mathcal{F}_{\mathrm{exc}}[n] = -\frac{1}{2\beta}\iint \Delta n(\boldsymbol{r})c(|\boldsymbol{r}-\boldsymbol{r}'|,\boldsymbol{\Omega},\boldsymbol{\Omega}';n_0)$$
$$\Delta n(\boldsymbol{r}')d\boldsymbol{r}d\boldsymbol{r}'d\boldsymbol{\Omega}d\boldsymbol{\Omega}' + \mathcal{F}_{\mathrm{B}}[n]$$

$$(n|v_{\mathrm{e}}^{\mathrm{MM}}|\rho) = -\int d\mathbf{r}_1 d\mathbf{r}_2 n_c(\mathbf{r}_1)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\rho(\mathbf{r}_2)$$

$$n_c(\boldsymbol{r}) = \iint n(\boldsymbol{r}',\boldsymbol{\Omega})\gamma(\boldsymbol{r}-\boldsymbol{r}',\boldsymbol{\Omega})d\mathbf{r}'d\boldsymbol{\Omega}$$

$$(v_{\mathrm{N}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n) = (w_{\mathrm{C}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n_c) + (w_{\mathrm{LJ}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n),$$

$$(w_{\mathrm{C}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n_c) = \int d\mathbf{r}n_c(\mathbf{r})\sum_A \frac{Z_A}{|\mathbf{R}_A-\mathbf{r}|}$$
$$(w_{\mathrm{LJ}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n) = \int d\tilde{\mathbf{Q}}n(\tilde{\mathbf{Q}})\sum_A \hat{\mathcal{W}}_A^{\mathrm{LJ}}(\mathbf{R}_A,\tilde{\mathbf{Q}})$$

$$v_{\mathrm{ext}}^{\mathrm{QM}}(\mathbf{r}) = \int d\mathbf{r}'n_c(\mathbf{r}')\frac{1}{|\mathbf{r}'-\mathbf{r}|}$$
$$v_{\mathrm{ext}}^{\mathrm{MM}}(\mathbf{r}) = \sum_A \frac{Z_A}{|\mathbf{R}_A-\mathbf{r}|} - \int d\mathbf{r}'\rho(\mathbf{r}')\frac{1}{|\mathbf{r}'-\mathbf{r}|}$$

$$(n|v_{\mathrm{e}}^{\mathrm{MM}}|\rho) = -\int d\mathbf{r}v_{\mathrm{ext}}^{\mathrm{QM}}(\mathbf{r})\rho(\mathbf{r})$$

$$(w_{\mathrm{C}}^{\mathrm{MM}}(\mathbf{R}^{\mathrm{N_N}}) \mid n_c) + (n|v_{\mathrm{e}}^{\mathrm{MM}}|\rho) = \int d\mathbf{r}v_{\mathrm{ext}}^{\mathrm{MM}}(\mathbf{r})n_c(\mathbf{r})$$

$$QR + 2e^- + 2H^+ \longrightarrow H_2QR.$$

$$QR + H_2Q \longrightarrow H_2QR + Q$$

$$E^\circ_{QR/H_2QR} = -\frac{\Delta_r G^\circ}{2F} + E^\circ_{Q/H_2Q},$$

$$\hat{\mathcal{W}}^{tot}_{NN}(\mathbf{R}^{N_N}) \approx \hat{\mathcal{W}}^{tot}_{NN}(\mathbf{R}_{eq}) + \frac{1}{2}\delta^\dagger_{\mathbf{R}^N\,N}\mathbf{h}\delta_{\mathbf{R}^N\,N},$$

$$\nabla_{\mathbf{R}^{N_N}}\hat{\mathcal{W}}^{tot}_{NN}(\mathbf{R}^{N_N})\big|_{\mathbf{R}^{N_N}=\mathbf{R}_{eq}} = 0,$$

$$\delta_{\mathbf{R}^{N_N}} = \mathbf{R}^{N_N} - \mathbf{R}_{eq}$$

$$\mathbf{h}_{ij} = \frac{\partial^2\hat{\mathcal{W}}^{tot}_{NN}(\mathbf{R}^{N_N})}{\partial\mathbf{R}_i\partial\mathbf{R}_j}\bigg|_{\mathbf{R}^N\,N=\mathbf{R}_{eq}}$$

$$\mathcal{U}_N[\hat{\boldsymbol{\rho}}_N] = \hat{\mathcal{W}}^{tot}_{NN}(\mathbf{R}_{eq}) + \sum_{k=1}^{N_\nu} \mathrm{Tr}_{QM}\{\hat{\boldsymbol{\rho}}_N\hat{h}_{\omega_k}\}$$

$$\hat{h}_{\omega_k} = -\frac{1}{2\mu_k}\frac{\partial}{\partial q_k^2} + \frac{1}{2}\mu_k(\omega_k)^2 q_k^2$$

$$\omega_k = \sqrt{\frac{\lambda_k}{\mu_k}},$$

$$\mathcal{Z}_{\tilde{\mathbf{Q}}^{N_c}} = e^{-\beta\hat{\mathcal{W}}^{tot}_{NN}(\mathbf{R}_{eq})}\prod_{k=1}^{N_\nu}\mathcal{Z}^k_{vib},$$

$$\mathcal{Z}^k_{vib} = \frac{e^{-\frac{\beta\omega_k}{2}}}{1-e^{-\beta\omega_k}}$$

$$\Omega = -\frac{1}{\beta}\log\left(\mathcal{Z}_{\tilde{\mathbf{Q}}^{N_c}}\right),$$

$$\left(\rho_{opt}(\mathbf{R}^{N_N}), n_{opt}(\mathbf{R}^{N_N})\right) = \underset{\rho,n}{\mathrm{argmin}}\, w^{eff}_N[\rho, n, \mathbf{R}^{N_N}].$$

$$\nabla_{\mathbf{R}^N\,N}\mathcal{W}^{eff}_N(\mathbf{R}^{N_N}) = \nabla_{\mathbf{R}^N\,N}\min_{\rho,n} w^{eff}_N[\rho, n, \mathbf{R}^{N_N}]$$
$$= \nabla_{\mathbf{R}^N\,N} w^{eff}_N[\rho_{opt}(\mathbf{R}^{N_N}), n_{opt}(\mathbf{R}^{N_N}), \mathbf{R}^{N_N}].$$

$$(\rho_{opt}(\mathbf{R}^{N_N}), n_{opt}(\mathbf{R}^{N_N}))\ (\rho_{opt}(\mathbf{R}^{N_N}), n_{opt}(\mathbf{R}^{N_N}))$$

$$\nabla_{\mathbf{R}^{N_N}}\mathcal{W}^{eff}_N(\mathbf{R}^{N_N}) = \left(\nabla_{\mathbf{R}^{N_N}} v_{Ne}(\mathbf{R}^{N_N}) \mid \rho_{opt}(\mathbf{R}^{N_N})\right)$$
$$+ \left(\nabla_{\mathbf{R}^{N_N}} v^{MM}_N(\mathbf{R}^{N_N}) \mid n_{opt}(\mathbf{R}^{N_N})\right).$$

$$\left(\nabla_{\mathbf{R}^{N_N}} v_{Ne}(\mathbf{R}^{N_N}) \mid \rho_{opt}(\mathbf{R}^{N_N})\right)$$

$$\left(\nabla_{\mathbf{R}^{N_N}} v_N^{MM}(\mathbf{R}^{N_N}) \mid n_{opt}(\mathbf{R}^{N_N})\right) = \int d\tilde{\mathbf{Q}} n_{opt}(\tilde{\mathbf{Q}}) \nabla_{\mathbf{R}^{N_N}} v_N^{MM}(\tilde{\mathbf{Q}}, \mathbf{R}^{N_N})$$

$$\frac{\partial^2 \mathcal{W}_N^{eff}(\mathbf{R}^{N_N})}{\partial \mathbf{R}_i \partial \mathbf{R}_j} = \mathbf{h}_{Ne}(\mathbf{R}_i, \mathbf{R}_j) + \mathbf{h}_N^{MM}(\mathbf{R}_i, \mathbf{R}_j) + \mathbf{h}_e^{MM}(\mathbf{R}_i, \mathbf{R}_j),$$

$$\mathbf{h}_{Ne}(\mathbf{R}_i, \mathbf{R}_j) = \left(\frac{\partial^2 v_{Ne}(\mathbf{R}^{N_N})}{\partial \mathbf{R}_i \partial \mathbf{R}_j}\middle| \rho_{opt}\right) + \left(\nabla_{\mathbf{R}_i} v_{Ne}(\mathbf{R}^{N_N}) \mid \nabla_{\mathbf{R}_j} \rho_{opt}\right),$$

$$\mathbf{h}_N^{MM}(\mathbf{R}_i, \mathbf{R}_j) = \left(\frac{\partial^2 v_N^{MM}(\mathbf{R}^{N_N})}{\partial \mathbf{R}_i \partial \mathbf{R}_j}\middle| n_{opt}\right) + \left(\nabla_{\mathbf{R}_i} v_N^{MM}(\mathbf{R}^{N_N}) \mid \nabla_{\mathbf{R}_j} n_{opt}\right),$$

$$\mathbf{h}_e^{MM}(\mathbf{R}_i, \mathbf{R}_j) = \left(\nabla_{\mathbf{R}_i} n_{opt} \middle| v_e^{MM} \middle| \nabla_{\mathbf{R}_j} \rho_{opt}\right).$$

$$\nabla_{\mathbf{R}^{N_N}} \frac{\delta}{\delta \rho(\mathbf{r})} w_N^{eff}[\rho_{opt}, n_{opt}, \mathbf{R}^{N_N}] = \langle \hat{\chi}^{el} \cdot \nabla_{\mathbf{R}^{N_N}} \rho_{opt} \rangle_{\mathbf{r}} + \langle \hat{\chi}_{el}^{MM} \cdot \nabla_{\mathbf{R}^{N_N}} n_{opt} \rangle_{\mathbf{r}}$$

$$\nabla_{\mathbf{R}^{N_N}} \frac{\delta}{\delta n(\tilde{\mathbf{Q}})} w_N^{eff}[\rho_{opt}, n_{opt}, \mathbf{R}^{N_N}] = \langle \hat{\chi}^{MM} \cdot \nabla_{\mathbf{R}^{N_N}} n_{opt} \rangle_{\mathbf{r}} + \left\langle \hat{\chi}_{MM}^{el} \cdot \nabla_{\mathbf{R}^{N_N}} \rho_{opt} \right\rangle_{\mathbf{r}}$$

$$\langle \hat{f} \cdot g \rangle_{\mathbf{r}} = \int d\mathbf{r}' f(\mathbf{r}, \mathbf{r}') g(\mathbf{r}')$$

$$\chi^{el}(\mathbf{r}, \mathbf{r}')^{-1} = -\frac{\delta^2}{\delta \rho(\mathbf{r}) \delta \rho(\mathbf{r}')} w_N^{eff}[\rho, n, \mathbf{R}^{N_N}]$$

$$\chi^{MM}(\tilde{\mathbf{Q}}, \tilde{\mathbf{Q}}')^{-1} = -\frac{\delta^2}{\delta n(\tilde{\mathbf{Q}}) \delta n(\tilde{\mathbf{Q}}')} w_N^{eff}[\rho, n, \mathbf{R}^{N_N}]$$

$$\chi_{el}^{MM}(\tilde{\mathbf{Q}}, \mathbf{r})^{-1} = -\frac{\delta^2}{\delta n(\tilde{\mathbf{Q}}) \delta \rho(\mathbf{r})} w_N^{eff}[\rho, n, \mathbf{R}^{N_N}]$$

$$\chi_{MM}^{el}(\mathbf{r}, \tilde{\mathbf{Q}})^{-1} = -\frac{\delta^2}{\delta \rho(\mathbf{r}) \delta n(\tilde{\mathbf{Q}})} w_N^{eff}[\rho, n, \mathbf{R}^{N_N}]$$

$$\frac{\partial^2 \mathcal{W}_N^{eff}(\mathbf{R}^{N_N})}{\partial \mathbf{R}_i \partial \mathbf{R}_j} \approx \mathbf{h}_{Ne}(\mathbf{R}_i, \mathbf{R}_j).$$

$$\langle \Phi_I | \hat{\boldsymbol{p}}_e | \Phi_I \rangle = -i\hbar \frac{\boldsymbol{P} \cdot \hat{\boldsymbol{d}}}{\boldsymbol{M}}$$

$$|\Psi_I\rangle = |\Phi_I\rangle - i\hbar \sum_{J \neq I} \frac{\langle \Phi_J | \sum_A \frac{\boldsymbol{P}^A \cdot \hat{\boldsymbol{d}}_A^A}{M_A} | \Phi_I \rangle}{E_I - E_J} |\Phi_J\rangle$$

$$\langle \Phi_I | \hat{\boldsymbol{d}}^A | \Phi_J \rangle \equiv \boldsymbol{d}_{IJ}^A$$

$$\langle \Psi_I | \hat{\boldsymbol{p}}_e | \Psi_I \rangle =$$

$$2\hbar \mathrm{Im} \sum_{J \neq I} \langle \Phi_I | \hat{\boldsymbol{p}}_e | \Phi_J \rangle \frac{\langle \Phi_J | \sum_A \frac{P^A \cdot \hat{\boldsymbol{d}}_A^A}{M_A} | \Phi_I \rangle}{E_I - E_J}$$

$$[\hat{H}_e, \hat{\boldsymbol{r}}_e] = -i\hbar \frac{\hat{\boldsymbol{p}}_e}{m_e},$$

$$(E_I - E_J) \langle \Phi_I | \hat{\boldsymbol{r}}_e | \Phi_J \rangle = -i\hbar \frac{1}{m_e} \langle \Phi_I | \hat{\boldsymbol{p}}_e | \Phi_J \rangle.$$

$$\langle \Psi_I | \hat{\boldsymbol{p}}_e | \Psi_I \rangle$$

$$= 2m_e \mathrm{Re} \sum_J \langle \Phi_I | \hat{\boldsymbol{r}}_e | \Phi_J \rangle \langle \Phi_J | \sum_A \frac{\boldsymbol{P}^A \cdot \hat{\boldsymbol{d}}^A}{M_A} \Bigg| \Phi(\bar{I}) \Bigg)$$

$$= 2m_e \mathrm{Re} \langle \Phi_I | \hat{\boldsymbol{r}}_e \sum_A \frac{\boldsymbol{P}^A \cdot \hat{\boldsymbol{d}}^A}{M_A} | \Phi_I \rangle$$

$$= 2m_e \mathrm{Re} \langle \Phi_I | \hat{\boldsymbol{r}}_e \left| \frac{d}{dt} \Phi_I \right\rangle$$

$$= m_e \frac{d}{dt} \langle \Phi_I | \hat{\boldsymbol{r}}_e | \Phi_I \rangle$$

$$\hat{H} = \frac{1}{2M_H} \hat{\boldsymbol{P}}_H^2 + \frac{1}{2m_e} \hat{\boldsymbol{p}}_e^2 - \frac{e^2}{|\boldsymbol{R}_H - \boldsymbol{r}_E|}$$

$$\hat{H}_{\mathrm{com}} = \frac{1}{2M_H + m_e} \hat{\boldsymbol{P}}_{\mathrm{com}}^2 + \frac{1}{2\mu} \hat{\boldsymbol{p}}_\mu^2 - \frac{e^2}{|\hat{\boldsymbol{r}}|}$$

$$E_n = \frac{P^2}{2M} - \frac{m_e e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2}$$

$$E_n^{\mathrm{com}} = \frac{P^2}{2(M + m_e)} - \frac{\mu e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2}$$

$$\mu = (M^{-1} + m_e^{-1})^{-1}$$

$$|\Psi_{\mathrm{el}}\rangle \approx \frac{1}{\sqrt{2}} (|\sigma\bar{\sigma}\rangle + |\sigma^*\bar{\sigma}^*\rangle)$$

$$\hat{H}_{\mathrm{el}} \left(\hat{U} \hat{H}_{\mathrm{el}} \hat{U}^\dagger = \hat{V}_{\mathrm{ad}} \right)$$

$$\hat{H}_{\mathrm{ad}} = \hat{U}^\dagger \hat{H} \hat{U} = \frac{(\hat{\boldsymbol{P}} - i\hbar \hat{\boldsymbol{d}})^2}{2M} + \hat{V}_{\mathrm{ad}}(\hat{\boldsymbol{R}})$$

$$\boldsymbol{d}_{IJ} = \langle \Phi_I | \frac{\partial}{\partial \boldsymbol{R}} | \Phi_J \rangle$$

$$\hat{H}_{\mathrm{BO}} = \frac{\hat{\boldsymbol{P}}^2}{2M} + \hat{V}_{\mathrm{ad}}(\hat{\boldsymbol{R}})$$

$$\hat{H}_{\mathrm{Shenvi}}(\boldsymbol{R}, \boldsymbol{P}) = \sum_{A,IJK} \frac{1}{2M_A} \left(\boldsymbol{P}_A \delta_{IJ} - \boldsymbol{d}_{IJ}^A \right) \cdot \left(\boldsymbol{P}_A \delta_{JK} - \boldsymbol{d}_{JK}^A \right) |\Phi_I\rangle\langle\Phi_K| + \sum_I E_I(\{\boldsymbol{R}\}) |\Phi_I\rangle\langle\Phi_I|.$$

$$\boldsymbol{d}_{IJ}^{A} = \frac{\langle \Phi_I | \nabla_A \hat{H} | \Phi_J \rangle}{E_J - E_I}$$

$$\hat{H}_{\mathrm{PS}}(\boldsymbol{R}, \boldsymbol{P}) =$$
$$\sum_A \frac{1}{2M_A} \left(\boldsymbol{P}_A - i\hbar \hat{\boldsymbol{\Gamma}}_A(\boldsymbol{R}) \right)^2 + \hat{H}_{el}(\boldsymbol{R})$$

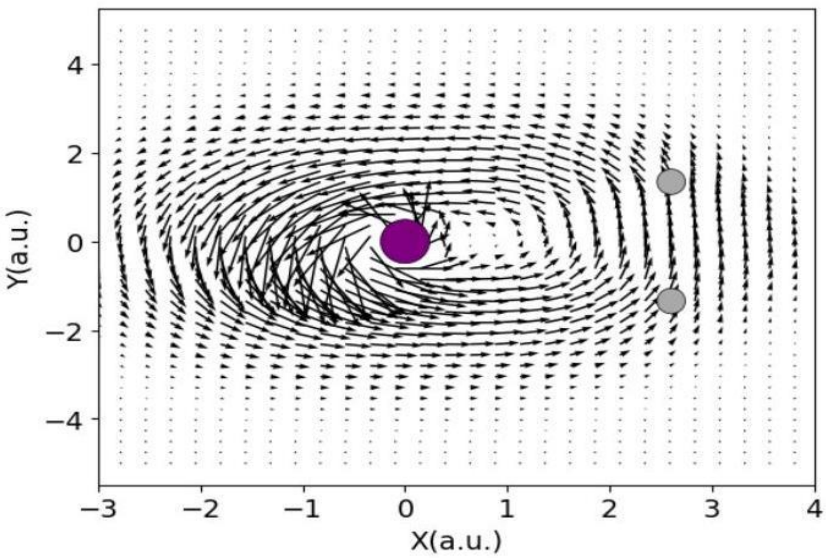
$$\hat{\boldsymbol{\Gamma}} = \hat{\boldsymbol{\Gamma}}' + \hat{\boldsymbol{\Gamma}}''$$

$$\hat{\boldsymbol{\Gamma}}_A' = \frac{-i}{2\hbar} (\theta_A(\hat{\boldsymbol{x}})\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\theta_A(\hat{\boldsymbol{x}}))$$
$$\hat{\boldsymbol{\Gamma}}_A'' = \sum_B \zeta_{AB} (\boldsymbol{R}_A - \boldsymbol{R}_B^0) \times \left(\boldsymbol{K}_B^{-1} \hat{\boldsymbol{J}}_B \right)$$
$$\hat{\boldsymbol{J}}_B = \frac{-i}{2\hbar} \left((\hat{\boldsymbol{x}} - \boldsymbol{R}_B) \times (\theta_B(\hat{\boldsymbol{x}})\hat{\boldsymbol{p}}) + (\theta_B(\hat{\boldsymbol{x}})\hat{\boldsymbol{p}}) \times (\hat{\boldsymbol{x}} - \boldsymbol{R}_B) + 2\theta_B(\hat{\boldsymbol{x}})\hat{\boldsymbol{s}} \right)$$
$$\boldsymbol{R}_B^0 = \frac{\sum_A \zeta_{AB} \boldsymbol{R}_B}{\sum_A \zeta_{AB}}$$
$$\boldsymbol{K}_B = \sum_A \zeta_{AB} (\boldsymbol{R}_A \boldsymbol{R}_A^T - \boldsymbol{R}_B^0 \boldsymbol{R}_B^{0T} - (\boldsymbol{R}_A \boldsymbol{R}_A^T - \boldsymbol{R}_B^{0T} \boldsymbol{R}_B^0) \mathcal{I}_3)$$

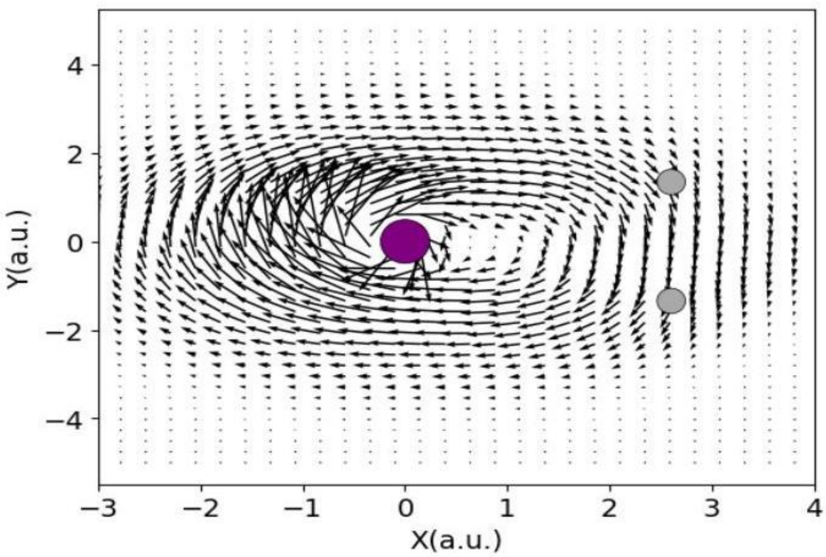
$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

$$\hat{H} = E_0(x, y)\mathbb{I} + \begin{pmatrix} \boldsymbol{g}z & \boldsymbol{h}x \\ \boldsymbol{h}x & -\boldsymbol{g}z \end{pmatrix}$$
$$E_{\pm} = E_0(x, y) \pm \sqrt{(\boldsymbol{g}x)^2 + (\boldsymbol{h}z)^2}$$

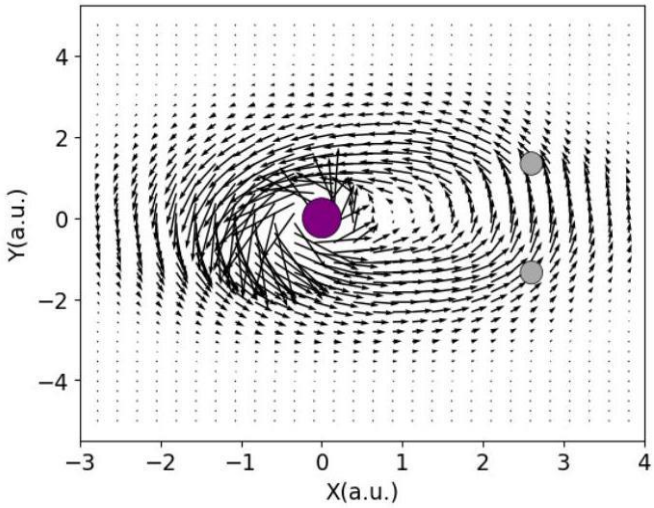
$$\hat{H} = E_0(x, y, z)\mathbb{I} + \begin{pmatrix} \boldsymbol{g}z & \boldsymbol{h}x - i\boldsymbol{f}y \\ \boldsymbol{h}x + i\boldsymbol{f}y & -\boldsymbol{g}z \end{pmatrix}$$
$$E_{\pm} = E_0(x, y, z) \pm \sqrt{(\boldsymbol{g}z)^2 + (\boldsymbol{h}x)^2 + (\boldsymbol{f}y)^2}(2$$



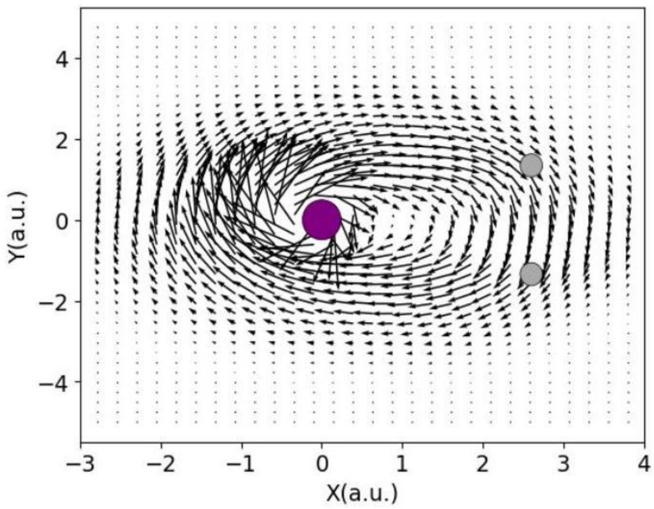
(a) S_0



(b) S_1



(a) Ψ_{CRHF}



(b) $\mathscr{T}\Psi_{CRHF}$

$$\mathbf{J} = \mathbf{L}_{\mathrm{el}} + \mathbf{L}_{\mathrm{nuc}} + \mathbf{S}$$

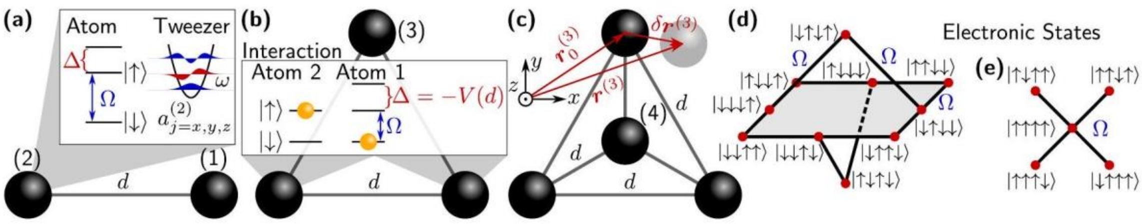
$$H^{(k)} = \Omega\sigma_x^{(k)} + \Delta n^{(k)} + \omega \sum_{j=x,y,z} \left(a_j^{(k)}\right)^{\dagger} a_j^{(k)}.$$

$$\sigma_x = |\downarrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow|$$

$$n = |\uparrow\rangle\langle\uparrow|$$

$$\delta r_j^{(k)} = x_0 \left(a_j^{(k)} + \left(a_j^{(k)}\right)^{\dagger}\right)/\sqrt{2}$$

$$H = \sum_{k=1}^{N} H^{(k)} + \sum_{k=1}^{N}\sum_{l=1}^{k-1} V\left(r^{(k,l)}\right) n^{(k)} n^{(l)},$$



$$\boldsymbol{r}^{(k)} = \boldsymbol{r}_0^{(k)} + \delta\boldsymbol{r}^{(k)}$$

$$\delta r_j^{(k)} = x_0\left(a_j^{(k)} + \left(a_j^{(k)}\right)^{\dagger}\right)/\sqrt{2}$$

$$V\left(r^{(k,l)}\right) \approx V\left(r_0^{(k,l)}\right) + \boldsymbol{G}^{(k,l)}\delta\boldsymbol{r}^{(k,l)}$$

$$+\frac{1}{2}\left(\delta\boldsymbol{r}^{(k,l)}\right)^{\mathrm{T}}\left(H_{\mathrm{a}}^{(k,l)} + H_{\mathrm{b}}^{(k,l)}\right)\delta\boldsymbol{r}^{(k,l)}$$

$$\delta\boldsymbol{r}^{(k,l)} = \delta\boldsymbol{r}^{(k)} - \delta\boldsymbol{r}^{(l)}$$

$$\boldsymbol{G}^{(k,l)} = V'\left(r_0^{(k,l)}\right)\frac{\left(\boldsymbol{r}_0^{(k,l)}\right)^{\mathrm{T}}}{r_0^{(k,l)}}$$

$$H_{\mathrm{a}}^{(k,l)} = V''\left(r_0^{(k,l)}\right)\frac{\boldsymbol{r}_0^{(k,l)}}{r_0^{(k,l)}} \otimes \frac{\left(\boldsymbol{r}_0^{(k,l)}\right)^{\mathrm{T}}}{r_0^{(k,l)}}$$

$$H_{\mathrm{b}}^{(k,l)} = \frac{V'\left(r_0^{(k,l)}\right)}{r_0^{(k,l)}}\left[1_3 - \frac{\boldsymbol{r}_0^{(k,l)}}{r_0^{(k,l)}} \otimes \frac{\left(\boldsymbol{r}_0^{(k,l)}\right)^{\mathrm{T}}}{r_0^{(k,l)}}\right]$$

$$\boldsymbol{r}_0^{(k,l)} = \boldsymbol{r}_0^{(k)} - \boldsymbol{r}_0^{(l)}$$

$$r_0^{(k,l)} = \left\|\boldsymbol{r}_0^{(k,l)}\right\|$$

$$\Delta = -V(d)$$

$$|\Delta| \gg |\Omega|\{|\downarrow\downarrow\rangle\}\{|\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle\}$$

$$|\downarrow\uparrow\rangle \overset{\Omega}{\longleftrightarrow} |\uparrow\uparrow\rangle \overset{\Omega}{\leftrightarrows} |\uparrow\downarrow\rangle$$

$$|+\rangle = (|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)/\sqrt{2}\{|+\rangle, |\uparrow\uparrow\rangle\}$$

$$b = \left(a^{(1)} - a^{(2)}\right)/\sqrt{2}$$

$$H_2 = \begin{bmatrix} \omega b^{\dagger}b & \sqrt{2}\Omega \\ \sqrt{2}\Omega & \omega b^{\dagger}b + \sqrt{2}\kappa\left(b + b^{\dagger}\right) + \xi\left(b + b^{\dagger}\right)^2 \end{bmatrix}.$$

$$H_{\mathrm{mol}} = \Omega\sum_{ss'} A_{ss'}|s\rangle\langle s'| + \sum_{s} h_s|s\rangle\langle s|$$

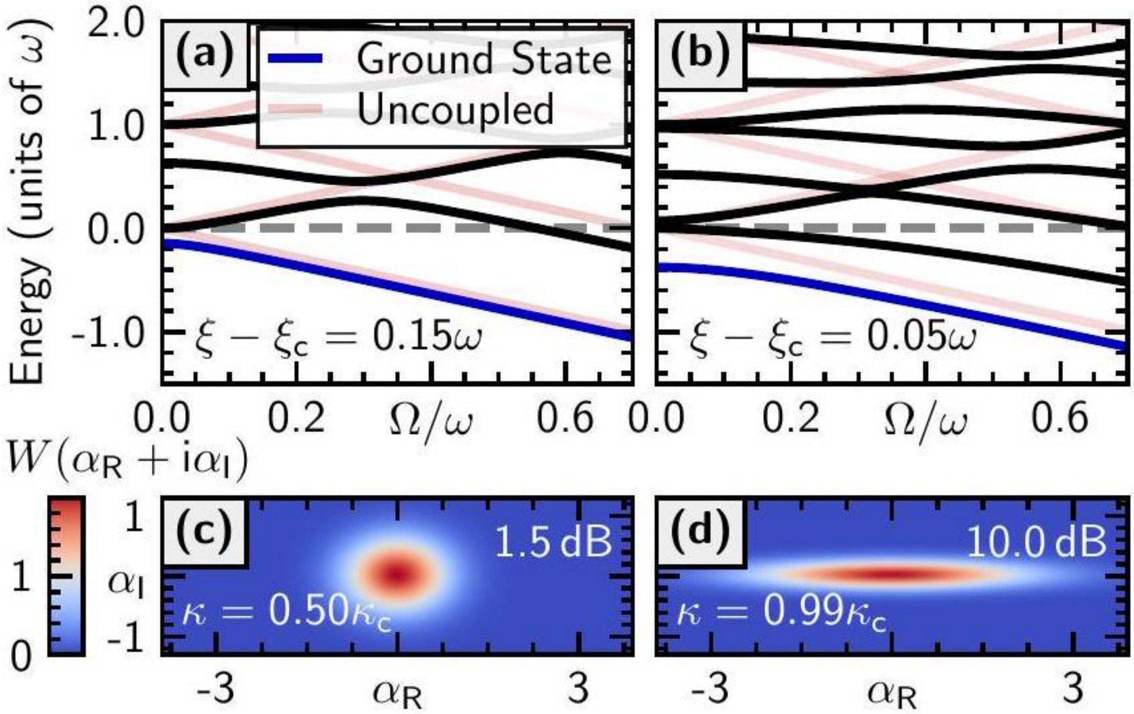
$$h_s = \omega \boldsymbol{b}_s^\dagger \boldsymbol{b}_s + \sqrt{2}\kappa \left(b_s^{\parallel} + \left(b_s^{\parallel}\right)^\dagger\right) + \xi \left(b_s^{\parallel} + \left(b_s^{\parallel}\right)^\dagger\right)^2$$
$$+ \frac{\nu\kappa}{\sqrt{2}}\left(b_s^{\perp,1} + \left(b_s^{\perp,1}\right)^\dagger\right)^2 + \frac{\nu\kappa}{\sqrt{2}}\left(b_s^{\perp,2} + \left(b_s^{\perp,2}\right)^\dagger\right)^2$$

$$b_{\mathrm{BT}} = (b + w b^\dagger)/\sqrt{1 - w^2}$$

$$w = 1 + \phi - \frac{\phi}{|\phi|}\sqrt{(1+\phi)^2 - 1}, \phi = \frac{\omega}{2\xi}.$$

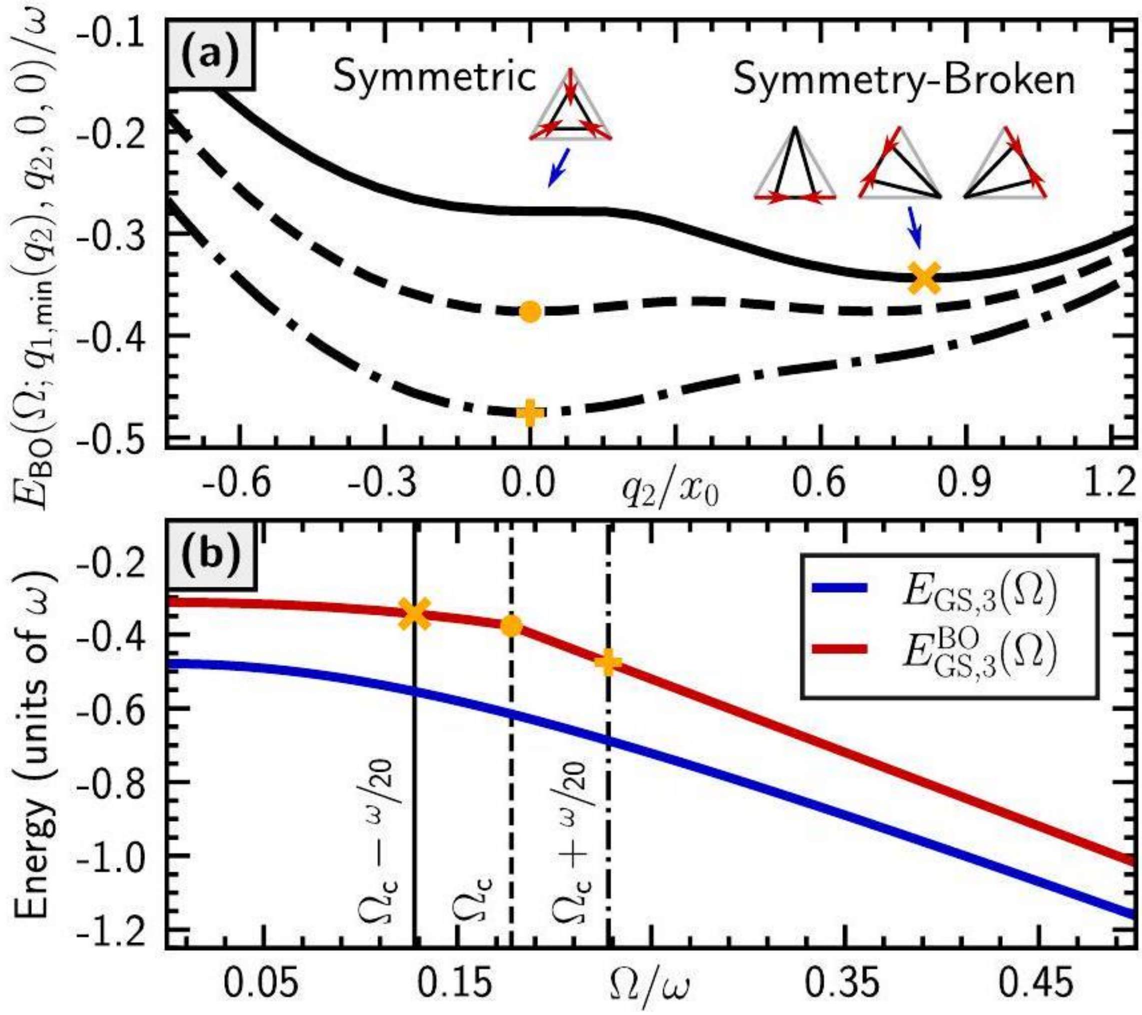
$$E_{\mathrm{GS},2} = \min\{\omega\varepsilon_2, 0\}$$

$$\varepsilon_2 = -\frac{2\kappa^2}{\omega^2}\frac{1}{1-\bar{\xi}} + \frac{1}{2}\sqrt{1-\bar{\xi}} - \frac{1}{2}, \bar{\xi} = \frac{\xi}{\xi_c}.$$



$$\varepsilon_4 = -\frac{2\kappa^2}{\omega^2}\frac{1}{1-\bar{\xi}} + \frac{1}{2}\sqrt{1-\bar{\xi}} + \sqrt{1-\bar{\kappa}} - \frac{3}{2}, \bar{\kappa} = \frac{\kappa}{\kappa_c}. \quad (12)$$

$$\kappa_c = -\omega/(2\sqrt{2}\nu) \mid \uparrow\uparrow\downarrow\downarrow\rangle \otimes |\mathrm{GS}\rangle$$



$$W(\alpha) = \frac{2}{\pi} \exp\left(-\bar{w}_+ \alpha_{\mathrm{R}}^2 - \bar{w}_- \alpha_{\mathrm{I}}^2\right), \bar{w}_\pm = 2\frac{1 \pm w}{1 \mp w} b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\perp,1}$$

$$\{|\downarrow\downarrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle\}$$

$$E_{\mathrm{BO}}(0; \boldsymbol{q}) = \frac{\omega}{2x_0^2}\boldsymbol{q}^2 + \frac{2\kappa}{x_0} q_\parallel + \frac{2\xi}{x_0^2} q_\parallel^2 + \frac{\sqrt{2}\nu\kappa}{x_0^2} q_\perp^2,$$

$$q_\parallel = (q_1 - q_2)/\sqrt{2} \text{ and } q_\perp = (q_3 + q_4)/\sqrt{2}$$

$$E_{\mathrm{GS},3} - E_{\mathrm{GS},3}^{\mathrm{BO}} = \frac{\omega}{2}\left[\sqrt{1 - \bar{\xi}} + \sqrt{1 - \bar{\kappa}} - 2\right]$$

$$R=\begin{bmatrix} \frac{1}{\sqrt{6}} & 0 & -\frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{6}} & -\frac{1}{2\sqrt{3}} & \frac{1}{\sqrt{6}} & -\frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{3}} & 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{3\sqrt{2}} & -\frac{1}{2\sqrt{6}} & -\frac{1}{6} & -\frac{\sqrt{2}}{3} & \frac{1}{6} & \frac{1}{6\sqrt{2}} & \frac{1}{\sqrt{6}} & -\frac{1}{3} & -\frac{1}{2\sqrt{3}} & 0 & \frac{1}{2} & 0 \\ -\frac{1}{6} & \frac{1}{2\sqrt{3}} & -\frac{\sqrt{2}}{3} & \frac{1}{6} & -\frac{1}{3\sqrt{2}} & -\frac{1}{6} & \frac{1}{2\sqrt{3}} & -\frac{1}{3\sqrt{2}} & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{2} \\ -\frac{1}{\sqrt{6}} & 0 & -\frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{6}} & \frac{1}{2\sqrt{3}} & -\frac{1}{\sqrt{6}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{3}} & 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{3\sqrt{2}} & -\frac{1}{2\sqrt{6}} & \frac{1}{6} & \frac{\sqrt{2}}{3} & \frac{1}{6} & \frac{1}{6\sqrt{2}} & -\frac{1}{\sqrt{6}} & -\frac{1}{3} & \frac{1}{2\sqrt{3}} & 0 & \frac{1}{2} & 0 \\ -\frac{1}{6} & \frac{1}{2\sqrt{3}} & \frac{\sqrt{2}}{3} & -\frac{1}{6} & -\frac{1}{3\sqrt{2}} & -\frac{1}{6} & -\frac{1}{2\sqrt{3}} & -\frac{1}{3\sqrt{2}} & -\frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{4} & 0 & 0 & \frac{1}{2\sqrt{2}} & 0 & -\frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{\sqrt{2}}{3} & -\frac{1}{2\sqrt{6}} & 0 & 0 & -\frac{1}{3} & -\frac{5}{6\sqrt{2}} & 0 & \frac{1}{6} & 0 & 0 & \frac{1}{2} & 0 \\ -\frac{1}{6} & -\frac{1}{\sqrt{3}} & 0 & 0 & -\frac{1}{3\sqrt{2}} & \frac{1}{3} & 0 & \frac{\sqrt{2}}{3} & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{\sqrt{3}} & -\frac{1}{2\sqrt{6}} & 0 & 0 & \frac{1}{2\sqrt{2}} & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{4} & 0 & 0 & 0 & \frac{1}{2\sqrt{2}} & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix},$$

$$\boldsymbol{a}=\left(a_x^{(1)},a_y^{(1)},a_z^{(1)},\dots,a_x^{(4)},a_y^{(4)},a_z^{(4)}\right)^{\mathrm{T}}$$

$$K=\begin{bmatrix} K^{(2,1)}+K^{(3,1)}+K^{(4,1)} & -K^{(2,1)} & -K^{(3,1)} & -K^{(4,1)} \\ -K^{(2,1)} & K^{(2,1)}+K^{(3,2)}+K^{(4,2)} & -K^{(3,2)} & -K^{(4,2)} \\ -K^{(3,1)} & -K^{(3,2)} & K^{(3,1)}+K^{(3,2)}+K^{(4,3)} & -K^{(4,3)} \\ -K^{(4,1)} & -K^{(4,2)} & -K^{(4,3)} & K^{(4,1)}+K^{(4,2)}+K^{(4,3)} \end{bmatrix}$$

$$K^{(k,l)}=H_{\mathrm{a}}^{(k,l)}+H_{\mathrm{b}}^{(k,l)}$$

$$U\left(\boldsymbol{r}^{(1)},\boldsymbol{r}^{(2)},\boldsymbol{r}^{(3)},\boldsymbol{r}^{(4)}\right)=V\left(r^{(2,1)}\right)+V\left(r^{(3,1)}\right)+V\left(r^{(3,2)}\right)+V\left(r^{(4,1)}\right)+V\left(r^{(4,2)}\right)+V\left(r^{(4,3)}\right),$$

$$\boldsymbol{r}^{(k,l)}=\left\|\boldsymbol{r}^{(k)}-\boldsymbol{r}^{(l)}\right\|$$

$$h_{|\uparrow\uparrow\downarrow\downarrow\rangle}=\omega\boldsymbol{a}^{\dagger}\boldsymbol{a}+\frac{x_0}{\sqrt{2}}\left[-\boldsymbol{G}^{(2,1)},\boldsymbol{G}^{(2,1)},\boldsymbol{0}^{\mathrm{T}},\boldsymbol{0}^{\mathrm{T}}\right]\left(\boldsymbol{a}+\left(\boldsymbol{a}^{\dagger}\right)^{\mathrm{T}}\right)+\frac{x_0^2}{4}\left(\boldsymbol{a}^{\dagger}+\boldsymbol{a}^{\mathrm{T}}\right)L^{(2,1)}\left(\boldsymbol{a}+\left(\boldsymbol{a}^{\dagger}\right)^{\mathrm{T}}\right)$$

$$=\omega\boldsymbol{b}^{\dagger}\boldsymbol{b}+\frac{x_0}{\sqrt{2}}\left[-\boldsymbol{G}^{(2,1)},\boldsymbol{G}^{(2,1)},\boldsymbol{0}^{\mathrm{T}},\boldsymbol{0}^{\mathrm{T}}\right]R\left(\boldsymbol{b}+\left(\boldsymbol{b}^{\dagger}\right)^{\mathrm{T}}\right)+\frac{x_0^2}{4}\left(\boldsymbol{b}^{\dagger}+\boldsymbol{b}^{\mathrm{T}}\right)R^{\mathrm{T}}L^{(2,1)}R\left(\boldsymbol{b}+\left(\boldsymbol{b}^{\dagger}\right)^{\mathrm{T}}\right).$$

$$L^{(2,1)}=\begin{bmatrix} K^{(2,1)} & -K^{(2,1)} & 0_3 & 0_3 \\ -K^{(2,1)} & K^{(2,1)} & 0_3 & 0_3 \\ 0_3 & 0_3 & 0_3 & 0_3 \\ 0_3 & 0_3 & 0_3 & 0_3 \end{bmatrix}$$

$$[L^{(k,l)}, L^{(k',l')}]R^{\mathrm{T}}_{|\uparrow\uparrow\downarrow\downarrow\rangle}(R^{\mathrm{T}}L^{(2,1)}R)R_{|\uparrow\uparrow\downarrow\downarrow\rangle}$$

$$\boldsymbol{b}_{|\uparrow\uparrow\downarrow\downarrow\rangle} = R^{\mathrm{T}}_{|\uparrow\uparrow\downarrow\downarrow}\boldsymbol{b}$$

$$h_{|\uparrow\uparrow\downarrow\downarrow\rangle} = |\uparrow\downarrow\downarrow\rangle$$

$$b^{\parallel}_{|\uparrow\uparrow\downarrow\downarrow\rangle} = \frac{1}{\sqrt{2}}\left(a_x^{(1)} - a_x^{(2)}\right), b^{\perp,1}_{|\uparrow\uparrow\downarrow\downarrow\rangle} = \frac{1}{\sqrt{2}}\left(a_y^{(1)} - a_y^{(2)}\right), b^{\perp,2}_{|\uparrow\uparrow\downarrow\downarrow\rangle} = \frac{1}{\sqrt{2}}\left(a_z^{(1)} - a_z^{(2)}\right)$$

$$h = \omega b^\dagger b + \lambda\left(b^\dagger + b\right) + \gamma\left(b^\dagger + b\right)^2$$

$$b_{\mathrm{BT}} = ub + vb^\dagger$$

$$b = u^* b^\dagger_{\mathrm{BT}} - v b_{\mathrm{BT}}$$

$$h = \left((\omega + 2\gamma)(|u|^2 + |v|^2) - 2\gamma(uv^* + u^*v)\right)b^\dagger_{\mathrm{BT}}b_{\mathrm{BT}} + \lambda\left((u - v)b^\dagger_{\mathrm{BT}} + (u^* - v^*)b_{\mathrm{BT}}\right)$$
$$+\left(f(u,v)b^{\dagger 2}_{\mathrm{BT}} + f^*(u,v)b^2_{\mathrm{BT}}\right) + (\omega + 2\gamma)|v|^2 + \gamma(1 - uv^* - u^*v).$$

$$f(u,v) = \gamma(u^2 + v^2) - (\omega + 2\gamma)uv$$

$$\gamma w^2 - (\omega + 2\gamma)w + \gamma = 0$$

$$w = \begin{cases} 1 + \phi \pm \sqrt{(1+\phi)^2 - 1}, & (1+\phi)^2 > 1 \\ 1 + \phi \pm \mathrm{i}\sqrt{1 - (1+\phi)^2}, & (1+\phi)^2 \le 1 \end{cases}, \phi = \frac{\omega}{2\gamma}.$$

$$u = \frac{1}{\sqrt{1 - w^2}}, v = \frac{w}{\sqrt{1 - w^2}}$$

$$w = 1 + \phi - \frac{\phi}{|\phi|}\sqrt{(1+\phi)^2 - 1}, \phi = \frac{\omega}{2\gamma}$$

$$H = \omega b^\dagger b + \sqrt{2}\kappa\left(b + b^\dagger\right) + \xi\left(b + b^\dagger\right)^2$$

$$H = \omega\sqrt{1 - \bar{\xi}}b^\dagger_{\mathrm{BT}}b_{\mathrm{BT}} + \frac{\sqrt{2}\kappa}{(1 - \bar{\xi})^{1/4}}\left(b_{\mathrm{BT}} + b^\dagger_{\mathrm{BT}}\right) + \frac{\omega}{2}\sqrt{1 - \bar{\xi}} - \frac{\omega}{2}, \bar{\xi} = \frac{\xi}{\xi_{\mathrm{c}}}.$$

$$D(b_{\mathrm{BT}}, \mu) = \exp\left(\mu b^\dagger_{\mathrm{BT}} - \mu^* b_{\mathrm{BT}}\right), \mu = -\frac{\sqrt{2}\kappa}{\omega}\frac{1}{(1 - \bar{\xi})^{3/4}}$$

$$D^\dagger(b_{\mathrm{BT}}, \mu)HD(b_{\mathrm{BT}}, \mu) = \omega\sqrt{1 - \bar{\xi}}b^\dagger_{\mathrm{BT}}b_{\mathrm{BT}} - \frac{2\kappa^2}{\omega}\frac{1}{1 - \bar{\xi}} + \frac{\omega}{2}\sqrt{1 - \bar{\xi}} - \frac{\omega}{2}$$

$$\rho_{\mathrm{gs}} = |\mathrm{gs}\rangle\langle\mathrm{gs}|$$

$$c = b^{\perp,1}_{|\uparrow\uparrow\downarrow\downarrow\rangle}$$

$$H = \omega c^\dagger c + \frac{\nu\kappa}{\sqrt{2}}\left(c + c^\dagger\right)^2$$

$$c_{\mathrm{BT}} = \left(c + wc^\dagger\right)/\sqrt{1 - w^2}$$

$$H=\omega\sqrt{1-\bar{\kappa}}c_{\mathrm{BT}}^{\dagger}c_{\mathrm{BT}}+\frac{\omega}{2}\sqrt{1-\bar{\kappa}}-\frac{\omega}{2},\bar{\kappa}=\frac{\kappa}{\kappa_{\mathrm{c}}}.$$

$$|\mathrm{gs}\rangle=|\mathrm{vac}\rangle_{c_{\mathrm{BT}}}$$

$$c_{\mathrm{BT}}=S^{\dagger}(c,\sigma)cS(c,\sigma),S(c,\sigma)=\exp\left(\frac{\sigma^{*}}{2}c^{2}-\frac{\sigma}{2}\left(c^{\dagger}\right)^{2}\right)$$

$$0=S^{\dagger}(c,\sigma)c|\mathrm{vac}\rangle_{c}=S^{\dagger}(c,\sigma)S(c,\sigma)c_{\mathrm{BT}}S^{\dagger}(c,\sigma)|\mathrm{vac}\rangle_{c}=c_{\mathrm{BT}}S^{\dagger}(c,\sigma)|\mathrm{vac}\rangle_{c}.$$

$$|\mathrm{vac}\rangle_{c_{\mathrm{BT}}}=S^{\dagger}(c,\sigma)|\mathrm{vac}\rangle_{c}$$

$$D(c,\beta)=\exp\left(\beta c^{\dagger}-\beta^{*}c\right)$$

$$f(\beta)=\mathrm{tr}\left(\rho_{\mathrm{gs}}D(c,\beta)\right)=\exp\left(-\frac{1}{2}\frac{|\beta+w\beta^{*}|}{1-w^{2}}\right)$$

$$W(\alpha)=\frac{1}{\pi^{2}}\int_{\mathbb{C}}\mathrm{d}\beta f(\beta)\mathrm{e}^{\beta^{*}\alpha-\alpha^{*}\beta}$$

$$h_{|\uparrow\uparrow\downarrow\downarrow\rangle}=\omega\boldsymbol{b}_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\dagger}\boldsymbol{b}_{|\uparrow\uparrow\downarrow\downarrow\rangle}+\sqrt{2}\kappa\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\parallel}+\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\parallel}\right)^{\dagger}\right)+\xi\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\parallel}+\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\parallel}\right)^{\dagger}\right)^{2}$$
$$+\frac{\nu\kappa}{\sqrt{2}}\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\perp,1}+\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\perp,1}\right)^{\dagger}\right)^{2}+\frac{\nu\kappa}{\sqrt{2}}\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\perp,2}+\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\perp,2}\right)^{\dagger}\right)^{2}.$$

$$b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\perp,j}\langle\mathrm{GS}|\left(b_{s}^{\perp,j}+\left(b_{s}^{\perp,j}\right)^{\dagger}\right)|\mathrm{GS}\rangle b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\parallel}$$

$$\frac{\delta}{x_{0}}=\frac{1}{\sqrt{2}}\langle\mathrm{gs}|b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\parallel}+\left(b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\parallel}\right)^{\dagger}|\mathrm{gs}\rangle,$$

$$H=\omega c^{\dagger}c+\sqrt{2}\kappa\left(c+c^{\dagger}\right)+\xi\left(c+c^{\dagger}\right)^{2},c\equiv b_{|\uparrow\uparrow\downarrow\downarrow\rangle}^{\dagger}$$

$$D^{\dagger}(c_{\mathrm{BT}},\mu)HD(c_{\mathrm{BT}},\mu)=\omega\sqrt{1-\bar{\xi}}c_{\mathrm{BT}}^{\dagger}c_{\mathrm{BT}}-\frac{2\kappa^{2}}{\omega}\frac{1}{1-\bar{\xi}}+\frac{\omega}{2}\sqrt{1-\bar{\xi}}-\frac{\omega}{2}$$

$$|\mathrm{gs}\rangle=D(c_{\mathrm{BT}},\mu)S^{\dagger}(c,\sigma)|\mathrm{vac}\rangle_{c}=D\left(S^{\dagger}(c,\sigma)cS(c,\sigma),\mu\right)S^{\dagger}(c,\sigma)|\mathrm{vac}\rangle_{c}=S^{\dagger}(c,\sigma)D(c,\mu)|\mathrm{vac}\rangle_{c}$$

$$\frac{\delta}{x_{0}}=\frac{1}{\sqrt{2}}\langle\mathrm{vac}|_{c}D^{\dagger}(c,\mu)S(c,\sigma)\left(c+c^{\dagger}\right)S^{\dagger}(c,\sigma)D(c,\mu)\mid\mathrm{vac}\rangle_{c}=\frac{1}{\sqrt{2}}\langle\mu|_{c}S(c,\sigma)\left(c+c^{\dagger}\right)S^{\dagger}(c,\sigma)\mid\mu\rangle_{c}$$

$$S^{\dagger}(\sigma,b)=S(-\sigma,b)$$

$$\frac{\delta}{x_{0}}=\frac{1}{\sqrt{2}}\langle\mathrm{gs}|\left(c+c^{\dagger}\right)|\mathrm{gs}\rangle=\frac{1}{\sqrt{2}}\sqrt{\frac{1-w}{1+w}}\langle\mu|_{c}\left(c+c^{\dagger}\right)\mid\mu\rangle_{c}=\frac{1}{\sqrt{2}}\sqrt{\frac{1-w}{1+w}}(\mu+\mu^{*})$$

$$\frac{\delta}{x_{0}}=-\frac{2\kappa}{\omega}\frac{1}{1-\bar{\xi}}$$

$$R = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & -\frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{\sqrt{3}} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ -\frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{\sqrt{3}} \\ 0 & 0 & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & \frac{1}{\sqrt{3}} \end{bmatrix}.$$

$$K = \begin{bmatrix} K^{(2,1)} + K^{(3,1)} & -K^{(2,1)} & -K^{(3,1)} \\ -K^{(2,1)} & K^{(2,1)} + K^{(3,2)} & -K^{(3,2)} \\ -K^{(3,1)} & -K^{(3,2)} & K^{(3,1)} + K^{(3,2)} \end{bmatrix}$$

$$\boldsymbol{a} = \left(a_x^{(1)}, a_y^{(1)}, a_x^{(2)}, a_y^{(2)}, a_x^{(3)}, a_y^{(3)}\right)^{\mathrm{T}}$$

$$|\uparrow\downarrow\downarrow\rangle \otimes |\mathrm{vac}\rangle_{\boldsymbol{b}}, |\downarrow\uparrow\downarrow\rangle \otimes |\mathrm{vac}\rangle_{\boldsymbol{b}}, |\downarrow\downarrow\uparrow\rangle \otimes |\mathrm{vac}\rangle_{\boldsymbol{b}}.$$

$$|\uparrow\uparrow\downarrow\rangle \otimes |gs\rangle_{\uparrow\uparrow\downarrow}, |\downarrow\uparrow\uparrow\rangle \otimes |gs\rangle_{\downarrow\uparrow\uparrow}, |\uparrow\downarrow\uparrow\rangle \otimes |gs\rangle_{\uparrow\downarrow\uparrow},$$

$$h_{|\uparrow\uparrow\downarrow\rangle} = \omega \boldsymbol{b}^\dagger \boldsymbol{b} + \sqrt{2}\kappa\left(b_{|\uparrow\uparrow\downarrow\rangle}^{\parallel} + \left(b_{|\uparrow\uparrow\downarrow\rangle}^{\parallel}\right)^\dagger\right) + \xi\left(b_{|\uparrow\uparrow\downarrow\rangle}^{\parallel} + \left(b_{|\uparrow\uparrow\downarrow\rangle}^{\parallel}\right)^\dagger\right)^2 + \frac{\nu\kappa}{\sqrt{2}}\left(b_{|\uparrow\uparrow\downarrow\rangle}^{\perp} + \left(b_{|\uparrow\uparrow\downarrow\rangle}^{\perp}\right)^\dagger\right)^2,$$

$$b_{|\uparrow\uparrow\downarrow\rangle}^{\parallel} = \frac{1}{\sqrt{2}}(b_1 - b_2) = \frac{1}{\sqrt{2}}\left(a_x^{(1)} - a_x^{(2)}\right), b_{|\uparrow\uparrow\downarrow\rangle}^{\perp} = \frac{1}{\sqrt{2}}(b_3 + b_4) = -\frac{1}{\sqrt{2}}\left(a_y^{(1)} - a_y^{(2)}\right).$$

$$\varepsilon_3 = -\frac{2\kappa^2}{\omega^2}\frac{1}{1-\bar{\xi}} + \frac{1}{2}\sqrt{1-\bar{\xi}} + \frac{1}{2}\sqrt{1-\bar{\kappa}} - 1$$

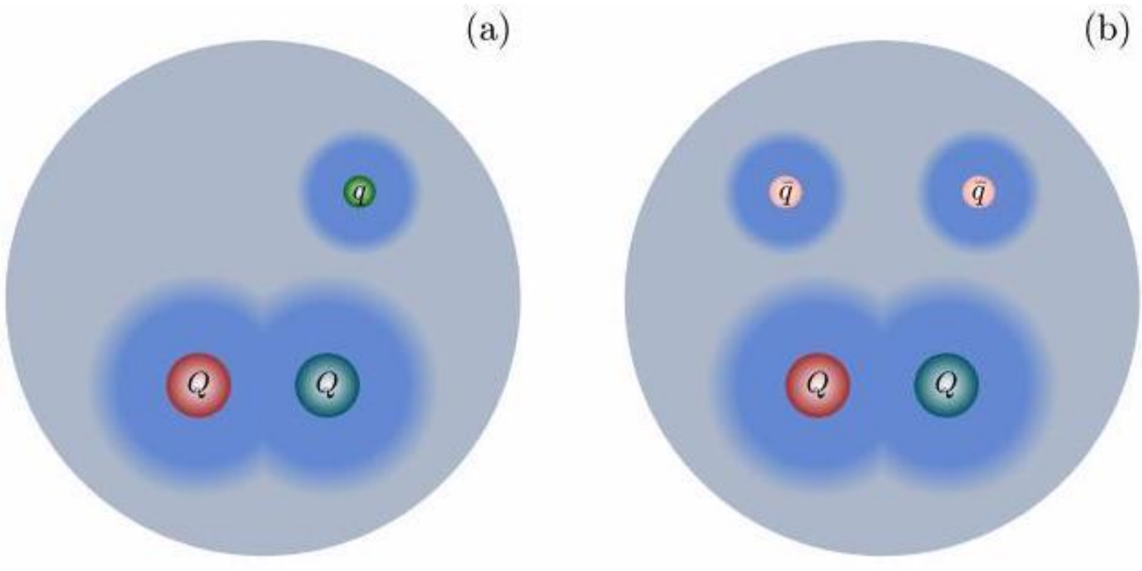
$$(\omega + 2\gamma)|v|^2 + \gamma(1 - uv^* - u^*v)$$

$$q_i = x_0\left(b_i + b_i^\dagger\right)/\sqrt{2}, i = 1,2,3,4$$

$$\begin{aligned} H_3 =& \Omega \sum_{ss'} B_{ss'}|s\rangle\langle s'| + \frac{\omega}{2}\left[\frac{\boldsymbol{q}^2}{x_0^2} + x_0^2\boldsymbol{p}^2\right] \\ &+ |\uparrow\uparrow\downarrow\rangle\langle\uparrow\uparrow\downarrow|\left[\frac{\sqrt{2}\kappa}{x_0}(q_1 - q_2) + \frac{\xi}{x_0^2}(q_1 - q_2)^2 + \frac{\nu\kappa}{\sqrt{2}x_0^2}(q_3 + q_4)^2\right] \\ &+ |\downarrow\uparrow\uparrow\rangle\langle\downarrow\uparrow\uparrow|\left[\frac{\sqrt{2}\kappa}{x_0}\left(q_1 + \frac{1}{2}q_2 - \frac{\sqrt{3}}{2}q_3\right) + \frac{\xi}{x_0^2}\left(q_1 + \frac{1}{2}q_2 - \frac{\sqrt{3}}{2}q_3\right)^2 + \frac{\nu\kappa}{\sqrt{2}x_0^2}\left(\frac{\sqrt{3}}{2}q_2 + \frac{1}{2}q_3 - q_4\right)^2\right] \\ &+ |\uparrow\downarrow\uparrow\rangle\langle\uparrow\downarrow|\left[\frac{\sqrt{2}\kappa}{x_0}\left(q_1 + \frac{1}{2}q_2 + \frac{\sqrt{3}}{2}q_3\right) + \frac{\xi}{x_0^2}\left(q_1 + \frac{1}{2}q_2 + \frac{\sqrt{3}}{2}q_3\right)^2 + \frac{\nu\kappa}{\sqrt{2}x_0^2}\left(-\frac{\sqrt{3}}{2}q_2 + \frac{1}{2}q_3 - q_4\right)^2\right]. \end{aligned}$$

$$E_{\mathrm{GS},3}^{\mathrm{BO}} = -\frac{2\kappa^2}{\omega}\frac{1}{1-\bar{\xi}}$$

$$E_{\mathrm{BO}}(\Omega; q_1, q_2, q_3 = 0, q_4 = 0)$$



$$H = \sum_{i=1}^{N} m_i + E + H_{ss}$$

$$H_{ss} = \sum_{i<j} 2\kappa_{ij}(s_i \cdot s_j)$$

$$H_t = H_h + H_l$$

$$H_h = \sum_{\text{heavy}} \frac{p_Q^2}{2m_Q} + V(\boldsymbol{x_A}, \boldsymbol{x_B})$$

$$H_l = \sum_{\text{light}} \frac{p_q^2}{2m_q} + V(\boldsymbol{x_A}, \boldsymbol{x_B}; \boldsymbol{x_1}, \boldsymbol{x_2})$$

$$\Psi = \psi(\boldsymbol{x_A}, \boldsymbol{x_B}) f(\boldsymbol{x_A}, \boldsymbol{x_B}; \boldsymbol{x_1}, \boldsymbol{x_2}),$$

$$\psi = \psi(\boldsymbol{x_A}, \boldsymbol{x_B})$$

$$f = f(\boldsymbol{x_A}, \boldsymbol{x_B}; \boldsymbol{x_1}, \boldsymbol{x_2})$$

$$\left(\sum_{\text{heavy}} \frac{p_Q^2}{2m_Q} + V_{\text{BO}}(\boldsymbol{x_A}, \boldsymbol{x_B}) \right) \psi = E\psi,$$

$$V_{\text{BO}}(\boldsymbol{x_A}, \boldsymbol{x_B}) = E_l(\boldsymbol{x_A}, \boldsymbol{x_B}) + V(\boldsymbol{x_A}, \boldsymbol{x_B}).$$

$$E_l = E_l(\boldsymbol{x_A}, \boldsymbol{x_B})$$

$$H_l f = E_l f$$

$$V(\boldsymbol{x_A}, \boldsymbol{x_B}) = \lambda_{Q_1 Q_2} \frac{\alpha_s}{r_{AB}} + V_{\text{conf}}$$

$$V_{\text{conf}} = k \times (r_{AB} - R_0) \times \theta(r_{AB} - R_0)$$

$$r_{AB} = |\boldsymbol{r_{AB}}| = |\boldsymbol{x_B} - \boldsymbol{x_A}|$$

$$\mu_1 = \left|(Q_1Q_2)^{\bar{3}}_0(q)^3_{\frac{1}{2}}\right\rangle,$$

$$\mu_2 = \left|(Q_1Q_2)^{\bar{3}}_1(q)^3_{\frac{1}{2}}\right\rangle.$$

$$\nu_1 = \left|(Q_1Q_2)^{\bar{3}}_1(q)^3_{\frac{1}{2}}\right\rangle.$$

$$(|(Q_1Q_2)(\bar{q}_3\bar{q}_4)\rangle)(|(Q_1\bar{q}_3)(Q_2\bar{q}_4)\rangle|(Q_1\bar{q}_4)(Q_2\bar{q}_3)\rangle)$$

$$3 \otimes 3 \rightarrow \bar{3} \oplus 6 \text{ and } \bar{3} \otimes \bar{3} \rightarrow 3 \oplus \bar{6}$$

$$\left|(Q_1Q_2)^{\bar{3}}(\bar{q}_3\bar{q}_4)^3\right\rangle \left|(Q_1Q_2)^6(\bar{q}_3\bar{q}_4)^{\bar{6}}\right\rangle$$

$$\left|(Q_1Q_2)^{\bar{3}}(\bar{q}_3\bar{q}_4)^3\right\rangle$$

$$\alpha_1 = \left|(Q_1Q_2)^{\bar{3}}_0(\bar{q}_3\bar{q}_4)^3_0\right\rangle \delta^S_{12}\delta^S_{34}$$

$$\alpha_2 = \left|(Q_1Q_2)^{\bar{3}}_1(\bar{q}_3\bar{q}_4)^3_1\right\rangle \delta^A_{12}\delta^A_{34}$$

$$\beta_1 = \left|(Q_1Q_2)^{\bar{3}}_0(\bar{q}_3\bar{q}_4)^3_1\right\rangle \delta^S_{12}\delta^A_{34}$$

$$\beta_2 = \left|(Q_1Q_2)^{\bar{3}}_1(\bar{q}_3\bar{q}_4)^3_0\right\rangle \delta^A_{12}\delta^S_{34}$$

$$\beta_3 = \left|(Q_1Q_2)^{\bar{3}}_1(\bar{q}_3\bar{q}_4)^3_1\right\rangle \delta^A_{12}\delta^A_{34}$$

$$\gamma_1 = \left|(Q_1Q_2)^{\bar{3}}_1(\bar{q}_3\bar{q}_4)^3_1\right\rangle \delta^A_{12}\delta^A_{34}$$

$$\left|(Q_1Q_2)^6(\bar{q}_3\bar{q}_4)^{\bar{6}}\right\rangle$$

$$\alpha_3 = \left|(Q_1Q_2)^6_0(\bar{q}_3\bar{q}_4)^{\bar{6}}_0\right\rangle \delta^A_{12}\delta^A_{34},$$

$$\alpha_4 = \left|(Q_1Q_2)^6_1(\bar{q}_3\bar{q}_4)^{\bar{6}}_1\right\rangle \delta^S_{12}\delta^S_{34}.$$

$$\beta_4 = \left|(Q_1Q_2)^6_0(\bar{q}_3\bar{q}_4)^{\bar{6}}_1\right\rangle \delta^A_{12}\delta^S_{34},$$

$$\beta_5 = \left|(Q_1Q_2)^6_1(\bar{q}_3\bar{q}_4)^{\bar{6}}_0\right\rangle \delta^S_{12}\delta^A_{34},$$

$$\beta_6 = \left|(Q_1Q_2)^6_1(\bar{q}_3\bar{q}_4)^{\bar{6}}_1\right\rangle \delta^S_{12}\delta^S_{34}.$$

$$\gamma_2 = \left|(Q_1Q_2)^6_1(\bar{q}_3\bar{q}_4)^{\bar{6}}_1\right\rangle \delta^S_{12}\delta^S_{34}.$$

$$\alpha_s(\mu) = \frac{\alpha_0}{\ln\left(\frac{\mu^2 + \mu_0^2}{\Lambda_0^2}\right)},$$

$$V_t = V(\boldsymbol{x_A}, \boldsymbol{x_B}) + V(\boldsymbol{x_A}, \boldsymbol{x_B}; \boldsymbol{x}),$$

$$V(\boldsymbol{x_A}, \boldsymbol{x_B}) = -\frac{2}{3}\frac{\alpha_s}{r_{AB}} + V_{\text{conf}},$$

$$V(\boldsymbol{x_A}, \boldsymbol{x_B}; \boldsymbol{x}) = -\frac{2}{3}\frac{\alpha_s'}{r_A} - \frac{2}{3}\frac{\alpha_s'}{r_B}.$$

$$H_l = -\frac{1}{2m_q}\nabla^2 - \frac{2}{3}\frac{\alpha_s'}{r_A} - \frac{2}{3}\frac{\alpha_s'}{r_B}.$$

$$R(r) = \frac{A^{\frac{3}{2}}}{\sqrt{\pi}} e^{-Ar},$$

$$f = \frac{R(r_A) + R(r_B)}{\sqrt{2(1+\mathcal{J})}},$$

$$\mathcal{J} = \int R(r_A)R(r_B)d\tau$$

$$E_l = \frac{\langle R(r_A), H_l R(r_A)\rangle + \langle R(r_B), H_l R(r_A)\rangle}{1+\mathcal{J}},$$

$$\langle R(r_B), H_l R(r_A)\rangle = \left(\frac{A}{m_q} - \frac{4}{3}\alpha_s'\right)\mathcal{I} - \frac{A^2}{2m_q}\mathcal{J}$$

$$\langle R(r_A), H_l R(r_A)\rangle = \frac{A^2}{2m_q} - \frac{2A}{3}\alpha_s' - \frac{2}{3}\alpha_s'\mathcal{K}$$

$$\mathcal{I} = \int \frac{R(r_A)R(r_B)}{r_A}d\tau = \int \frac{R(r_A)R(r_B)}{r_B}d\tau$$

$$\mathcal{K} = \int \frac{R^2(r_A)}{r_B}d\tau = \int \frac{R^2(r_B)}{r_A}d\tau$$

$$V_{\text{BO}}(r_{AB}) = -\frac{2}{3}\frac{\alpha_s}{r_{AB}} + V_{\text{conf}} + E_l.$$

$$M(\Xi_{cc}^{++})_{\frac{1}{2}^+} = 2m_c + m_n + E + \frac{1}{2}(\kappa_{cc})^{\bar{3}} - 2(\kappa_{nc})^{\bar{3}}.$$

$$E = 19.7\text{MeV}, R_0 = 4.12\text{GeV}^{-1}.$$

$$\left|(Q_1Q_2)^{\bar{3}}(\bar{q}_3\bar{q}_4)^3\right\rangle Q_1Q_2\bar{q}_3\bar{q}_4 (Q_1Q_2)^{\bar{3}}(\bar{q}_3\bar{q}_4)^3 \bar{3} \otimes 3 \rightarrow 1$$

$$V_t = V(\boldsymbol{x_A}, \boldsymbol{x_B}) + V(\boldsymbol{x_A}, \boldsymbol{x_B}; \boldsymbol{x_1}, \boldsymbol{x_2}),$$

$$V(\boldsymbol{x_A}, \boldsymbol{x_B}) = -\frac{2}{3}\frac{\alpha_s}{r_{AB}} + V_{\text{conf}}$$

$$V(\boldsymbol{x_A}, \boldsymbol{x_B}; \boldsymbol{x_1}, \boldsymbol{x_2}) = -\frac{2}{3}\frac{\alpha_s''}{r_{12}} - \frac{1}{3}\frac{\alpha_s'}{r_{A1}} - \frac{1}{3}\frac{\alpha_s'}{r_{A2}} - \frac{1}{3}\frac{\alpha_s'}{r_{B1}} - \frac{1}{3}\frac{\alpha_s'}{r_{B2}}$$

$$H_{\bar{q}_3} = -\frac{1}{2m_{\bar{q}_3}}\nabla^2 - \frac{1}{3}\frac{\alpha_s'}{r_{A1}} - \frac{1}{3}\frac{\alpha_s'}{r_{B1}}$$

$$f_{\bar{q}_3} = \frac{R(r_{A1}) + R(r_{B1})}{\sqrt{2(1+\mathcal{J})}}.$$

$$E_{\bar{q}_3} = \frac{\langle R(r_{A1}), H_{\bar{q}_3} R(r_{A1})\rangle + \langle R(r_{B1}), H_{\bar{q}_3} R(r_{A1})\rangle}{1+\mathcal{J}},$$

$$\langle R(r_{B1}), H_{\bar{q}_3} R(r_{A1})\rangle = \left(\frac{A}{m_{\bar{q}_3}} - \frac{2}{3}\alpha_s'\right)\mathcal{I} - \frac{A^2}{2m_{\bar{q}_3}}\mathcal{J},$$

$$\langle R(r_{A1}), H_{\bar{q}_3} R(r_{A1})\rangle = \frac{A^2}{2m_{\bar{q}_3}} - \frac{A}{3}\alpha_s' - \frac{1}{3}\alpha_s'\mathcal{K}.$$

$$H_{\text{pert}} = -\frac{2}{3}\frac{\alpha_s''}{r_{12}}.$$

$$f = \frac{f(3,4)}{\sqrt{\mathcal{N}}} = \frac{f_{\bar{q}_3} f_{\bar{q}_4}}{\sqrt{\mathcal{N}}},$$

$$\mathcal{N} = \int_{-\infty}^{\infty} |f(3,4)|^2 d\tau$$

$$\Delta E = \langle f | H_{\text{pert}} | f \rangle.$$

$$\left|(Q_1Q_2)^{\bar{3}}(\bar{q}_3\bar{q}_4)^3\right\rangle$$

$$V_{\text{BO}}(r_{AB}) = -\frac{2}{3}\frac{\alpha_s}{r_{AB}} + V_{\text{conf}} + E_l,$$

$$E_l = E_{\bar{q}_3} + E_{\bar{q}_4} + \Delta E.$$

$$\left|(Q_1Q_2)^6(\bar{q}_3\bar{q}_4)^{\bar{6}}\right\rangle$$

$$(\bar{q}_3\bar{q}_4)^{\bar{6}}\ 6 \otimes \bar{6} \to 1$$

$$\left|(Q_1Q_2)^{\bar{3}}(\bar{q}_3\bar{q}_4)^3\right\rangle$$

$$\langle H_{ss}\rangle = \frac{1}{2}(\kappa_{cc})^{\bar{3}} - \frac{3}{2}(\kappa_{nn})^{\bar{3}} = -150.8\text{MeV}.$$

$$\langle H_{ss}\rangle = \frac{3}{4}(\kappa_{cc})^{\bar{3}} - \frac{1}{4}(\kappa_{nn})^{\bar{3}} = -20.2\text{MeV}.$$

$$E = 75.6\text{MeV}, R_0 = 2.95\text{GeV}^{-1}.$$

$$E = -54.9\text{MeV}, R_0 = 5.25\text{GeV}^{-1}$$

$$\left|(cc)_0^6(\bar{u}\bar{d})_1^{\bar{6}}\right\rangle$$

$$H_{mol} = -\sum_{j=1}^{N}\frac{1}{2}\Delta_{x_j} - \sum_{j=1}^{M}\frac{1}{2m_j}\Delta_{y_j} + V_e(x) + V_{en}(x,y) + V_n(y),$$

$$x = (x_1, \dots, x_N) \in \mathbb{R}^{3N}$$

$$y = (y_1, \dots, y_M) \in \mathbb{R}^{3M}$$

$$L^2_{\text{p.sym}}\left(\mathbb{R}^{3(N+M)}\right)L^2\left(\mathbb{R}^{3(N+M)}\right)$$

$$H_{bo}(y) = -\sum_{j=1}^{N}\frac{1}{2}\Delta_{x_j} + V_e(\cdot) + V_{en}(\cdot,y) + V_n(y), \text{ on } L_x^2 = L^2_{\text{sym}}\left(\mathbb{R}^{3N}\right),$$

$$K = -\sum_{j=1}^{M}\frac{1}{2m_j}\Delta_{y_j} + E(y), \text{ on } L_y^2 = L^2(\mathbb{R}^{3M}).$$

$$\begin{cases} i\partial_s\Psi = H_{mol}\Psi, \\ \Psi|_{s=0} = \Psi_0, \end{cases}$$

$$\Psi_0 \in L^2_{\text{sym}}\left(\mathbb{R}^{3(N+M)}\right)$$

$$\begin{cases} i\partial_s\psi = K\psi, \\ \psi|_{s=0} = \psi_0 \in L_y^2. \end{cases} \text{ in } L_y^2,$$

$$\kappa^2 := \frac{m_e}{\min_j m_j} = \frac{1}{\min_j m_j},$$

$$\begin{cases} i\kappa\partial_t\Psi = H_{mol}\Psi, \text{ in } L^2_{x,y} \\ \Psi|_{t=0} = \Psi_0 \in L^2_{x,y} \end{cases}$$

$$\mathcal{H} = L^2(\mathbb{R}^m, \mathcal{H}_{el})$$

$$\Psi = \int_{\mathbb{R}^m}^{\oplus}\Psi(y)dy$$

$$\langle\Psi,\Phi\rangle = \int_{\mathbb{R}^m}\langle\Psi(y),\Phi(y)\rangle_{\mathcal{H}_{el}}dy, \Psi, \Phi \in \mathcal{H}$$

$$\mathcal{H} = \int_{\mathbb{R}^m}^{\oplus}\mathcal{H}_{el}dy$$

$$(A\Psi)(y) = A(y)\Psi(y), y \in \mathbb{R}^m, \Psi \in \mathcal{H}$$

$$A = \int_{\mathbb{R}^m}^{\oplus}A(y)dy$$

$$H_\kappa = -\kappa^2\Delta_y + H_{bo}, \text{ with } H_{bo} = \int_{\mathbb{R}^m}^{\oplus} H(y)dy$$

$$\begin{cases} i\kappa\partial_t\Psi = H_\kappa\Psi, \text{ in } \mathcal{H}, \\ \Psi|_{t=0} = \Psi_0 \in \mathcal{H}. \end{cases}$$

$$t \mapsto \Psi(t) = \int_{\mathbb{R}^m}^{\oplus} \Psi(y,t)dy$$

$$f(y,t) := \langle \psi_\circ(y), \Psi(y,t)\rangle_{\mathcal{H}_{el}}.$$

$$\begin{cases} i\kappa\partial_t f = h_{\text{eff}}^{\kappa} f \\ f|_{t=0} = f_0 \in L_y^2 \end{cases}$$

$$f \in C(\mathbb{R}, L^2(\mathbb{R}^m))$$

$$U_t = e^{-iH_\kappa t/\kappa}$$

$$T = -\kappa^2\Delta_y, \text{ in } \mathbb{R}^m$$

$$(\psi_\circ f)(y) = \psi_\circ(y)f(y) \text{ and } \langle t\rangle = (1+|t|^2)^{1/2}$$

$$F: H_{\kappa,y}^s\mathcal{H}_{el} \to H_{\kappa,y}^{s'}\mathcal{H}_{el} \text{ is } O_{\mathcal{L}_{s,s'}}(a)$$

$$\|F\phi\|_{H_{k,y}^s\mathcal{H}_{el}} \le C\|\phi\|_{H_{k,y}^{s'}\mathcal{H}_{el}}, \forall\phi \in H_{k,y}^s\mathcal{H}_{el}.$$

$$U_t\psi_\circ f = \psi_\circ\left(e^{-ih_{\text{eff}}t/\kappa} f\right) + O_{\mathcal{L}_{2,0}}(\kappa\langle t\rangle^3)$$

$$h_{\text{eff}} = T + E + \kappa^2 v$$

$$v(y) := \frac{1}{2}\left\|\nabla_y\psi_\circ\right\|_{\mathcal{H}_{el}}^2.$$

$$O_{\mathcal{L}_{2,0}}(\kappa\langle t\rangle^3)\Psi(t) = \psi_\circ f(t)$$

$$i\kappa\partial_t f = h_{\text{eff}} f,\ f|_{t=0} = f_0$$

$$\bar{R} = \bar{P}((H_{\text{bo}} - E)|_{\text{Ran}\bar{P}})^{-1}\bar{P},$$

$$P = \int_{\mathbb{R}^m}^{\oplus} P(y)dy$$

$$\bar{H} = \bar{P}H_\kappa\bar{P},$$

$$\bar{U}_t = e^{-i\bar{H}t/\kappa}, t \in \mathbb{R}.$$

$$Q_P: C(I, L_y^2) \to C(I, \mathcal{H})$$

$$(Q_P f)(t) := \psi_\circ f(t) - \frac{i}{\kappa}\int_0^t \bar{U}_{t-s}\bar{P}H_\kappa P\psi_\circ f(s)ds, t \in I$$

$$f(t)(y) = f(y,t)$$

$$\Psi(t)(y) = \Psi(y,t) \in \mathcal{H}_{el}$$

$$\Psi_0 = \psi_\circ f_0$$

$$\mathcal{H} = L^2(\mathbb{R}^m, \mathcal{H}_{el})$$

$$f(t) := \langle \psi_\circ, \Psi(t) \rangle_{\mathcal{H}_{el}}$$

$$i\kappa\partial f = h_{\text{eff}}^{\kappa} f, f(0) = f_0$$

$$h_{\text{eff}}^{\kappa} = T + E + \kappa^2 v + w^{\kappa},$$

$$f \in C\big(\mathbb{R}, L^2(\mathbb{R}^m)\big)$$

$$w^{\kappa}[f](t) = -\frac{i}{\kappa}\int_0^t \langle \psi_\circ, PT\bar{P}\bar{U}_{t-s}\bar{P}TP\psi_\circ f(s)\rangle_{\mathcal{H}_{el}} ds$$

$$Q_P f(0) = \psi_\circ f_0$$

$$f_0 \in H_{\kappa,y}^{s+2n}$$

$$B_\tau^{s+2n+2} := L^\infty\big(0,\tau; H_{\kappa,y}^{s+2n+2}\big)$$

$$w^{\kappa}[f](t) = \sum_{j=1}^{n-1} (-i\kappa)^{j+1}\big(w_j f(t) - \tilde{w}_j(t) f_0\big) + (-i\kappa)^{n+1} w_n^{\kappa}[f](t),$$

$$\big\|w_j u\big\|_{H_{\kappa,y}^s} \lesssim \|u\|_{H_{\kappa,y}^{s+j+1}}, \forall u \in H_{\kappa,y}^{s+j+1}$$

$$\big\|\tilde{w}_j(t)u\big\|_{H_{\kappa,y}^s} \lesssim e^{C\tau}\|u\|_{H_{\kappa,y}^{s+2j}}, \forall u \in H_{\kappa,y}^{s+2j}, 0 \le t \le \tau$$

$$\|w_n^{\kappa}[f](t)\|_{H_{\kappa,y}^s} \lesssim e^{C\tau}\left(\|f\|_{B_\tau^{s+2n+2}} + \|f_0\|_{H_{\kappa,y}^{s+2n}}\right), 0 \le t \le \tau$$

$$\Psi(t) = Q_P\tilde{f}(t) + O_{\mathcal{L}_{7,0}}(\kappa^2 e^{Ct})$$

$$\mathcal{H} = L^2(\mathbb{R}^m, \mathcal{H}_{el})$$

$$\Psi(0) = \psi_\circ f_0$$

$$f_0 \in H_{\kappa,y}^7$$

$$\kappa_0 = \kappa_0\left(\delta, m, \left\|\nabla_{y_j} H_{bo}\right\|, \dots, \left\|\nabla_{y_k}\psi_\circ\right\|, \dots\right)$$

$$\left\|\Psi(t) - Q_P\tilde{f}(t)\right\| \leqslant \kappa^2 C e^{C\tau}\|f_0\|_{H_{\kappa,y}^7}, 0 \leqslant t \le \tau$$

$$i\kappa\partial_t\tilde{f} = h_{\text{eff}}^{(2)}\tilde{f}, h_{\text{eff}}^{(2)} := T + E + \kappa^2 v - \kappa^2 w_1,$$

$$\tilde{f}\big|_{t=0} = f_0$$

$$w_1 = -\frac{1}{\kappa^2}\langle \psi_\circ, PT\bar{P}\bar{R}\bar{P}TP\psi_\circ\rangle_{\mathcal{H}_{el}}, w_1 = O_{\mathcal{L}_{s+2,s}}(1)$$

$$D_y := -i\kappa\partial_y, D^\alpha = \prod_{j=1}^{m} D_{y_j}^{\alpha_j}$$

$$\partial_y^\alpha = \partial_{y_1}^{\alpha_1} \dots \partial_{y_m}^{\alpha_m}$$

$$\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{N}^m$$

$$|\alpha| = \sum_{j=1}^{m} \alpha_j$$

$$L_y^2 \equiv L^2(\mathbb{R}^m)$$

$$H_{\kappa,y}^s = \left\{ \phi \in L^2(\mathbb{R}^m) : \|\phi\|_{H_y^{s,\kappa}}^2 = \sum_{|\alpha|=s} \left\| D_y^\alpha \phi \right\|_{L_y^2}^2 + \|\phi\|_{L_y^2}^2 < \infty \right\}$$

$$\langle \phi, (H(y) + \gamma)\phi \rangle \geq \gamma \|\phi\|^2, \phi \in \mathcal{H}$$

$$\left\| \partial_y^\alpha H(y) \right\|_{\mathcal{L}(\mathcal{H}_{el})} \leqslant C(\alpha), \forall \alpha \text{ with } 1 \leqslant |\alpha| \leqslant k_A \text{ and } y \in \mathbb{R}^m$$

$$\mathcal{D}(H_\kappa) = H_y^{2,\kappa} \otimes \mathcal{H}_{el} \cap L_y^2 \otimes \mathcal{D}_\circ$$

$$H(y)\psi_\circ(y) = E(y)\psi_\circ(y), \|\psi_\circ(y)\|_{\mathcal{H}_{el}} = 1, \forall y \in \mathbb{R}^m$$

$$(P\Psi)(y) = \psi_\circ(y)\langle \psi_\circ(y), \Psi(y) \rangle_{\mathcal{H}_{el}}.$$

$$\mathcal{H} = L^2(\mathbb{R}^m, \mathcal{H}_{\mathrm{el}})$$

$$\psi_\circ \otimes L_y^2$$

$$\inf_{y \in \mathbb{R}^m} \{ |\xi - E(y)| ; \xi \in \sigma(H(y)) \setminus \{E(y)\} \} \geqslant \delta > 0$$

$$L^2\left(\mathbb{R}^{3(M+N)}\right) L^2(\mathbb{R}^{3M}, \mathcal{H}_{el}) \mathcal{H}_{el} = L^2(\mathbb{R}^{3N})$$

$$H_{mol} = T + H_{\mathrm{bo}}, \text{ with } H_{bo} = \int_{\mathbb{R}^{3M}}^{\oplus} H(y) dy$$

$$\mathcal{H}_{el} = L_x^2 \equiv L^2(\mathbb{R}^{3N}) L_y^2$$

$$H(y) = -\sum_{j=1}^{N} \frac{1}{2} \Delta_{x_j} + V_e(x) + V_{en}(x, y) + V_n(y)$$

$$T = -\sum_{j=1}^{M} \frac{1}{2m_j} \Delta_{y_j} = -\kappa^2 \sum_{j=1}^{M} \frac{1}{2m_j'} \Delta_{y_j}, m_j' = \kappa^2 m_j = \frac{m_j}{\min_k m_k}$$

$$(y, \tilde{y}) = 2 \sum_{j=1}^{M} m_j' y_j \cdot \tilde{y}_j$$

$$T = -\kappa^2 \Delta_y,$$

$$V_e(x) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{e^2}{|x_i - x_j|}.$$

$$\rho \in C_c^\infty(\mathbb{R}^3), \rho \geqslant 0$$

$$V_n(y) = \sum_{i=1}^{M-1} \sum_{j=i+1}^{M} \int_{\mathbb{R}^6} \frac{e^2 Z_i Z_j \rho(z - y_i)\rho(z' - y_j)}{|z - z'|} dzdz'$$

$$V_{en}(x, y) = -\sum_{i=1}^{M} \sum_{j=1}^{N} \int_{\mathbb{R}^3} \frac{e^2 Z_i \rho(z - y_i)}{|z - x_j|} dz.$$

$$x \mapsto V_{en}(x,\cdot)$$

$$V_{en}(x,\cdot) \in L_y^\infty$$

$$x \in \mathbb{R}^{3N}$$

$$m = 3M \text{ and } \mathcal{H}_{el} = L^2(\mathbb{R}^{3N})$$

$$h_{\text{eff}} = T + E + \kappa^2 v$$

$$v(y) := \frac{1}{2} \|\nabla_y \psi_\circ\|_{\mathcal{H}_{el}}^2$$

$$\Psi_0 = \psi_\circ f_0$$

$$\Psi = \Psi(t) L^2\left(\mathbb{R}^{3(N+M)}\right) \Psi(0) = \Psi_0$$

$$f(t) := \langle \psi_\circ, \Psi(t) \rangle_{L_x^2}$$

$$f_0 \in H_{\kappa,y}^{s+2n} B_\tau^{s+2n+2}$$

$$f_0 \in H_{\kappa,y}^{s+7}$$

$$a\kappa_0 = \kappa_0\left(\delta, M, \left\|\nabla_{y_j} V\right\|, \dots, \|\nabla_{y_k} \psi_\circ\|, \dots\right) > 0$$

$$\partial_y^\alpha H(y) = \partial_y^\alpha (V_n(y) + V_{en}(x, y))$$

$$\bar{R} = \bar{P}\{(H_{\text{bo}} - E)|_{\text{Ran}\bar{P}}\}^{-1} \bar{P}$$

$$L_y^2 = L^2(\mathbb{R}^m) \text{ and } \mathcal{H} = L^2(\mathbb{R}^m, \mathcal{H}_{el}) = L_y^2 \mathcal{H}_{el}$$

$$H_{\kappa,y}^s \mathcal{H}_{el} = H_{\kappa,y}^s(\mathbb{R}^m) \otimes \mathcal{H}_{el} = H_{\kappa,y}^s(\mathbb{R}^m, \mathcal{H}_{el}),$$

$$\mathcal{L}_{r,s} = \mathcal{L}\left(H_y^{r,\kappa} \mathcal{H}_{el}, H_{\kappa,y}^s \mathcal{H}_{el}\right)$$

$$B_T^s = L^\infty\left(0, T; H_{\kappa,y}^s\right)$$

$$\|g\|_{B_T^s} = \sup_{t \in [0,T]} \|g(t)\|_{H_{\kappa,y}^s}.$$

$$U_t P = U_t^P P + O_{\mathcal{L}_{2,0}}(\kappa\langle t\rangle^3)$$

$$U_t^P = e^{-iH^P t/\kappa} \text{ and } H^P = PHP, \text{ so } H^P(\phi f) = \phi(h_{\text{eff}} f)$$

$$U_t J = J\tilde{U}t + O\mathcal{L}_{2,0}(\kappa\langle t\rangle^3)$$

$$J: \psi_\circ \otimes f \mapsto \psi_\circ f \text{ and } \tilde{U}t = e^{-i\tilde{H}t/\kappa} \text{ with } \tilde{H}(\psi \circ\otimes f) = \psi_\circ \otimes h_{\text{eff}} f, \text{ i.e., } \tilde{H} = 1 \otimes h_{\text{eff}}$$

$$v = \|\nabla_y \psi_\circ\|_{\mathcal{H}_{el}}^2 - \frac{i}{\kappa}\sum_{j=1}^{m} \left(a_j D_{y_j} + D_{y_j} a_j\right),$$

$$a_j := \left\langle \psi_\circ, \nabla_{y_j} \psi_\circ \right\rangle_{\mathcal{H}_{el}}$$

$$\text{Re}\langle \psi_\circ, \nabla_y \psi_\circ\rangle_{\mathcal{H}_{el}} = \frac{1}{2}\nabla_y \|\psi_\circ\|_{\mathcal{H}_{el}}^2 = 0$$

$$\bar{R} = \bar{P}\{(H_{\text{bo}} - E)|_{\text{Ran}\bar{P}}\}^{-1}\bar{P}$$

$$e^{At} = \partial_t(e^{At}(A-B)^{-1}e^{-Bt})e^{Bt} - e^{At}S$$

$$S = (A-B)^{-1}[A,B](A-B)^{-1}$$

$$e^{Dt} = \partial_t(D^{-1}e^{Dt})$$

$$\begin{aligned}\partial_t(e^{At}(A-B)^{-1}e^{-Bt}) &= e^{At}A(A-B)^{-1}e^{-Bt} - e^{At}(A-B)^{-1}Be^{-Bt} \\ &= e^{At}e^{-Bt} + e^{At}[A,(A-B)^{-1}]e^{-Bt}\end{aligned}$$

$$S = [(A-B)^{-1}, A]$$

$$1 = (A-B)(A-B)^{-1} \text{ and } 1 = (A-B)^{-1}(A-B)$$

$$\begin{aligned}[(A-B)^{-1}, A] &= (A-B)^{-1}[A, A-B](A-B)^{-1} \\ &= -(A-B)^{-1}[A,B](A-B)^{-1} =: -S\end{aligned}$$

$$\begin{aligned}\int_0^t G_s e^{As} F_s ds =& G_s e^{As} R F_s|_{s=0}^{s=t} + \int_0^t G_s e^{As} S F_s ds \\ &- \int_0^t (G_s' e^{As} R F_s + G_s e^{As} R[BF_s + F_s'])ds\end{aligned}$$

$$G(s)e^{As}F(s) = G(s)\frac{d}{ds}[e^{As}Re^{-Bs}]e^{Bs}F(s) + G(s)e^{As}SF(s).$$

$$e^{-Bs}\frac{d}{ds}[e^{Bs}F_s] = e^{-Bs}[Be^{Bs}F_s + e^{Bs}F_s'] = BF_s + F_s'$$

$$e^{-At} = e^{-Bt}\partial_t(e^{Bt}(A-B)^{-1}e^{-At}) + Se^{-At}$$

$$\begin{aligned}\int_0^t F_s e^{-As} G_s ds =& F_s R e^{-As} G_s|_{s=0}^{s=t} - \int_0^t F_s S e^{-As} G_s ds \\ &- \int_0^t ([F_s' - F_s B] R e^{-As} G_s + F_s R e^{-As} G_s')ds\end{aligned}$$

$$D(t) := (U_t - U_t^P)P, t \geq 0$$

$$P = \int_{\mathbb{R}^m}^{\oplus} P(y)dy, \text{with } P(y) = |\psi_\circ(y)\rangle\langle\psi_\circ(y)|$$

$$P\Psi = \int^{\oplus} \psi_\circ(y)\langle\psi_\circ(y), \Psi(y)\rangle_{\mathcal{H}_{el}} dy$$

$$e^{As} = e^{i\bar{H}s/\kappa} =: \bar{U}_{-s}, \bar{H} = \bar{P}H_\kappa\bar{P}$$

$$e^{Bs} = e^{i\bar{K}s/\kappa} =: \bar{V}_{-s}, \bar{K} = \bar{P}K\bar{P}, K = E + T.$$

$$(A - B)^{-1} = -i\kappa\bar{P}(\bar{H}_{bo} - \bar{E})^{-1}\bar{P} =: -i\kappa\bar{R}$$

$$E(y) \in \rho(H(y)|_{\mathrm{Ran}\bar{P}}), \forall y \in \mathbb{R}^m,$$

$$E(\cdot) \in C_b^{k_A}(\mathbb{R}^m), P(\cdot) \in C_b^{k_A}\left(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el})\right).$$

$$\|\bar{R}\|_{\mathcal{L}(\mathrm{Ran}\bar{P})} \leqslant \frac{1}{\delta}, \bar{R} = O_{\mathcal{L}_{s,s}}(1)$$

$$\bar{R} = \int_{\mathbb{R}^m}^{\oplus} \bar{R}(y)dy$$

$$\bar{R}(\cdot) \in C_b^{k_A}\left(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el})\right)$$

$$PKP\psi_\circ g = \psi_\circ(K + \kappa^2 v)g$$

$$t \mapsto \Psi(t) \in \mathcal{H}$$

$$H^P\Psi = \psi_\circ h_{\mathrm{eff}} f$$

$$h_{\mathrm{eff}} = T + E + \kappa^2 v$$

$$U_t^P\Psi = \psi_\circ e^{-ih_{\mathrm{eff}}t/\kappa} f$$

$$f = \langle\psi_\circ, \Psi\rangle_{\mathcal{H}_{el}} \text{ and } h_{\mathrm{eff}} = T + E + \kappa^2 v$$

$$P(\psi_\circ g) = \psi_\circ g$$

$$[T, \psi_\circ]g = T(\psi_\circ g) - \psi_\circ T g$$

$$KP\psi_\circ g = K\psi_\circ g = \psi_\circ(E + T)g + [T, \psi_\circ]g.$$

$$PKP\psi_\circ g = P\psi_\circ(E + T)g + P[T, \psi_\circ]g = P\psi_\circ Kg + P[T, \psi_\circ]g = \psi_\circ Kg + \langle\psi_\circ, [T, \psi_\circ]\rangle_{\mathcal{H}_{el}} g,$$

$$[T, \psi_\circ]g = -\kappa^2(\Delta_y\psi_\circ)g - 2i\kappa(\nabla_y\psi_\circ)D_y g$$

$$\begin{aligned}
\langle\psi_\circ, [T, \psi_\circ]\rangle_{\mathcal{H}_{el}} g &= -\kappa^2\langle\psi_\circ, \Delta_y\psi_\circ\rangle_{\mathcal{H}_{el}} g - 2i\kappa\langle\psi_\circ, \nabla_y\psi_y\rangle_{\mathcal{H}_{el}} D_y g \\
&= \langle\psi_\circ, \nabla_y(\nabla_y\psi_\circ)\rangle_{\mathcal{H}_{el}} - 2i\kappa\langle\psi_\circ, \nabla_y\psi_y\rangle_{\mathcal{H}_{el}} D_y g \\
&= \nabla_y\langle\psi_\circ, \nabla_y\psi_\circ\rangle_{\mathcal{H}_{el}} - \langle\nabla_y\psi_\circ, \nabla_y\psi_\circ\rangle_{\mathcal{H}_{el}} - 2i\kappa\langle\psi_\circ, \nabla_y\psi_y\rangle_{\mathcal{H}_{el}} D_y g \\
&= -\kappa^2(\nabla_y a) + \kappa^2\|\nabla_y\psi_\circ\|_{\mathcal{H}_{el}}^2 - 2i\kappa a D_y g
\end{aligned}$$

$$y \mapsto a(y) := \langle \psi_y, \nabla_y \psi_y \rangle_{\mathcal{H}_{el}}$$

$$\Delta_y \psi_\circ = \nabla_y \cdot (\nabla_y \psi_\circ) \|\psi_\circ\|^2_{\mathcal{H}_{el}} = 1$$

$$a = \langle \psi_\circ, \nabla_y \psi_\circ \rangle_{\mathcal{H}_{el}} = \frac{1}{2} \nabla_y \|\psi_\circ\|^2_{\mathcal{H}_{el}} = 0$$

$$\langle \psi_\circ, [T, \psi_\circ] \rangle_{\mathcal{H}_{el}} g = \kappa^2 \|\nabla_y \psi_\circ\|^2_{\mathcal{H}_{el}} g$$

$$PKP\psi_\circ g = \psi_\circ K g + \kappa^2 \|\nabla_y \psi_\circ\|^2_{\mathcal{H}_{el}} g$$

$$t \mapsto \Psi(t) \in \mathcal{H}$$

$$P\Psi = \psi_\circ f$$

$$H^P \Psi = PHP\Psi = P(K - E + H_{bo})\psi_\circ f = \psi_\circ (K + \kappa^2 v) f + P(-E + H_{bo})\psi_\circ f$$

$$PH_{bo}\psi_\circ f = PH_{bo}\psi_\circ f = P(H_{bo}\psi_\circ) f = PE\psi_\circ f$$

$$P(-E + H_{bo})\psi_\circ f = e^{-ih_{\text{eff}} t/\kappa}$$

$$\Psi(t) = U_t^P \psi_0 f_0$$

$$i\kappa \partial_t \Psi(t) = H^P \Psi(t) = \psi_\circ h_{\text{eff}} f(t)$$

$$f(t) := \langle \psi_\circ, \Psi(t) \rangle_{\mathcal{H}_{el}}$$

$$i\kappa \partial_t f(t) = \langle \psi_\circ, H^P \Psi(t) \rangle = h_{\text{eff}} f(t)$$

$$(U_t - U_t^P)P = U_t X_t$$

$$X_t := -\int_0^t Y_s \bar{U}_{-s} X U_s^P \, ds, \text{ with } Y_s := \mathbf{1} + \int_0^s U_{-a} X^* \bar{U}_a \, da$$

$$X_t = i\kappa U_{-s} \bar{R} X U_s^P |_0^t - i\kappa \int_0^t U_{-s} X^* \bar{R} X P U_s^P \, ds - i\kappa \int_0^t U_{-s} X_2 U_s^P \, ds$$

$$X_2 = \frac{i}{\kappa} SX + \frac{i}{\kappa} \bar{R}(\bar{K}X - XK^P), S = \bar{R}[H_{bo} - E, T]\bar{R}$$

$$(U_t - U_t^P)P = -U_t(U_{-t}U_t^P - 1)P = -U_t \int_0^t \frac{d}{ds}(U_{-s}U_s^P)P ds$$
$$= -\frac{i}{\kappa} \int_0^t U_{t-s}(H - PHP)PU_s^P \, ds$$

$$U_s^P P = P U_s^P$$

$$H_\kappa = H_{\text{bo}} + T[H_{\text{bo}}, P]$$

$$(H_\kappa - H^P)P = \bar{P} H_\kappa P = \bar{P} T P$$

$$X_t = -\int_0^t U_{-s} X U_s^P \, ds, X := \frac{i}{\kappa} \bar{P} T P$$

$$U_{-s}\bar{P} = \bar{U}_{-s}\bar{P} + \frac{i}{\kappa}\int_0^s U_{-s+r}PH\bar{P}\bar{U}_{-r}dr$$

$$-\frac{i}{\kappa}PH\bar{P} = -\frac{i}{\kappa}PT\bar{P} = X^*$$

$$U_{-s}\bar{P} = Y_s\bar{U}_{-s}\bar{P}, Y_s = \mathbf{1} + \int_0^s U_{-a}X^*\bar{U}_a da$$

$$G_s = Y_s, A = \frac{i}{\kappa}\bar{H}, B = \frac{i}{\kappa}\bar{K}$$

$$X_t = i\kappa Y_s\bar{U}_{-s}\bar{R}XU_s^P|_0^t - \int_0^t Y_s\bar{U}_{-s}SXPU_s^P ds$$
$$-i\kappa\int_0^t \left[(\partial_s Y_s)\bar{U}_{-s}\bar{R}XU_s^P + Y_s\bar{U}_{-s}\bar{R}\left(\frac{i}{\kappa}\bar{K}XU_s^P + \partial_s(XU_s^P)\right)\right]ds$$

$$H^P = K^P \equiv PKP$$

$$\frac{i}{\kappa}\bar{K}XU_s^P + \partial_s(XU_s^P) = \frac{i}{\kappa}(\bar{K}X - XK^P)U_s^P$$

$$Y_s\bar{U}_{-s}\bar{P} = U_{-s}\bar{P}$$

$$(\partial_s Y_s)\bar{U}_{-s}\bar{P} = U_{-s}X^*$$

$$X = \frac{i}{\kappa}\bar{P}TP$$

$$X^* = -\frac{i}{\kappa}PT\bar{P}$$

$$S = \bar{R}\big((H_{bo} - E)\bar{P}K - K\bar{P}(H_{bo} - E)\big)\bar{R} = \bar{R}\big((H_{bo} - E)K - K(H_{bo} - E)\big)\bar{R}$$
$$= \bar{R}[H_{bo} - E, K]\bar{R}$$

$$[H_{bo} - E, K] = [H_{bo} - E, T] \;\square$$

$$S = O_{\mathcal{L}_{s+1,s}}(\kappa), X_2 = O_{\mathcal{L}_{2,0}}(1)$$

$$X_t = O_{\mathcal{L}_{2,0}}(\kappa\langle t\rangle^3).$$

$$[H_{bo}, T][E, T]\; O_{\mathcal{L}_{s+1,s}}(\kappa)$$

$$S = \bar{R}([H_{bo}, T] - [E, T])\bar{R}$$

$$\bar{R} = O_{\mathcal{L}_{s,s}}(1),$$

$$X = \tfrac{i}{\kappa}\bar{P}[T, P]P \text{ and } X^* = \tfrac{i}{\kappa}P[T, P]\bar{P}$$

$$U_t = O_{\mathcal{L}_{s,s}}(\langle t\rangle^s), U_t^P = O_{\mathcal{L}_{s,s}}(\langle t\rangle^s),$$

$$O_{\mathcal{L}_{2,0}}(\kappa\langle t\rangle^3)X^\circ = \frac{i}{\kappa}[T, P]X = \bar{P}X^\circ P$$

$$X_2 = \frac{i}{\kappa} S\bar{P}X^{\circ}P + \frac{i}{\kappa}\bar{R}[X^{\circ},[K,P]-K]PU_s^P = O_{\mathcal{L}_{2,0}}(1),$$

$$X_t = O_{\mathcal{L}_{2,0}}(\kappa\langle t\rangle^3)\ \square$$

$$U_t(\psi_{\circ}f) - \psi_{\circ}e^{ih_{\text{eff}}t/k}f = (U_t - U_t^P)P\Psi.$$

$$(U_t - U_t^P)P\Psi = U_t X_t \Psi,$$

$$\Psi \in H^2_{\kappa,y}\mathcal{H}_{el}$$

$$\|X_t\Psi\|_{H^2_{\kappa,y}}\mathcal{H}_{el} \leq C\kappa\langle t\rangle^3\|\Psi\|_{L^2_{\kappa,y}}\mathcal{H}_{el}.$$

$$\left\|U_t(\psi_{\circ}f) - \psi_{\circ}e^{ih_{\text{eff}}t/k}f\right\|_{H^2_{\kappa,y}}\mathcal{H}_{el} = \|U_tX_t\Psi\|_{H^2_{\kappa,y}}\mathcal{H}_{el} \lesssim \|X_t\Psi\|_{H^2_{\kappa,y}}\mathcal{H}_{el} \lesssim C\kappa\langle t\rangle^3\|\Psi\|_{L^2_{\kappa,y}}\mathcal{H}_{el}.$$

$$X_t = O_{\mathcal{L}_{2,0}}(\kappa\langle t\rangle^3)$$

$$\phi(t) := P\Psi(t) \text{ and } \bar{\phi}(t) := \bar{P}\Psi(t)$$

$$\begin{cases} i\kappa\partial_t\phi = H^P\phi + PT\bar{\phi}, & \underline{\phi(0) = P\Psi_0} \\ i\kappa\partial_t\bar{\phi} = \bar{H}\bar{\phi} + \bar{P}T\phi, & \bar{\phi}(0) = \bar{P}\Psi_0. \end{cases}$$

$$i\kappa\partial_t\phi = PH_\kappa\Psi.$$

$$\begin{aligned} PH_\kappa\psi = PH_\kappa(\phi + \bar{\phi}) = PH_\kappa\phi + P(T + H_{bo})\bar{\phi} &= (PH_\kappa P)P\phi + PT\bar{\phi} + PH_{bo}\bar{P}\psi \\ &= H^P\phi + PT\bar{\phi} \end{aligned}$$

$$i\kappa\partial_t\phi = H^P\phi + PT\bar{\phi}$$

$$PH_{bo}\bar{P} = 0 = \bar{P}H_{bo}P$$

$$PH\bar{P} = PT\bar{P} \text{ and } \bar{P}HP = \bar{P}TP$$

$$\phi(y,t) = \psi_{\circ}(y)f(y,t)$$

$$\bar{\phi}(0) = \bar{P}\Psi(0) = \bar{P}(\psi_0 f_0) = 0$$

$$i\kappa\partial_t\bar{\phi} = \bar{H}\bar{\phi} + \bar{P}T\phi, \phi(0) = 0.$$

$$\bar{U}_t = \epsilon^{-i\bar{H}t/\kappa}, t \in \mathbb{R}$$

$$\bar{\phi}(t) = -\frac{i}{\kappa}\int_0^t \bar{U}_{t-s}\bar{P}T\phi(s)ds$$

$$i\kappa\partial_t\phi = H^P\phi + \mathcal{K}\phi,$$

$$(\mathcal{K}\phi)(t) = -\frac{i}{\kappa}PT\bar{P}\int_0^t \bar{U}_{t-s}\bar{P}TP\phi(s)ds$$

$$(\mathcal{K}\phi)(x,y,t) = \psi_{\circ}(x,y)w^\kappa[f](y,t)$$

$$(\mathcal{K}\phi)(y,t) = -\frac{i}{\kappa}\psi_\circ(y)\left\langle\psi_\circ(y), PT\bar{P}\int_0^t \bar{U}_{t-s}\bar{P}TP\psi_\circ(y)f(s)ds\right\rangle_{\mathcal{H}_{el}}$$

$$= \psi_\circ(y)\left(-\frac{i}{\kappa}\int_0^t \langle\psi_\circ(y), PT\bar{P}\bar{U}_{t-s}\bar{P}TP\psi_\circ(y)\rangle_{\mathcal{H}_{el}} f(s)ds\right)$$

$$\Psi|_{t=0} = \psi_\circ(x,y)f_0(y)$$

$$i\kappa\partial_t\Psi = \psi_\circ(i\kappa\partial_t f) + \bar{H}\Psi_1 + \bar{P}T\psi_\circ f = \psi_\circ(E + T + \kappa^2 v)f + \psi_\circ w^\kappa[f] + \bar{H}\Psi_1 + \bar{P}T\psi_\circ f$$

$$\Psi_1 := -\frac{i}{\kappa}\int_0^t \bar{U}_{t-s}\bar{P}T\psi_\circ f ds$$

$$P\Psi = \psi_\circ f$$

$$\psi_\circ(E + T + \kappa^2 v)f = H^P\Psi.$$

$$\psi_\circ w^\kappa[f] = PT\Psi_1 = PH\bar{P}\Psi.$$

$$\bar{P}HP = \bar{P}TP\psi_\circ f = P\Psi$$

$$\bar{P}T\psi_\circ f = \bar{P}HP\Psi$$

$$(PHP + PH\bar{P} + \bar{P}H\bar{P} + \bar{P}HP)\Psi = H\Psi$$

$$\Psi_0(x,y) = \psi_\circ(x,y)f_0(y)$$

$$X = \frac{i}{\kappa}\bar{P}TP$$

$$X^* = -\frac{i}{\kappa}PT\bar{P}$$

$$w^\kappa[f](t) = -i\kappa\langle\psi_o, X^*(A_t f)(t)\rangle_{\mathcal{H}_{el}}$$

$$(A_t f)(t) = \int_0^t \bar{U}_{t-r}X\psi_\circ f(r)dr$$

$$(A_t^Y f)(t) = \int_0^t \bar{U}_{t-r}Y\psi_\circ f(r)dr$$

$$(A_t^Y f)(t) = -i\kappa[\bar{R}Y\psi_\circ f(t) - \bar{U}_t\bar{R}Y\psi_\circ f_0] - i\kappa\left(A_t^{\bar{R}YX^*}A_{(\cdot)}^X f\right)(t) + i\kappa\left(A_t^{W[Y]}f\right)(t),$$

$$W[Y] = \frac{i}{\kappa}SY + \frac{i}{\kappa}\bar{R}(\bar{K}Y - YK^P)P,$$

$$W[\cdot]X = \frac{i}{\kappa}\bar{P}TP$$

$$\begin{cases} X_1 & = \frac{i}{\kappa}\bar{P}TP \\ X_j & = \frac{i}{\kappa}SX_{j-1} + \frac{i}{\kappa}\bar{R}\left(K\bar{P}X_{j-1} - X_{j-1}PK\right)P, j \geqslant 2 \end{cases}$$

$G_s = 1, A = \frac{i}{\kappa}\bar{H}, B = \frac{i}{\kappa}\bar{K}$, and $F_s = Y\psi_\circ f(s)$

$$(A_t^Y f)(t) = \bar{U}_{t-r}\bar{R}Y\psi_\circ f(r)|_{r=0}^{r=t} + \int_0^t \bar{U}_{t-r}SY\psi_\circ f(r)dr - \int_0^t \bar{U}_{t-r}\bar{R}C_r dr$$

$$S = \bar{R}[\bar{H}_{bo} - \bar{E}, \bar{K}]\bar{R} \text{ and } \bar{R} = \bar{P}(\bar{H}_{bo} - \bar{E})^{-1}\bar{P}$$

$$C_r := \frac{i}{\kappa}\bar{K}Y\psi_\circ f(r) + \frac{\partial}{\partial r}(Y\psi_\circ f(r))$$

$$-i\kappa C_r = \bar{K}Y\psi_\circ f(r) - Y\psi_\circ(i\kappa\partial_r f(r)) = \bar{K}Y\psi_\circ f(r) - Y\psi_\circ(K + \kappa^2 v)f(r) - Y\psi_\circ w^\kappa[f](r).$$

$$\psi_\circ w^\kappa[f](r) = -i\kappa X^*(A_r^X f)(r)$$

$$-i\kappa C_r = (\bar{K}Y - YK^P)\psi_\circ f(r) - i\kappa Y X^*(A_r^X f)(r)$$

$$(A_t^X f)(t) = -i\kappa[\bar{R}X\psi_\circ f(t) - \bar{U}_t\bar{R}X\psi_\circ f_0] - i\kappa\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^X f\right)(t) + i\kappa\left(A_t^{X_2} f\right)(t)$$

$$w^\kappa[f](t) = (-i\kappa)^2(w_1 f(t) - \tilde{w}_1(t)f_0) + (-i\kappa)^3 w_2^\kappa[f](t)$$

$$w_1 f(t) = \langle\psi_\circ, X^*\bar{R}X\psi_\circ f(t)\rangle_{\mathcal{H}_{el}}$$
$$\tilde{w}_1(t)f_0 = \langle\psi_\circ, X^*\bar{U}_t\bar{R}X\psi_\circ f_0\rangle_{\mathcal{H}_{el}}$$

$$w_2^\kappa[f](t) = (w_2 f(t) - \tilde{w}_2(t)f_0) + \int_0^t \langle\psi_\circ, X^*\bar{U}_{t-r}(X_3 + \bar{R}XX^*\bar{R}X)\psi_\circ f(r)\rangle_{\mathcal{H}_{el}} dr$$
$$+ \int_0^t \int_0^r \langle\psi_\circ, X^*\bar{U}_{t-r}\bar{R}X_2X^*\bar{U}_{r-s}X\psi_\circ f(s)\rangle_{\mathcal{H}_{el}} dsdr$$
$$+ \int_0^t \int_0^r \langle\psi_\circ, X^*\bar{U}_{t-r}\bar{R}XX^*\bar{U}_{r-s}X_2\psi_\circ f(s)\rangle_{\mathcal{H}_{el}} dsdr$$
$$+ \int_0^t \int_0^r \int_0^s \left\langle\psi_\circ, X^*\bar{U}_{t-r}\bar{R}XX^*\bar{U}_{r-s}\bar{R}XX^*\bar{U}_{s-q}X\psi_\circ f(q)\right\rangle_{\mathcal{H}_{el}} dqdsdr$$

$$w_2 f(t) = \langle\psi_\circ, X^*\bar{R}X_2\psi_\circ f(t)\rangle_{\mathcal{H}_{el}}$$

$$\tilde{w}_2(t)f_0 = \langle\psi_\circ, X^*\bar{U}_t\bar{R}X_2\psi_\circ f_0\rangle_{\mathcal{H}_{el}} - \int_0^t \langle\psi_\circ, X^*\bar{U}_{t-r}\bar{R}XX^*\bar{U}_r\bar{R}X\psi_\circ f_0\rangle_{\mathcal{H}_{el}} dr$$

$$X = \frac{i}{\kappa}\bar{P}[T,P]P, X^* = \frac{i}{\kappa}P[T,P]\bar{P}$$

$$X_2 = -\frac{1}{\kappa^2}S\bar{P}[T,P]P - \frac{1}{\kappa^2}\bar{R}[[T,P],[T,P]-K]P,$$
$$X_3 = -\frac{i}{\kappa^3}S^2\bar{P}[T,P]P - \frac{i}{\kappa^3}\bar{R}[S,[T,P]-K][T,P]P - \frac{i}{\kappa^3}\bar{R}S[[T,P],[T,P]-K]P$$
$$-\frac{i}{\kappa^3}S\bar{R}[[T,P],[T,P]-K]P - \frac{i}{\kappa^3}\bar{R}[\bar{R},[T,P]-K][[T,P],[T,P]-K]P$$
$$-\frac{i}{\kappa^3}\bar{R}^2[[[T,P],[T,P]-K],[T,P]-K].$$

$$\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^X f\right)(t)A_{(\cdot)}^X f$$

$$\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^X f\right)(t) = (-i\kappa)\left(A_t^{\bar{R}XX^*\bar{R}X} f\right)(t) - (-i\kappa)\left(A_t^{\bar{R}XX^*}\bar{U}_{(\cdot)}\right)(t)\bar{R}X\psi_\circ f_0$$
$$-(-i\kappa)\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{X_2} f\right)(t) + (-i\kappa)\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{\bar{R}XX^*}A_{(\cdot)}^X f\right)(t).$$

$$\left(A_t^{X_2} f\right)(t)$$

$$\left(A_t^{X_2}f\right)(t) = -(-i\kappa)(\bar{R}X_2\psi_\circ f(t) - \bar{U}_t\bar{R}X_2\psi_\circ f_0) + (-i\kappa)\left(A_t^{\bar{R}X_2X^*}A_{(\cdot)}^{X}f\right)(t)$$
$$-(-i\kappa)\left(A_t^{X_3}f\right)(t)$$

$$(A_t^X f)(t) = -i\kappa(\bar{R}X\psi_\circ f(t) - \bar{U}_t\bar{R}X\psi_\circ f_0) - (-i\kappa)^2(\bar{R}X_2\psi_\circ f(t) - \bar{U}_t\bar{R}X_2\psi_\circ f_0)$$
$$-(-i\kappa)^2\left(A_t^{\bar{R}XX^*}\bar{U}_{(\cdot)}\right)(t)\bar{R}X\psi_\circ f_0 + (-i\kappa)^2\left(A_t^{X_3+\bar{R}XX^*\bar{R}X}f\right)(t)$$
$$+(-i\kappa)^2\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{X_2}f\right)(t) + (-i\kappa)^2\left(A_t^{\bar{R}X_2X^*}A_{(\cdot)}^{X}f\right)(t)$$
$$+(-i\kappa)^2\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{\bar{R}XX^*}A_{(\cdot)}^{X}f\right)(t).$$

$$w^\kappa[f](t) = (-i\kappa)^2(w_1 f(t) - \tilde{w}_1(t)f_0) + (-i\kappa)^3 w_2^\kappa[f](t),$$

$$w_1 f(t) = \langle\psi_\circ, X^*\bar{R}X\psi_\circ f(t)\rangle_{\mathcal{H}_{el}},$$
$$\tilde{w}_1(t)f_0 = \langle\psi_\circ, X^*\bar{U}_t\bar{R}X\psi_\circ f_0\rangle_{\mathcal{H}_{el}},$$
$$w_2^\kappa[f](t) = -\left(\langle\psi_\circ, X^*\bar{R}X_2\psi_\circ f(t)\rangle_{\mathcal{H}_{el}} - \langle\psi_\circ, X^*\bar{U}_t\bar{R}X_2\psi_\circ f_0\rangle_{\mathcal{H}_{el}}\right)$$
$$-\left\langle\psi_\circ, X^*\left(A_t^{\bar{R}XX^*}\bar{U}_{(\cdot)}\right)(t)\bar{R}X\psi_\circ f_0\right\rangle_{\mathcal{H}_{el}}$$
$$+\left\langle\psi_\circ, X^*\left(A_t^{X_3+\bar{R}XX^*\bar{R}X}f\right)(t)\right\rangle_{\mathcal{H}_{el}} + \left\langle\psi_\circ, X^*\left(A_t^{\bar{R}X_2X^*}A_{(\cdot)}^{X}f\right)(t)\right\rangle_{\mathcal{H}_{el}}$$
$$+\left\langle\psi_\circ, X^*\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{X_2}f\right)(t)\right\rangle_{\mathcal{H}_{el}} + \left\langle\psi_\circ, X^*\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{\bar{R}XX^*}A_{(\cdot)}^{X}f\right)(t)\right\rangle_{\mathcal{H}_{el}}.$$

$$(A_t^X f)(t) = \sum_{j=1}^{n} -(-i\kappa)^j\left[L_j\psi_\circ f(t) - \tilde{L}_j(t)\psi_\circ f_0\right] + (-i\kappa)^n\mathcal{R}_n[f](t),$$

$$\mathcal{R}_n[f](t) = \left(A_t^{Y_n}f\right)(t) + \sum_{j=2}^{n}\sum_{l=1}^{N(n,j)}\left(A_t^{Y_{n,j}^{l,j}}A_{(\cdot)}^{Y_{n,j}^{l,j-1}}A_{(\cdot)}^{Y_{n,j}^{l,j-2}}\dots A_{(\cdot)}^{Y_{n,j}^{l,1}}f\right)(t)$$

$$+\left(A_t^{\bar{R}XX^*}\left(\prod_{1}^{n-1}A_{(\cdot)}^{\bar{R}XX^*}\right)A_{(\cdot)}^{X}f\right)(t),$$

$$N(n+1,j) = N(n,j-1) + N(n,j) + N(n,j+1)$$

$$L_{n+1} = \bar{R}Y_n, n \geqslant 0$$

$$Y_n = -W(Y_{n-1}) + \sum_{l=1}^{N(n-1,2)} Y_{n,2}^{l,2}\bar{R}Y_{n,2}^{l,1}, Y_1 := X$$

$$W(Y_{n-1}) = \frac{i}{\kappa}SY_{n-1} + \frac{i}{\kappa}\bar{R}(\bar{K}Y_{n-1} - Y_{n-1}K^P)$$

$$\tilde{L}_{n+1}(t) = \bar{U}_t\bar{R}Y_n - \sum_{j=2}^{n}\sum_{l=1}^{N(n,j)}\left(A_t^{Y_{n,j}^{l,j}}A_{(\cdot)}^{Y_{n,j}^{l,j-1}}A_{(\cdot)}^{Y_{n,j}^{l,j-2}}\dots\bar{U}_{(\cdot)}\right)(t)Y_{n,j}^{l,1}$$
$$-\left(A_t^{\bar{R}XX^*}\left(\prod_{1}^{n-1}A_{(\cdot)}^{\bar{R}XX^*}\right)\bar{U}_{(\cdot)}\right)(t)\bar{R}X$$

$$\left(A_t^{Y_{n,j}^{l,j}}A_{(\cdot)}^{Y_{n,j}^{l,j-1}}\dots A_{(\cdot)}^{Y_{n,j}^{l,2}}A_{(\cdot)}^{Y_{n,j}^{l,1}}f\right)(t),$$

$$A_{(\cdot)}^{Y_{n,j}^{l,1}} f = Y_{n,j}^{l,1}$$

$$\left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} A_{(\cdot)}^{Y_{n,j}^{l,1}} f\right)(t) = (-i\kappa)\left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}\bar{R}Y_{n,j}^{l,1}} f\right)(t)$$
$$-(-i\kappa)\left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} \bar{U}(\cdot)\right)(t)\bar{R}Y_{n,j}^{l,1}\psi_\circ f_0$$
$$-(-i\kappa)\left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} A_{(\cdot)}^{W\left(Y_{n,j}^{l,1}\right)} f\right)(t)$$
$$+(-i\kappa)\left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} A_{(\cdot)}^{\bar{R}Y_{n,j}^{l,1}X^*} A_{(\cdot)}^{X} f\right)(t).$$

$$w^\kappa[f](t) = \sum_{j=1}^{n-1} -(-i\kappa)^{j+1}\left(w_j f(t) - \tilde{w}_j(t) f_0\right) + (-i\kappa)^{n+1} w_n^\kappa[f](t)$$

$$w_j f(t) = \langle \psi_\circ, X^* L_j \psi_\circ f(t)\rangle_{\mathcal{H}_{el}},$$
$$\tilde{w}_j(t) f_0 = \langle \psi_\circ, X^* \tilde{L}_j(t) \psi_\circ f_0\rangle_{\mathcal{H}_{el}},$$
$$w_n^\kappa[f](t) = -(w_n f(t) - \tilde{w}_n(t) f_0) + \langle \psi_\circ, X^* \mathcal{R}_n[f](t)\rangle_{\mathcal{H}_{el}}.$$

$$X_j = O_{\mathcal{L}_{s+j,s}}(1)$$

$$(\partial_y^{\alpha_1} H_{bo}), (\partial_y^{\alpha_2} P), (\partial_y^{\alpha_3} E), \text{and } \bar{R},$$

$$A = \sum_{0 \leqslant |\alpha| \leqslant k} c_\alpha B_\alpha D^\alpha = O_{\mathcal{L}_{s+k,s}}(1),$$

$$C_1 C_2 = \sum_{|\alpha| \leqslant k, |\beta| \leqslant l} B_\alpha D^\alpha B_\beta D^\beta = \sum_{|\alpha| \leqslant k, |\beta| \leqslant l} B_\alpha B_\beta D^{\alpha+\beta} + \sum_{|\alpha| \leqslant k, |\beta| \leqslant l} B_\alpha [D^\alpha, B_\beta] D^\beta$$

$$[D^\alpha, B_\beta] \in \mathcal{C}^{|\alpha|-1}$$

$$B = O_{\mathcal{L}_{s,s}}(1), \frac{i}{\kappa}[B, [T,P] - T] \in \mathcal{C}^1$$

$$\frac{i}{\kappa}[B, [T,P] - T] = O_{\mathcal{L}_{s+1,s}}(1)$$

$$[T,P] - T = -\kappa^2(\Delta_y P) - 2i\kappa(\nabla_y P)D - D^2.$$

$$X^\circ = \frac{i}{\kappa}[T,P] \in \mathcal{C}^1 \text{ and } X^\circ = O_{\mathcal{L}_{s+1,s}}(1) \text{ for } s \leqslant k_A - 1$$

$$X_{n+1} = \frac{i}{\kappa} S X_n + \frac{i}{\kappa}\bar{R}(K\bar{P}X_n - X_n P K)P$$

$$X_{n+1} = \frac{i}{\kappa} S X_n^\circ P + \frac{i}{\kappa}\bar{R}(K\bar{P}X_n^\circ - X_n^\circ P K)P$$

$$X_{n+1} = \frac{i}{\kappa} S X_n^\circ P + \frac{i}{\kappa}\bar{R}[X_n^\circ, [K,P] - K]P$$

$$X_{n+1}=\frac{i}{\kappa}SX_n^\circ P+\frac{i}{\kappa}\bar{R}[X_n^\circ,[T,P]-T]P-\frac{i}{\kappa}\bar{R}[X_n^\circ,E]P$$

$$X_{n+1}^\circ=\frac{i}{\kappa}SX_n^\circ+\frac{i}{\kappa}\bar{R}[X_n^\circ,[T,P]-T]-\frac{i}{\kappa}\bar{R}[X_n^\circ,E]$$

$$\begin{aligned}[X_n^\circ,[T,P]-T]&=\sum_{0\leqslant|\alpha|\leqslant n}[B_\alpha D^\alpha,[T,P]-T]\\&=\sum_{0\leqslant|\alpha|\leqslant n}[B_\alpha,[T,P]-T]D^\alpha+B_\alpha[D^\alpha,[T,P]-T]\end{aligned}$$

$$[D^\alpha,[T,P]-T]=[D^\alpha,[T,P]]\in\mathcal{C}^{|\alpha|}$$

$$\left[X_j^\circ,[T,P]-T\right]\in\mathcal{C}^{|\alpha|+1}$$

$$X_n^\circ=\sum_{0\leqslant|\alpha|\leqslant n}B_\alpha D^\alpha$$

$$[X_n^\circ,E]=\sum_{0\leqslant|\alpha|\leqslant n}B_\alpha[D^\alpha,E]$$

$$L_n=O_{\mathcal{L}_{s+n,s}}(1),\tilde{L}_n(t)=O_{\mathcal{L}_{s+2n-1,s}}(e^{Ct})$$

$$\|\mathcal{R}_n[f](t)\|_{H^s_{\kappa,y}}\lesssim e^{C\tau}\|f\|_{B_\tau^{s+2n+1}}$$

$$\bar{R}=O_{\mathcal{L}_{s,s}}(1),X=O_{\mathcal{L}_{s+1,s}}$$

$$\bar{U}_t=O_{\mathcal{L}_{s,s}}(e^{Ct})$$

$$L_1=\bar{R}X=O_{\mathcal{L}_{s+1,s}}(1),L_1(t)=\bar{U}_t\bar{R}X=O_{\mathcal{L}_{s+1,s}}(e^{Ct})$$

$$X_2=O_{\mathcal{L}_{s+2,s}}(1)\text{ and }X^*=O_{\mathcal{L}_{s+1,s}}(1)$$

$$\|(A_t^Y f)(t)\|_{H^s_{\kappa,y}}\leqslant\int_0^t e^{C(t-s)}\|Y\psi_\circ f(r)\|_{H^s_{\kappa,y}}dr\leqslant e^{C\tau}\|f\|_{B_\tau^{s+j}}$$

$$\mathcal{R}_1[f](t)=-i\kappa\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^X f\right)(t)+i\kappa\left(A_t^{X_2}f\right)(t),$$

$$L_2=\bar{R}X_2=O_{\mathcal{L}_{s+2,s}}(1)$$

$$\left\|\left(A_t^{\bar{R}XX^*}\bar{U}_{(\cdot)}\right)(t)u\right\|_{H^s_{\kappa,y}}\leqslant\int_0^t e^{C(t-r)}\|\bar{R}XX^*\bar{U}_r u\|_{H^s_{\kappa,y}}dr\lesssim e^{Ct}\|u\|_{H^{s+2}_{\kappa,y}}$$

$$\tilde{L}_2(t)=\bar{U}_t\bar{R}X_2-\left(A_t^{\bar{R}XX^*}\bar{U}_{(\cdot)}\right)(t)\bar{R}X=O_{\mathcal{L}_{s+3,s}}(e^{Ct})$$

$$\begin{aligned}\mathcal{R}_2[f](t)=&\left(A_t^{X_3+\bar{R}XX^*\bar{R}X}f\right)(t)+\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{X_2}f\right)(t)+\left(A_t^{\bar{R}X_2X^*}A_{(\cdot)}^X f\right)(t)\\&+\left(A_t^{\bar{R}XX^*}A_{(\cdot)}^{\bar{R}XX^*}A_{(\cdot)}^X f\right)(t)\end{aligned}$$

$$X_3=O_{\mathcal{L}_{s+3,s}}\left(A_t^{Y_1}\dots A_{(\cdot)}^{Y_n}u\right)(t)$$

$$1, \left(A_t^{X_3+\bar{R}XX^*\bar{R}X} f\right)(t) 2, \left(A_t^{\bar{R}XX^*} A_{(\cdot)}^{X_2} f\right)(t) + \left(A_t^{\bar{R}X_2X^*} A_{(\cdot)}^{X} f\right)(t) 3, \left(A_t^{\bar{R}XX^*} A_{(\cdot)}^{\bar{R}XX^*} A_{(\cdot)}^{X} f\right)(t)$$

$$\sum_{l=1}^{N(n,j)} \left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} A_{(\cdot)}^{Y_{n,j}^{l,1}} f\right)(t) = O_{\mathcal{L}_{s+n+j+1}}(e^{Ct}).$$

$$A_{(\cdot)}^{Y_{n,j}^{l,1}} f = Y_{n,j}^{l,1}$$

$$\sum_{l=1}^{N(n,j)} \left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} A_{(\cdot)}^{Y_{n,j}^{l,1}} f\right)(t)$$

$$= (-i\kappa) \sum_{l=1}^{N(n,j)} \left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}\bar{R}Y_{n,j}^{l,1}} f\right)(t)$$

$$-(-i\kappa) \sum_{l=1}^{N(n,j)} \left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} \bar{U}_{(\cdot)}\right)(t) \bar{R} Y_{n,j}^{l,1} \psi_\circ f_0$$

$$-(-i\kappa) \sum_{l=1}^{N(n,j)} \left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} A_{(\cdot)}^{W\left(Y_{n,j}^{l,1}\right)} f\right)(t)$$

$$+(-i\kappa) \sum_{l=1}^{N(n,j)} \left(A_t^{Y_{n,j}^{l,j}} A_{(\cdot)}^{Y_{n,j}^{l,j-1}} \dots A_{(\cdot)}^{Y_{n,j}^{l,2}} A_{(\cdot)}^{\bar{R}Y_{n,j}^{l,1}X^*} A_{(\cdot)}^{X} f\right)(t).$$

$$\left(A_t^{\bar{R}XX^*} \left(\prod_1^{n-2} A_{(\cdot)}^{\bar{R}XX^*}\right) \bar{U}_{(\cdot)}\right)(t) \bar{R} X = O_{\mathcal{L}_{s+2n-1}}(e^{Ct})$$

$$\left\| \left(A_t^{\bar{R}XX^*} \left(\prod_1^{n-1} A_{(\cdot)}^{\bar{R}XX^*}\right) A_{(\cdot)}^{X} f\right)(t) \right\|_{H_{\kappa,y}^s} \lesssim e^{Ct} \|f\|_{B_t^{s+2n+1}}$$

$$\|w_n f(t)\|_{H_{\kappa,y}^s} \lesssim \|f(t)\|_{H_{\kappa,y}^{s+n+1}}, \|\tilde{w}_n(t) f_0\|_{H_{\kappa,y}^s} \lesssim e^{Ct} \|f_0\|_{H_{\kappa,y}^{s+2n}}$$

$$\|w_n^\kappa[f](t)\|_{H_{\kappa,y}^s} \lesssim e^{C\tau} \left(\|f_0\|_{H_{\kappa,y}^{s+2n}} + \|f\|_{B_\tau^{s+2n+2}}\right)$$

$$\|w_n f(t)\|_{H_{\kappa,y}^s} \lesssim \|X^* L_n \psi_\circ f\|_{H_{\kappa,y}^s} \mathcal{H}_{el}$$

$$X^* = \frac{i}{\kappa} P[T, P]\bar{P} = O_{\mathcal{L}_{s+1,s}}$$

$$\|w_n^\kappa[f](t)\|_{H_{\kappa,y}^s} \lesssim \|f(t)\|_{H_{\kappa,y}^{s+n+1}} + e^{C\tau} \left(\|f_0\|_{H_{\kappa,y}^{s+2n}} + \|f\|_{B_\tau^{s+2n+2}}\right)$$

$$\|f(t)\|_{H_{\kappa,y}^{s+n+1}} \leqslant \|f\|_{B_t^{s+n+1}} \lesssim \|f\|_{B_t^{s+2n+2}}$$

$$\Psi(t) - \left(Q_P \tilde{f}\right)(t)$$

$$\Psi(0) = \psi_\circ f_0$$

$$\Psi(t) = (Q_P f)(t) = \psi_\circ f(t) + \int_0^t \bar{U}_{t-s} X^* \psi_\circ f(s) ds$$

$$X^* = -\frac{i}{\kappa}\bar{P}H_\kappa P$$

$$\Psi(t) - \left(Q_P\tilde{f}\right)(t) = \psi_\circ(f(t) - \tilde{f}(t)) + \int_0^t \bar{U}_{t-s}X^*\psi_\circ(f(s) - \tilde{f}(s))ds$$

$$\psi_\circ(f(t) - \tilde{f}(t)) = O_{\mathcal{L}_{s+6,s}}(\kappa^2 e^{C\tau})$$

$$A = \frac{i}{\kappa}\bar{H}, B = \frac{i}{\kappa}\bar{K}$$

$$e^{As} = e^{i\bar{H}s/\kappa} =: \bar{U}_s, \bar{H} = \bar{P}H_\kappa\bar{P}, e^{Bs} = e^{i\bar{K}s/\kappa} =: \bar{V}_s, \bar{K} = \bar{P}K\bar{P},$$

$$(A - B)^{-1} = -i\kappa\bar{P}(\bar{H}_{bo} - \bar{E})^{-1}\bar{P} =: -i\kappa\bar{R}.$$

$$0 < \kappa < \sqrt{\frac{2}{\tilde{C}\sqrt{m(m+1)}}}, \tilde{C} = \tilde{C}\left(\delta, \left\|\nabla_{y_j}H_{bo}\right\|, \dots\right)$$

$$\|w_1 u\| \leqslant \tilde{C}\|u\|_{H_y^{2,\kappa}}$$

$$H_\kappa^{(2)}: \mathrm{Ran}P \to \mathrm{Ran}P$$

$$H_\kappa^{(2)}(\psi_\circ f) = \psi_\circ\left(h_{\mathrm{eff}}^{(2)} f\right)$$

$$U_t^{(2)} = e^{-iH_\kappa^{(2)}t/\kappa}$$

$$U_t^{(2)}\Psi = \psi_\circ e^{-ih_{\mathrm{eff}}^{(2)}t/\kappa} g$$

$$g = \langle\psi_\mathrm{o}, \Psi\rangle_{\mathcal{H}_{\mathrm{el}}}$$

$$\|u\|_{H_y^{2,\kappa}} \leqslant \frac{\sqrt{m(m+1)}}{2}\|Tu\| + \|u\|.$$

$$\|w_1 u\| \leqslant \tilde{C}\|u\|_{H_y^{2,\kappa}}$$

$$\|w_1 u\| \leqslant \tilde{C}\frac{\sqrt{m(m+1)}}{2}\|Tu\| + \tilde{C}\|u\|,$$

$$\mathcal{D}(T) = H_y^{2,\kappa}$$

$$\left\|\nabla_{y_j}P\right\| \leqslant \frac{1}{\delta}\left\|\nabla_{y_j}H_{bo}\right\|$$

$$\psi_\circ(f(t) - \tilde{f}(t))$$

$$X^* = -\frac{i}{\kappa}PT\bar{P}$$

$$\psi_\circ(f(t) - \tilde{f}(t)) = U_t^{(2)}Z_t\bar{R}X\psi_\circ f_0 - \kappa^2\int_0^t U_{t-r}^{(2)}\psi_\circ w_2^\kappa[f](r)dr$$

$$Z_t = -i\kappa \int_0^t U_{-r}^{(2)} X^* \bar{U}_r dr$$

$$Z_t = -\kappa^2 U_{-r}^{(2)} \bar{R} X \bar{U}_r \Big|_{r=0}^{r=t} - \kappa^2 \int_0^t U_{-r}^{(2)} X_{(2)} \bar{U}_r dr$$

$$X_{(2)} = (X_2)^* - i\kappa\psi_\circ w_1 \langle \psi_\circ, X^*(\cdot)\rangle_{\mathcal{H}_{\text{el}}} \cdot$$

$$h_{\text{eff}} f(t) = h_{\text{eff}}^{(2)} f(t) + \kappa^2 \tilde{w}_1(t) f_0 + i\kappa^3 w_2^\kappa [f](t)$$

$$\psi_\circ (f(t) - \tilde{f}(t)) = -i\kappa \int_0^t U_{t-r}^{(2)} \psi_\circ \tilde{w}_1(r) f_0 dr - \kappa^2 \int_0^t U_{t-r}^{(2)} \psi_\circ w_2^\kappa [f](r) dr$$

$$U_{t-r}^{(2)} \psi_\circ \tilde{w}_1(r) f_0 = U_{t-r}^{(2)} X^* \bar{U}_t \bar{R} X \psi_\circ f_0$$

$$F_r = U_{t-r}^{(2)} X^* \text{ and } G_r = 1$$

$$F_r' = \frac{i}{\kappa} U_{t-r}^{(2)} H_\kappa^{(2)} X^*$$

$$Z_t = -\kappa^2 U_{t-r}^{(2)} X^* \bar{R} \bar{U}_r \Big|_{r=0}^{r=t} + i\kappa \int_0^t U_{t-r}^{(2)} X^* S \bar{U}_r dr - i\kappa \int_0^t U_{t-r}^{(2)} \left(H_\kappa^{(2)} X^* - X^* \bar{K} \right) \bar{R}_{\bar{U}} \bar{U}_r dr$$

$$X_{(2)} = -\frac{i}{\kappa} X^* S - \frac{i}{\kappa} \left(H_\kappa^{(2)} X^* - X^* \bar{K} \right) \bar{R}$$

$$g \in L_y^2, H_\kappa^{(2)} \psi_\circ g = K^P \psi_\circ g - \kappa^2 \psi_\circ w_1 g$$

$$Z_t = O_{\mathcal{L}_{s+2,s}}(\kappa^2 e^{Ct})$$

$$\|f\|_{B_\tau^s} \leqslant C \langle \tau \rangle^s \|f_0\|_{H_{\kappa,y}^s}$$

$$\psi_\circ w_1 \langle \psi_\circ, X^*(\cdot)\rangle_{\mathcal{H}_{el}} = O_{\mathcal{L}_{s+2,s}}$$

$$X_{(2)} = O_{\mathcal{L}s+2,s}(1)$$

$$\bar{U}_t = O_{\mathcal{L}_{s,s}}(e^{Ct})$$

$$X = O_{\mathcal{L}_{s+1,s}}(1) \text{ and } \bar{R} = O_{\mathcal{L}_{s,s}}(1)$$

$$\psi_\circ f(t) = P(Q_P f)(t)$$

$$i\kappa \partial_t Q_P f(t) = H_\kappa Q_P f(t)$$

$$(Q_P f)(0) = \psi_\circ f_0$$

$$\psi_\circ f(t) = P(Q_P f)(t) = P U_t \psi_\circ f_0$$

$$P = O_{\mathcal{L}_{s,s}}$$

$$\|f(t)\|_{B_\tau^s} = \sup_{0 \leqslant t \leqslant \tau} \|\psi_\circ f(t)\|_{\mathcal{H}_{el} H_{\kappa,y}^s} \lesssim \sup_{0 \leqslant t \leqslant \tau} \|U_t \psi_\circ f_0\|_{\mathcal{H}_{el} H_{\kappa,y}^s}$$

$$U_t = O_{\mathcal{L}_{s,s}}(\langle t\rangle^s)$$

$$\Psi(t) - (Q_P\tilde{f})(t) = \psi_\circ(f(t) - \tilde{f}(t)) + \int_0^t \bar{U}_{t-s}X^*\psi_\circ(f(s) - \tilde{f}(s))ds$$

$$\psi_\circ(f(t) - \tilde{f}(t)) = U_t^{(2)}Z_t\bar{R}X\psi_\circ f_0 - \kappa^2 \int_0^t U_{t-r}^{(2)}\psi_\circ w_2^\kappa[f](r)dr$$

$$U_t^{(2)} = O_{\mathcal{L}_{s,s}}(\langle t\rangle^s)$$

$$\|w_2^\kappa[f](t)\| \lesssim e^{C\tau}\|f_0\|_{H_{\kappa,y}^{s+6}}, 0 \le t \le \tau$$

$$\left\|\psi_\circ(f(t) - \tilde{f}(t))\right\|_{H_{\kappa,y}^s} \lesssim \kappa^2\langle t\rangle^s\|f_0\|_{H_{\kappa,y}^{s+3}} + \kappa^2 e^{C\tau}\|f_0\|_{H_{\kappa,y}^{s+6}} \lesssim \kappa^2 e^{C\tau}\|f_0\|_{H_{\kappa,y}^{s+6}}, 0 \leqslant t \leqslant \tau$$

$$\text{Ran } P \subset \mathcal{H} = L^2(\mathbb{R}^m, \mathcal{H}_{el})$$

$$\text{Ran}P = \{g(y)\psi_\circ(y): \forall g(y) \in L^2(\mathbb{R}^m)\}$$

$$\psi_\circ = \int_{\mathbb{R}^m}^{\oplus} \psi_\circ(y)dy$$

$$P(y) = \frac{1}{2\pi i}\oint_{\Gamma(\tilde{y})} R(z,y)dz, \forall y \in U(\tilde{y})$$

$$\inf_{y\in U(\tilde{y})} \text{dist}(\Gamma(\tilde{y}), \sigma(H(y))) \geqslant \frac{\delta}{4}$$

$$\sup_y \left\|\partial_y^\alpha \psi_\circ(y)\right\|_{\mathcal{H}_{el}} \leqslant C \text{ for all multi-index } |\alpha| \leqslant k_A$$

$$P(y), y, \tilde{y} \in \mathbb{R}^m$$

$$P(\tilde{y})\psi_\circ(\tilde{y}) = \psi_\circ(\tilde{y})$$

$$P(\cdot) \in C_b^k(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el}))$$

$$\nu(y) = \langle\psi_\circ(\tilde{y}), P(y)\psi_\circ(\tilde{y})\rangle_{\mathcal{H}_{el}}, \mu(y) = \langle H(y)\psi_\circ(\tilde{y}), P(y)\psi_\circ(\tilde{y})\rangle_{\mathcal{H}_{el}}$$

$$\inf_{y\in\mathbb{R}^m} \nu(y) > 0$$

$$E(y) = \nu(y)^{-1}\mu(y), \psi_\circ(y) = \nu(y)^{-\frac{1}{2}}P(y)\psi_\circ(\tilde{y})$$

$$\partial_y^\alpha H_{bo} = \int_{\mathbb{R}^m}^{\oplus} \partial_y^\alpha H(y)dy$$

$$E(y), \bar{H}_{\text{bo}} - \bar{E}$$

$$\bar{H}_{\text{bo}} = \int_{\mathbb{R}^m}^{\oplus} \bar{H}(y)dy \geqslant \int_{\mathbb{R}^m}^{\oplus} E_1(y)\bar{P}(y)dy$$

$$E_1(y) := \inf(\sigma(H(y)) \setminus \{E(y)\})$$

$$\Psi := \int_{\mathbb{R}^m}^{\oplus} \Psi(y)dy$$

$$\langle \Psi, (\bar{H}_{\mathrm{bo}} - \bar{E})\Psi \rangle \geqslant \int_{\mathbb{R}^m}^{\oplus} \langle \Psi(y), (\bar{H}(y) - \bar{E}(y))\Psi(y) \rangle dy \geqslant \int_{\mathbb{R}^m}^{\oplus} \langle \Psi(y), (E_1(y) - E(y))\Psi(y) \rangle dy$$
$$\geqslant \int_{\mathbb{R}^m}^{\oplus} \delta \|\Psi(y)\|_{\mathcal{H}_{el}}^2 dy$$

$$\int_{\mathbb{R}^m}^{\oplus} \|\Psi(y)\|_{\mathcal{H}_{el}}^2 dy = \|\Psi\|^2$$

$$\langle \Psi, (\bar{H}_{\mathrm{bo}} - \bar{E})\Psi \rangle \geqslant \delta \|\Psi\|^2$$

$$\|(\bar{H}_{\mathrm{bo}} - \bar{E})^{-1}\| \leqslant \frac{1}{\mathrm{dist}\big(0, \sigma(\bar{H}_{\mathrm{bo}} - \bar{E})\big)}$$

$$\bar{R}(y) = \bar{P}(y)(\bar{H}(y) - \bar{E}(y))^{-1}\bar{P}(y)$$

$$\bar{R}(\cdot) \in C_b^k\big(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el})\big)$$

$$\bar{P}(y) = \mathbf{1} - P(y)$$

$$\bar{P}(\cdot) \in C_b^k\big(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el})\big)$$

$$\partial_y^\alpha \bar{P}(y) = -\partial_y^\alpha P(y)$$

$$\bar{H}(y) = \bar{P}(y)H(y)\bar{P}(y) = H(y)\bar{P}(y)$$

$$\partial_y^\alpha \bar{H}(y) = \partial_y^\alpha (H(y)\bar{P}(y)) = -\sum_{0 \leqslant \beta \leqslant \alpha} \binom{\alpha}{\beta} \left(\partial_y^\beta H(y)\right) \left(\partial_y^{\alpha-\beta} P(y)\right)$$

$$\beta \leqslant \alpha \text{ if } \beta_j \leqslant \alpha_j \text{ for all } j = 1, \dots, m \text{ and } \binom{\alpha}{\beta} := \binom{\alpha_1}{\beta_1} \dots \binom{\alpha_m}{\beta_m}$$

$$H(y)\partial_y^\alpha P(y)$$

$$\inf_{y \in U(\tilde{y})} \mathrm{dist}(\Gamma(\tilde{y}), \sigma(H(y))) \geqslant \frac{\delta}{4}$$

$$H(y)\partial_y^\alpha P(y) = \frac{1}{2\pi i} \oint_{\Gamma(\tilde{y})} H(y)\partial_y^\alpha R(z, y)dz$$

$$H(y)R(z, y) = 1 + zR(z, y)$$

$$H(\cdot)\partial_y^\alpha P(\cdot) \in C_b^{k-|\alpha|}\big(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el})\big)$$

$$\partial_y^\alpha \bar{H}_{bo}(\cdot) \in C_b^{k-|\alpha|}\big(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el})\big).$$

$$\bar{R}(\cdot) \in C_b^k\big(\mathbb{R}^m, \mathcal{L}(\mathcal{H}_{el})\big)$$

$$D^s\bar{R}(y) = [D^s, \bar{R}(y)] + \bar{R}(y)D^s$$

$$\bar{R}(\cdot) \in C_b^k(\mathbb{R}^m, \mathcal{L}(\mathrm{Ran}\bar{P}))$$

$$D_{y_j} := -i\kappa \partial_{y_j}, D^{\alpha} = \prod_{j=1}^{m} D_{y_j}^{\alpha_j}$$

$$\left\| -\kappa^2 \Delta_y \phi \right\| \leqslant \| H_\kappa \phi \| + C \| \phi \|, \phi \in \mathcal{D}(H_\kappa)$$

$$2\mathrm{Re}\left\langle -\kappa^2 \Delta_y \phi, \tilde{H}_{bo} \phi \right\rangle$$

$$\tilde{H}_{bo} = H_{bo} + \gamma$$

$$-\kappa^2 \Delta_y = \left(i\kappa \nabla_y \right)^2$$

$$\left\langle -\kappa^2 \Delta_y \phi, \tilde{H}_{bo} \phi \right\rangle = \left\langle i\kappa \nabla_y \phi, \tilde{H}_{bo} \left(i\kappa \nabla_y \phi \right) \right\rangle + \left\langle i\kappa \nabla_y \phi, \left(i\kappa \nabla_y H_{bo} \right) \phi \right\rangle \geqslant \left\langle i\kappa \nabla_y \phi, i\kappa \left(\nabla_y H_{bo} \right) \phi \right\rangle$$

$$2\mathrm{Re}\left\langle -\kappa^2 \Delta_y \phi, \tilde{H}_{bo} \phi \right\rangle \geqslant 2\mathrm{Re}\left\langle i\kappa \nabla_y \phi, i\kappa \left(\nabla_y H_{bo} \right) \phi \right\rangle.$$

$$\begin{aligned} \left\langle \phi, i\kappa \left(\nabla_y H_{bo} \right) \psi \right\rangle = \left\langle \phi, i\kappa \nabla_y \left(H_{bo} \psi \right) - H_{bo} \left(i\kappa \nabla_y \psi \right) \right\rangle &= \left\langle H_{bo} \left(i\kappa \nabla_y \phi \right) - i\kappa \nabla_y \left(H_{bo} \phi \right), \psi \right\rangle dy \\ &= \left\langle -i\kappa \left(\nabla_y H_{bo} \right) \phi, \psi \right\rangle \end{aligned}$$

$$\begin{aligned} \overline{\left\langle i\kappa \nabla_y \phi, i\kappa \left(\nabla_y H_{bo} \right) \phi \right\rangle} = \left\langle i\kappa \left(\nabla_y H_{bo} \right) \phi, i\kappa \nabla_y \phi \right\rangle &= \left\langle \left(-\kappa^2 \Delta_y H_{bo} \right) \phi, \phi \right\rangle + \left\langle i\kappa \left(\nabla_y H_{bo} \right) \left(i\kappa \nabla_y \phi \right), \phi \right\rangle \\ &= \left\langle \left(-\kappa^2 \Delta_y H_{bo} \right) \phi, \phi \right\rangle - \left\langle i\kappa \nabla_y \phi, i\kappa \left(\nabla_y H_{bo} \right) \phi \right\rangle \end{aligned}$$

$$2\mathrm{Re}\left\langle i\kappa \nabla_y \phi, i\kappa \left(\nabla_y H_{bo} \right) \phi \right\rangle = 2\mathrm{Re}\left\langle \left(-\kappa^2 \Delta_y H_{bo} \right) \phi, \phi \right\rangle.$$

$$2\mathrm{Re}\left\langle -\kappa^2 \Delta_y \phi, \tilde{H}_{bo} \phi \right\rangle \geqslant -C\kappa^2 \| \phi \|^2$$

$$2\mathrm{Re}\left\langle -\kappa^2 \Delta_y \phi, \tilde{H}_{bo} \phi \right\rangle + C \| \phi \|^2 \geqslant 0.$$

$$\begin{aligned} \left\| -\kappa^2 \Delta_y \phi \right\|^2 &\leqslant \left\| -\kappa^2 \Delta_y \phi \right\|^2 + \left\| \tilde{H}_{bo} \phi \right\|^2 + 2\mathrm{Re}\left\langle -\kappa^2 \Delta_y \phi, \tilde{H}_{bo} \phi \right\rangle + C \| \phi \|^2 \\ &= \left\| \left(-\kappa^2 \Delta_y + \tilde{H}_{bo} \right) \phi \right\|^2 + C \| \phi \|^2 \\ &\leqslant \left(\left\| \left(-\kappa^2 \Delta_y + H_{bo} \right) \phi \right\| + \left(\sqrt{C} + |\gamma| \right) \| \phi \| \right)^2 \end{aligned}$$

$$H^P = P H_\kappa P, \bar{H} = \bar{P} H_\kappa \bar{P}$$

$$\mathcal{D}(H^P) = H_y^{2,\kappa} \otimes \psi_\circ \text{ and } \mathcal{D}(\bar{P}) = \bar{P} \mathcal{D}(H_\kappa)$$

$$H_{\mathrm{diag}} := H^P + \bar{H}$$

$$\mathcal{H} = L^2(\mathbb{R}^m, \mathcal{H}_{el})$$

$$\mathcal{D}\left(H_{\mathrm{diag}} \right) = \mathcal{D}(H_\kappa)$$

$$H_{diag} = H - \Lambda, \text{where } \Lambda = P H_\kappa \bar{P} + \bar{P} H_\kappa P$$

$$H_\kappa = -\kappa^2 \Delta_y + H_{bo} \text{ and } P H_{bo} \bar{P} = H_{bo} P \bar{P} = 0$$

$$P H_\kappa \bar{P} = -\kappa^2 P \Delta_y \bar{P} = \sum_{j=1}^{m} P D_{y_j}^2 \bar{P}$$

$$P D_{y_j}^2 \bar{P} = P \left[D_{y_j}^2, \bar{P} \right]$$

$$P\left[D_{y_j}^2,\bar{P}\right]=P\left(D_{y_j}\left(D_{y_j}\bar{P}\right)+\left(D_{y_j}\bar{P}\right)D_{y_j}\right)=P\left(D_{y_j}^2\bar{P}\right)+2P\left(D_{y_j}\bar{P}\right)D_{y_j}$$

$$\|\bar{P}H_\kappa P\phi\|^2\leqslant C_1\sum_1^m\left\|-i\kappa\partial_{y_j}\phi\right\|^2+C_2\|\phi\|^2$$

$$-\kappa^2\Delta_y PH_\kappa\bar{P}-\kappa^2\Delta_y\bar{P}H_\kappa P=(PH_\kappa\bar{P})^*$$

$$\Lambda=\bar{P}H_\kappa P+PH_\kappa\bar{P}$$

$$\mathcal{D}(H^P)=H_y^{2,\kappa}\otimes\psi_\circ$$

$$u_\pm\in\mathcal{D}(\bar{H})\text{ and }v_\pm\in\mathcal{D}(H^P)$$

$$(\bar{H}\pm i)u_\pm=f,(H^P\pm i)v_\pm=g.$$

$$\left(H_{\text{diag}}+i\right)w=h$$

$$H_{\text{diag}}=\bar{H}+H^P$$

$$H^P u+iu=Ph,\bar{H}v+iv=\bar{P}h$$

$$f\in\operatorname{Ran}\bar{P}\text{ and }g\in\operatorname{Ran}P$$

$$\langle f,[A,T]g\rangle=\langle A^*f,Tg\rangle-\langle T^*f,Ag\rangle,$$

$$A=\int_{\mathbb{R}^m}^{\oplus}A(y)dy$$

$$F=\int_{\mathbb{R}^m}^{\oplus}F(y)dy$$

$$[A,F]=\int_{\mathbb{R}^m}^{\oplus}[A(y),F(y)]dy$$

$$F(y)=f(y)f:\mathbb{R}^m\to\mathbb{C}$$

$$[A,F]=0$$

$$\left[D_{y_j},A\right]=\int_{\mathbb{R}^m}^{\oplus}\left(D_{y_j}A(y)\right)dy\ \forall j$$

$$F(y)\in C_b^k\left(\mathbb{R}^m,\mathcal{L}_{s_1,s_2}\right)$$

$$[D_{y_i}^k,F(y)]=\sum_{j=0}^{k-1}\binom{k}{k-j}(-i\kappa)^{k-j}(\partial_{y_i}^{k-j}F(y))D_{y_i}^j$$

$$\alpha=(\alpha_1,\dots,\alpha_m)\text{ with }|\alpha|\leqslant k$$

$$[D^\alpha,F(y)]=\sum_{\substack{0\leqslant\beta\leqslant\alpha\\ \beta\neq\alpha}}\binom{\alpha}{\alpha-\beta}(-i\kappa)^{|\alpha-\beta|}\left(\partial_y^{\alpha-\beta}F(y)\right)D_y^\beta,$$

$\beta \leqslant \alpha$ if $\beta_j \leqslant \alpha_j$ for all $j = 1, \dots, m$ and $\binom{\alpha}{\beta} := \binom{\alpha_1}{\beta_1} \dots \binom{\alpha_m}{\beta_m}$

$$F = \int_{\mathbb{R}^m}^{\oplus} F(y)dy$$

$$[D^\alpha, F] = \sum_{\substack{0 \leqslant \beta \leqslant \alpha \\ \beta \neq \alpha}} \binom{\alpha}{\alpha - \beta} (-i\kappa)^{|\alpha-\beta|} \left(\partial_y^{\alpha-\beta} F\right) D_y^\beta,$$

$$\partial_y^{\alpha-\beta} F = \int_{\mathbb{R}^m}^{\oplus} \left(\partial_y^{\alpha-\beta} F(y)\right) dy$$

$$\bar{P}(K\bar{P}X^\circ - X^\circ PK)P = \bar{P}[X^\circ, [K, P] - K]P$$

$$\bar{P}(K\bar{P}X^\circ - X^\circ PK)P = \bar{P}(KX^\circ + [K, \bar{P}]X^\circ - X^\circ K - X^\circ[P, K])P.$$

$$KX^\circ - X^\circ K = -[X^\circ, K]$$

$$[K, \bar{P}] = -[K, P] \text{ and } -[P, K] = [K, P]$$

$$[K, \bar{P}]X^\circ - X^\circ[P, K] = [X^\circ, [K, P]]$$

$$1 \leqslant |\alpha| = s \leqslant k$$

$$[iH_\kappa, D^\alpha] = O_{\mathcal{L}_{s-1,0}}(\kappa)$$
$$\left[i\bar{H}, \overline{D^\alpha}\right] = O_{\mathcal{L}_{s,0}}(\kappa)$$

$$[iH_\kappa, D^\alpha] = -[D^\alpha, iH_\kappa]$$

$$\langle f, [iH_\kappa, D^\alpha]g\rangle := \langle D^\alpha f, iH_\kappa g\rangle - \langle iH_\kappa f, D^\alpha g\rangle$$

$$f, g \in \mathcal{D}(H_\kappa) \cap H_{\kappa,y}^s \mathcal{H}_{el}$$

$$\left[i\bar{H}, \overline{D^\alpha}\right] = -\left[\overline{D^\alpha}, i\bar{H}\right]$$

$$\left\langle f, \left[i\bar{H}, \overline{D^\alpha}\right]g\right\rangle := \left\langle \overline{D^\alpha} f, i\bar{H} g\right\rangle - \left\langle i\bar{H} f, \overline{D^\alpha} g\right\rangle$$

$$f, g \in \mathcal{D}(\bar{H}) \cap \bar{P} H_{\kappa,y}^s \mathcal{H}_{el}$$

$$f, g \in H_{\kappa,y}^s \mathcal{H}_{el} \cap \mathcal{D}(H_\kappa) = H_{\kappa,y}^{s+2} \mathcal{H}_{el} \cap L_y^2 \mathcal{D},$$
$$\langle D^\alpha f, iH_\kappa g\rangle - \langle iH_\kappa f, D^\alpha g\rangle = \langle f, [D^\alpha, iH_\kappa]g\rangle.$$

$$H_\kappa = T + H_{bo}$$

$$T = -\kappa^2 \Delta_y$$

$$\alpha, [D^\alpha, T] = \left[D^\alpha, -\kappa^2 \Delta_y\right] = 0$$

$$[D^\alpha, H_\kappa] = [D^\alpha, H_{bo}]$$

$$[D^\alpha, H_{bo}] = \sum_{\substack{0 \leqslant \beta \leqslant \alpha \\ \beta \neq \alpha}} \binom{\alpha}{\alpha - \beta} (-i\kappa)^{|\alpha-\beta|} \left(\partial_y^{\alpha-\beta} H_{bo}\right) D_y^\beta$$

$$\partial_y^{\alpha-\beta} H_{bo} = \int_{\mathbb{R}^m}^{\oplus} \left(\partial_y^{\alpha-\beta} H(y)\right) dy$$

$$\left(\partial_y^{\alpha-\beta} H(y)\right) = O$$

$$[D^\alpha, H_\kappa] = \sum_{j=0}^{|\alpha|-1} O_{\mathcal{L}_{j,0}}\left(\kappa^{|\alpha|-j}\right) = O_{\mathcal{L}_{|\alpha|-1,0}}(\kappa)$$

$$\|\phi\|_{H_y^{j,\kappa}\mathcal{H}_{el}} \lesssim \|\phi\|_{H_y^{n,\kappa}\mathcal{H}_{el}}$$

$$f, g \in \bar{P} H^s_{\kappa,y}\mathcal{H}_{el} \cap \mathcal{D}(\bar{H}) = \bar{P} H_y^{s+2,\kappa}\mathcal{H}_{el} \cap L_y^2 \mathcal{D}_{el}$$

$$\left\langle \overline{D^\alpha} f, i\bar{H} g\right\rangle - \left\langle i\bar{H} f, \overline{D^\alpha} g\right\rangle = \left\langle f, \left[\overline{D^\alpha}, i\bar{H}\right] g\right\rangle.$$

$$\left[\overline{D^\alpha}, i\bar{H}\right] = \left[\overline{D^\alpha}, i\bar{H}_{bo}\right] + \left[\overline{D^\alpha}, i\bar{T}\right]$$

$$\bar{H}_{bo} = \bar{P} H_{bo} \bar{P} = H_{bo}\bar{P} = \bar{P} H_{bo}$$

$$\left[\overline{D^\alpha}, i\bar{H}_{bo}\right] = \bar{P} D^\alpha \bar{P} H_{bo} \bar{P} - \bar{P} H_{bo} \bar{P} D^\alpha \bar{P} = i\bar{P}(D^\alpha H_{bo} - H_{bo} D^\alpha)\bar{P} = i\bar{P}[D^\alpha, H_{bo}]\bar{P}$$

$$\left[\overline{D^\alpha}, i\bar{H}_{bo}\right] = O_{\mathcal{L}_{|\alpha|-1,0}}(\kappa)$$

$$T = \sum_{j=1}^{m} D_{y_j}^2$$

$$\left[\overline{D^\alpha}, i\bar{T}\right] = i\sum_{j=1}^{m} \left[\overline{D^\alpha}, \overline{D_{y_j}^2}\right]$$

$$\left[\overline{D^\alpha}, \overline{D_{y_j}^2}\right]$$

$$\left[\overline{D^\alpha}, i\bar{T}\right] = i\sum_{j=1}^{m} \bar{P}\left[[D^\alpha, P], \left[D_{y_j}^2, P\right]\right]\bar{P}$$

$$[D^\alpha, P] = \sum_{\substack{0 \leqslant \beta \leqslant \alpha \\ \beta \neq \alpha}} \binom{\alpha}{\alpha-\beta} (-i\kappa)^{|\alpha-\beta|} \left(\partial_y^{\alpha-\beta} P\right) D_y^\beta$$

$$\left[D_{y_j}^2, P\right] = -\kappa^2 \left(\partial_{y_j}^2 P\right) - 2i\kappa \left(\partial_{y_j} P\right) D_{y_j}$$

$$\partial_y^\gamma P = O$$

$$|\gamma| \leqslant k\left[\overline{D^\alpha}, i\bar{T}\right]$$

$$\left[\overline{D^\alpha}, i\bar{T}\right] = \sum_{\substack{0 \leqslant \beta \leqslant \alpha, \beta \neq \alpha \\ j=1,\dots,m}} O(\kappa^3)\bar{P}\left[\left(\partial_y^{\alpha-\beta} P\right) D_y^\beta, \left(\partial_{y_j}^2 P\right)\right]\bar{P} + O(\kappa^2)\bar{P}\left[\left(\partial_y^{\alpha-\beta} P\right) D_y^\beta, \left(\partial_{y_j} P\right) D_{y_j}\right]\bar{P}$$

$$\left[\left(\partial_y^{\alpha-\beta} P\right), \left(\partial_{y_j} P\right)\right] \neq |\beta| = |\alpha| - 1$$

$$\left[\overline{D^\alpha}, i\bar{T}\right] = O_{\mathcal{L}_{|\alpha|,0}}(\kappa^2)$$

$$\left[\overline{D^\alpha}, i\bar{H}\right] = O_{\mathcal{L}_{|\alpha|-1,0}}(\kappa) + O_{\mathcal{L}_{|\alpha|,0}}(\kappa^2)$$

$$\left[\overline{D^\alpha}, \overline{D_{y_j}^2}\right] = \bar{P}\left(D^\alpha \bar{P} D_{y_j}^2 - D_{y_j}^2 \bar{P} D^\alpha\right)\bar{P}$$

$$\left[\overline{D^\alpha}, \overline{D_{y_j}^2}\right] = \bar{P}\left(\left[D^\alpha, D_{y_j}^2\right] - D^\alpha P D_{y_j}^2 + D_{y_j}^2 P D^\alpha\right)\bar{P}$$

$$\left[\overline{D^\alpha}, \overline{D_{y_j}^2}\right] = \bar{P}\left(D_{y_j}^2 P D^\alpha - D^\alpha P D_{y_j}^2\right)\bar{P}$$

$$\bar{P} D_{y_j}^2 P = \bar{P}\left[D_{y_j}^2, P\right] \text{ and } P D^\alpha \bar{P} = [P, D^\alpha]\bar{P} = -[D^\alpha, P]\bar{P}$$

$$\bar{P} D_{y_j}^2 P D^\alpha \bar{P} = -\bar{P}\left[D_{y_j}^2, P\right][D^\alpha, P]\bar{P}$$

$$-\bar{P} D^\alpha P D_{y_j}^2 \bar{P} = \bar{P}[D^\alpha, P]\left[D_{y_j}^2, P\right]\bar{P}$$

$$\left[\overline{D^\alpha}, \overline{D_{y_j}^2}\right] = \bar{P}\left(-\left[D_{y_j}^2, P\right][D^\alpha, P] + [D^\alpha, P]\left[D_{y_j}^2, P\right]\right) = \bar{P}\left[[D^\alpha, P], \left[D_{y_j}^2, P\right]\right]\bar{P}$$

$$[D^\alpha, \bar{R}] = O_{\mathcal{L}_{s+|\alpha|-1,s}}(\kappa)$$

$$[H_{bo}, [T, P]] = O_{\mathcal{L}_{s+1,s}}(\kappa)$$

$$[D^\alpha, [T, P]] = O_{\mathcal{L}_{s+|\alpha|,s}}(\kappa^2)$$

$$\|[D^\alpha, H_{bo}]\phi\|_{H_{\kappa,y}^s \mathcal{H}_{el}}^2 = \|[D^\alpha, H_{bo}]\phi\|^2 + \sum_{|\beta|=s} \left\|D^\beta [D^\alpha, H_{bo}]\phi\right\|^2$$

$$[D^\alpha, H_{bo}] = \sum_{\substack{0\leqslant\gamma\leqslant\alpha\\ \gamma\neq\alpha}} \binom{\alpha}{\alpha-\gamma} (-i\kappa)^{|\alpha-\gamma|} \int_{\mathbb{R}^m}^{\oplus} \left(\partial_y^{\alpha-\gamma} H(y)\right) dy D_y^\gamma = O_{\mathcal{L}_{|\alpha|-1,0}}(\kappa)$$

$$D^\beta [D^\alpha, H_{bo}] = \left[D^\beta, [D^\alpha, H_{bo}]\right] + [D^\alpha, H_{bo}] D^\beta$$

$$D^\beta [D^\alpha, H_{bo}] = \left[D^\beta, [D^\alpha, H_{bo}]\right] + O_{\mathcal{L}_{s+|\alpha|-1,0}}(\kappa)$$

$$\left[D^\beta, [D^\alpha, H_{bo}]\right] = \sum_{\substack{0\leqslant\gamma\leqslant\alpha\\ \gamma\neq\alpha}} \binom{\alpha}{\alpha-\gamma} (-i\kappa)^{|\alpha-\gamma|} [D^\beta, (\partial_y^{\alpha-\gamma} H_{bo})] D^\gamma$$

$$[D^\beta, (\partial_y^{\alpha-\gamma} H_{bo})]$$

$$[D^\beta, (\partial_y^{\alpha-\gamma} H_{bo})] = \sum_{\substack{0\leqslant\sigma\leqslant\beta\\ \sigma\neq\beta}} \binom{\beta}{\beta-\sigma} (-i\kappa)^{|\beta-\sigma|} \left(\partial_y^{\alpha+\beta-\gamma-\sigma} H_{bo}\right) D^\sigma$$

$$\left[D^{\beta},[D^{\alpha},H_{bo}]\right]=\sum_{\substack{0\leqslant\gamma\leqslant\alpha\\ \gamma\neq\alpha}}\sum_{\substack{0\leqslant\sigma\leqslant\beta\\ \sigma\neq\beta}}\binom{\alpha}{\alpha-\gamma}\binom{\beta}{\beta-\sigma}(-i\kappa)^{|\alpha-\gamma|+|\beta-\sigma|}\left(\partial_y^{\alpha+\beta-\gamma-\sigma}H_{bo}\right)D^{\gamma+\sigma}$$
$$=O_{\mathcal{L}_{s+|\alpha|-2,0}}(\kappa^2)$$

$$\|f\|_{H_y^{s+|\alpha|-2,\kappa}}\lesssim\|f\|_{H_y^{s+|\alpha|-1,\kappa}}$$

$$D^s[H_{bo},T]=O_{\mathcal{L}_{s+|\alpha|-2,0}}(\kappa^2)+O_{\mathcal{L}_{s+|\alpha|-1,0}}(\kappa)=O_{\mathcal{L}_{s+|\alpha|-1,0}}(\kappa)$$

$$\|[H_{bo},T]\phi\|^2_{H^s_{\kappa,y}}\lesssim\kappa^2\|\phi\|^2_{H_y^{|\alpha|-1,\kappa}}+\kappa^2\|\phi\|^2_{H_y^{s+|\alpha|-1,\kappa}}\lesssim\kappa^2\|\phi\|^2_{H_y^{s+|\alpha|-1,\kappa}}$$

$$[D^{\alpha},\bar{R}]=D^{\alpha}\bar{R}-\bar{R}D^{\alpha}=\left[\overline{D^{\alpha}},\bar{R}\right]+PD^{\alpha}\bar{R}-\bar{R}D^{\alpha}P$$

$$\overline{D^{\alpha}}:=\bar{P}D^{\alpha}\bar{P}$$

$$PD^{\alpha}\bar{P}=[P,D^{\alpha}]\bar{P}=O_{\mathcal{L}_{s+|\alpha|-1,s}}(\kappa)$$

$$\bar{R}=O_{\mathcal{L}_{s,s}}(\kappa)$$

$$PD^{\alpha}\bar{R}=O_{\mathcal{L}_{s+|\alpha|-1,s}}(\kappa)=\bar{R}D^{\alpha}P$$

$$\bar{P}(H_{bo}-E)\bar{R}=\bar{P}=\bar{R}(H_{bo}-E)\bar{P}$$

$$\left[\overline{D^{\alpha}},\bar{R}\right]=\bar{R}\left[\bar{H}_{bo}-\bar{E},\overline{D^{\alpha}}\right]\bar{R}$$

$$\bar{R}\bar{P}=\bar{R}=\bar{P}\bar{R}$$

$$[H_{bo}-E,\bar{P}]=0$$

$$\left[\overline{D^{\alpha}},\bar{R}\right]=\bar{R}\big((H_{bo}-E)\bar{P}D^{\alpha}-D^{\alpha}\bar{P}(H_{bo}-E)\big)\bar{R}=\bar{R}\big((H_{bo}-E)D^{\alpha}-D^{\alpha}(H_{bo}-E)\big)\bar{R}$$
$$=\bar{R}([H_{bo}-E,D^{\alpha}])\bar{R}$$

$$[H_{bo},D^{\alpha}][E,D^{\alpha}]O_{\mathcal{L}_{s+|\alpha|-1,s}}(\kappa)$$

$$\left[\overline{D^{\alpha}},\bar{R}\right]=O_{\mathcal{L}_{s+|\alpha|-1,s}}(\kappa)$$

$$[D^{\alpha},\bar{R}]O_{\mathcal{L}_{s+|\alpha|-1,s}}(\kappa)$$

$$[T,P]=[D^2,P]=-i\kappa D\left(\nabla_yP\right)-i\kappa\left(\nabla_yP\right)D$$

$$[[T,P],H_{bo}]=-i\kappa\left[D\left(\nabla_yP\right),H_{bo}\right]-i\kappa\left[\left(\nabla_yP\right)D,H_{bo}\right]$$

$$\left[D\left(\nabla_yP\right),H_{bo}\right]=[D,H_{bo}]\left(\nabla_yP\right)+D\left[\left(\nabla_yP\right),H_{bo}\right]$$

$$\left[\left(\nabla_yP\right),H_{bo}\right]\neq0$$

$$\left[\left(\nabla_yP\right),H_{bo}\right]=\left(\nabla_yP\right)H_{bo}-H_{bo}\left(\nabla_yP\right)$$
$$=\nabla_y(PH_{bo})-P\left(\nabla_yH_{bo}\right)-\nabla_y(H_{bo}P)+\left(\nabla_yH_{bo}\right)P$$

$$H_{bo}P=PH_{bo},\ \text{then}\ \nabla_y(PH_{bo})-\nabla_y(H_{bo}P)=0$$

$$[(\nabla_y P), H_{bo}] = [(\nabla_y H_{bo}), P]$$

$$[[T, P], H_{bo}]O_{\mathcal{L}_{s+1,s}}(\kappa)$$

$$[D^\alpha, [T, P]] = -i\kappa D[D^\alpha, (\nabla_y P)] - i\kappa[D^\alpha, (\nabla_y P)]D$$

$$[D^\alpha, (\nabla_y P)] = O_{\mathcal{L}_{s+|\alpha|-1,s}}(\kappa)$$

$$[D^\alpha, [T, P]] = O_{\mathcal{L}_{s+|\alpha|,s}}(\kappa^2)$$

$$S\bar{P}[T, P]P + \bar{R}[[T, P], [K, P] - K]P = O_{\mathcal{L}_{s+2,s}}(\kappa^2)$$

$$\bar{P}[T, P]P = O_{\mathcal{L}_{s+1,s}}(\kappa)$$

$$S = O_{\mathcal{L}_{s+1,s}}(\kappa)$$

$$S\bar{P}[T, P]P = O_{\mathcal{L}_{s+2,s}}(\kappa^2)$$

$$\bar{R}[[T, P], [K, P] - K]P$$

$$\bar{R} = O_{\mathcal{L}_{s,s}}$$

$$[[T, P], [K, P] - K] = [[T, P], [T, P] - T - E] = -[[T, P], T] - [[T, P], E]$$

$$[[T, P], T] = O_{\mathcal{L}_{s+2,s}}(\kappa^2)$$

$$[[T, P], E] = O_{\mathcal{L}_{s+2,s}}(\kappa^2)$$

$$[T, P] = [D^2, P] = [D, P]D + D[D, P]$$

$$[D, P] = O(\kappa)$$

$$[E, [D, P]] = -i\kappa[E, (\nabla_y P)] = i\kappa[P, (\nabla_y E)] = \nabla_y E(\nabla_y E)(y)$$

$$\begin{aligned}[E, [T, P]] &= [E, [D, P]]D + [D, P][E, D] + [E, D][D, P] + D[E, [D, P]] \\ &= [D, P][E, D] + [E, D][D, P]\end{aligned}$$

$$[E, D] = i\kappa(\nabla_y E) = O(\kappa)$$

$$[E, [T, P]] = O(\kappa^2)$$

$$\bar{R}[[T, P], [K, P] - K]PO_{\mathcal{L}_{s+2,s}}(\kappa^2)$$

$$U_t = e^{-iHt/\kappa}, \bar{U}_t = e^{-i\bar{H}t/\kappa}, U_t^P = e^{-iPH_\kappa Pt/\kappa}.$$

$$\mathcal{H} = L_y^2 \mathcal{H}_{el} \mathrm{Ran}\bar{P}$$

$$\|U_t \phi\|_{H^s_{\kappa,y}} \mathcal{H}_{el} \leqslant C\langle t\rangle^s \|\phi\|_{H^s_{\kappa,y}} \mathcal{H}_{el}.$$

$$\|\bar{U}_t \phi\|_{H^s_{\kappa,y}} \mathcal{H}_{el} \leqslant C_s e^{C_s|t|} \|\phi\|_{H^s_{\kappa,y}} \mathcal{H}_{el}.$$

$$H_{\kappa,C} = \frac{i}{\kappa} H_\kappa - C, \mathcal{D}(H_{\kappa,C}) = \mathcal{D}(H_\kappa)$$
$$H_{\bar{C}} = \frac{i}{\kappa} \bar{H} - \bar{C}, \mathcal{D}(H_{\bar{C}}) = \mathcal{D}(\bar{H})$$

$$\mathrm{Re}\left\langle \left(\frac{i}{\kappa} H_\kappa - C\right)\phi, \phi \right\rangle_{H^s_{\kappa,}\mathcal{H}_{el}} \leqslant 0 \text{ and } \mathrm{Re}\left\langle \left(\frac{i}{\kappa} \bar{H} - \bar{C}\right)\phi, \phi \right\rangle_{H^s_{\kappa,y}} \mathcal{H}_{el} \leqslant 0, \forall \phi \in H^s_{\kappa,y}\mathcal{H}_{el}.$$

$$D^\alpha_y\left(\frac{i}{\kappa} H_\kappa\right) = \left[D^\alpha_y, \frac{i}{\kappa} H_\kappa\right] + \frac{i}{\kappa} H_\kappa D^\alpha_y$$

$$\left\langle \frac{i}{\kappa} H_\kappa \phi, \phi \right\rangle_{H^s_{\kappa,y}} \mathcal{H}_{el} = \sum_{|\alpha|=s} \left\langle D^\alpha_y\left(\frac{i}{\kappa} H_\kappa\right)\phi, D^\alpha_y \phi \right\rangle + \left\langle \frac{i}{\kappa} H_\kappa \phi, \phi \right\rangle$$
$$= \sum_{|\alpha|=s} \left\langle \left[D^\alpha_y, \frac{i}{\kappa} H_\kappa\right]\phi, D^\alpha_y \phi \right\rangle + \left\langle \left(\frac{i}{\kappa} H_\kappa\right) D^\alpha_y \phi, D^\alpha_y \phi \right\rangle + \left\langle \frac{i}{\kappa} H_\kappa \phi, \phi \right\rangle$$

$$\mathrm{Re}\left\langle \frac{i}{\kappa} H_\kappa \phi, \phi \right\rangle_{H^s_{\kappa,y}} \mathcal{H}_{el} = \sum_{|\alpha|=s} \mathrm{Re}\left\langle \left[D^\alpha_y, \frac{i}{\kappa} H_\kappa\right]\phi, D^\alpha_y \phi \right\rangle.$$

$$\left[D^\alpha_y, \frac{i}{\kappa} H_\kappa\right] = O_{\mathcal{L}_{s-1,0}}$$

$$\mathrm{Re}\left\langle \frac{i}{\kappa} H_\kappa \phi, \phi \right\rangle_{H^s_{\kappa,y}} \mathcal{H}_{el} \leqslant C\|\phi\|^2_{H^s_{\kappa,y}} \mathcal{H}_{el},$$

$$H_{\kappa,C} = \frac{i}{\kappa} H_\kappa - C_0\text{-}\ H^s_{\kappa,y}\mathcal{H}_{el} U_t|_{H^s_{\kappa,y}} \mathcal{H}_{el}$$
$$\|U_t\phi\|_{H^s_{\kappa,y}} \mathcal{H}_{el} \lesssim e^{Ct}\|\phi\|_{H^s_{\kappa,y}} \mathcal{H}_{el}.$$

$$t \mapsto D(t) := U_{-t} D^\alpha U_t$$

$$U_{-t} D^\alpha U_t \phi = D^\alpha \phi + U_{-t}[D^\alpha, U_t]\phi = D^\alpha \phi + \int_0^t U_{-s}\left[\frac{i}{\kappa} H_\kappa, D^\alpha\right] U_s \phi ds.$$

$$D_{y_j} U_t = U_t D_{y_j} + \left[D_{y_j}, U_t\right]$$

$$\|U_t\phi\|_{H^{1,\kappa}_y \mathcal{H}_{el}} \leqslant \sum_{j=1}^m \left\|D_{y_j} U_t \phi\right\| + \|U_t \phi\|$$
$$\leqslant \sum_{j=1}^m \left\|D_{y_j}\phi\right\| + \left\|\left[D_{y_j}, U_t\right]\phi\right\| + \|\phi\| \lesssim \|\phi\|_{H^{1,\kappa}_y \mathcal{H}_{el}} + \sum_{j=1}^m \left\|\left[D_{y_j}, U_t\right]\phi\right\|^2$$

$$\left[D_{y_j}, U_t\right] = \int_0^t U_{t-r}\left[D_{y_j}, \frac{-i}{\kappa} H\right] U_r dr = O(|t|)$$

$$\|U_t\phi\|_{H^{n+1,\kappa}_y \mathcal{H}_{el}} \leqslant \sum_{|\alpha|=n+1} \|D^\alpha_y U_t \phi\| + \|U_t \phi\|$$
$$\leqslant \sum_{|\alpha|=n+1} \|D^\alpha_y \phi\| + \|[D^\alpha_y, U_t]\phi\| + \|\phi\| \lesssim \|\phi\|_{H^{n+1,\kappa}_y \mathcal{H}_{el}} + \sum_{|\alpha|=n+1} \|[D^\alpha_y, U_t]\phi\|.$$

$$[D^\alpha, U_t] = \int_0^t U_{t-r}\left[D^\alpha, \frac{-i}{\kappa}H\right]U_r dr = \int_0^t U_{t-r}O_{\mathcal{L}_{n,0}}(1)U_r dr$$

$$O_{\mathcal{L}_{n},0}(1)U_r = O_{\mathcal{L}_{n},0}((1+|r|)^n)$$

$$[D^\alpha, U_t] = O_{\mathcal{L}_{n,0}}((1+|t|)^{n+1})$$

$$\|\phi\|_{H_y^{n,\kappa}\mathcal{H}_{el}} \lesssim \|\phi\|_{H_y^{n+1,\kappa}\mathcal{H}_{el}}$$

$$\operatorname{Re}\left\langle\frac{i}{\kappa}\bar{H}\phi, \phi\right\rangle_{H^s_{\kappa,y}}\mathcal{H}_{el} = \sum_{|\alpha|=s}\operatorname{Re}\left\langle D_y^\alpha\left(\frac{i}{\kappa}\bar{H}\right)\phi, D_y^\alpha\phi\right\rangle,$$

$$\operatorname{Re}\left\langle\frac{i}{\kappa}\bar{H}\phi, \phi\right\rangle = 0$$

$$\left\langle D_y^\alpha\left(\frac{i}{\kappa}\bar{H}\right)\phi, D_y^\alpha\phi\right\rangle = \left\langle D_y^\alpha(P+\bar{P})\left(\frac{i}{\kappa}\bar{H}\right)\phi, D_y^\alpha(P+\bar{P})\phi\right\rangle = \left\langle D_y^\alpha\bar{P}\left(\frac{i}{\kappa}\bar{H}\right)\phi, D_y^\alpha\bar{P}\phi\right\rangle$$

$$\overline{D_y^\alpha}\left(\frac{i}{\kappa}\bar{H}\right) = \left[\overline{D_y^\alpha}, \left(\frac{i}{\kappa}\bar{H}\right)\right] + \left(\frac{i}{\kappa}\bar{H}\right)\overline{D_y^\alpha}$$

$$\operatorname{Re}\left\langle\left(\frac{i}{\kappa}\bar{H}\right)\overline{D_y^\alpha}\phi, \overline{D_y^\alpha}\phi\right\rangle = 0$$

$$\operatorname{Re}\left\langle D_y^\alpha\left(\frac{i}{\kappa}\bar{H}\right)\phi, D_y^\alpha\phi\right\rangle = \operatorname{Re}\left\langle\overline{D_y^\alpha}\left(\frac{i}{\kappa}\bar{H}\right)\phi, \overline{D_y^\alpha}\phi\right\rangle + \operatorname{Re}\left\langle PD_y^\alpha\bar{P}\left(\frac{i}{\kappa}\bar{H}\right)\phi, PD_y^\alpha\bar{P}\phi\right\rangle$$

$$\operatorname{Re}\left\langle\frac{i}{\kappa}\bar{H}\phi, \phi\right\rangle_{H^s_{\kappa,y}}\mathcal{H}_{el} = \sum_{|\alpha|=s}\operatorname{Re}(I_1^\alpha + I_2^\alpha),$$

$$I_1^\alpha := \left\langle\overline{D_y^\alpha}\left(\frac{i}{\kappa}\bar{H}\right)\phi, \overline{D_y^\alpha}\phi\right\rangle, I_2^\alpha := \left\langle PD_y^\alpha\bar{P}\left(\frac{i}{\kappa}\bar{H}\right)\phi, PD_y^\alpha\bar{P}\phi\right\rangle.$$

$$\left[\overline{D_y^\alpha}, \frac{i}{\kappa}\bar{H}\right]O_{\mathcal{L}_{s,0}}$$

$$\|\phi\|_{H_y^{s-1,\kappa}\mathcal{H}_{el}} \lesssim \|\phi\|_{H^s_{\kappa,y}}\mathcal{H}_{el}$$

$$\operatorname{Re}I_1^\alpha = \operatorname{Re}\left\langle\left[\overline{D_y^\alpha}, \left(\frac{i}{\kappa}\bar{H}\right)\right]\phi, \overline{D_y^\alpha}\phi\right\rangle \leqslant C\|\phi\|_{H_y^{s-1,\kappa}\mathcal{H}_{el}}\|\phi\|_{H^s_{\kappa,y}\mathcal{H}_{el}} \leqslant C\|\phi\|^2_{H^s_{\kappa,y}\mathcal{H}_{el}}.$$

$$\bar{H} = \bar{H}_{bo} + \bar{T}$$

$$T = -\kappa^2\Delta_y$$

$$D_y^\alpha H_{bo} = [D_y^\alpha, H_{bo}] + H_{bo}D_y^\alpha$$

$$PD_y^\alpha\bar{P}\left(\frac{i}{\kappa}\bar{H}\right) = \frac{i}{\kappa}PD_y^\alpha\bar{P}H_{bo}\bar{P} + \frac{i}{\kappa}PD_y^\alpha\bar{P}T\bar{P} = \frac{i}{\kappa}P[D_y^\alpha, H_{bo}]\bar{P} + \frac{i}{\kappa}PH_{bo}D_y^\alpha\bar{P} + PD_y^\alpha\bar{P}T\bar{P},$$

$$PD_y^\alpha\bar{P}H_{bo}\bar{P} = PD_y^\alpha H_{bo}\bar{P} = P[D_y^\alpha, H_{bo}]\bar{P} + H_{bo}PD_y^\alpha\bar{P}$$

$$PD_y^\alpha\bar{P}\left(\frac{i}{\kappa}\bar{H}\right) = \frac{i}{\kappa}H_{bo}PD_y^\alpha\bar{P} + \frac{i}{\kappa}P[D_y^\alpha, H_{bo}]\bar{P} + \frac{i}{\kappa}PD_y^\alpha\bar{P}T\bar{P}.$$

$$\mathrm{Re} I_2^\alpha = \mathrm{Re}\left\langle \frac{i}{\kappa} P\left[D_y^\alpha, H_{bo}\right]\bar{P}\phi, PD_y^\alpha \bar{P}\phi \right\rangle + \mathrm{Re}\left\langle \frac{i}{\kappa} PD_y^\alpha \bar{P} T \bar{P}\phi, PD_y^\alpha \bar{P}\phi \right\rangle,$$

$$\mathrm{Re}\left\langle \frac{i}{\kappa} H_{bo} PD_y^\alpha \bar{P}\phi, PD_y^\alpha \bar{P}\phi \right\rangle = 0$$

$$P\left[D_y^\alpha, H_{bo}\right]\bar{P} = \sum_{\substack{0 \leqslant \beta \leqslant \alpha \\ \beta \neq \alpha}} \binom{\alpha}{\alpha - \beta} (-i\kappa)^{|\alpha-\beta|} P\left(\partial_y^{\alpha-\beta} H_{bo}\right) D_y^\beta \bar{P} = O_{\mathcal{L}_{s-1,0}}(\kappa)$$

$$PD_y^\alpha \bar{P} = \left[P, D_y^\alpha\right]\bar{P} = -\sum_{\substack{0 \leqslant \beta \leqslant \alpha \\ \beta \neq \alpha}} \binom{\alpha}{\alpha - \beta} (-i\kappa)^{|\alpha-\beta|} \left(\partial_y^{\alpha-\beta} P\right) D_y^\beta \bar{P} = O_{\mathcal{L}_{s-1,0}}(\kappa)$$

$$\mathrm{Re}\left\langle \frac{i}{\kappa} P\left[D_y^\alpha, H_{bo}\right]\bar{P}\phi, PD_y^\alpha \bar{P}\phi \right\rangle \leqslant C\kappa \|\phi\|^2_{H_y^{s-1,\kappa}\mathcal{H}_{el}} \leqslant C\kappa \|\phi\|^2_{H^s_{\kappa,y}\mathcal{H}_{el}},$$

$$\mathrm{Re}\left\langle \frac{i}{\kappa} PD_y^\alpha \bar{P} T \bar{P}\phi, PD_y^\alpha \bar{P}\phi \right\rangle \leqslant C\kappa \|\phi\|^2_{H^s_{\kappa}\mathcal{H}_{el}},$$

$$\mathrm{Re} I_2^\alpha = \mathrm{Re}\left\langle PD_y^\alpha \bar{P}\left(\frac{i}{\kappa}\bar{H}\right)\phi, PD_y^\alpha \bar{P}\phi \right\rangle \leqslant C\kappa \|\phi\|^2_{H^s_{\kappa,y}}\mathcal{H}_{el},$$

$$\mathrm{Re}\left\langle \frac{i}{\kappa}\bar{H}\phi, \phi \right\rangle_{H^s_{\kappa,y}} \mathcal{H}_{el} \leqslant \bar{C} \|\phi\|^2_{H^s_{\kappa,y}}\mathcal{H}_{el},$$

$$\frac{i}{\kappa}\bar{H} - \bar{C}\bar{U}_t|_{\bar{P}H^s_{\kappa,y}\mathcal{H}_{el}}$$

$$h_{\text{eff}} = T + E + \kappa^2 v$$

$$U_t^P \Psi(x, y) = \psi_\circ(x, y) e^{-ih_{\text{eff}} t/\kappa} f(y),$$

$$f(y) = \langle \psi_\circ(x, y), \Psi(x, y) \rangle_{\mathcal{H}_{el}}$$

$$h_{\text{eff}} = T + E + \kappa^2 v$$

$$\Psi \in H^s_{\kappa,y}\mathcal{H}_{el} f \in H^s_{\kappa,y}$$

$$\|U_t^P \phi\|_{H^s_{\kappa,y}\mathcal{H}_{el}} \leqslant C\langle t\rangle^s \|\phi\|_{H^s_{\kappa,y}\mathcal{H}_{el}}$$

$$\left\|e^{-ih_{\text{eff}} t/\kappa}\phi\right\|_{H^s_{\kappa,y}} \lesssim \langle t\rangle^s \|\phi\|_{H^s_{\kappa,y}}$$

$$\tilde{\phi}_A = M_A{}^B \xi_B, \qquad \tilde{\phi}^A = (M^{-1})^A{}_B \phi^B$$
$$\tilde{\bar{\chi}}_{A'} = M^*{}_{A'}{}^{B'} \bar{\chi}_{B'}, \quad \tilde{\bar{\chi}}^{A'} = (M^{-1})^*{}_{B'} \bar{\chi}^{B'}$$

$$\sigma^0 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$\bar{\sigma}^{aA'A} = \epsilon^{A'B'} \epsilon^{AB} \sigma^a_{BB'}$$

$$\left(\sigma^a\bar{\sigma}^b+\sigma^b\bar{\sigma}^a\right)_A^{\ B}=-2\eta^{ab}\delta_A^B$$
$$\left(\bar{\sigma}^a\sigma^b+\bar{\sigma}^b\sigma^a\right)_{B'}^{\ A'}=-2\eta^{ab}\delta_{B'}^{A'}$$

$$\gamma^a=\begin{pmatrix}0 & \sigma^a\\ \bar{\sigma}^a & 0\end{pmatrix}$$

$$\Phi=\begin{pmatrix}\phi_A\\ \bar{\chi}^{A'}\end{pmatrix}$$

$$\gamma_c^0=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix},\gamma_c^j=\begin{pmatrix}0 & \sigma^j\\ -\sigma^j & 0\end{pmatrix}$$

$$\Gamma_W=X\Gamma_c X^{-1},X=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}$$

$$I_{\text{ferm}}=-\frac{i}{2}\int d^4xe\left(\bar{\phi}^{A'}e_{AA'}^{\mu}D_\mu\phi^A+\bar{\chi}^{A'}e_{AA'}^{\mu}D_\mu\chi^A\right)+\text{ H.c.}$$
$$-\frac{m}{\sqrt{2}}\int d^4xe\left(\chi_A\phi^A+\bar{\phi}^{A'}\bar{\chi}_{A'}\right)$$

$$e_{AA'}^{\mu}D_\mu\phi^A=i\frac{m}{\sqrt{2}}\bar{\chi}_{A'}$$
$$e_{AA'}^{\mu}D_\mu\chi^A=i\frac{m}{\sqrt{2}}\bar{\phi}_{A'}$$
$$e_{AA'}^{\mu}D_\mu\bar{\phi}^{A'}=-i\frac{m}{\sqrt{2}}\chi_A$$
$$e_{AA'}^{\mu}D_\mu\bar{\chi}^{A'}=-i\frac{m}{\sqrt{2}}\phi_A$$

$$ds^2=-N_0(x^0)(dx^0)^2+a^2(x^0)d\Omega_3^2$$

$$d\Omega_3^2=d\chi^2+\sin^2\chi(d\theta^2+\sin^2\theta d\phi^2)$$

$$V=\left(\frac{\ell_o}{2}\right)^3a^3\equiv\ell^3a^3$$

$$n_{AA'}e^{BA'j(3)}D_j\text{ and }n_{AA'}e^{AB'j(3)}D_j,$$

$$-in_{AA'}e^{BA'j(3)}D_j\rho_B^{nq}(\mathbf{x})=+\lambda_n\rho_A^{nq}(\mathbf{x})$$
$$-in_{AA'}e^{BA'j(3)}D_j\bar{\sigma}_B^{nq}(\mathbf{x})=-\lambda_n\bar{\sigma}_A^{nq}(\mathbf{x})$$

$$-in_{AA'}e^{AB'j(3)}D_j\bar{\rho}_{B'}^{nq}(\mathbf{x})=-\lambda_n\bar{\rho}_{A'}^{nq}(\mathbf{x})$$
$$-in_{AA'}e^{AB'j(3)}D_j\sigma_{B'}^{qq}(\mathbf{x})=+\lambda_n\sigma_{A'}^{nq}(\mathbf{x})$$

$$\int d\mu\rho_A^{np}n^{AA'}\sigma_{A'}^{mq}=0$$
$$\int d\mu\bar{\rho}_{A'}^{np}n^{AA'}\bar{\sigma}_A^{mq}=0$$
$$\int d\mu\rho_A^{np}n^{AA'}\bar{\rho}_{A'}^{mq}=\delta^{nm}\delta^{pq}$$
$$\int d\mu\bar{\sigma}_A^{np}n^{AA'}\sigma_{A'}^{mq}=\delta^{nm}\delta^{pq}$$

$$d\mu = \sin^2 \chi \sin \theta d\chi d\theta d\phi$$

$$\begin{aligned}
\phi_A(x) &= \frac{a^{-\frac{3}{2}}}{2\pi} \sum_{npq} \alpha_n^{pq} \left(m_{np}(x^0) \rho_A^{nq}(\mathbf{x}) + \bar{r}_{np}(x^0) \bar{\sigma}_A^{nq}(\mathbf{x}) \right), \\
\bar{\phi}_{A'}(x) &= \frac{a^{-\frac{3}{2}}}{2\pi} \sum_{npq} \alpha_n^{pq} \left(\bar{m}_{np}(x^0) \bar{\rho}_{A'}^{nq}(\mathbf{x}) + r_{np}(x^0) \sigma_{A'}^{nq}(\mathbf{x}) \right), \\
\chi_A(x) &= \frac{a^{-\frac{3}{2}}}{2\pi} \sum_{npq} \beta_n^{pq} \left(s_{np}(x^0) \rho_A^{nq}(\mathbf{x}) + \bar{t}_{np}(x^0) \bar{\sigma}_A^{nq}(\mathbf{x}) \right), \\
\bar{\chi}_{A'}(x) &= \frac{a^{-\frac{3}{2}}}{2\pi} \sum_{npq} \beta_n^{pq} \left(\bar{s}_{np}(x^0) \bar{\rho}_{A'}^{nq}(\mathbf{x}) + t_{np}(x^0) \sigma_{A'}^{nq}(\mathbf{x}) \right).
\end{aligned}$$

$$\alpha_n^{pq} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \text{ and } \beta_n^{pq} = \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}$$

$$\begin{aligned}
I_{\text{ferm}} = \sum_{np} \int dt N_0 \Big[\frac{i}{2N_0} & (\bar{m}_{np}\dot{m}_{np} + m_{np}\dot{\bar{m}}_{np} + \bar{s}_{np}\dot{s}_{np} + s_{np}\dot{\bar{s}}_{np} \\
& + \bar{t}_{np}\dot{t}_{np} + t_{np}\dot{\bar{t}}_{np} + \bar{r}_{np}\dot{r}_{np} + r_{np}\dot{\bar{r}}_{np}) \\
& + \lambda_n a^{-1} (\bar{m}_{np} m_{np} + \bar{s}_{np} s_{np} + \bar{t}_{np} t_{np} + \bar{r}_{np} r_{np}) \\
& - m (r_{np} t_{np} + \bar{t}_{np} \bar{r}_{np} + s_{np} m_{np} + \bar{m}_{np} \bar{s}_{np}) \Big]
\end{aligned}$$

$$I_{np} = \int dt N_0 \left(\frac{i}{2N_0} (\bar{x}\dot{x} + x\dot{\bar{x}} + \bar{y}\dot{y} + y\dot{\bar{y}}) + \frac{\lambda_n}{a} (\bar{x}x + \bar{y}y) - m(yx + \bar{x}\bar{y}) \right)$$

$$\begin{aligned}
I_{\text{ferm}} &= \sum_{np} \left[I_{np}(m_{np}, \bar{m}_{np}, s_{np}, \bar{s}_{np}) + I_{np}(r_{np}, \bar{r}_{np}, t_{np}, \bar{t}_{np}) \right] \\
&=: \sum_{np} I_{np}(x, y, \bar{x}, \bar{y})
\end{aligned}$$

$$\begin{aligned}
i\frac{\dot{x}}{N_0} + \nu x - m\bar{y} &= 0 \\
i\frac{\dot{\bar{x}}}{N_0} - \nu\bar{x} + my &= 0 \\
i\frac{\dot{y}}{N_0} + \nu y + m\bar{x} &= 0 \\
i\frac{\dot{\bar{y}}}{N_0} - \nu\bar{y} - mx &= 0
\end{aligned}$$

$$\nu(x^0) = a^{-1}(x^0)\left(n + \frac{3}{2}\right) \equiv \lambda_n a^{-1}(x^0)$$

$$\frac{1}{N_0}\frac{d}{dt}\left(\frac{\dot{x}}{N_0}\right) + \left(\frac{\dot{\nu}}{iN_0} + \nu^2 + m^2\right)x = 0$$

$$\frac{1}{N_0}\frac{d}{dt}\left(\frac{\dot{\bar{x}}}{N_0}\right) + \left(-\frac{\dot{\nu}}{iN_0} + \nu^2 + m^2\right)\bar{x} = 0$$

$$H_{np}(x, \bar{x}, y, \bar{y}) = N_0[\nu(x\bar{x} + y\bar{y}) + m(yx + \bar{x}\bar{y})]$$

$$[x,\bar{x}]^* = -i \text{ and } [y,\bar{y}]^* = -i$$

$$H_{\text{ferm}} = \sum_{np} \left[H_{np}\left(m_{np},\bar{m}_{np},s_{np},\bar{s}_{np}\right) + H_{np}\left(r_{np},\bar{r}_{np},t_{np},\bar{t}_{np}\right)\right]$$
$$=: \sum_{np} H_{np}(x,\bar{x},y,\bar{y})$$

$$H_{\text{geo}} + H_{\text{ferm}} \approx 0$$

$$H_{\text{geo}} = H_{\text{grav}} + H_T$$

$$\{\hat{x},\hat{\bar{x}}\} = 1 \text{ and } \{\hat{y},\hat{\bar{y}}\} = 1$$

$$\bar{x} \to \hat{\bar{x}} = \partial/\partial x \text{ and } \bar{y} \to \hat{\bar{y}} = \partial/\partial y$$

$$\psi(x,y) \equiv \psi(m,s,r,t)$$

$$i\hbar\partial_{x^0}\psi(x^0;x,y) = \sum_{np} \hat{H}_{np}(x,y)\psi(x^0;x,y)$$

$$\hat{H}_{np} = N_0[\nu(\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m(\widehat{\bar{y}x} + \widehat{\bar{x}\bar{y}})]$$

$$N_\tau = N(\tau) = a^3$$

$$\hat{H}_{np}^{(\tau)} = \lambda_n a^2(\widehat{x\bar{x}} + \widehat{y\bar{y}}) + ma^3(\widehat{\bar{y}x} + \widehat{\bar{x}\bar{y}})$$
$$= \lambda_n \ell^{-2} V^{2/3}(\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m\ell^{-3}V(\widehat{\bar{y}x} + \widehat{\bar{x}\bar{y}})$$

$$\psi(x,p) = \prod_{np} \psi_{np}\left(m_{np},s_{np},r_{np},t_{np}\right)$$

$$\langle\psi_1,\psi_2\rangle = \int \overline{\psi_1(x,y)}\psi_2(x,y)e^{-x\bar{x}-y\bar{y}}dxd\bar{x}dyd\bar{y}$$

$$\int dx = 0, \int xdx = 1, \int d\bar{x} = 0, \int \bar{x}d\bar{x} = 1$$

$$\hat{H}_{np}^{(\tau)}\psi_{np} = E_{np}\psi_{np}$$

$$\mathcal{H}_{\text{ferm}} = \bigotimes_{np} \mathcal{H}_{np}$$

$$x\bar{x} \to \frac{1}{2}\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)$$

$$\hat{H}_{np}^{(\tau)} = \lambda_n \ell^{-2} V^{\frac{2}{3}}(\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m\ell^{-3}V(\widehat{\bar{y}x} + \widehat{\bar{x}\bar{y}})$$
$$= \lambda_n \ell^{-2} V^{\frac{2}{3}}\left(-1 + x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}\right) + m\ell^{-3}V\left(yx + \frac{\partial^2}{\partial x\partial y}\right)$$

$$\left[\frac{\lambda_n}{\ell^2}V^{2/3}\left(-1 + x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}\right) + \frac{m}{\ell^3}V\left(yx + \frac{\partial^2}{\partial x\partial y}\right)\right]\psi_{np}(x,y) = E_{np}\psi_{np}(x,y)$$

$$E_{np}^{(0)} = -w_n: \quad \psi_{np}^{(0)} = \mathrm{N}_n^{(0)}\left(1 + \frac{m\ell^{-3}V}{\lambda_n \ell^{-2}V^{2/3} + w_n}xy\right)$$
$$E_{np}^{(1)} = 0: \quad \psi_{np}^{(1)} = \mathrm{N}_n^{(1)}x$$
$$E_{np}^{(2)} = 0: \quad \psi_{np}^{(2)} = \mathrm{N}_n^{(2)}y$$
$$E_{np}^{(3)} = +w_n: \quad \psi_{np}^{(3)} = \mathrm{N}_n^{(3)}\left(1 + \frac{m\ell^{-3}V}{\lambda_n \ell^{-2}V^{2/3} - w_n}xy\right)$$

$$w_n = \sqrt{\frac{\lambda_n^2}{\ell^4}V^{\frac{4}{3}} + \frac{m^2}{\ell^6}V^2}$$

$$\mathrm{N}_n^{(0)} = \left(\frac{\lambda_n \ell^{-2}V^{2/3} + w_n}{2w_n}\right)^{\frac{1}{2}}, \ \mathrm{N}_n^{(1)} = \mathrm{N}_n^{(2)} = 1, \ \mathrm{N}_n^{(3)} = \left(\frac{\lambda_n \ell^{-2}V^{2/3} - w_n}{2w_n}\right)^{\frac{1}{2}}$$

$$\psi_{np}(x,y) = \sum_{I=0}^{3} a_I \psi_{np}^{(I)}(x,y)$$

$$\hat{H}_{np}^{(\tau)} = \lambda_n \ell^{-2}V^{\frac{2}{3}}(\widehat{x\bar{x}} + \widehat{y\bar{y}})$$

$$N_0 H_{\mathrm{geo}} = N_0\left(H_T + H_{\mathrm{grav}}\right) \approx 0$$

$$H_{\mathrm{grav}} = -\frac{3}{8\pi G}\frac{\sqrt{p}}{\gamma^2}\left[\left(c - \frac{\ell_o}{a_o}\right)^2 - \frac{\gamma^2 \ell_o^2}{a_o^2}\right]$$

$$|p| = a^2\ell_o^2/4 = a^2\ell^2$$

$$q_{ij} = {}^{o}q_{ij}|p|\ell_o^{-2}$$

$$\{c,p\} = \frac{8\pi G\gamma}{3}$$

$$V = \ell^3 a^3 = |p|^{3/2}$$

$$H_T = \frac{P_T^2}{2V}$$

$$\square\, T = (P_T/\ell^3)\tau$$

$$H_{\mathrm{geo}}^{(\tau)} := N_\tau H_{\mathrm{geo}} = \frac{P_T^2}{2\ell^3} - \frac{3}{8\pi G}\frac{1}{\gamma^2\ell^3}V^{2/3}\left[\left(c - \frac{\ell_o}{2}\frac{2}{a_o}\right)^2 - \frac{\gamma^2\ell_o^2}{4}\frac{4}{a_o^2}\right]V^{2/3}$$
$$=: \frac{P_T^2}{2\ell^3} + H_{\mathrm{grav}}^{(\tau)} \approx 0$$

$$\hat{H}_{\mathrm{geo}}^{(\tau)}\Psi_o(v,T) = \left(\frac{\hat{P}_T^2}{2\ell^3} + \hat{H}_{\mathrm{grav}}^{(\tau)}\right)\Psi_o(v,T) \approx 0$$

$$\hat{H}_{\mathrm{grav}}^{(\tau)} = \frac{1}{16\pi G\ell^3}\hat{V}^{\frac{1}{2}}e^{if\ell_o}\sin(\bar{\mu}c)\hat{A}\sin(\bar{\mu}c)e^{-if\ell_o}\hat{V}^{\frac{1}{2}}$$
$$-\frac{1}{16\pi G\ell^3}\hat{V}^{\frac{1}{2}}\left(\sin^2\left(\frac{\bar{\mu}\ell_o}{2}\right) - \frac{\bar{\mu}^2\ell_o^2}{4} - \frac{\ell_o^2}{9|K^2 v|^{2/3}}\right)\hat{A}\hat{V}^{\frac{1}{2}}$$

$$\bar{\mu} = \sqrt{\Delta}|p|^{-1/2}$$

$$\Delta \equiv (2\sqrt{3}\pi\gamma)\ell_{\mathrm{Pl}}^2$$

$$\hat{V} = |\hat{p}|^{3/2}$$

$$\hat{V}|v\rangle = \left(\frac{8\pi\gamma}{6}\right)^{3/2}\frac{|v|}{K}\ell_{\mathrm{Pl}}^3|v\rangle$$

$$K = 2\sqrt{2}/(3\sqrt{3\sqrt{3}})$$

$$\begin{aligned}\hat{A}\Psi_o(v) &= \frac{24i\,\mathrm{sgn}(\mu)}{8\pi\gamma^3\bar{\mu}^3\ell_{\mathrm{Pl}}^2}\left[\sin\left(\frac{\bar{\mu}c}{2}\right)\hat{V}\cos\left(\frac{\bar{\mu}c}{2}\right) - \cos\left(\frac{\bar{\mu}c}{2}\right)\hat{V}\sin\left(\frac{\bar{\mu}c}{2}\right)\right]\Psi_o(v)\\ &= -\frac{27K}{4}\sqrt{\frac{8\pi}{6}\frac{\ell_{\mathrm{Pl}}}{\gamma^{3/2}}}|v|\big||v-1|-|v+1|\big|\Psi_o(v)\end{aligned}$$

$$\hat{P}_T = -i\hbar(\partial/\partial T)$$

$$\hat{H}_{\mathrm{geo}}^{(\tau)}\Psi_o(v,T) = -\frac{\hbar^2}{2\ell^3}\left(\partial_T^2 - \frac{2\ell^3}{\hbar^2}\hat{H}_{\mathrm{grav}}^{(\tau)}\right)\Psi_o(v,T) = 0$$

$$\partial_T^2\Psi_o(v,T) = -\Theta\Psi_o(v,T)$$

$$\Psi_o(v) \in \mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$$

$$\begin{aligned}\Theta\Psi_o(v) &= -\frac{2\ell^3}{\hbar^2}\hat{H}_{\mathrm{grav}}^{(\tau)}\Psi_o(v)\\ &=: (\Theta_0 + \Theta_1)\Psi_o(v)\end{aligned}$$

$$\begin{aligned}\Theta_0\Psi_o(v) &= \frac{3\pi G}{4}\Big[(v+2)\sqrt{v(v+4)}\Psi_o(v+4) - 2v\Psi_o(v)\\ &\quad + (v-2)\sqrt{v(v-4)}\Psi_o(v-4)\Big]\\ \Theta_1\Psi_o(v) &= \frac{3\pi G}{2}\left[\left(\sin^2\left(\frac{\bar{\mu}\ell_o}{2}\right) - \frac{\bar{\mu}^2\ell_o^2}{4}\right)v^2 - \frac{\ell_o^2}{9}\left(\frac{v}{K}\right)^{4/3}\right]\Psi_o(v).\end{aligned}$$

$$\mathcal{H}_{\mathrm{kin}}^{o} = L^2\left(\overline{\mathbb{R}}, d\mu_{\mathrm{Bohr}}\right) \otimes L^2(\mathbb{R}, dT)$$

$$L^2\left(\overline{\mathbb{R}}, d\mu_{\mathrm{Bohr}}\right)$$

$$-i\hbar\partial_T\Psi_o(v,T) = \hbar\sqrt{\Theta}\Psi_o(v,T) =: \hat{H}_o\Psi_o(v,T)$$

$$\langle\Psi_o \mid \Psi_o'\rangle_\varepsilon = \sum_{v\in\mathcal{L}_\varepsilon}\overline{\Psi_o(v,T_0)}\Psi_o'(v,T_0)$$

$$\mathcal{L}_\varepsilon = \mathcal{L}_{|\varepsilon|} \cup \mathcal{L}_{-|\varepsilon|}$$

$$H_{\mathrm{tot}} = H_{\mathrm{geo}}^{(\tau)} + H_{\mathrm{ferm}}^{(\tau)}$$

$$\hat{H}_{\text{tot}}\Psi = \left[\hat{H}^{(\tau)}_{\text{geo}} \otimes \mathbb{I} + \sum_{np} \hat{H}^{(\tau)}_{np}(x,y)\right]\Psi$$

$$\hat{H}^{(\tau)}_{np} = \left[\lambda_n \ell^{-2}\hat{V}^{2/3} \otimes (\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m\ell^{-3}\hat{V} \otimes (\widehat{\bar{y}x} + \widehat{\bar{x}y})\right]$$

$$\hat{H}_{\text{tot}}\Psi = \left[-\frac{\hbar^2}{2\ell^3}(\partial_T^2 + \Theta) \otimes \mathbb{I} + \sum_{np} \hat{H}^{(\tau)}_{np}(x,y)\right]\Psi$$

$$\begin{aligned}\Psi := &\sum_{np} \Psi_{np}(T, v, m_{np}, s_{np}, r_{np}, t_{np}) \\ &= \Psi_o(T,v) \otimes \prod_{np} \psi_{np}(T, m_{np}, s_{np}) \otimes \psi_{np}(T, r_{np}, t_{np}) \\ &=: \Psi_o(T,v) \otimes \prod_{np} \psi_{np}(T,x,y)\end{aligned}$$

$$\Psi_{np} = \Psi_o \otimes \psi_{np}$$

$$-\hbar^2 \partial_T^2 \Psi_{np} = \left[\hat{H}_o^2 - 2\ell^3 \hat{H}^{(\tau)}_{np}\right]\Psi_{np}$$

$$-i\hbar\partial_T \Psi_{np} = \left[\hat{H}_o^2 - 2\ell^3 \hat{H}^{(\tau)}_{np}\right]^{\frac{1}{2}}\Psi_{np}$$

$$\begin{aligned}-i\hbar\partial_T \Psi_{np} &\approx \left[\hat{H}_o - \ell^3 \hat{H}_o^{-\frac{1}{2}} \hat{H}^{(\tau)}_{np} \hat{H}_o^{-\frac{1}{2}}\right]\Psi_{np} \\ &=: \left(\hat{H}_o - \hat{H}^{(T)}_{np}\right)\Psi_{np}\end{aligned}$$

$$\mathcal{H}_{\text{phys}} \equiv \mathcal{H}^{o}_{\text{kin}} \otimes \mathcal{H}_{np}$$

$$\begin{aligned}\left\langle \Psi_{np}, \Psi'_{np}\right\rangle_\varepsilon = &\sum_{\varepsilon \in \mathcal{L}_\varepsilon} \int dx d\bar{x} dy d\bar{y} e^{-x\bar{x} - y\bar{y}} \\ &\times \overline{\Psi_{np}(T_0, v; x, y)}\Psi'_{np}(T_0, v; x, y)\end{aligned}$$

$$\Psi^{(np)}_{\text{int}}(v,x,y,T) = e^{-(i\hat{H}_o/\hbar)(T-T_0)}\Psi_{np}(v,x,y,T)$$

$$\Psi_o(v,T) = e^{(i\hat{H}_o/\hbar)(T-T_0)}\Psi_o(v,T_0)$$

$$\Psi^{(np)}_{\text{int}}(v,x,y,T) = \Psi_o(v,T_0) \otimes \psi_{np}(x,y,T)$$

$$\begin{aligned}i\hbar\partial_T \psi_{np} = &\left\langle \hat{H}^{(T)}_{np}\right\rangle_o \psi_{np} \\ &= \left[\lambda_n \ell^{-2}\left\langle \hat{H}_o^{-\frac{1}{2}} \hat{V}^{\frac{2}{3}} \hat{H}_o^{-\frac{1}{2}}\right\rangle_o (\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m\ell^{-3}\left\langle \hat{H}_o^{-\frac{1}{2}} \hat{V} \hat{H}_o^{-\frac{1}{2}}\right\rangle_o (\widehat{\bar{y}x} + \widehat{\bar{x}y})\right]\psi_{np} \\ &=: \left[\lambda_n \langle\hat{\alpha}\rangle_o(\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m\langle\hat{\beta}\rangle_o(\widehat{\bar{y}x} + \widehat{\bar{x}y})\right]\psi_{np}\end{aligned}$$

$$\hat{\alpha}(T) := \ell^{-2}\hat{H}_o^{-\frac{1}{2}}\hat{V}^{2/3}(T)\hat{H}_o^{-\frac{1}{2}} \text{ and } \hat{\beta}(T) := \ell^{-3}\hat{H}_o^{-\frac{1}{2}}\hat{V}(T)\hat{H}_o^{-\frac{1}{2}}$$

$$\hat{V}(T) = e^{-(i\hat{H}_o/\hbar)(T-T_0)}\hat{V}(T_0)e^{(i\hat{H}_o/\hbar)(T-T_0)}$$

$$\bar{g}_{\mu\nu}dx^\mu dx^\nu = -\bar{N}_T^2(T)dT^2 + \bar{a}^2(T)d\Omega_3^2$$

$$i\hbar\partial_T\psi_{np} = \bar{N}_T[\lambda_n\bar{a}^{-1}(\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m(\widehat{\bar{y}x} + \widehat{\bar{x}\bar{y}})]\psi_{np}$$

$$\lambda_n\bar{N}_T\bar{a}^{-1} = \lambda_n\ell^{-2}\left\langle \hat{H}_o^{-\frac{1}{2}}\hat{V}^{2/3}\hat{H}_o^{-\frac{1}{2}}\right\rangle_o$$

$$m\bar{N}_T = m\ell^{-3}\left\langle \hat{H}_o^{-\frac{1}{2}}\hat{V}\hat{H}_o^{-\frac{1}{2}}\right\rangle_o$$

$$\bar{N}_T(T) = \ell^{-3}\left\langle \hat{H}_o^{-\frac{1}{2}}\hat{V}(T)\hat{H}_o^{-\frac{1}{2}}\right\rangle_o$$

$$\bar{a}(T) = \ell^{-1}\frac{\left\langle \hat{H}_o^{-\frac{1}{2}}\hat{V}(T)\hat{H}_o^{-\frac{1}{2}}\right\rangle_o}{\left\langle \hat{H}_o^{-\frac{1}{2}}\hat{V}^{2/3}(T)\hat{H}_o^{-\frac{1}{2}}\right\rangle_o}$$

$$\frac{\bar{N}_T}{\bar{a}} = \ell^{-2}\left\langle \hat{H}_o^{-\frac{1}{2}}\hat{V}^{2/3}(T)\hat{H}_o^{-\frac{1}{2}}\right\rangle_o$$

$$g_{\mu\nu} \to \Omega^2(x^\sigma)g_{\mu\nu}$$

$$d\bar{T} \equiv \frac{\bar{N}_T}{\bar{a}}dT = \ell^{-2}\left\langle \hat{H}_o^{-\frac{1}{2}}\hat{V}^{2/3}(T)\hat{H}_o^{-\frac{1}{2}}\right\rangle_o dT$$

$$\bar{g}_{\mu\nu}dx^\mu dx^\nu = \bar{a}^2(T)[-d\bar{T}^2 + d\Omega_3^2]$$

$$\bar{g}'_{\mu\nu}dx^\mu dx^\nu = -d\bar{T}^2 + d\Omega_3^2$$

$$\psi_{np}^{(I)}\left(E_n^{(0)} = -w_n; \psi_{np}^{(0)}\right)\left(\psi_{np}^{(1,2)}\right)\left(E_n^{(3)} = +w_n; \psi_{np}^{(3)}\right)\left(\psi_{np}^{(0)} \to \psi_{np}^{(3)}\right)$$

$$\tilde{\Psi}_{np}(T,v;x,y) = \tilde{\Psi}_{np}^o(T,v) \otimes \psi_{np}(T,x,y)$$

$$\begin{aligned}\hat{H}_{\text{tot}}\tilde{\Psi}_{np}^o &= \left[\hat{H}_{\text{geo}}^{(\tau)} + \left\langle \hat{H}_{np}^{(T)}(v)\right\rangle_\psi\right]\tilde{\Psi}_{np}^o \\ &= \left[-\frac{\hbar^2}{2\ell^3}(\partial_T^2 + \Theta) + \left\langle \hat{H}_{np}^{(T)}(v)\right\rangle_\psi\right]\tilde{\Psi}_{np}^o\end{aligned}$$

$$\hat{E}_n(v) = \left\langle \hat{H}_{np}^{(T)}(v)\right\rangle_\psi = \pm\sqrt{\frac{\lambda_n^2}{\ell^4}\hat{V}^{\frac{4}{3}} + \frac{m^2}{\ell^6}\hat{V}^2}$$

$$\begin{aligned}-\partial_T^2\tilde{\Psi}_n^o &= \left[\Theta - \frac{2\ell^3}{\hbar^2}\hat{E}_n\right]\tilde{\Psi}_n^o \\ &=: (\Theta + \Theta_n)\tilde{\Psi}_n^o = \tilde{\Theta}_n\tilde{\Psi}_n^o\end{aligned}$$

$$\Theta_n = -\frac{2\ell^3}{\hbar^2}\hat{E}_n$$

$$\Theta = -(2\ell^3/\hbar^2)\hat{H}_{\text{grav}}^{(\tau)}$$

$$-i\hbar\partial_T\tilde{\Psi}_n^o = [\hat{H}_o^2 - 2\ell^3\hat{E}_n]^{\frac{1}{2}}\tilde{\Psi}_n^o$$

$$-i\hbar\partial_T\tilde{\Psi}_n^o(T,v) \approx \left[\hat{H}_o - \hat{E}_n^{(T)}\right]\tilde{\Psi}_n^o(T,v)$$

$$\begin{aligned}\hat{E}_n^{(T)}(v) &:= \ell^3\hat{H}_o^{-\frac{1}{2}}\hat{E}_n(v)\hat{H}_o^{-\frac{1}{2}} \\ &= \pm\left(\lambda_n^2\ell^2\hat{H}_o^{-1}\hat{V}^{\frac{4}{3}}\hat{H}_o^{-1} + m^2\hat{H}_o^{-1}\hat{V}^2\hat{H}_o^{-1}\right)^{1/2}\end{aligned}$$

$$\lambda_n\ell\hat{H}_o^{-1/2}\hat{V}^{\frac{2}{3}}\hat{H}_o^{-1/2}m\hat{H}_o^{-1/2}\hat{V}\hat{H}_o^{-1/2}$$

$$\Theta_n = (2\ell^3/\hbar^2)|\hat{E}_n| > 0$$

$$\Theta_n = -(2\ell^3/\hbar^2)|\hat{E}_n| < 0$$

$$\Theta_n - (4\ell^3/\hbar^2)|\hat{E}_n| + (4\ell^3/\hbar^2)|\hat{E}_n|$$

$$\Theta e_k(v) = \omega_k^2 e_k(v), \text{ with } \langle e_k \mid e_{k'}\rangle = \delta_{k,k'}.$$

$$\Psi_o(v,T) = \sum_k c_k^o e_k(v)e^{i\omega_k T}$$

$$[\Theta + \Theta_n]e_k^{(n)}(v) = \left(\omega_k^{(n)}\right)^2 e_k^{(n)}(v), \text{ with } \left\langle e_k^{(n)} \mid e_{k'}^{(n)}\right\rangle = \delta_{k,k'}$$

$$U_{\text{eff}}(v) = U_o(v) + \Theta_n(v)$$

$$U_{\text{eff}}(v_{\text{b}}) = \omega_k^2[U_{\text{eff}}(v) < \omega_k^2][U_{\text{eff}}(v) > \omega_k^2]$$

$$\rho_T - |\rho_n| = \rho_{\text{cr}}$$

$$U_{\text{eff}} = U_o(v) - |\Theta_n(v)| < U_o(v)$$

$$\Delta\Theta_n = -(4\ell^3/\hbar^2)|\hat{E}_n|$$

$$\Delta\Theta_n = +(4\ell^3/\hbar^2)|\hat{E}_n|$$

$$\Theta_n(v) \sim \pm\lambda_n\ell^{-2}\hat{V}^{2/3}$$

$$\Theta_n(v) \sim \pm m\ell^{-3}\hat{V}$$

$$\left|e_k^{(n)}\right\rangle = \underline{N}_k\left[|e_k\rangle + \left|\delta e_k^{(n)}\right\rangle\right]$$

$$\tilde{\Psi}_n^o(v,T) = \sum_k c_k^{(n)}e_k^{(n)}(v)e^{i\omega_k T}$$

$$\tilde{\Psi}_n^o(v,T) = \sum_k c_k e_k(v) e^{i\omega_k T} + \sum_k c_k \delta e_k^{(n)}(v) e^{i\omega_k T}$$
$$=: \Psi_o(v,T) + \delta\Psi_n(v,T)$$

$$c_k = c_k^{(n)} = c_k^o$$

$$\tilde{\Psi}_{np} = \tilde{\Psi}_n^o \otimes \psi_{np}$$

$$-i\hbar\partial_T \tilde{\Psi}_{np} = \left(\hat{H}_o - \hat{H}_{np}^{(T)}\right) \tilde{\Psi}_{np}$$

$$i\hbar\partial_T \psi_{np} = \left[\lambda_n \ell^{-2} \left\langle \hat{H}_o^{-\frac{1}{2}} \hat{V}^{\frac{2}{3}} \hat{H}_o^{-\frac{1}{2}} \right\rangle (\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m\ell^{-3} \left\langle \hat{H}_o^{-\frac{1}{2}} \hat{V} \hat{H}_o^{-\frac{1}{2}} \right\rangle (\widehat{\bar{y}x} + \widehat{\bar{x}\bar{y}}) \right] \psi_{np}$$

$$\tilde{\Psi}_n^o = \Psi_o + \delta\Psi_n$$

$$\langle \hat{O} \rangle = \langle \hat{O} \rangle_o + \langle \hat{O} \rangle_n$$

$$\langle \hat{O} \rangle_n := \langle \Psi_o | \hat{O} | \delta\Psi_n \rangle + \langle \delta\Psi_n | \hat{O} | \Psi_o \rangle + \langle \delta\Psi_n | \hat{O} | \delta\Psi_n \rangle$$

$$\delta\Psi_n(v,T) = \sum_k c_k \delta e_k^{(n)}(v) e^{i\omega_k T}$$

$$i\hbar\partial_T \psi_{np} = \left[\lambda_n (\langle\hat{\alpha}\rangle_o + \langle\hat{\alpha}\rangle_n)(\widehat{x\bar{x}} + \widehat{y\bar{y}}) + m\left(\langle\hat{\beta}\rangle_o + \langle\hat{\beta}\rangle_n\right)(\widehat{\bar{y}x} + \widehat{\bar{x}\bar{y}})\right]\psi_{np}$$

$$\tilde{g}_{\mu\nu} dx^\mu dx^\nu = -\tilde{N}_T^2(T) dT^2 + \tilde{a}^2(T) d\Omega_3^2$$

$$\lambda_n \tilde{N}_T \tilde{a}^{-1} = \lambda_n \langle \hat{\alpha}(T) \rangle_o \left(1 + \delta_n^{(1)}\right)$$
$$m\tilde{N}_T = m \langle \hat{\beta}(T) \rangle_o \left(1 + \delta_n^{(2)}\right)$$

$$\delta_n^{(1)}(T) \equiv \frac{\langle \hat{\alpha}(T) \rangle_n}{\langle \hat{\alpha}(T) \rangle_o} \text{ and } \delta_n^{(2)}(T) \equiv \frac{\langle \hat{\beta}(T) \rangle_n}{\langle \hat{\beta}(T) \rangle_o}$$

$$\tilde{N}_T(T) = \bar{N}_T(T) F_n(T)$$
$$\tilde{a}(T) = \bar{a}(T) G_n(T)$$

$$F_n \equiv \left[\left(1 + \delta_n^{(1)}\right)\left(1 + \delta_n^{(2)}\right)^3\right]^{\frac{1}{4}}$$

$$G_n \equiv \left(\frac{1 + \delta_n^{(2)}}{1 + \delta_n^{(1)}}\right)^{\frac{1}{4}}$$

$$\frac{\tilde{N}_T}{\tilde{a}} = \langle \hat{\alpha}(T) \rangle_o \left(1 + \delta_n^{(1)}\right)$$

$$\tilde{g}_{\mu\nu} dx^\mu dx^\nu = \tilde{a}^2(T)\left[-d\tilde{T}^2 + d\Omega_3^2\right]$$
$$=: \tilde{a}^2(T) \tilde{g}'_{\mu\nu} dx^\mu dx^\nu$$

$$d\tilde{T} \equiv \frac{\tilde{N}_T}{\tilde{a}} dT = \left(1 + \delta_n^{(1)}\right) d\bar{T}$$

$$\epsilon_{\mathbf{k}}^{(s)}(v) = \left(s + \frac{1}{2}\right)\hbar k \hat{V}^{-1/3}$$

$$\rho_n(T) = \left\langle :V^{-1(T)E_n^{(T)}}: \right\rangle$$

$$\rho_n \approx 2\lambda_n \ell \left\langle \hat{H}_o^{-1/2}\hat{V}^{-1/3}(T)\hat{H}_o^{-1/2} \right\rangle \sim \langle \hat{V}^{-1/3}\rangle_o \langle \hat{H}_o^{-1}\rangle_o$$

$$\hat{H}_o \Psi_o = P_T^2 \Psi_o$$

$$\langle \hat{H}_o^{-1}\rangle_o = P_T^{-2} = \text{const.}$$

$$\rho_n = m\langle \hat{H}_o^{-1}\rangle_o \approx \text{const.}$$

$$P_T = V_\mathrm{b}\sqrt{2\rho_\mathrm{crit}}$$

$$P_T \approx 10^8 \ell_\mathrm{Pl}^3 \sqrt{0.82\rho_\mathrm{Pl}} \sim 9 \times 10^7$$

$$\langle \hat{H}_o^{-1}\rangle_o \sim 10^{-15}$$

$$\langle \hat{H}_o^{-1}\rangle_o \sim 10^{-19}$$

$$\Lambda_\mathrm{eff} = 8\pi G \rho_n = 8\pi G m \langle \hat{H}_o^{-1}\rangle_o$$

$$\Lambda_\mathrm{eff} \sim 6 \times 10^{-33}$$

$$\psi_{np}(x,y) = c_0 + c_1 x + c_2 y + c_3 xy$$

$$\lambda_n \ell^{-2} V^{\frac{2}{3}}(-c_0 + c_3 xy) + m\ell^{-3}V(c_3 - c_0 xy) = E_{np}(c_0 + c_1 x + c_2 y + c_3 xy)$$

$$\left(\lambda_n \ell^{-2} V^{\frac{2}{3}} + E_{np}\right) c_0 = m\ell^{-3} V c_3$$

$$\left(\lambda_n \ell^{-2} V^{\frac{2}{3}} - E_{np}\right) c_3 = m\ell^{-3} V c_0$$

$$E_{np} c_1 = 0 \;\Rightarrow\; c_1 = 0 \text{ or } E_{np} = 0$$

$$E_{np} c_2 = 0 \;\Rightarrow\; c_2 = 0 \text{ or } E_{np} = 0$$

$$\begin{pmatrix} \lambda_n \ell^{-2} V^{\frac{2}{3}} + E_{np} & -m\ell^{-3}V \\ -m\ell^{-3}V & \lambda_n \ell^{-2} V^{\frac{2}{3}} - E_{np} \end{pmatrix} \begin{pmatrix} c_0 \\ c_3 \end{pmatrix} = 0$$

$$E_{np}^{(\pm)} = \pm\sqrt{\lambda_n^2 \ell^{-4} V^{\frac{4}{3}} + m^2 \ell^{-6} V^2} \equiv \pm w_n$$

$$c_0 = \frac{m\ell^{-3}V}{\lambda_n \ell^{-2} V^{\frac{2}{3}} + E_{np}} c_3, \text{ with } E_{np}^{(\pm)} = \pm w_n$$

$$E_{np} = +w_n: \quad c_3 = \frac{m\ell^{-3}V}{\lambda_n \ell^{-2} V^{\frac{2}{3}} - w_n} c_0$$

$$E_{np} = -w_n: \quad c_3 = \frac{m\ell^{-3}V}{\lambda_n \ell^{-2} V^{\frac{2}{3}} + w_n} c_0$$

$$\psi_{np}^{(\pm)} = c_0 \left(1 + \frac{m\ell^{-3}V}{\lambda_n \ell^{-2} V^{\frac{2}{3}} \mp w_n} xy \right)$$

$$E_{np} = 0: \psi_{np} = c_1 x \text{ or } \psi_{np} = c_2 y$$

$$\Theta_0 \Psi_o(v) = -\frac{1}{8\pi G\hbar^2} \left[\hat{V}^{\frac{1}{2}} e^{if\ell_o} \sin(\bar{\mu}c) \hat{A} \sin(\bar{\mu}c) e^{-if\ell_o} \hat{V}^{\frac{1}{2}} \right] \Psi_o(v)$$

$$\Theta_1 \Psi_o(v) = \frac{1}{8\pi G\hbar^2} \hat{V}^{\frac{1}{2}} \left[\sin^2\left(\frac{\bar{\mu}\ell_o}{2}\right) - \frac{\bar{\mu}^2 \ell_o^2}{4} - \frac{\ell_o^2}{9|K^2 v|^{2/3}} \right] \hat{A} \hat{V}^{\frac{1}{2}} \Psi_o(v)$$

$$\begin{aligned} \sin(\bar{\mu}c)\Psi_o(v) &= \frac{1}{2i}\left(e^{i\bar{\mu}c} - e^{-i\bar{\mu}c}\right)\Psi_o(v) \\ &= \frac{1}{2i}[\Psi_o(v+2) - \Psi_o(v-2)] \\ \cos(\bar{\mu}c)\Psi_o(v) &= \frac{1}{2}\left(e^{i\bar{\mu}c} + e^{-i\bar{\mu}c}\right)\Psi_o(v) \\ &= \frac{1}{2}[\Psi_o(v+2) + \Psi_o(v-2)] \end{aligned}$$

$$\hat{A}\Psi_o(v) = C_A(v)\Psi_o(v)$$

$$C_A(v) \equiv \frac{27K}{4} \sqrt{\frac{8\pi}{6} \frac{\ell_{\text{Pl}}}{\gamma^{3/2}}} |v| \big| |v+1| - |v-1| \big|$$

$$\Psi_1(v) \equiv \hat{V}^{\frac{1}{2}} \Psi_o(v) = \sqrt{C_V(v)} \Psi_o(v)$$

$$C_V(v) \equiv \left(\frac{8\pi\gamma}{6}\right)^{\frac{3}{2}} \frac{\ell_{\text{Pl}}^3}{K} |v|$$

$$\begin{aligned} \Psi_2(v) &\equiv \sin(\bar{\mu}c) e^{-if\ell_o} \Psi_1(v) \\ &= \frac{1}{2i} \sqrt{C_V(v)} e^{-if\ell_o} [\Psi_o(v+2) - \Psi_o(v-2)] \end{aligned}$$

$$\begin{aligned} \hat{A}\Psi_2(v) &= \frac{1}{2i} \sqrt{C_V(v)} e^{-if\ell_o} \hat{A} [\Psi_o(v+2) - \Psi_o(v-2)] \\ &= \frac{1}{2i} \sqrt{C_V(v)} e^{-if\ell_o} [C_A(v+2)\Psi_o(v+2) - C_A(v-2)\Psi_o(v-2)]. \end{aligned}$$

$$\begin{aligned} \Psi_3 &\equiv e^{if\ell_o} \sin(\bar{\mu}c) \hat{A} \Psi_2(v) \\ &= -\frac{1}{4} \sqrt{C_V(v)} [C_A(v+2)(\Psi_o(v+4) - \Psi_o(v)) \\ &\qquad - C_A(v-2)(\Psi_o(v) - \Psi_o(v-4))] \end{aligned}$$

$$\begin{aligned}\Theta_0\Psi_o(v) &= -\frac{1}{8\pi G\hbar^2}\hat{V}^{\frac{1}{2}}\Psi_3(v)\\ &= \frac{1}{32\pi G\hbar^2}\sqrt{C_V(v)}\hat{V}^{\frac{1}{2}}[C_A(v+2)(\Psi_o(v+4)-\Psi_o(v))\\ &\quad -C_A(v-2)(\Psi_o(v)-\Psi_o(v-4))]\\ &= \frac{1}{32\pi G\hbar^2}\sqrt{C_V(v)}[C_A(v+2)\left(\sqrt{C_V(v+4)}\Psi_o(v+4)-\sqrt{C_V(v)}\Psi_o(v)\right)\\ &\quad -C_A(v-2)\left(\sqrt{C_V(v)}\Psi_o(v)-\sqrt{C_V(v-4)}\Psi_o(v-4)\right)]\\ &= \frac{3\pi G}{8}\left[C^+(v)\Psi_o(v+4)+C^0(v)\Psi_o(v))+C^-(v)\Psi_o(v-4)\right]\end{aligned}$$

$$\begin{aligned}C^+(v) &= |v+2|||v+3|-|v+1||\sqrt{|v||v+4|}\\ C^0(v) &= -(|v+2|||v+3|-|v+1||+|v-2|||v-1|-|v-3||)|v|,\\ C^-(v) &= |v-2|||v-1|-|v-3||\sqrt{|v||v-4|}.\end{aligned}$$

$$\begin{aligned}\Psi_4(v) &\equiv \hat{A}\hat{V}^{\frac{1}{2}}\Psi_o(v) = \hat{A}\Psi_1\\ &= \sqrt{C_V(v)}C_A(v)\Psi_o(v)\end{aligned}$$

$$\begin{aligned}\Psi_5(v) &\equiv \left(\sin^2\left(\frac{\bar{\mu}\ell_o}{2}\right)-\frac{\bar{\mu}^2\ell_o^2}{4}-\frac{\ell_o^2}{9|K^2v|^{2/3}}\right)\Psi_4(v)\\ &= \sqrt{C_V(v)}C_A(v)\left(\sin^2\left(\frac{\bar{\mu}\ell_o}{2}\right)-\frac{\bar{\mu}^2\ell_o^2}{4}-\frac{\ell_o^2}{9|K^2v|^{2/3}}\right)\Psi_o(v)\end{aligned}$$

$$\begin{aligned}\Theta_1\Psi_o(v) &= \frac{1}{8\pi G\hbar^2}\hat{V}^{\frac{1}{2}}\Psi_5(v)\\ &= \frac{3\pi G}{2}|v|^2||v+1|-|v-1||\left(\sin^2\left(\frac{\bar{\mu}\ell_o}{2}\right)-\frac{\bar{\mu}^2\ell_o^2}{4}-\frac{\ell_o^2}{9|K^2v|^{2/3}}\right)\Psi_o(v).\end{aligned}$$

$$H = -\sum_{a=1}^{2N}\frac{1}{2m_a}\nabla^2_{\mathbf{x}_a}+\frac{1}{2}\sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{a,b=1}^{2N}\frac{q_aq_b}{|\mathbf{x}_a-\mathbf{x}_b+\mathbf{n}L|},$$

$$\Psi(\mathbf{X}) = \Phi(\mathbf{R})\det[\phi_a(\mathbf{r}_i \mid \mathbf{X})]e^{-U(\mathbf{X})}$$

$$\Phi(\mathbf{R}) = \prod_I \varphi\left(\left|\mathbf{R}_I-\mathbf{R}_I^{(0)}\right|\right)$$

$$\phi_{\mathbf{k}}^{\sigma}(\mathbf{r}_i) = \sum_{\mathbf{n}\in\mathbb{Z}^3}\sum_{I=1}^{N}e^{i\mathbf{k}\cdot(\mathbf{R}_I+\mathbf{n}L)}\chi(\mathbf{r}_i^{\sigma}-\mathbf{R}_I-\mathbf{n}L),$$

$$\mathbf{r}_i \to \mathbf{r}_i + W\mathbf{y}_i^{(b)}$$

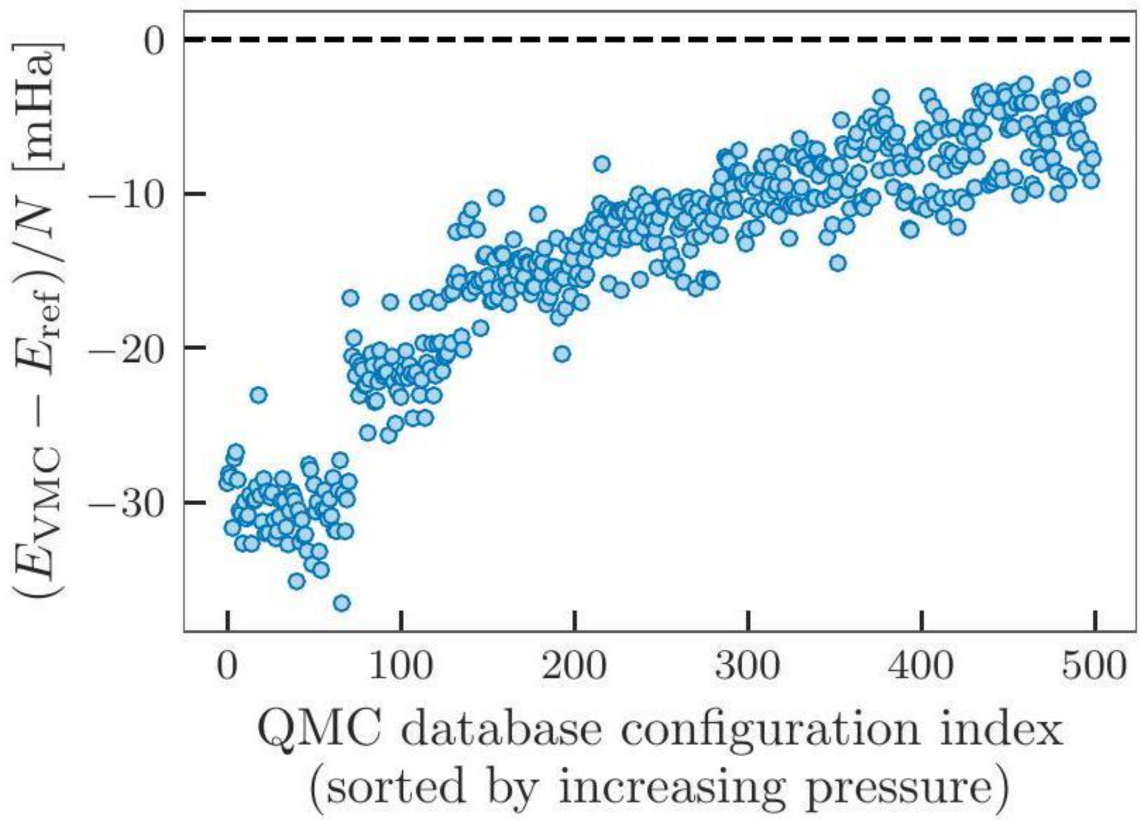
$$U(\mathbf{x}) \to U(\mathbf{x}) + \sum_{i<j}\left[w\mathrm{MLP}\left(\mathbf{Y}_{ij}^{(b)}\right)\right]$$

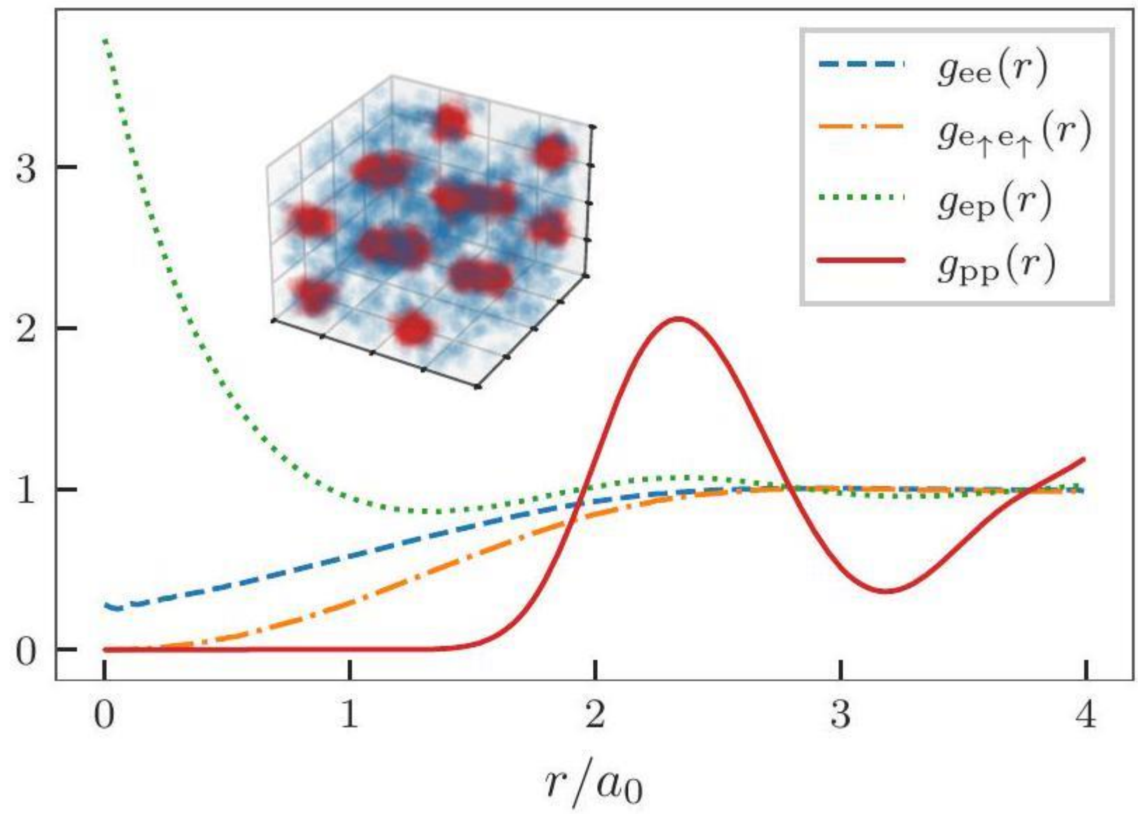
$$\Psi(\mathbf{r}_1+L\mathbf{e}_\alpha,\dots,\mathbf{r}_N,\mathbf{R}) = e^{i\theta_\alpha}\Psi(\mathbf{r}_1,\dots,\mathbf{r}_N,\mathbf{R}),$$

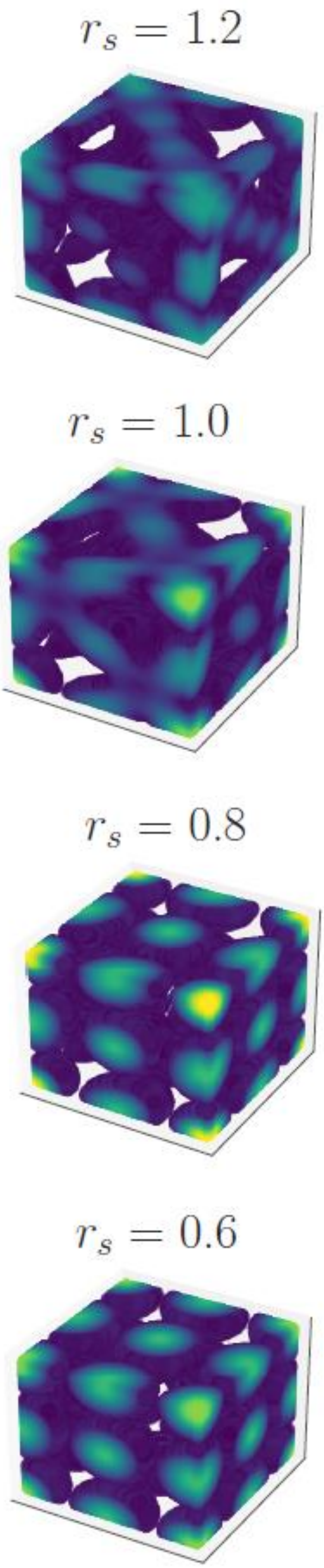
$$\boldsymbol{\theta} \equiv \left(\theta_x,\theta_y,\theta_z\right) = \mathbf{0}$$

$$\mathbf{k} = (2\pi\mathbf{m}+\boldsymbol{\theta})/L$$

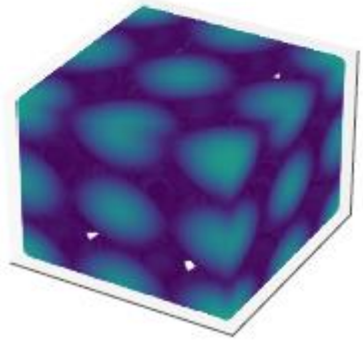
$$E_{\text{global}}(\boldsymbol{\alpha}) = \int d\mathbf{R}\mathcal{P}(\mathbf{R}) \frac{\langle \Psi_{\boldsymbol{\alpha}}(\mathbf{R}) | H_{\mathbf{R}} | \Psi_{\boldsymbol{\alpha}}(\mathbf{R}) \rangle}{\langle \Psi_{\boldsymbol{\alpha}}(\mathbf{R}) \mid \Psi_{\boldsymbol{\alpha}}(\mathbf{R}) \rangle}$$



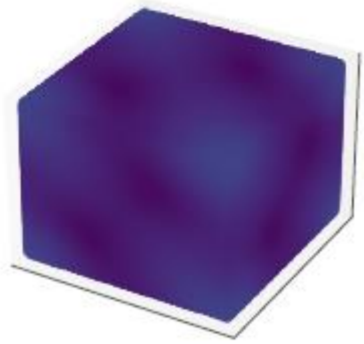



$r_s = 1.2$
$r_s = 1.0$
$r_s = 0.8$
$r_s = 0.6$

$r_s = 0.4$



$r_s = 0.2$



$$a_0^p \equiv a_0 m_e / m_p$$

$$a^p / a_0^p \simeq 1836 r_s$$

$$E_{\text{global}}(\boldsymbol{\alpha}) = \frac{1}{M} \sum_{I=1}^{M} \frac{\langle \Psi_{\boldsymbol{\alpha}}(\mathbf{R}_I) | H_{\mathbf{R}_I} | \Psi_{\boldsymbol{\alpha}}(\mathbf{R}_I) \rangle}{\langle \Psi_{\boldsymbol{\alpha}}(\mathbf{R}_I) \mid \Psi_{\boldsymbol{\alpha}}(\mathbf{R}_I) \rangle}$$

$$\mathcal{S} \boldsymbol{\delta\theta} = -\eta \mathbf{F},$$

$$\mathcal{F}_k = \int d\mathbf{R} \mathcal{P}(\mathbf{R}) F_k(\mathbf{R})$$

$$F_k(\mathbf{R}) = -2\mathrm{Re}\{\langle H_{\mathbf{R}} O_k^{\dagger}(\mathbf{R}) \rangle - \langle H_{\mathbf{R}} \rangle \langle O_k^{\dagger}(\mathbf{R}) \},$$

$$P_{\boldsymbol{\alpha}}(\mathbf{r} \mid \mathbf{R}) = |\langle \Psi_{\boldsymbol{\alpha}}(\mathbf{R}) \mid \mathbf{r} \rangle|^2 / \langle \Psi_{\boldsymbol{\alpha}}(\mathbf{R}) \mid \Psi_{\boldsymbol{\alpha}}(\mathbf{R}) \rangle$$

$$O_k(\mathbf{R}) = \partial \ln \Psi_{\boldsymbol{\alpha}}(\mathbf{r}, \mathbf{R}) / \partial \alpha_k$$

$$\mathcal{S}_{kl} = \int d\mathbf{R} \mathcal{P}(\mathbf{R}) S_{kl}(\mathbf{R})$$

$$S_{kl}(\mathbf{R}) = \mathrm{Re}\{\langle O_k^{\dagger}(\mathbf{R}) O_l(\mathbf{R}) \rangle - \langle O_k^{\dagger}(\mathbf{R}) \rangle \langle O_l(\mathbf{R}) \rangle\}.$$

$$\begin{aligned} \mathbf{I}_{ij} &= [\sin(2\pi \mathbf{r}_{ij}/L), \cos(2\pi \mathbf{r}_{ij}/L), |\sin(\pi \mathbf{r}_{ij}/L)|, s_i s_j] \in \mathbb{R}^{2d+2} \\ \mathbf{I}_{iI} &= [\sin(2\pi \mathbf{r}_{iI}/L), \cos(2\pi \mathbf{r}_{iI}/L), |\sin(\pi \mathbf{r}_{iI}/L)|] \in \mathbb{R}^{2d+1} \end{aligned}$$

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \mathbf{r}_{iI} = \mathbf{r}_i - \mathbf{R}_I$$

$$\mathbf{h}_i^{(0)}, \mathbf{H}_{ij}^{(0)}, \mathbf{H}_{iI}^{(0)} \quad \rhd h$$

$$\mathbf{y}_i^{(0)} = \mathbf{h}_i^{(0)} \quad \rhd h$$

$$\mathbf{Y}_{ij}^{(0)} = \left[\mathbf{I}_{ij}, \mathbf{H}_{ij}^{(0)}\right], \mathbf{Y}_{iI}^{(0)} = \left[\mathbf{I}_{iI}, \mathbf{H}_{iI}^{(0)}\right] \quad \Delta 2d + 2 + h, 2d + 1 + h$$

$$Q_{ep}^{(\ell)}, K_{ep}^{(\ell)}$$

$$\mathbf{Q}_{iI}^{(\ell)} = Q_{ep}^{(\ell)} \mathbf{Y}_{iI}^{(\ell)}, \mathbf{K}_{iI}^{(\ell)} = K_{ep}^{(\ell)} \mathbf{Y}_{iI}^{(\ell)}$$

$$\rhd \dim\left(\mathbf{Y}_{iI}^{(\ell)}\right) \times a$$

$$\mathbf{W}_{iI}^{(\ell)} = \mathrm{MLP}_{ep,1}^{(\ell)}\left(\mathbf{Q}^{(\ell)} \mathbf{K}^{(\ell)} / \sqrt{a}\right)_{iI}$$

$$\mathbf{M}_{iI}^{(\ell)} = \mathbf{W}_{iI}^{(\ell)} \odot \mathrm{MLP}_{ep,2}^{(\ell)}\left(\mathbf{Y}_{iI}^{(\ell)}\right)$$

$$\mathbf{H}_{iI}^{(\ell+1)} = \mathrm{MLP}_{ep,3}^{(\ell)}\left(\left[\mathbf{Y}_{iI}^{(\ell)}, \mathbf{M}_{iI}^{(\ell)}\right]\right)$$

$$\mathbf{Y}_{iI}^{(\ell+1)} = \left[\mathbf{I}_{iI}, \mathbf{H}_{iI}^{(\ell+1)}\right]$$

$$Q_{ee}^{(\ell)}, K_{ee}^{(\ell)}$$

$$\mathbf{Q}_{ij}^{(\ell)} = Q_{ee}^{(\ell)} \mathbf{Y}_{ij}^{(\ell)}, \mathbf{K}_{ij}^{(\ell)} = K_{ee}^{(\ell)} \mathbf{Y}_{ij}^{(\ell)}$$

$$\rhd \dim\left(\mathbf{Y}_{ij}^{(\ell)}\right) \times a$$

$$\mathbf{W}_{ij}^{(\ell)} = \mathrm{MLP}_{ee,1}^{(\ell)}\left(\mathbf{Q}^{(\ell)} \mathbf{K}^{(\ell)} / \sqrt{a}\right)_{ij}$$

$$\mathbf{M}_{ij}^{(\ell)} = \mathbf{W}_{ij}^{(\ell)} \odot \mathrm{MLP}_{ee,2}^{(\ell)}\left(\mathbf{Y}_{ij}^{(\ell)}\right)$$

$$\mathbf{C}_i^{(\ell)} = \sum_I \mathrm{MLP}_{ee,3}\left(\mathbf{Y}_{iI}^{(\ell+1)}\right)$$

$$\mathbf{C}_{ij}^{(\ell)} = \sum_I \mathrm{MLP}_{ee,4}\left(\mathbf{Y}_{iI}^{(\ell+1)}\right) \odot \mathrm{MLP}_{ee,5}\left(\mathbf{Y}_{jI}^{(\ell+1)}\right)$$

$$\mathbf{h}_i^{(\ell+1)} = \mathrm{MLP}_{ee,6}^{(\ell)}\left(\left[\mathbf{h}_i^{(\ell)}, \sum_j \mathbf{M}_{ij}^{(\ell)}, \mathbf{C}_i^{(\ell)}\right]\right)$$

$$\mathbf{H}_{ij}^{(\ell+1)} = \mathrm{MLP}_{ee,7}^{(\ell)}\left(\left[\mathbf{Y}_{ij}^{(\ell)}, \mathbf{M}_{ij}^{(\ell)}, \mathbf{C}_{ij}^{(\ell)}\right]\right)$$

$$\mathbf{y}_i^{(\ell+1)} = \mathbf{h}_i^{(\ell+1)}$$

$$\mathbf{Y}_{ij}^{(\ell+1)} = \left[\mathbf{I}_{ij}, \mathbf{H}_{ij}^{(\ell+1)}\right]$$

$$\mathbf{y}_i^{(b)}, \mathbf{Y}_{ij}^{(b)}, \mathbf{Y}_{iI}^{(b)}$$

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \mathbf{V}(x), \mathbf{V}(x) = \begin{pmatrix} V_0(x) & \Delta \\ \Delta & V_1(x) \end{pmatrix},$$

$$\hat{\mathcal{P}}_{\mathrm{P}}^{\mathrm{BO}} = \Theta(\hat{x}),$$

$$\hat{\mathcal{P}}_{\mathrm{P}}^{\mathrm{GR}} = |1\rangle\langle 1| = \Theta(|1\rangle\langle 1| - |0\rangle\langle 0|) = \Theta(-\hat{\sigma}_z).$$

$$\begin{aligned}\hat{\mathcal{P}}_{\mathrm{P}}(\alpha) &= \Theta(\hat{x} - x_\alpha \hat{\sigma}_z) \\ &= \Theta(\hat{x} - x_\alpha)|0\rangle\langle 0| + \Theta(\hat{x} + x_\alpha)|1\rangle\langle 1| \\ &= \hat{\mathcal{P}}_{\mathrm{n}}^{0}(\alpha)\hat{\mathcal{P}}_{\mathrm{e}}^{0} + \hat{\mathcal{P}}_{\mathrm{n}}^{1}(\alpha)\hat{\mathcal{P}}_{\mathrm{e}}^{1} \\ &= \hat{\mathcal{P}}_{\mathrm{P}}^{0}(\alpha) + \hat{\mathcal{P}}_{\mathrm{P}}^{1}(\alpha)\end{aligned}$$

$$\begin{aligned}\hat{\mathcal{P}}_{\mathrm{n}}^{\phi}(\alpha) &= \Theta\big(\hat{x} - (-1)^{\phi} x_\alpha\big) \\ \hat{\mathcal{P}}_{\mathrm{e}}^{\phi} &= |\phi\rangle\langle\phi|\end{aligned}$$

$$\hat{\mathcal{F}}(\alpha) = \frac{\mathrm{i}}{\hbar}\big[\hat{\mathcal{H}}, \hat{\mathcal{P}}_{\mathrm{P}}(\alpha)\big].$$

$$\hat{\mathcal{F}}(\alpha) = \hat{\mathcal{F}}_{\mathrm{n}}(\alpha) + \hat{\mathcal{F}}_{\mathrm{e}}(\alpha),$$

$$\begin{aligned}\hat{\mathcal{F}}_{\mathrm{n}}(\alpha) &= \hat{\mathcal{F}}_{\mathrm{n}}^{0}(\alpha)\hat{\mathcal{P}}_{\mathrm{e}}^{0} + \hat{\mathcal{F}}_{\mathrm{n}}^{1}(\alpha)\hat{\mathcal{P}}_{\mathrm{e}}^{1} \\ \hat{\mathcal{F}}_{\mathrm{e}}(\alpha) &= \hat{\mathcal{F}}_{\mathrm{e}}^{0}\hat{\mathcal{P}}_{\mathrm{n}}^{0}(\alpha) + \hat{\mathcal{F}}_{\mathrm{e}}^{1}\hat{\mathcal{P}}_{\mathrm{n}}^{1}(\alpha)\end{aligned}$$

$$\begin{aligned}\hat{\mathcal{F}}_{\mathrm{n}}^{\phi}(\alpha) &= \frac{1}{2m}\big[\hat{p}\delta\big(\hat{x} - (-1)^{\phi}x_\alpha\big) + \delta\big(\hat{x} - (-1)^{\phi}x_\alpha\big)\hat{p}\big] \\ \hat{\mathcal{F}}_{\mathrm{e}}^{\phi} &= \frac{\mathrm{i}\Delta}{\hbar}[|\phi\rangle\langle\bar{\phi}| - |\bar{\phi}\rangle\langle\phi|]\end{aligned}$$

$$kZ_{\mathrm{R}} = \int_{-\infty}^{\infty} \mathrm{d}t C(t;\alpha),$$

$$C(t;\alpha) = \frac{1}{2}\mathrm{Tr}\big[\hat{\mathcal{F}}(\alpha)\mathrm{e}^{-\hat{\mathcal{H}}(\tau-\mathrm{i}t)/\hbar}\hat{\mathcal{F}}(\alpha)\mathrm{e}^{-\hat{\mathcal{H}}(\beta\hbar-\tau+\mathrm{i}t)/\hbar}\big].$$

$$\begin{aligned}c(t;\alpha) = \mathrm{Tr}\big[&\hat{\mathcal{F}}(\alpha)\mathrm{e}^{-\hat{\mathcal{H}}(\tau-\mathrm{i}t)/2\hbar}\hat{\mathcal{P}}_{\mathrm{R}}(\alpha)\mathrm{e}^{-\hat{\mathcal{H}}(\tau-\mathrm{i}t)/2\hbar} \\ &\times \hat{\mathcal{F}}(\alpha)\mathrm{e}^{-\hat{\mathcal{H}}(\beta\hbar-\tau+\mathrm{i}t)/2\hbar}\hat{\mathcal{P}}_{\mathrm{P}}(\alpha)\mathrm{e}^{-\hat{\mathcal{H}}(\beta\hbar-\tau+\mathrm{i}t)/2\hbar}\big].\end{aligned}$$

$$c(t;\alpha) = c_{\mathrm{nn}}(t;\alpha) + c_{\mathrm{ne}}(t;\alpha) + c_{\mathrm{en}}(t;\alpha) + c_{\mathrm{ee}}(t;\alpha).$$

$$\begin{aligned}c_{\gamma'\gamma''}(t;\alpha) = \mathrm{Tr}\big[&\hat{\mathcal{F}}_{\gamma'}\mathrm{e}^{-\hat{\mathcal{H}}(\tau-\mathrm{i}t)/2\hbar}\hat{\mathcal{P}}_{\mathrm{R}}\mathrm{e}^{-\hat{\mathcal{H}}(\tau-\mathrm{i}t)/2\hbar} \\ &\times \hat{\mathcal{F}}_{\gamma''}\mathrm{e}^{-\hat{\mathcal{H}}(\beta\hbar-\tau+\mathrm{i}t)/2\hbar}\hat{\mathcal{P}}_{\mathrm{P}}\mathrm{e}^{-\hat{\mathcal{H}}(\beta\hbar-\tau+\mathrm{i}t)/2\hbar}\big],\end{aligned}$$

$$Z = \mathrm{Tr}\big[\mathrm{e}^{-\beta\hat{\mathcal{H}}}\big].$$

$$Z = \lim_{N\to\infty} \Lambda^{-N} \int \mathrm{d}\mathbf{x}\mathrm{e}^{-S(\mathbf{x})/\hbar}$$

$$\Lambda = \sqrt{2\pi\beta_N\hbar^2/m}$$

$$S(\mathbf{x}) = S_{\mathrm{free}}(\mathbf{x}) - \hbar\ln\left(\mathrm{Tr}[\mathbf{M}_0\mathbf{M}_1 \ldots \mathbf{M}_{N-1}]\right)$$

$$S_{\mathrm{free}}(\mathbf{x}) = \sum_{i=1}^{N} \frac{m}{2\beta_N\hbar}|x_i - x_{i-1}|^2$$

$$\mathbf{M}_i = \mathrm{e}^{-\beta_N\mathbf{V}(x_i)}$$

$$Z \sim \Lambda^{-N}\sqrt{\frac{(2\pi\hbar)^N}{\det_N \nabla^2 S}}\mathrm{e}^{-S(\tilde{\mathbf{x}})/\hbar}$$

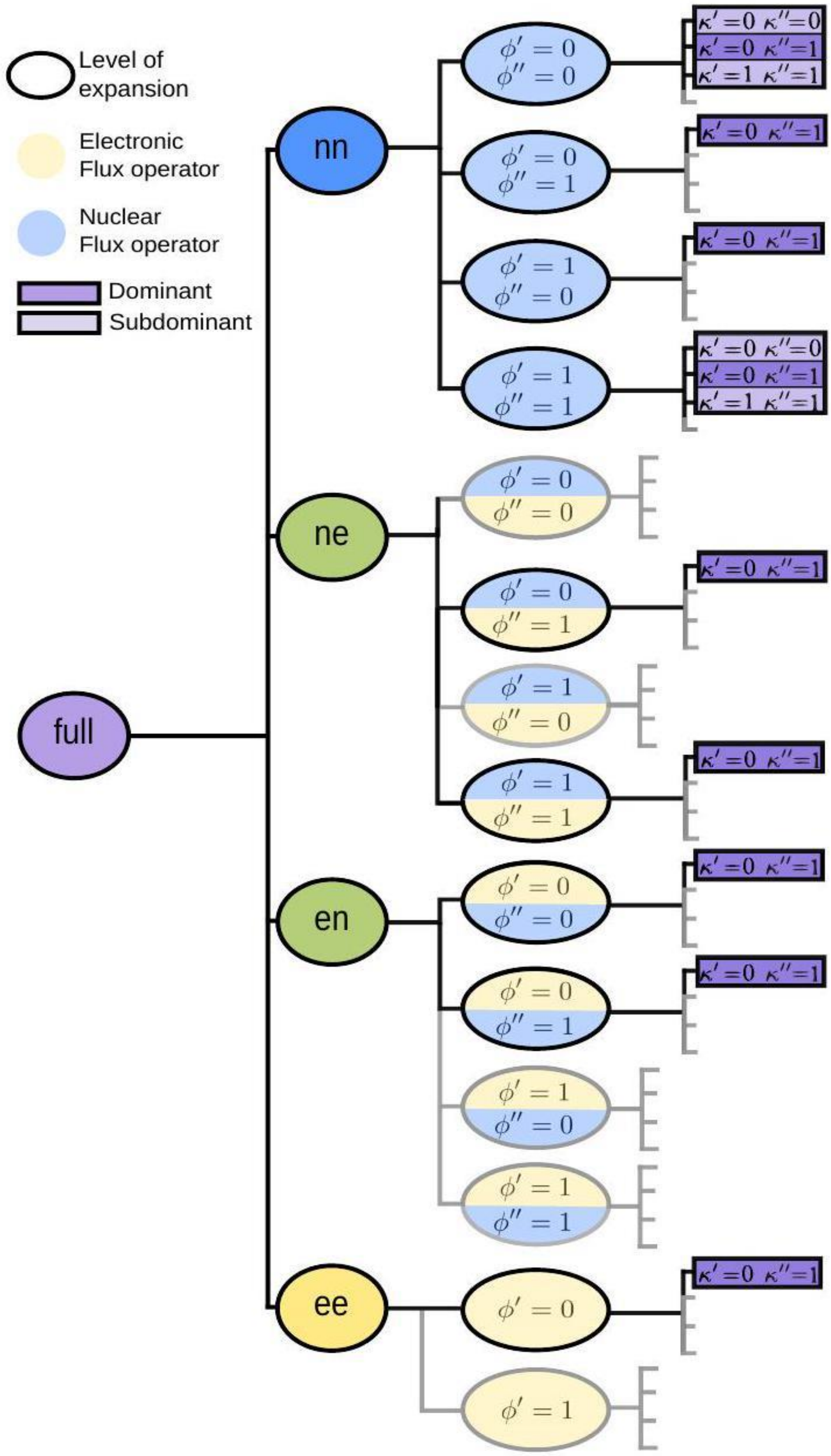
$$P_\delta(x_\alpha) = \mathrm{Tr}\left[\mathrm{e}^{-\tau\hat{\mathcal{H}}/\hbar}\delta(\hat{x} - x_\alpha)\mathrm{e}^{-(\beta\hbar-\tau)\hat{\mathcal{H}}/\hbar}\right].$$

$$P_\delta(x_\alpha) = \Lambda^{-N}\int \mathrm{d}\mathbf{x}\mathrm{e}^{-S(\mathbf{x})/\hbar}\delta\left(x_{N_\tau} - x_\alpha\right)$$

$$P_\delta(x_\alpha) \sim \Lambda^{-N}\sqrt{\frac{(2\pi\hbar)^{N-1}}{\det_{N-1}\nabla^2 S}}\mathrm{e}^{-S(\tilde{\mathbf{x}})/\hbar}$$

$$S(\mathbf{x}) = S_{\text{free}}(\mathbf{x}) - \hbar\ln\left(\mathrm{Tr}\left[\mathbf{M}_0^{1/2}\hat{\mathcal{F}}_\mathrm{e}^{\phi'}\mathbf{M}_0^{1/2}\mathbf{M}_1\cdots \mathbf{M}_{N_\tau/2}^{1/2}\hat{\mathcal{P}}_\mathrm{e}^{\kappa'}\mathbf{M}_{N_\tau/2}^{1/2}\cdots\mathbf{M}_{N_\tau}^{1/2}\hat{\mathcal{F}}_\mathrm{e}^{\phi''}\mathbf{M}_{N_\tau}^{1/2}\cdots \mathbf{M}_{(N_\tau+N)/2}^{1/2}\hat{\mathcal{P}}_\mathrm{e}^{\kappa''}\mathbf{M}_{(N_\tau+N)/2}^{1/2}\cdots\mathbf{M}_{N-1}\right]\right)$$

$$\mathbf{M}_i^{1/2} = \mathrm{e}^{-\beta_N\mathbf{V}(x_i)/2}$$



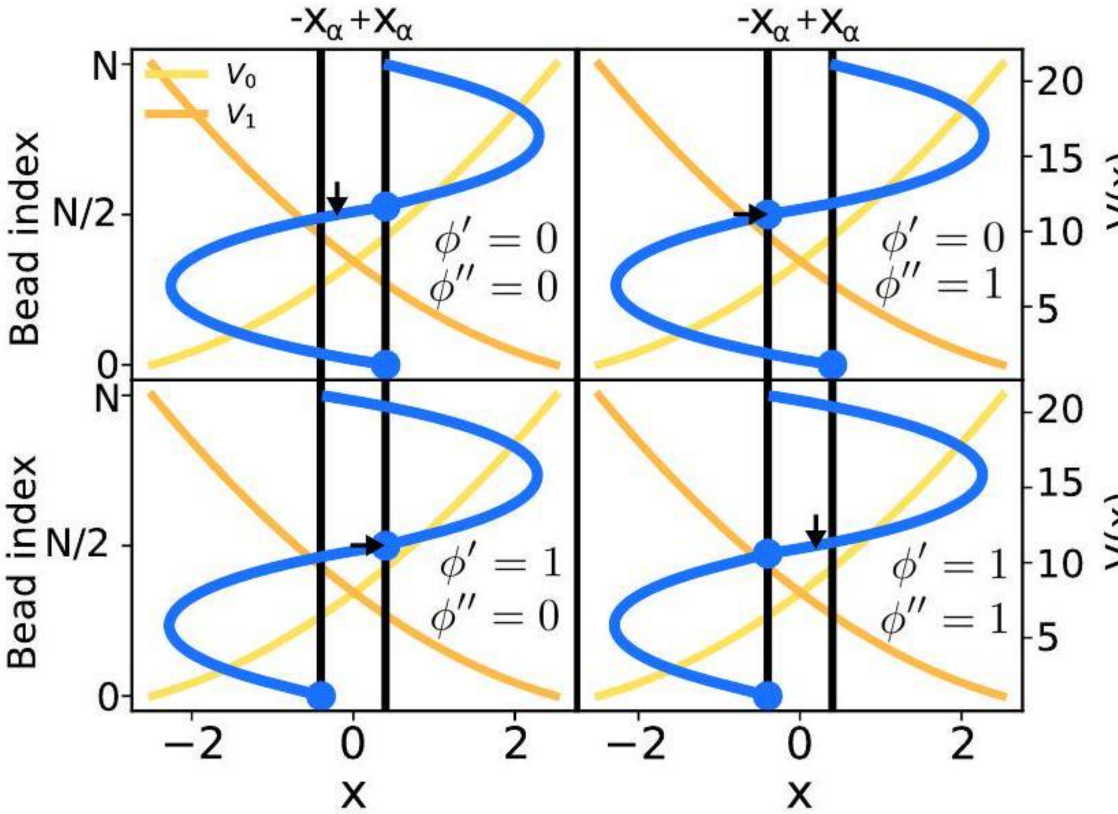
$$c_{\gamma'\gamma''}(t) = \sum_{\phi'\phi''\kappa'\kappa''} c_{\gamma'\gamma''}^{\phi'\phi''\kappa'\kappa''}(t),$$

$$c_{\text{ee}}(t) = \sum_{\phi'\kappa'\kappa''} c_{\text{ee}}^{\phi'\kappa'\kappa''}(t).$$

$$c_{\mathrm{nn}}^{\phi'\phi''\kappa'\kappa''}(t) = \mathrm{Tr}\left[\hat{\mathcal{F}}_{\mathrm{n}}^{\phi'}\hat{\mathcal{P}}_{\mathrm{e}}^{\phi'}\hat{K}'\hat{\mathcal{P}}_{\mathrm{R}}^{\kappa'}\hat{K}'\hat{\mathcal{F}}_{\mathrm{n}}^{\phi''}\hat{\mathcal{P}}_{\mathrm{e}}^{\phi''}\hat{K}''\hat{\mathcal{P}}_{\mathrm{P}}^{\kappa''}\hat{K}''\right],$$

$$\hat{K}' = \mathrm{e}^{-\hat{\mathcal{H}}(\tau-\mathrm{i}t)/2\hbar}$$

$$\hat{K}'' = \mathrm{e}^{-\hat{\mathcal{H}}(\beta\hbar-\tau+\mathrm{i}t)/2\hbar}$$



$$\hat{\mathcal{F}}_{\mathrm{e}}^{0} = -\hat{\mathcal{F}}_{\mathrm{e}}^{1}$$

$$\hat{\mathcal{F}}_{\mathrm{e}} = \hat{\mathcal{F}}_{\mathrm{e}}^{0}\hat{\mathcal{P}}_{\mathrm{n}}^{0} + \hat{\mathcal{F}}_{\mathrm{e}}^{1}\hat{\mathcal{P}}_{\mathrm{n}}^{1} = \hat{\mathcal{F}}_{\mathrm{e}}^{1}\left(\hat{\mathcal{P}}_{\mathrm{n}}^{1} - \hat{\mathcal{P}}_{\mathrm{n}}^{0}\right)$$

$$c_{\mathrm{ne}}^{\phi'\phi''\kappa'\kappa''}(t) = (-1)^{\phi''}\frac{\mathrm{i}\Delta}{\hbar}\mathrm{Tr}\left[\hat{\mathcal{F}}_{\mathrm{n}}^{\phi'}\hat{\mathcal{P}}_{\mathrm{e}}^{\phi'}\hat{K}'\hat{\mathcal{P}}_{\mathrm{R}}^{\kappa'}\hat{K}'\right.$$
$$\left.\times\,|\bar{\phi}''\rangle\langle\phi''|\left(\hat{\mathcal{P}}_{\mathrm{n}}^{1} - \hat{\mathcal{P}}_{\mathrm{n}}^{0}\right)\hat{K}''\hat{\mathcal{P}}_{\mathrm{P}}^{\kappa''}\hat{K}''\right]$$

$$c_{\mathrm{ee}}^{\phi'\kappa'\kappa''}(t) = \frac{\Delta^2}{\hbar^2}\mathrm{Tr}\left[|\bar{\phi}'\rangle\langle\phi'|\left(\hat{\mathcal{P}}_{\mathrm{n}}^{1} - \hat{\mathcal{P}}_{\mathrm{n}}^{0}\right)\hat{K}'\hat{\mathcal{P}}_{\mathrm{R}}^{\kappa'}\hat{K}'\right.$$
$$\left.\times\left(|\phi'\rangle\langle\bar{\phi}'| - |\bar{\phi}'\rangle\langle\phi'|\right)\left(\hat{\mathcal{P}}_{\mathrm{n}}^{1} - \hat{\mathcal{P}}_{\mathrm{n}}^{0}\right)\hat{K}''\hat{\mathcal{P}}_{\mathrm{P}}^{\kappa''}\hat{K}''\right]$$

$$kZ_{\mathrm{R}} \sim \sum_{\chi}\sqrt{2\pi\hbar}\left(-\frac{\mathrm{d}^2 S^{\chi}}{\mathrm{d}\tau^2}\right)^{-1/2} c^{\chi}(0)$$

$$V_0(x) = \begin{cases}\frac{1}{2}m\omega^2(x+x_0)^2 & \text{for } x > -x_0\\ 0 & \text{otherwise}\end{cases}$$
$$V_1(x) = \begin{cases}\frac{1}{2}m\omega^2(x-x_0)^2 & \text{for } x < x_0\\ 0 & \text{otherwise}\end{cases}$$

$$P_\Theta(x_\alpha) = \mathrm{Tr}\left[\mathrm{e}^{-\tau\hat{\mathcal{H}}/\hbar}\Theta(\hat{x} - x_\alpha)\mathrm{e}^{-(\beta\hbar-\tau)\hat{\mathcal{H}}/\hbar}\right]$$
$$= \Lambda^{-N}\int \mathrm{d}\mathbf{x}\mathrm{e}^{-S(\mathbf{x})/\hbar}\Theta\left(x_{N_\tau} - x_\alpha\right)$$

$$P_\Theta(x_\alpha) \sim \Lambda^{-N}\sqrt{\frac{(2\pi\hbar)^{N-1}}{\det_{N-1}\nabla^2 S}}\mathrm{e}^{-S(\tilde{\mathbf{x}})/\hbar}$$
$$\times \int \mathrm{d}x_{N_\tau}\Theta\left(x_{N_\tau} - x_\alpha\right)\exp\left(-\frac{\left(x_{N_\tau} - \tilde{x}_{N_\tau}\right)^2}{2\sigma^2}\right)$$

$$x_{N_\tau}\sigma^2 = \hbar\left(\left.\frac{\mathrm{d}^2 S}{\mathrm{d}x_{N_\tau}^2}\right|_{x_{N_\tau}=\tilde{x}_{N_\tau}}\right)^{-1}$$

$$\int_{L_A}^{L_B} \mathrm{d}x\mathrm{e}^{-\frac{(x-\mu)^2}{2\sigma^2}}$$
$$= \frac{\sqrt{2\pi\sigma^2}}{2}\left(\mathrm{erf}\left(\frac{L_B - \mu}{\sqrt{2\sigma^2}}\right) - \mathrm{erf}\left(\frac{L_A - \mu}{\sqrt{2\sigma^2}}\right)\right)$$

$$g = \left.\frac{\partial S\left(x_{N_\tau}, \mathbf{x}'\right)}{\partial x_{N_\tau}}\right|_{\tilde{x}_{N_\tau},\tilde{\mathbf{x}}'}$$

$$\mathbf{H} = \left.\begin{pmatrix} \frac{\partial^2 S\left(x_{N_\tau}, \mathbf{x}'\right)}{\partial x_{N_\tau}^2} & \frac{\partial^2 S\left(x_{N_\tau}, \mathbf{x}'\right)}{\partial x_{N_\tau}\partial \mathbf{x}'} \\ \frac{\partial^2 S\left(x_{N_\tau}, \mathbf{x}'\right)}{\partial \mathbf{x}'\partial x_{N_\tau}} & \frac{\partial^2 S\left(x_{N_\tau}, \mathbf{x}'\right)}{\partial \mathbf{x}'\partial \mathbf{x}'} \end{pmatrix}\right|_{\tilde{x}_{N_\tau},\tilde{\mathbf{x}}'}$$

$$S\left(x_{N_\tau}, \mathbf{x}'\right) \sim \tilde{S} + g\Delta x_{N_\tau} + \frac{1}{2}\begin{pmatrix}\Delta x_{N_\tau} \\ \Delta \mathbf{x}'\end{pmatrix}^T \mathbf{H}\begin{pmatrix}\Delta x_{N_\tau} \\ \Delta \mathbf{x}'\end{pmatrix}$$

$$\Delta x_{N_\tau} = x_{N_\tau} - \tilde{x}_{N_\tau}$$

$$\Delta \mathbf{x}' = \mathbf{x}' - \tilde{\mathbf{x}}'$$

$$P_\Theta(x_\alpha) \sim \int_{x_\alpha}^{\infty} \mathrm{d}x_{N_\tau}\int_{-\infty}^{\infty} \mathrm{d}\mathbf{x}'\mathrm{e}^{-\tilde{S}/\hbar - g\Delta x_{N_\tau}/\hbar}$$
$$\times\ \mathrm{e}^{-\frac{1}{2\hbar}\left(\Delta x_{N_\tau}H_{11}\Delta x_{N_\tau} + \Delta\mathbf{x}'\mathbf{H}_{22}\Delta\mathbf{x}' + \Delta x_{N_\tau}\mathbf{H}_{12}\Delta\mathbf{x}' + \Delta\mathbf{x}'\mathbf{H}_{21}\Delta x_{N_\tau}\right)}$$
$$= \sqrt{\frac{(2\pi\hbar)^{N-1}}{\det_{N-1}\mathbf{H}_{22}}}\mathrm{e}^{-\tilde{S}/\hbar}$$
$$\times \int_{x_\alpha}^{\infty} \mathrm{d}x_{N_\tau}\mathrm{e}^{-\frac{1}{\hbar}g\Delta x_{N_\tau} - \frac{1}{2\hbar}\Delta x_{N_\tau}\left(H_{11} - \mathbf{H}_{12}\mathbf{H}_{22}^{-1}\mathbf{H}_{21}\right)\Delta x_{N_\tau}}$$

$$P_{\Theta,\Theta}(x_\alpha, x_\alpha) =$$
$$\Lambda^{-N}\int \mathrm{d}\mathbf{x}\mathrm{e}^{-S(\mathbf{x})/\hbar}\Theta(x_0 - x_\alpha)\Theta\left(x_{N_\tau} - x_\alpha\right)$$

$$p_0 = \frac{\partial S}{\partial x_0}\bigg|_{\tilde{x}} = m\frac{\tilde{x}_0 - \tilde{x}_1}{\beta_N \hbar},$$

$$c_{\rm nn}^{1,1,0,0}(t) = \mathrm{Tr}\left[\hat{\mathcal{F}}_{\rm n}^1 \hat{\mathcal{P}}_{\rm e}^1 \hat{K}' \hat{\mathcal{P}}_{\rm R}^0 \hat{K}' \hat{\mathcal{F}}_{\rm n}^1 \hat{\mathcal{P}}_{\rm e}^1 \hat{K}'' \hat{\mathcal{P}}_{\rm P}^0 \hat{K}''\right].$$

$$c_{\rm nn}^{1,1,0,0}(t) = \frac{1}{4m^2}\Big(\mathrm{Tr}\left[\delta(\hat{x}+x_\alpha)\hat{p}\hat{\mathcal{P}}_{\rm e}^1\hat{K}'\hat{\mathcal{P}}_{\rm R}^0\hat{K}'\hat{p}\delta(\hat{x}+x_\alpha)\hat{\mathcal{P}}_{\rm e}^1\hat{K}''\hat{\mathcal{P}}_{\rm P}^0\hat{K}''\right]$$

$$+\mathrm{Tr}\left[\delta(\hat{x}+x_\alpha)\hat{p}\hat{\mathcal{P}}_{\rm e}^1\hat{K}'\hat{\mathcal{P}}_{\rm R}^0\hat{K}'\delta(\hat{x}+x_\alpha)\hat{p}\hat{\mathcal{P}}_{\rm e}^1\hat{K}''\hat{\mathcal{P}}_{\rm P}^0\hat{K}''\right]$$
$$+\mathrm{Tr}\left[\hat{p}\delta(\hat{x}+x_\alpha)\hat{\mathcal{P}}_{\rm e}^1\hat{K}'\hat{\mathcal{P}}_{\rm R}^0\hat{K}'\hat{p}\delta(\hat{x}+x_\alpha)\hat{\mathcal{P}}_{\rm e}^1\hat{K}''\hat{\mathcal{P}}_{\rm P}^0\hat{K}''\right]$$
$$+\mathrm{Tr}\left[\hat{p}\delta(\hat{x}+x_\alpha)\hat{\mathcal{P}}_{\rm e}^1\hat{K}'\hat{\mathcal{P}}_{\rm R}^0\hat{K}'\delta(\hat{x}+x_\alpha)\hat{p}\hat{\mathcal{P}}_{\rm e}^1\hat{K}''\hat{\mathcal{P}}_{\rm P}^0\hat{K}''\right]\Big)$$

$$\mathrm{Tr}\left[\delta(\hat{x}+x_\alpha)\hat{p}\hat{\mathcal{P}}_{\rm e}^1\hat{K}'\hat{\mathcal{P}}_{\rm R}^0\hat{K}'\hat{p}\delta(\hat{x}+x_\alpha)\hat{\mathcal{P}}_{\rm e}^1\hat{K}''\hat{\mathcal{P}}_{\rm P}^0\hat{K}''\right]$$
$$\sim \hbar^2 \frac{\mathrm{d}}{\mathrm{d}x_0}\frac{\mathrm{d}}{\mathrm{d}x_{N_\tau}} I_1 I_2$$

$$\mathbf{x}' = \left\{x_1, \dots x_{N_\tau/2-1}, x_{N_\tau/2+1}, \dots x_{N_\tau-1}, x_{N_\tau+1}, \dots x_{(N_\tau+N)/2-1}, x_{(N_\tau+N)/2+1}, \dots, x_{N-1}\right\}$$

$$I_1 = \int_{-\infty}^{x_\alpha} \mathrm{d}x_{N_\tau/2} \int_{x_\alpha}^{\infty} \mathrm{d}x_{(N+N_\tau)/2} \mathrm{e}^{-g\Delta x_{(N+N_\tau)/2}/\hbar} \mathrm{e}^{-\frac{1}{2\hbar}\Delta x_{N_\tau/2}^2 (H_{11} - \mathbf{H}_{12}\mathbf{H}_{22}^{-1}\mathbf{H}_{21})},$$

$$g = \frac{\partial S}{\partial x_{(N+N_\tau)/2}}\bigg|_{\tilde{x}} H_{11} = \frac{\partial^2 S}{\partial x_{N_\tau/2}^2} \mathbf{H}_{12} = \frac{\partial^2 S}{\partial x_{N_\tau/2}\partial \mathbf{x}'} \mathbf{H}_{21} = \frac{\partial^2 S}{\partial \mathbf{x}' \partial x_{N_\tau/2}}. \mathbf{H}_{22}$$

$$I_2 = \mathrm{e}^{-S(\tilde{\mathbf{x}})/\hbar} \int_{-\infty}^{\infty} \mathrm{d}\mathbf{x}' \mathrm{e}^{-\frac{1}{2\hbar}\Delta \mathbf{x}' \mathbf{H}_{22} \Delta \mathbf{x}'}$$

$$\hbar^2 \frac{\mathrm{d}}{\mathrm{d}x_0}\frac{\mathrm{d}}{\mathrm{d}x_{N_\tau}} I_1 I_2 \sim \frac{\mathrm{d}S}{\mathrm{d}x_0}\frac{\mathrm{d}S}{\mathrm{d}x_{N_\tau}} I_1 I_2 - \hbar \frac{\mathrm{d}S}{\mathrm{d}x_0}\frac{\mathrm{d}I_1}{\mathrm{d}x_{N_\tau}} I_2 - \hbar \frac{\mathrm{d}S}{\mathrm{d}x_{N_\tau}}\frac{\mathrm{d}I_1}{\mathrm{d}x_0} I_2 - \hbar \frac{\mathrm{d}^2 S}{\mathrm{d}x_0\, \mathrm{d}x_{N_\tau}} I_1 I_2 + \hbar^2 \frac{\mathrm{d}^2 I_1}{\mathrm{d}x_0\, \mathrm{d}x_{N_\tau}} I_2$$

$$\hbar \frac{\mathrm{d}I_1}{\mathrm{d}x_0} \sim -\left(\frac{\mathrm{d}g}{\mathrm{d}x_0}\right) \int_{-\infty}^{x_\alpha} \mathrm{d}x_{N_\tau/2} \int_{x_\alpha}^{\infty} \mathrm{d}x_{(N+N_\tau)/2} \Delta_{x_{(N+N_\tau)/2}} \mathrm{e}^{-g\Delta x_{(N+N_\tau)/2}/\hbar - \frac{1}{2\hbar}\Delta x_{N_\tau/2}^2 (H_{11} - \mathbf{H}_{12}\mathbf{H}_{22}^{-1}\mathbf{H}_{21})}.$$

$$\hbar^2 \frac{\mathrm{d}^2 I_1}{\mathrm{d}x_0\, \mathrm{d}x_{N_\tau}} \sim \left(\frac{\mathrm{d}g}{\mathrm{d}x_0}\right)\left(\frac{\mathrm{d}g}{\mathrm{d}x_{N_\tau}}\right) \int_{-\infty}^{x_\alpha} \mathrm{d}x_{N_\tau/2} \int_{x_\alpha}^{\infty} \mathrm{d}x_{(N+N_\tau)/2} \Delta_{x_{(N+N_\tau)/2}}^2 \mathrm{e}^{-g\Delta x_{(N+N_\tau)/2}/\hbar - \frac{1}{2\hbar}\Delta x_{N_\tau/2}^2 (H_{11} - \mathbf{H}_{12}\mathbf{H}_{22}^{-1}\mathbf{H}_{21})},$$

$$\frac{\mathrm{d}^2 g}{\mathrm{d}x_0\, \mathrm{d}x_{N_\tau}}$$

$$\frac{\mathrm{d}}{\mathrm{d}x_0}\frac{\partial S}{\partial x_{(N+N_\tau)/2}} = \frac{\partial^2 S}{\partial x_0 \partial x_{(N+N_\tau)/2}} + \frac{\partial^2 S}{\partial x_0 \partial \mathbf{x}'}\frac{\mathrm{d}\mathbf{x}'}{\mathrm{d}x_0}.$$

$$\frac{\mathrm{d}\mathbf{x}'}{\mathrm{d}x_0}$$

$$\frac{\partial^2 S}{\partial \mathbf{x}'^2}\frac{\mathrm{d}\mathbf{x}'}{\mathrm{d}x_0} = -\frac{\partial^2 S}{\partial x_0 \partial \mathbf{x}'}.$$

$$H_{SR} = -a_0 \frac{g\alpha^2}{2m_e} \sum_A \sum_i \frac{Z_A}{|\hat{\boldsymbol{r}}_i - \boldsymbol{R}_A|^3} \left((\hat{\boldsymbol{r}}_i - \boldsymbol{R}_A) \times \left(\frac{1}{M_A} \boldsymbol{P}_A \right) \right) \cdot \hat{\boldsymbol{s}}_i$$

$$H_{\text{SO}}^{(1)} = a_0 \frac{g\alpha^2}{4m_e^2} \sum_A \sum_i \frac{Z_A}{|\hat{\boldsymbol{r}}_i - \boldsymbol{R}_A|^3} ((\hat{\boldsymbol{r}}_i - \boldsymbol{R}_A) \times \hat{\boldsymbol{p}}_i) \cdot \hat{\boldsymbol{s}}_i$$

$$H_{\text{SO}}^{(2)} = -a_0 \frac{g\alpha^2}{4m_e^2} \sum_{ij} \frac{1}{|\hat{\boldsymbol{r}}_i - \hat{\boldsymbol{r}}_j|^3} \left((\hat{\boldsymbol{r}}_i - \hat{\boldsymbol{r}}_j) \times \hat{\boldsymbol{p}}_i \right) \cdot \hat{s}_i$$

$$H_{\text{SOO}}^{(2)} = a_0 \frac{g\alpha^2}{2m_e^2} \sum_{ij} \frac{1}{|\hat{\boldsymbol{r}}_i - \hat{\boldsymbol{r}}_j|^3} \left((\hat{\boldsymbol{r}}_i - \hat{\boldsymbol{r}}_j) \times \hat{\boldsymbol{p}}_j \right) \cdot \hat{\boldsymbol{s}}_i$$

$$H_{\text{SR}} = \omega \cdot \hat{\boldsymbol{j}} = \omega \cdot (\hat{\boldsymbol{l}} + \hat{\boldsymbol{s}})$$

$$\omega = \frac{|\boldsymbol{P}|}{M|\boldsymbol{R}|}$$

$$\hat{H}_{\text{Shenvi}}(\boldsymbol{R}, \boldsymbol{P}) = \sum_{A,ijk} \frac{1}{2M_A} (\boldsymbol{P}_A \delta_{ij} - \boldsymbol{d}_{ij}^A) \cdot (\boldsymbol{P}_A \delta_{jk} - \boldsymbol{d}_{jk}^A) |\Phi_i\rangle\langle\Phi_k| + \sum_i E_i(\{\boldsymbol{R}\}) |\Phi_i\rangle\langle\Phi_i|.$$

$$\hat{H}_{el} |\Phi_i\rangle = E_i |\Phi_i\rangle$$

$$\boldsymbol{d}_{ij}^A = \langle \Phi_i | \frac{\partial}{\partial \boldsymbol{R}_a} | \Phi_j \rangle$$

$$-i\hbar \sum_A \boldsymbol{d}_{jk}^A + \langle \Phi_j | \hat{\boldsymbol{p}} | \Phi_k \rangle = 0,$$

$$\sum_A \boldsymbol{\nabla}_A \boldsymbol{d}_{jk}^B = 0$$

$$-i\hbar \sum_A \boldsymbol{R}_A \times \boldsymbol{d}_{jk}^A + \langle \Phi_j | \hat{\boldsymbol{l}} | \Phi_k \rangle = 0,$$

$$-\sum_A \left(\boldsymbol{R}_A \times \boldsymbol{\nabla}_A \boldsymbol{d}_{jk}^{B\beta} \right)_\alpha = \sum_\gamma \epsilon_{\alpha\beta\gamma} \boldsymbol{d}_{jk}^{B\gamma},$$

$$\left[\hat{H}_{el}, \hat{\boldsymbol{p}} - i\hbar \sum_A \boldsymbol{\nabla}_A \right] = 0$$

$$\left[\hat{H}_{el}, \hat{\boldsymbol{l}} - i\hbar \sum_A \boldsymbol{R}_A \times \boldsymbol{\nabla}_A \right] = 0$$

$$\hat{H}_{\text{PS}}(\boldsymbol{R}, \boldsymbol{P}) = \sum_A \frac{1}{2M_A} \left(\boldsymbol{P}_A - i\hbar \hat{\boldsymbol{\Gamma}}_A(\{\boldsymbol{R}\}) \right)^2 + \hat{H}_{el}(\{\boldsymbol{R}\}).$$

If the $\hat{\boldsymbol{\Gamma}}$ operator satisfies the analogues of Eqs. 7-10,

$$-i\hbar\sum_A \hat{\boldsymbol{\Gamma}}_A + \hat{\boldsymbol{p}} = 0,$$

$$\left[-i\hbar\sum_B \frac{\partial}{\partial \boldsymbol{R}_B} + \hat{\boldsymbol{p}}, \hat{\boldsymbol{\Gamma}}_A\right] = 0,$$

$$-i\hbar\sum_A \boldsymbol{R}_A \times \hat{\boldsymbol{\Gamma}}_A + \hat{\boldsymbol{l}} = 0,$$

$$\left[-i\hbar\sum_B \left(\boldsymbol{R}_B \times \frac{\partial}{\partial \boldsymbol{R}_B}\right)_\gamma + \hat{\boldsymbol{l}}_\gamma, \hat{\boldsymbol{\Gamma}}_{A\delta}\right] = i\hbar\sum_\alpha \epsilon_{\alpha\gamma\delta}\hat{\boldsymbol{\Gamma}}_{A\alpha},$$

$$\hat{\boldsymbol{p}} \equiv \sum_i \hat{\boldsymbol{p}}_i$$

$$\hat{\boldsymbol{l}}_\gamma \hat{\boldsymbol{\Gamma}}_{A\delta} = \sum_i \boldsymbol{l}_\gamma(\hat{\boldsymbol{r}}_i)\boldsymbol{\Gamma}_{A\delta}(\hat{\boldsymbol{r}}_i)$$

$$\hat{\boldsymbol{\Gamma}} = \hat{\boldsymbol{\Gamma}}' + \hat{\boldsymbol{\Gamma}}''$$

$$\hat{\boldsymbol{\Gamma}}'_A = \frac{-i}{2\hbar}\left(\theta_A(\hat{\boldsymbol{r}})\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\theta_A(\hat{\boldsymbol{r}})\right)$$

$$\hat{\boldsymbol{\Gamma}}''_A = \sum_B \zeta_{AB}(\boldsymbol{R}_A - \boldsymbol{R}_B^0) \times \left(\boldsymbol{K}_B^{-1}\hat{\boldsymbol{J}}_B\right)$$

$$\hat{\boldsymbol{J}}_B = \hat{\boldsymbol{J}}_B^{(l)} = \frac{-i}{2\hbar}\left((\hat{\boldsymbol{r}} - \boldsymbol{R}_B) \times (\theta_B(\hat{\boldsymbol{r}})\hat{\boldsymbol{p}}) + (\theta_B(\hat{\boldsymbol{r}})\hat{\boldsymbol{p}}) \times (\hat{\boldsymbol{r}} - \boldsymbol{R}_B)\right)$$

$$\boldsymbol{R}_B^0 = \frac{\sum_A \zeta_{AB}\boldsymbol{R}_B}{\sum_A \zeta_{AB}}$$

$$\boldsymbol{K}_B = \sum_A \zeta_{AB}\left(\boldsymbol{R}_A\boldsymbol{R}_A^T - \boldsymbol{R}_B^0\boldsymbol{R}_B^{0T} - (\boldsymbol{R}_A\boldsymbol{R}_A^T - \boldsymbol{R}_B^{0T}\boldsymbol{R}_B^0)\mathcal{I}_3\right),$$

$$\theta_A(\hat{\boldsymbol{r}}) = \frac{Z_A e^{-(\hat{\boldsymbol{r}} - \boldsymbol{R}_A)^2/\sigma^2}}{\sum_B Z_B e^{-(\hat{\boldsymbol{r}} - \boldsymbol{R}_B)^2/\sigma^2}}$$

$$\zeta_{AB} = M_A e^{-(\boldsymbol{R}_A - \boldsymbol{R}_B)^2/8\sigma^2}$$

$$\sum_A \frac{1}{2M_A}\left(\boldsymbol{P}_A - i\hbar\hat{\boldsymbol{\Gamma}}_A(\{\boldsymbol{R}\})\right)^2 = \sum_A \frac{|\boldsymbol{P}_A|^2}{2M_{tot}} - \frac{1}{M_{tot}}\sum_A \boldsymbol{P}_A \cdot \hat{\boldsymbol{p}} + \frac{|\hat{\boldsymbol{p}}|^2}{2M_{tot}}$$

$$-\sum_A \frac{1}{M_A}\left((\boldsymbol{R}_A - \boldsymbol{R}_{\mathrm{CM}}) \times \boldsymbol{P}_A\right) \cdot \boldsymbol{K}_{\mathrm{CM}}^{-1} \cdot \left(\hat{\boldsymbol{l}}_{\mathrm{CM}}\right)$$

$$+\frac{1}{2}\hat{\boldsymbol{l}}_{\mathrm{CM}} \cdot \boldsymbol{K}_{\mathrm{CM}}^{-1} \cdot \hat{\boldsymbol{l}}_{\mathrm{CM}}$$

$$-i\hbar\sum_A \boldsymbol{R}_A \times \hat{\boldsymbol{\Gamma}}_A + \hat{\boldsymbol{l}} + \hat{\boldsymbol{s}} = 0$$

$$\left[-i\hbar\sum_B \left(\boldsymbol{R}_B \times \frac{\partial}{\partial \boldsymbol{R}_B}\right)_\gamma + \hat{\boldsymbol{l}}_\gamma + \hat{\boldsymbol{s}}_\gamma, \hat{\boldsymbol{\Gamma}}_{A\delta}\right] = i\hbar\sum_\alpha \epsilon_{\alpha\gamma\delta}\hat{\boldsymbol{\Gamma}}_{A\alpha}$$

$$\hat{\boldsymbol{J}}_B = \frac{-i}{2\hbar}\left((\hat{\boldsymbol{r}} - \boldsymbol{R}_B) \times (\theta_B(\hat{\boldsymbol{r}})\hat{\boldsymbol{p}}) + (\theta_B(\hat{\boldsymbol{r}})\hat{\boldsymbol{p}}) \times (\hat{\boldsymbol{r}} - \boldsymbol{R}_B) + 2\theta_B(\hat{\boldsymbol{r}})\hat{\boldsymbol{s}}\right)$$
$$\equiv \hat{\boldsymbol{J}}_B^{(l)} + \hat{\boldsymbol{J}}_B^{(s)}$$
$$\hat{\boldsymbol{J}}_B^{(s)} = -\frac{i}{\hbar}\theta_B(\hat{\boldsymbol{r}})\hat{\boldsymbol{s}}$$

$$\hat{\boldsymbol{\Gamma}}_A''^{(s)} \equiv \sum_B \zeta_{AB}(\boldsymbol{R}_A - \boldsymbol{R}_B^0) \times \left(\boldsymbol{K}_B^{-1}\hat{\boldsymbol{J}}_B^{(s)}\right)$$

$$-i\hbar\boldsymbol{P} \cdot \hat{\boldsymbol{\Gamma}}_A''^{(s)}/M$$

$$\hat{H}_{\mathrm{PS}}\psi = E_{PS}\psi$$

$$E_{PS} = \langle\psi|\hat{H}_{\mathrm{PS}}|\psi\rangle$$

$$\frac{\partial E_{PS}}{\partial \boldsymbol{R}} = 0$$
$$\frac{\partial E_{PS}}{\partial \boldsymbol{P}} = 0$$

$$H = \boldsymbol{P}^2/2M + V$$

$$\dot{\boldsymbol{R}} = \frac{\partial E_{PS}}{\partial \boldsymbol{P}}$$

$$\sum_A \frac{\partial E_{\mathrm{PS}}}{\partial \boldsymbol{P}_A} = \sum_A \frac{\boldsymbol{P}_A}{M_A} - \frac{i\hbar\langle\hat{\boldsymbol{\Gamma}}_A\rangle}{M_A}$$

$$\boldsymbol{P}_A^{\min} = i\hbar\langle\hat{\boldsymbol{\Gamma}}_A\rangle,$$

$$\langle\hat{\boldsymbol{p}}\rangle = i\hbar\sum_A \langle\hat{\boldsymbol{\Gamma}}_A\rangle = \sum_A \boldsymbol{P}_A^{\min}$$
$$\langle\hat{\boldsymbol{l}} + \hat{\boldsymbol{s}}\rangle = i\hbar\sum_A \langle\boldsymbol{R}_A \times \hat{\boldsymbol{\Gamma}}_A\rangle = \sum_A \boldsymbol{R}_A^{\min} \times \boldsymbol{P}_A^{\min}$$

$$\boldsymbol{P}/M = \boldsymbol{v}\langle\phi_A|\hat{\theta}_A|\phi_B\rangle\mathbf{L}_{CM}\mathbf{K}_{CM}^{-1}\boldsymbol{v}$$

$$\sum_A \frac{1}{M_A}\left((\boldsymbol{R}_A - \boldsymbol{R}_{\mathrm{CM}}) \times \boldsymbol{P}_A\right) \cdot \boldsymbol{K}_{\mathrm{CM}}^{-1} \cdot \left(\hat{\boldsymbol{l}}_{\mathrm{CM}}\right) \to \mathbf{L}_{CM} \cdot K_{\mathrm{CM}}^{-1} \cdot \left(\hat{\boldsymbol{l}}_{\mathrm{CM}} + \hat{\boldsymbol{s}}\right)$$

$$|\phi_A\chi_A\rangle|\phi_B\chi_B\rangle\langle\phi_A\chi_A|\boldsymbol{P} \cdot \hat{\boldsymbol{\Gamma}}''|\phi_B\chi_B\rangle \propto \frac{v}{R}\langle\phi_A \mid \phi_B\rangle\langle\chi_A|\hat{\boldsymbol{s}}_z|\chi_B\rangle$$

$$\langle m_s = -1|\hat{H}_{\mathrm{PS}}|m_s = +1\rangle$$

$$\hat{\boldsymbol{\Gamma}}\sum_A i\hbar\langle\boldsymbol{R}_A \times \hat{\boldsymbol{\Gamma}}_A\rangle_z = \langle\hat{\boldsymbol{s}}_z\rangle$$

$$\sum_A \langle\boldsymbol{R}_A \times \hat{\boldsymbol{\Gamma}}_A\rangle_z(\beta, P) = \tanh\left(C\beta^2\frac{P}{M}\right)$$

$$E = E_1 + E_2$$
$$E_1 = \frac{1}{2}m(r_1 - R_1)^2(\omega_s - \omega_f)^2 + \frac{1}{2}mr_1^2\omega_f^2 + \frac{1}{2}M_1R_1^2\omega_f^2$$
$$E_2 = \frac{1}{2}m(r_2 - R_2)^2(\omega_s - \omega_f)^2 + \frac{1}{2}mr_2^2\omega_f^2 + \frac{1}{2}M_2R_2^2\omega_f^2$$

$$E_1 = \frac{1}{2}\left(m(r_1 - R_1)^2\omega_s^2 - 2m(r_1 - R_1)^2\omega_s \cdot \omega_f + m(r_1 - R_1)\omega_f^2 + mr_1^2\omega_f^2 + MR_1^2\omega_f^2\right)$$

$$\langle \hat{\boldsymbol{s}} \rangle = \lim_{r_1 \to R_1} I\omega_s = m(r_1 - R_1)^2\omega_s$$

$$\frac{1}{2}m(r_1 - R_1)^2\omega_s^2$$

$$E_1 = \frac{1}{2}\left(-2\hbar\langle \hat{\boldsymbol{s}} \rangle\omega_f + MR_1^2\omega_f^2 + mR_1^2\omega_f^2\right)$$

$$\omega_{f,\min} = \frac{\hbar\langle \hat{\boldsymbol{s}} \rangle}{2(m+M)R_1^2}$$

$$\frac{P_{\min}}{M} = \omega_{f,\min}R = \frac{\hbar\langle \hat{\boldsymbol{s}} \rangle}{2(m+M)R}$$

$$\hat{H}'_{BH} \propto \frac{\hbar^2 \boldsymbol{d} \cdot \boldsymbol{P}}{M}$$

$$\beta_{vib} = \frac{Z\alpha^2}{(m_e/M)^{3/4}}$$
$$\beta_{rot} = \frac{Z\alpha^2}{(m_e/M)}$$

$$\beta_{vib} = \frac{2^{3/4}Z^{7/4}\alpha^2}{(m_e/M_H)^{3/4}} = 0.025Z^{7/4}$$
$$\beta_{rot} = \frac{2Z^2\alpha^2}{(m_e/M_H)} = 0.20Z^2$$

$$\hat{H}_{\mathrm{CBO}} = \hat{H}_{el} + \sum_{c=1}^{N_M} \frac{\omega_c^2}{2}\left(\hat{q}_c - \frac{\hat{d}_c}{\omega_c}\right)^2$$

$$\hat{d}_c = \boldsymbol{\lambda}_c \cdot \hat{\boldsymbol{\mu}} = \boldsymbol{\lambda}_c \cdot (\hat{\boldsymbol{\mu}}_{el} + \boldsymbol{\mu}_{nuc}) \text{ with } \boldsymbol{\lambda}_c = \boldsymbol{e}_c\lambda_c = \boldsymbol{e}_c\sqrt{\frac{4\pi}{\mathcal{V}_c}}$$

$$\boldsymbol{\lambda}_c = \boldsymbol{e}_c \frac{\lambda_0}{\sqrt{N_{mol}}}$$

$$|\Psi(\boldsymbol{\kappa})\rangle = e^{\hat{\kappa}}|\Psi_0\rangle$$

$$\hat{\kappa} = \sum_a^{occ}\sum_r^{virt}\left(\kappa_{ar}\hat{a}_a^\dagger\hat{a}_r - \kappa_{ar}\hat{a}_r^\dagger\hat{a}_a\right)$$

$$E_{\mathrm{CBO}}(\boldsymbol{\kappa}) = \langle\Psi(\boldsymbol{\kappa})|\hat{H}_{\mathrm{CBO}}|\Psi(\boldsymbol{\kappa})\rangle$$

$$\langle\hat{\boldsymbol{\mu}}\rangle_{\text{CBO}} = \langle\Psi(\boldsymbol{\kappa})|\hat{\boldsymbol{\mu}}_{el}|\Psi(\boldsymbol{\kappa})\rangle + \boldsymbol{\mu}_{nuc} = -\sum_{a}^{occ}\langle a|\hat{\boldsymbol{r}}|a\rangle + \sum_{A}^{N_{nuc}} Z_A\boldsymbol{R}_A$$

$$\langle\alpha_{ij}\rangle = \frac{\partial\langle\hat{\mu}_i\rangle}{\partial F_j} = \frac{\partial^2 E}{\partial F_i \partial F_j}$$

$$\hat{H}_{\text{CBO}}^{\boldsymbol{F}} = \hat{H}_{el} + \sum_{c=1}^{N_M}\frac{\omega_c^2}{2}\left(\hat{q}_c - \frac{\hat{d}_c}{\omega_c}\right)^2 - (\hat{\boldsymbol{\mu}} + \boldsymbol{\mu}_{nuc})\boldsymbol{F}$$

$$E_{\text{CBO}}^{\boldsymbol{F}}(\boldsymbol{\kappa}) = \langle\Phi(\boldsymbol{\kappa})|\hat{H}_{\text{CBO}}^{\text{ext}}|\Phi(\boldsymbol{\kappa})\rangle$$

$$\langle\hat{\boldsymbol{\mu}}\rangle_{\text{CBO}}^{\boldsymbol{F}} = \langle\Phi(\boldsymbol{\kappa})|\hat{\boldsymbol{\mu}}|\Phi(\boldsymbol{\kappa})\rangle\langle\boldsymbol{\alpha}\rangle_{\text{CBO}}^{\text{num}}$$

$$\langle\alpha_{ij}\rangle_{\text{CBO}}^{\text{num}} \approx \frac{\langle\hat{\mu}_i\rangle_{\text{CBO}}^{\text{F}_\text{j}} - \langle\hat{\mu}_i\rangle_{\text{CBO}}^{-\text{F}_\text{j}}}{2F_j}$$

$$\langle\alpha_{ij}\rangle_{\text{CBO}}^{\text{pphf}} = -\left[\frac{\partial^2 E_{\text{CBO}}^0}{\partial F_i \partial F_j} + \sum_{a}^{occ}\sum_{r}^{virt}\left.\frac{\partial^2 E_{\text{CBO}}^0}{\partial F_i \partial \kappa_{ar}}\right|_{\kappa=0}\frac{\partial\kappa_{ar}}{\partial F_j}\right]\langle\boldsymbol{\alpha}\rangle_{\text{CBO}}^{\text{cphf}}$$

$$E_{\text{CBO}}^0 = \langle\Psi(\boldsymbol{\kappa})|\hat{H}_{\text{cbo}}^{\text{ext}}|\Psi(\boldsymbol{\kappa})\rangle$$

$$\left.\frac{\partial^2 E_{\text{CBO}}^0}{\partial F_i \partial \kappa_{ar}}\right|_{\boldsymbol{\kappa}=0} = 2\frac{\langle\Psi_a^r|\hat{H}_{\text{CBO}}^{\text{ext}}|\Psi(\boldsymbol{\kappa})\rangle}{\partial F_i} = -2\langle r|\hat{\mu}_i|a\rangle.$$

$$\sum_{b}^{occ}\sum_{s}^{virt}(A_{ar,bs} + B_{ar,bs})\frac{\partial\kappa_{ar}}{\partial F_j} = \langle r|\hat{\mu}_j|a\rangle.$$

$$A_{ar,bs} = (\epsilon_r - \epsilon_a)\delta_{rs}\delta_{ab} + \langle rb \mid as\rangle - \langle rb \mid sa\rangle + \sum_{c}^{N_M}\langle r|\hat{d}_c|a\rangle\langle b|\hat{d}_c|s\rangle - \langle r|\hat{d}_c|s\rangle\langle b|\hat{d}_c|a\rangle$$

$$B_{ar,bs} = \langle rs \mid ab\rangle - \langle rs \mid ba\rangle + \sum_{c}^{N_M}\langle r|\hat{d}_c|s\rangle\langle a|\hat{d}_c|b\rangle - \langle r|\hat{d}_c|b\rangle\langle s|\hat{d}_c|a\rangle.$$

$$\langle\alpha_{ij}\rangle_{\text{CBO}}^{\text{cphf}} = 2\boldsymbol{\mu}_i^T(\boldsymbol{A} + \boldsymbol{B})^{-1}\boldsymbol{\mu}_j,$$

$$\mu_{i,ar} = \langle r|\hat{\mu}_i|a\rangle(\,\boldsymbol{A} + \boldsymbol{B}\,)\big(A_{ar,bs} + B_{ar,bs}\big)\langle\boldsymbol{\alpha}\rangle_{\text{CBO}}^{\text{cphf}}$$

$$\nabla_k\boldsymbol{\alpha}_{ij} = \sum_{n=1}^{N_A+N_M}\left(\nabla^{ij}\langle\boldsymbol{\alpha}\rangle_{\text{CBO}}\right)_n \cdot \frac{\boldsymbol{Q}_n^k}{\sqrt{M_n}}$$

$$\bar{\alpha}_k = \left(\nabla_k\boldsymbol{\alpha}_{xx} + \nabla_k\boldsymbol{\alpha}_{yy} + \nabla_k\boldsymbol{\alpha}_{zz}\right)/3$$

$$\gamma_k^2 = \left(\nabla_k \boldsymbol{\alpha}_{xx} - \nabla_k \boldsymbol{\alpha}_{yy}\right)^2/2 + \left(\nabla_k \boldsymbol{\alpha}_{yy} - \nabla_k \boldsymbol{\alpha}_{zz}\right)^2/2 + (\nabla_k \boldsymbol{\alpha}_{zz} - \nabla_k \boldsymbol{\alpha}_{xx})^2/2$$
$$+3\left(\left(\nabla_k \boldsymbol{\alpha}_{xy}\right)^2 + \left(\nabla_k \boldsymbol{\alpha}_{yz}\right)^2 + (\nabla_k \boldsymbol{\alpha}_{xz})^2\right)$$

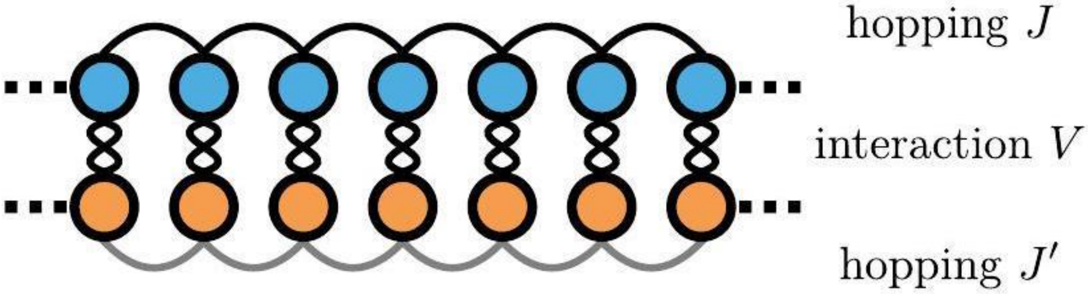
$$S_k = 45\bar{\alpha}_k^2 + 7\gamma_k^2$$

$$\Delta|\mu(N_{mol}, \lambda_0)| = \frac{|\mu_{N_{mol}}(\lambda_c)|}{N_{mol}} - |\mu_1(\lambda_0)|$$
$$\Delta\bar{\alpha}(N_{mol}, \lambda_0) = \frac{\bar{\alpha}_{N_{mol}}(\lambda_c)}{N_{mol}} - \bar{\alpha}_1(\lambda_0)$$

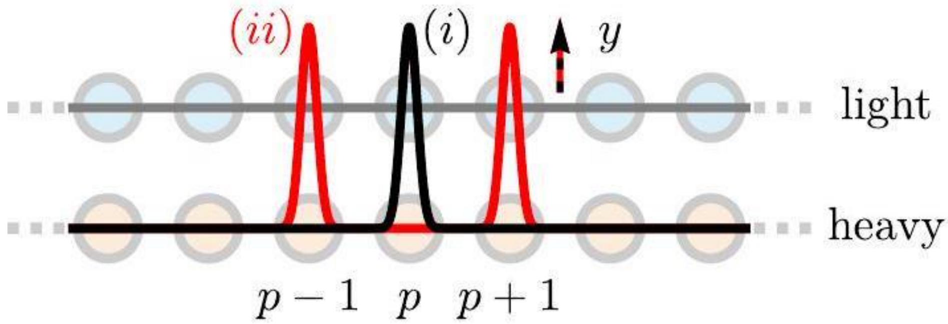
$$\mathcal{H} = \sum_{i=1}^{L} \left(-J \cdot \hat{c}_i^\dagger \hat{c}_{i+1} - J' \cdot \hat{d}_i^\dagger \hat{d}_{i+1} \right.$$
$$\left. +V \cdot \hat{c}_i^\dagger \hat{c}_i \hat{n}_i \right) + \text{h.c.}$$
$$\hat{c}_i^\dagger (\hat{c}_i) \hat{d}_i^\dagger (\hat{d}_i) \hat{n}_i = \hat{d}_i^\dagger \hat{d}_i$$

$$d = \sum_{m=0}^{L} \binom{2L}{m} . L$$

$$|\Psi\rangle = |\Psi_{\text{eq}}\rangle + y \cdot |\Psi_{\text{neq}}\rangle$$
$$= \left(e^{-\beta\mathcal{H}} + y \cdot e^{-\frac{\beta\mathcal{H}}{2}} \mathcal{A}_i e^{-\frac{\beta\mathcal{H}}{2}}\right) |\Psi_{\text{r}}\rangle.$$



b) Initial State Occupations



$$\mathcal{A}_1 = \hat{n}_p$$

$$p = \frac{L}{2}$$

$$\mathcal{A}_2 = \hat{n}_{p-1} + \hat{n}_{p+1}$$

$$D(t)\Sigma(t) = \sqrt{\langle \hat{r}^2(t)\rangle - \langle \hat{r}(t)\rangle^2}$$

$$D(t) = \frac{\mathrm{d}}{\mathrm{d}t}\Sigma(t)$$

$$\Sigma(t) = \sqrt{\sum_{i=1}^{L} i^2 \cdot n_i(t) - \left(\sum_{i=1}^{L} i \cdot n_i(t)\right)^2}$$

$$n_i(t) \sim \langle \hat{n}_i(t)\rangle - n_{\mathrm{bg}}$$

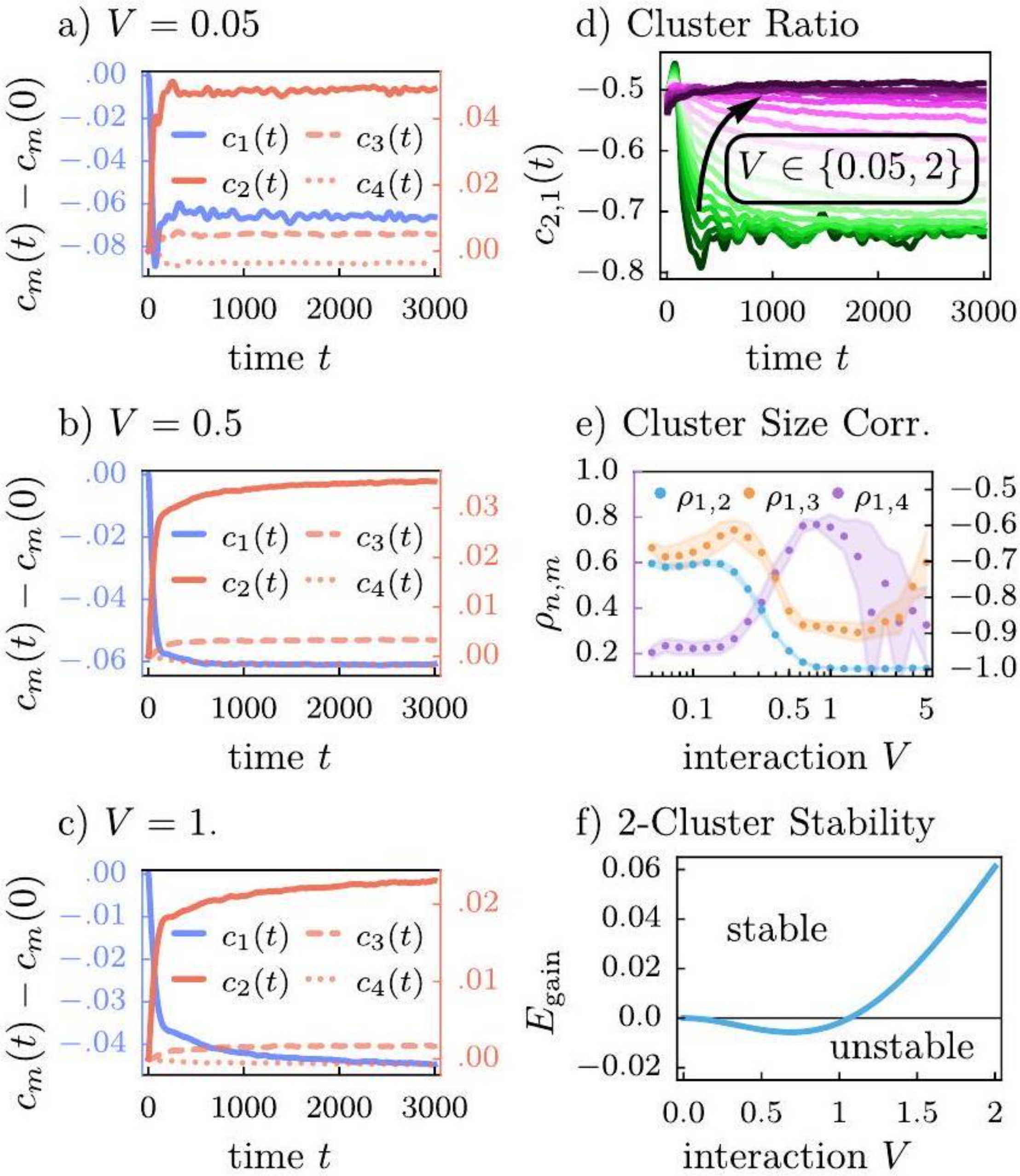
$$\sum_i n_i(t) = n_{\mathrm{bg}}$$

$$\mathcal{C}_m = \sum_{i=1}^{L} (1 - \hat{n}_{i-1})(1 - \hat{n}_{i+m}) \prod_{j=0}^{m-1} \hat{n}_{i+j}$$

$$c_m(t) = \mathrm{Tr}(\rho_{\mathrm{H}}(t) \cdot \mathcal{C}_m)$$

$$\rho_{\mathrm{H}}(t) = \mathrm{Tr}_{\mathrm{L}}(|\Psi(t)\rangle\langle\Psi(t)|)$$

$$c_{n,m}(t) = \frac{c_n(t) - c_n(0)}{c_m(t) - c_m(0)}, \rho_{n,m} = \frac{\mathrm{cov}_t(c_n(t), c_m(t))}{\sigma_t(c_n(t)) \cdot \sigma_t(c_m(t))}$$



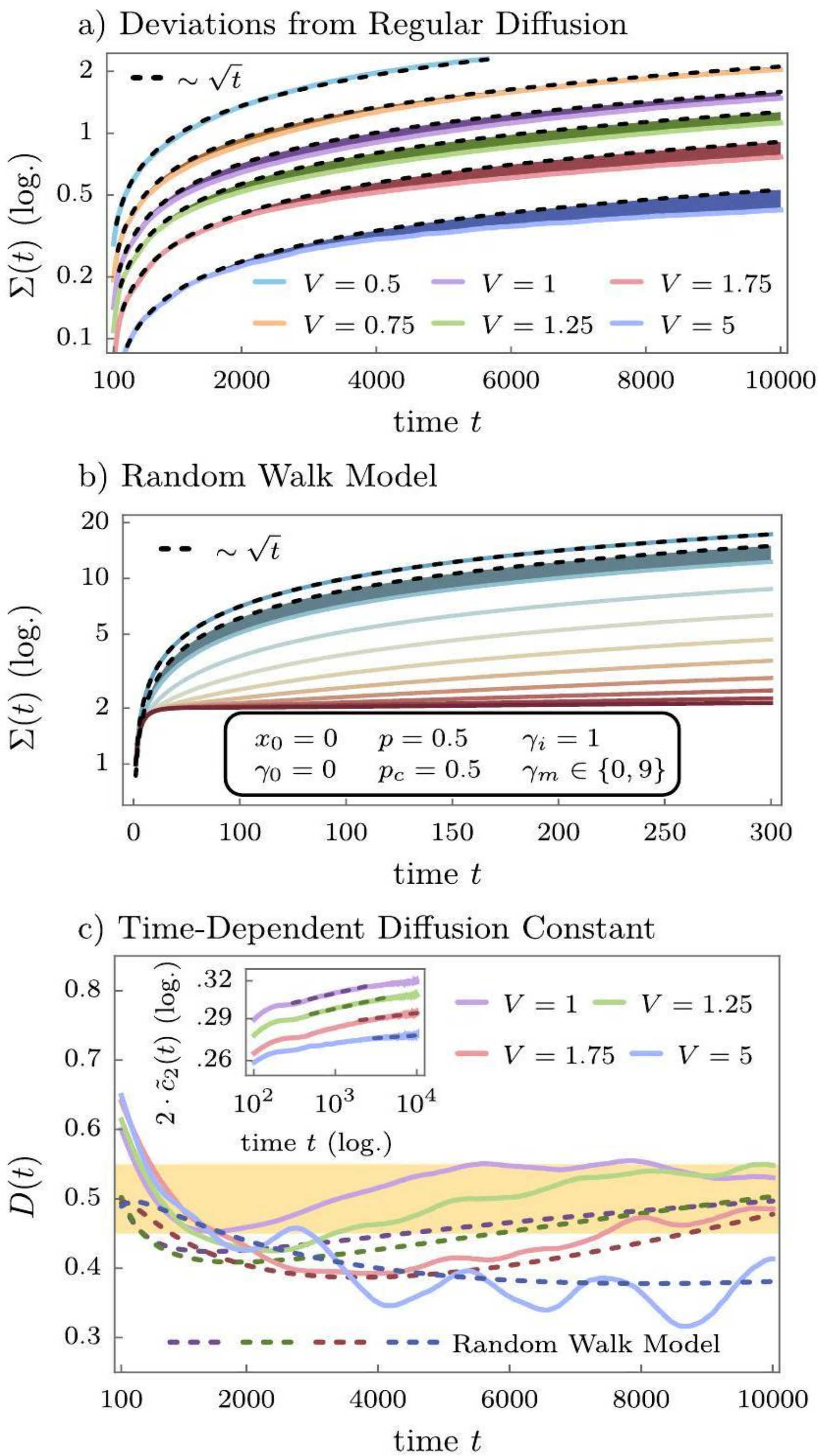
$$\mathcal{H}'|\phi_n[\chi_m]\rangle \otimes |\chi_m\rangle = \varepsilon_n[\chi_m]|\phi_n[\chi_m]\rangle \otimes |\chi_m\rangle.$$

$|\chi_m\rangle|\phi_n[\chi_m]\rangle$

$\varepsilon_0[\chi_m]E_{\text{gain}}$

$$E_{\text{gain}} = \varepsilon_0[\chi_{\text{free}}] - \varepsilon_0[\chi_{\text{pair}}]\begin{cases} > 0 & : \text{stable} \\ \leq 0 & : \text{unstable} \end{cases}$$

$|\chi_{\text{free}}\rangle|\chi_{\text{pair}}\rangle$



$$\{p^{1+\gamma_t}, p^{1+\gamma_t}, 1-2p^{1+\gamma_t}\}: x_{t+1} = x_t + \{-1,+1,0\}$$

$$\{p_c, 1-p_c\}: \gamma_{t+1} = \gamma_t + \gamma_i \cdot \{1,0\}$$

$$\gamma_i \text{ if } \gamma_{t+1} < \gamma_m$$

$$\tilde{c}_m(t) y \to \infty c_m(t) \tilde{c}_m(t) \sum_m \tilde{c}_m(t) = 1 \forall t$$

$$\partial_\mu \phi(x) = \lim_{a \to 0} \big(\phi(x^\mu + a) - \phi(x^\mu)\big)/a$$

$$\delta / \delta X^\mu(\xi)$$

$$\{X^\mu(\xi)\}_{\mu=0}^{D-1} : S^p \to \Sigma_D$$

$$\xi = \{\xi^i\}_{i=1}^{p}$$

$$h_{ij}(\xi) := \frac{\partial X^\mu(\xi)}{\partial \xi^i} \frac{\partial X^\nu(\xi)}{\partial \xi^j} g_{\mu\nu}(X(\xi)), h(\xi) := \det(h_{ij}) \geq 0$$

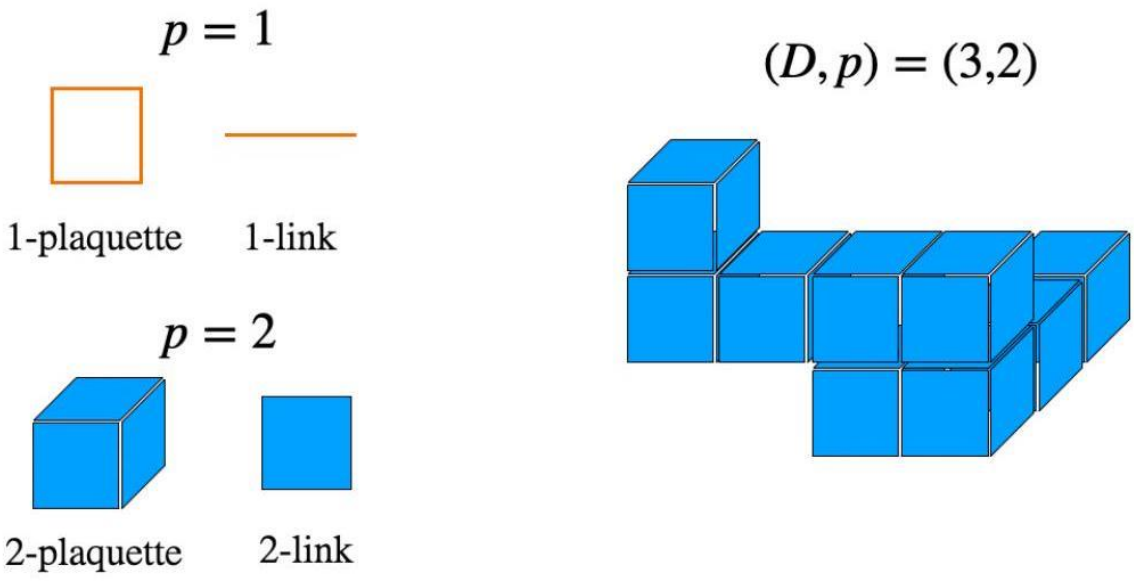
$$\mathrm{Vol}[C_p] = \int_{S^p} d^p \xi \sqrt{h(\xi)} = \int_{C_p} E_p$$

$$E_p = \frac{1}{p! \sqrt{h(\xi)}} \{X^{\mu_1}, \cdots, X^{\mu_p}\} dX_{\mu_1} \wedge \cdots \wedge dX_{\nu_p}$$

$$\{X^{\mu_1}, \cdots, X^{\mu_p}\} = \epsilon^{i_1 \cdots i_p} \frac{\partial X^{\mu_1}(\xi)}{\partial \xi^{i_1}} \cdots \frac{\partial X^{\mu_p}(\xi)}{\partial \xi^{i_p}}$$

$$\{X^{\mu_1}, \cdots, X^{\mu_p}\}\left\{X_{\mu_1}, \cdots, X_{\mu_p}\right\} = p!\, h(\xi)$$

$$\{X^\mu, X^{\mu_2}, \cdots, X^{\mu_p}\}\left\{X^\nu, X_{\mu_2}, \cdots, X_{\mu_p}\right\} = (p-1)!\, h(\xi) \frac{\partial X^\mu(\xi)}{\partial \xi^i} \frac{\partial X^\nu(\xi)}{\partial \xi^j} h^{ij}(\xi)$$



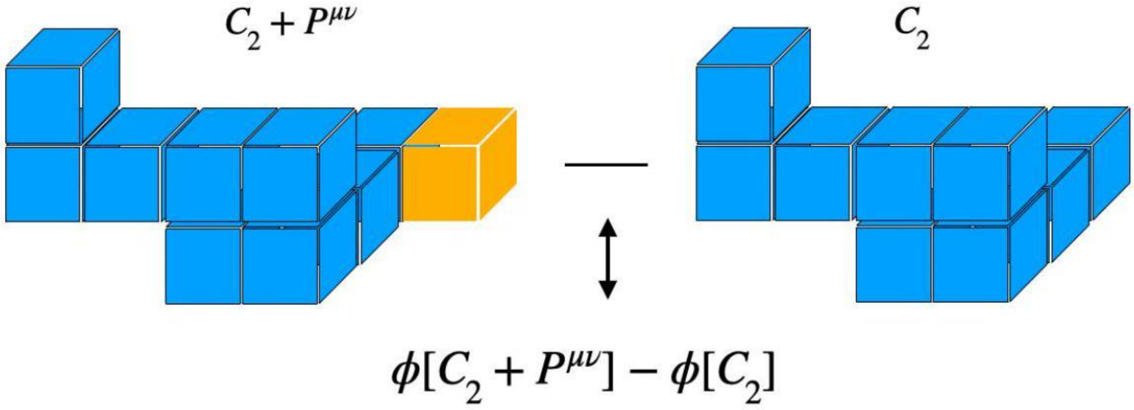
$$\phi[C_p] = \phi[\{X^\mu(\xi)\}]$$

$$\phi[\{X'^\mu(\xi)\}] = \phi[\{X^\mu(\xi)\}] \quad \text{(spacetime diffeomorphism)}$$
$$\phi[\{X^\mu(\xi')\}] = \phi[\{X^\mu(\xi)\}] \quad \text{(reparametrization)}$$

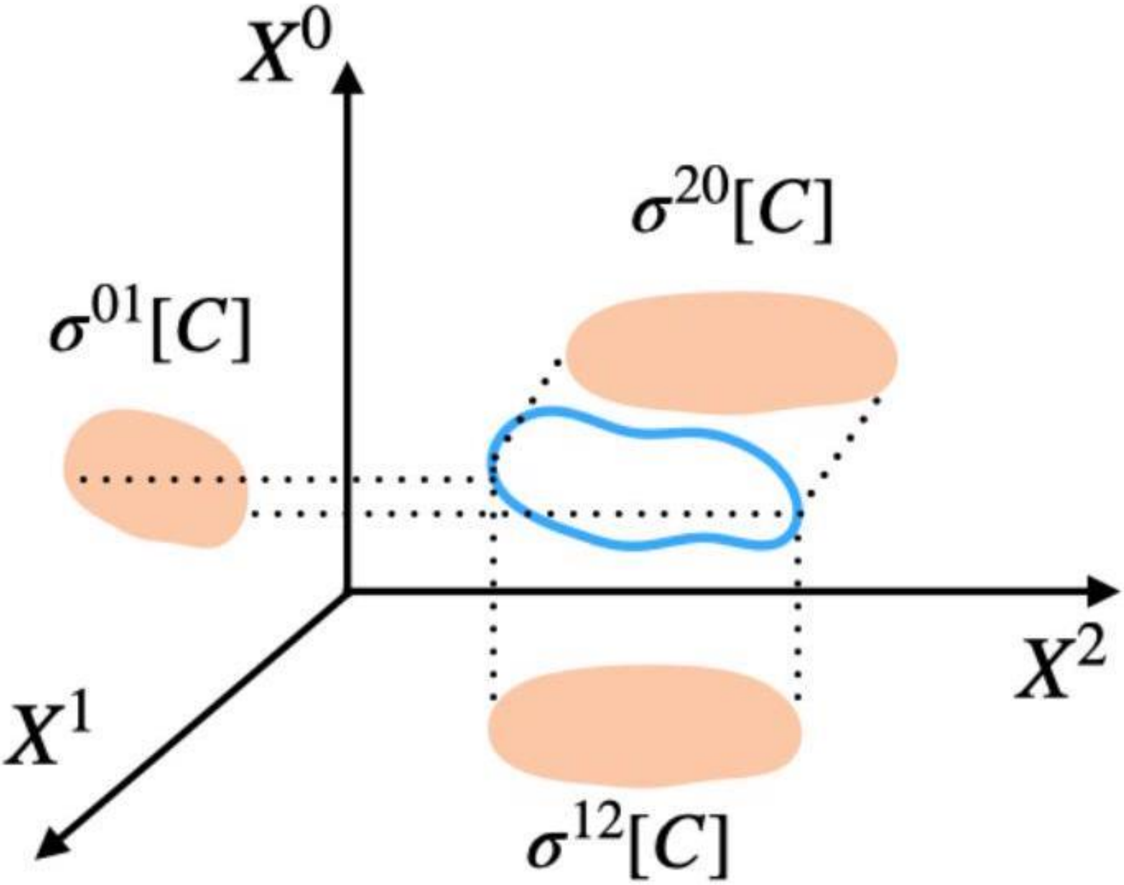
$$\phi[C_p] = \phi\left(\left\{\int_{C_p} A_p^{(a)}\right\}_a\right)$$

$$\delta C_p = \{\delta X^{\mu}(\xi)\}_{\mu=0}^{D-1}$$

$$\delta\phi[C_p] = \int_{S^p} d^p\xi\, \delta X^{\mu}(\xi)\, \frac{\delta\phi[C_p]}{\delta X^{\mu}(\xi)}.$$



$$\frac{\delta\phi[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\hat{\imath})} := \frac{\phi[C_p + P^{\mu_1\cdots\mu_{p+1}}(\hat{\imath})] - \phi[C_p]}{a^{p+1}}$$



$$\begin{aligned} \delta\phi[C_p] &= \frac{1}{(p+1)!} \int_{\delta D_{p+1}} dX^{\mu_1} \wedge \cdots \wedge dX^{\mu_{p+1}} \frac{\delta\phi[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)} \\ &= \frac{1}{(p+1)!} \sigma^{\mu_1\cdots\mu_{p+1}}[\delta C_p(\xi)] \frac{\delta\phi[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)} \end{aligned}$$

$$\sigma^{\mu_1\cdots\mu_{p+1}}[C_p] = \int_{D_{p+1}} dX^{\mu_1} \wedge \cdots \wedge dX^{\mu_{p+1}} = \frac{1}{(p+1)!}\int_{C_p} X^{[\mu_1}(\xi)dX^{\mu_2} \wedge \cdots \wedge dX^{\mu_{p+1}]}$$

$$A^{[\mu_1\mu_2\cdots\mu_p]} := \sum_{\sigma\in S_p} \mathrm{sgn}(\sigma) A^{\sigma(\mu_1)\sigma(\mu_2)\cdots\sigma(\mu_p)}$$

$$\delta/\delta X^\mu(\xi) \text{ and } \delta/\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)$$

$$\frac{\delta}{\delta X^\mu(\xi)} = \frac{1}{p!}\{X^{\nu_1},\cdots,X^{\nu_p}\}\frac{\delta}{\delta\sigma^{\mu\nu_1\cdots\nu_p}(\xi)}$$

$$\delta/\delta X^\mu(\xi)$$

$$Y^\mu(\xi) := X^\mu(\xi) - x^\mu_{\mathrm{CM}},$$

$$x^\mu_{\mathrm{CM}} := \frac{1}{\mathrm{Vol}[C_p]}\int_{S^p} d^p\xi\sqrt{h(\xi)}X^\mu(\xi)$$

$$\phi[C_p]x^\mu_{\mathrm{CM}} \to x^\mu_{\mathrm{CM}} + \delta x^\mu_{\mathrm{CM}}$$

$$\frac{\delta}{\delta X^\mu(\xi)} = \frac{\partial}{\partial x^\mu_{\mathrm{CM}}} + \frac{1}{p!}\{X^{\nu_1},\cdots,X^{\nu_p}\}\frac{\delta}{\delta\sigma^{\mu\nu_1\cdots\nu_p}(\xi)} + \cdots$$

$$\frac{\delta}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\left(\int_{C_p} A_p\right) = F_{\mu_1\cdots\mu_{p+1}}(X(\xi))$$

$$F_{p+1}(X) = \frac{1}{(p+1)!}F_{\mu_1\cdots\mu_{p+1}}(X)dX^{\mu_1} \wedge \cdots \wedge dX^{\mu_{p+1}} := dA_p(X)$$

$$\frac{\delta \mathrm{Vol}[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)} = \left(dE_p(\xi)\right)_{\mu_1\cdots\mu_{p+1}}$$

$$\frac{\delta}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)} = \left(dE_p(\xi)\right)_{\mu_1\cdots\mu_{p+1}}\frac{\partial}{\partial\mathrm{Vol}[C_p]}$$

$$\int_{S^p}\frac{d^p\xi}{\sqrt{h(\xi)}}\frac{\delta\phi^*[C_p]}{\delta X^\mu(\xi)}\frac{\delta\phi[C_p]}{\delta X_\mu(\xi)}, \int_{S^p} d^p\xi\sqrt{-h(\xi)}\frac{\delta\phi^*[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\frac{\delta\phi[C_p]}{\delta\sigma_{\mu_1\cdots\mu_{p+1}}(\xi)}$$

$$\int_{S^p}\frac{d^p\xi}{\sqrt{h(\xi)}}\{X^{\nu_1},\cdots,X^{\nu_p}\}\{X^{\lambda_1},\cdots,X^{\lambda_p}\}\frac{\delta\phi^*[C_p]}{\delta\sigma^{\mu\nu_1\cdots\nu_p}(\xi)}\frac{\delta\phi[C_p]}{\delta\sigma_\mu{}^{\lambda_1\cdots\lambda_p}(\xi)}$$

$$S[\phi] = -\mathcal{N}\int [dC_p]\left[\frac{1}{\mathrm{Vol}[C_p]^2}\frac{\partial\phi^*[C_p]}{\partial x^\mu_{\mathrm{CM}}}\frac{\partial\phi[C_p]}{\partial x_{\mathrm{CM}\mu}} + \frac{1}{\mathrm{Vol}[C_p]}\int_{S^p} d^p\xi\sqrt{-h(\xi)}\frac{\delta\phi^*[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\frac{\delta\phi[C_p]}{\delta\sigma_{\mu_1\cdots\mu_{p+1}}(\xi)} + V(\phi[C_p],\phi^*[C_p])\right]$$

$$V(\phi[C_p],\phi^*[C_p])$$

$$\|\delta X\|^2 := \int_{S^p} d^p\xi\sqrt{-h(\xi)}\delta X^\mu(\xi)\delta X_\mu(\xi)$$

$$\int_{\Sigma_D} \star 1 \in \int [dC_p]$$

$$\int [dC_p] = \int_{\Sigma_D} \star 1 \int [dY]$$

$$V(\phi[C_p], \phi^*[C_p])$$

$$\phi^*[C_p]\phi[C_p]$$

$$\phi[C_p] \rightarrow e^{i\int_{C_p}\Lambda_p}\phi[C_p], d\Lambda_p = 0,$$

$$\phi[C_p] \rightarrow e^{i\theta}\phi[C_p]$$

$$\phi[C_p] \rightarrow e^{i\int_{C_p}\Lambda_p}\phi[C_p], d\Lambda_p \neq 0,$$

$$\delta S = -\mathcal{N}\int [dC_p]\frac{i}{\mathrm{Vol}[C_p](p+1)!}\int_{S^p} d^p\xi\sqrt{h(\xi)}\left(\frac{\delta\phi^*[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\phi[C_p] - \phi^*[C_p]\frac{\delta\phi[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\right)(d\Lambda_p)_{\mu_1\cdots\mu_{p+1}}$$
$$= -\int_{\Sigma_D} d\Lambda_p \wedge \star J_{p+1}$$

$$J_{p+1}(X) = \mathcal{N}\int [dC_p]\frac{i}{\mathrm{Vol}[C_p](p+1)!}\int_{S^p} d^p\xi\sqrt{h(\xi)}\left(\frac{\delta\phi^*[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\phi[C_p] - \phi^*[C_p]\frac{\delta\phi[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\right)$$
$$\times\frac{\delta^{(D)}(X - X(\xi))}{\sqrt{-g(X(\xi))}}dX^{\mu_1}\wedge\cdots\wedge dX^{\mu_{p+1}}$$

$$d\star J_{p+1}(x_{\mathrm{CM}}) = 0,$$

$$\phi[C_p] \rightarrow e^{i\theta(x_{\mathrm{CM}})}\phi[C_p]$$

$$J_1(x_{\mathrm{CM}}) = \mathcal{N}\int [dY]\frac{i}{\mathrm{Vol}[C_p]^2}\left(\frac{\partial\phi^*[C_p]}{\partial x^\mu_{\mathrm{CM}}}\phi[C_p] - \phi^*[C_p]\frac{\partial\phi[C_p]}{\partial x^\mu_{\mathrm{CM}}}\right)dx^\mu_{\mathrm{CM}}$$

$$i\left(\partial_\mu\phi^*(x_{\mathrm{CM}})\phi(x_{\mathrm{CM}}) - \phi^*(x_{\mathrm{CM}})\partial_\mu\phi(x_{\mathrm{CM}})\right)dx^\mu_{\mathrm{CM}}$$

$$V(\phi[C_p], \phi^*[C_p])g\phi[C_p]^N + \mathrm{h.c.}$$

$$\phi[C_p] \rightarrow e^{\frac{i}{N}\int_{C_p}\Lambda_p}\phi[C_p] \text{ with } d\Lambda_p = 0, \int_{C_p}\Lambda_p \in 2\pi\mathbb{Z}$$

$$\phi[C_p] \rightarrow e^{\frac{2\pi i}{N}n}\phi[C_p], n \in \mathbb{Z}$$

$$\frac{1}{(p+1)!}\int_{S^p} d^p\xi\frac{\delta}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\frac{\sqrt{h(\xi)}}{\mathrm{Vol}[C_p]}\frac{\delta\phi[C_p]}{\delta\sigma_{\mu_1\cdots\mu_{p+1}}(\xi)} - \frac{\delta V(\phi[C_p], \phi^*[C_p])}{\delta\phi^*[C_p]} = 0$$

$$V(\phi[C_p], \phi^*[C_p])$$

$$\mathrm{Vol}[C_p] \rightarrow \infty$$

$$\phi[C_p] = \frac{1}{\sqrt{2}}f(\mathrm{Vol}[M_{p+1}])$$

$$\mathrm{Vol}[M_{p+1}] = \int_{M_{p+1}} E_p = \frac{1}{(p+1)!}\int_{M_{p+1}} (E_{p+1})_{\mu_1\cdots\mu_{p+1}} dX^{\mu_1}\wedge\cdots\wedge dX^{\mu_{p+1}}$$

$$f''(z) - q(z)f'(z) - \frac{\delta V(f)}{\delta f(z)} = 0, z = \mathrm{Vol}[M_{p+1}]$$

$$q(z) = \frac{1}{(p+1)!}\int_{S^p} d^p\xi \frac{\delta}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\left(\frac{\sqrt{h(\xi)}}{\mathrm{Vol}[C_p]}E^{\mu_1\cdots\mu_{p+1}}(\xi)\right)$$

$$V(\phi[C_p], \phi^*[C_p])$$

$$f''(z) - T_p^2 f(z) \approx 0$$

$$V(\phi[C_p], \phi^*[C_p]) \approx T_p^2\phi[C_p]\phi^*[C_p]$$

$$\phi[C_p] \approx \frac{1}{\sqrt{2}}\exp\left(-T_p\times\mathrm{Vol}[M_{p+1}]\right) \text{ for } z\to\infty$$

$$\langle\phi[C_p]\rangle = v/\sqrt{2} \neq 0$$

$$\phi[C_p] = \frac{v}{\sqrt{2}}\exp\left(i\varphi(x_{\mathrm{CM}}) + i\int_{C_p} A_p\right)$$

$$\varphi(x_{\mathrm{CM}}) \sim \varphi(x_{\mathrm{CM}}) + 2\pi$$

$$\begin{aligned} \varphi &\to \varphi + \theta, \theta\in\mathbb{R} \\ A_p &\to A_p + \Lambda_p, d\Lambda_p = 0 \end{aligned}$$

$$S_{\mathrm{eff}}[\varphi, A_p] = -\frac{v^2}{2}\int_{\Sigma_D}\left[d\varphi\wedge\star\, d\varphi + F_{p+1}\wedge\star\, F_{p+1}\right]$$

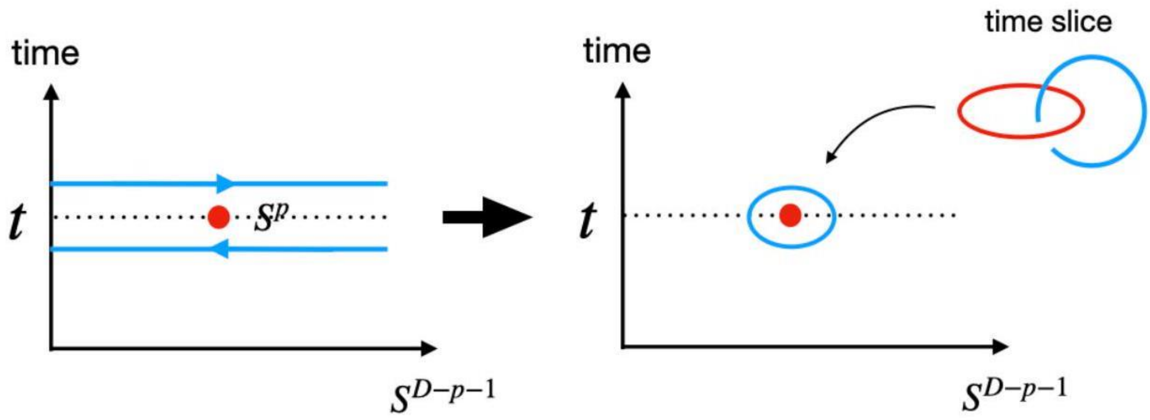
$$dd\varphi = 0, dF_{p+1} = 0$$

$$Q_{D-2} = \frac{1}{2\pi}\int_{C_1} d\varphi \in\mathbb{Z}, Q_{D-p-2} = \frac{1}{2\pi}\int_{C_{p+1}} F_{p+1} \in\mathbb{Z}$$

$$S_{\mathrm{eff}} = \frac{N}{2\pi}\int_{\Sigma_D} H_{D-1}\wedge d\varphi + \frac{N}{2\pi}\int_{\Sigma_D} B_{D-p-1}\wedge dA_p$$

$$\begin{aligned} H_{D-1} &\to H_{D-1} + \frac{1}{N}\Lambda_{D-1}, d\Lambda_{D-1} = 0, \int_{C_{D-1}}\Lambda_{D-1}\in 2\pi\mathbb{Z} \\ B_{D-p-1} &\to B_{D-p-1} + \frac{1}{N}\Lambda_{D-p-1}, d\Lambda_{D-p-1} = 0, \int_{C_{D-p-1}}\Lambda_{D-p-1}\in 2\pi\mathbb{Z} \end{aligned}$$

$$\begin{aligned} U_0(C_{D-1}) &= \exp\left(i\int_{C_{D-1}} H_{D-1}\right), U_p(C_{D-p-1}) = \exp\left(i\int_{C_{D-p-1}} B_{D-p-1}\right), \\ U_{D-1}(P, P') &= \exp\left(i\left(\varphi(P) - \varphi(P')\right)\right), U_{D-p-1}(C_p) = \exp\left(i\int_{C_p} A_p\right), \end{aligned}$$



$$\Sigma_{D-1} = \mathbb{R}^{D-1}$$

$$\langle U_0(C_{D-1})\rangle = \langle U_p(C_{D-p-1})\rangle = \langle U_{D-p-1}(C_p)\rangle = 1$$

$$\Sigma_{D-1} = S^p \times S^{D-p-1}$$

$$C_{D-p-1} = S^{D-p-1}$$

$$U_p(S^{D-p-1}) \text{ and } U_{D-p-1}(S^p)$$

$$U_p(S^{D-p-1})U_{D-p-1}(S^p)U_p^{-1}(S^{D-p-1}) = e^{i\frac{2\pi}{N}}U_{D-p-1}(S^p)$$

$$U_p(S^{D-p-1})|\Omega\rangle = e^{i\theta}|\Omega\rangle, \theta \in \mathbb{R},$$

$$|\Omega'\rangle := U_{D-p-1}(S^p)|\Omega\rangle$$

$$U_p(S^{D-p-1})|\Omega'\rangle = e^{i\theta+i\frac{2\pi}{N}}|\Omega'\rangle$$

$$\int \left[dC_p^{(1)}\right]\int \left[dC_p^{(2)}\right]\int \left[dC_p^{(3)}\right]\delta\left(C_p^{(1)}+C_p^{(2)}+C_p^{(3)}\right)\phi\left[C_p^{(1)}\right]\phi\left[C_p^{(2)}\right]\phi\left[C_p^{(3)}\right] + \text{h.c.}$$

$$\delta\left(C_p^{(1)}+C_p^{(2)}+C_p^{(3)}\right)C_p^{(1)} = -C_p^{(2)} - C_p^{(3)}$$

$$\begin{aligned} &\delta(C_p^{(1)}+C_p^{(2)}+C_p^{(3)})\phi[C_p^{(1)}]\phi[C_p^{(2)}]\phi[C_p^{(3)}] \\ \to\ &\delta(C_p^{(1)}+C_p^{(2)}+C_p^{(3)})e^{i\int_{C_p^{(1)}+C_p^{(2)}+C_p^{(3)}}\Lambda_p}\phi[C_p^{(1)}]\phi[C_p^{(2)}]\phi[C_p^{(3)}] \\ &= \delta(C_p^{(1)}+C_p^{(2)}+C_p^{(3)})\phi[C_p^{(1)}]\phi[C_p^{(2)}]\phi[C_p^{(3)}]\ , \end{aligned}$$

$$i\lambda\int [dC_p]\frac{1}{\text{Vol}[C_p]}\int_{S^p} d^p\xi\sqrt{h(\xi)}D_{p+1}\phi[C_p]\wedge\cdots\wedge D_{p+1}\phi[C_p] + \text{h.c.}$$

$$D_{p+1}\phi[C_p] := \frac{1}{(p+1)!}\frac{\delta\phi[C_p]}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}dX^{\mu_1}\wedge\cdots\wedge dX^{\mu_{p+1}}$$

$$\lambda\int_{\Sigma_D}\sin(M\varphi)F_{p+1}\wedge\cdots\wedge F_{p+1}$$

$$V(\phi[C_p], \phi^*[C_p])$$

$$S_{\text{eff}} \approx \frac{N}{2\pi}\int_{\Sigma_D} H_{D-1} \wedge d\varphi + \frac{N}{2\pi}\int_{\Sigma_D} B_{D-p-1} \wedge dA_p + \lambda \int_{\Sigma_D} \sin{(M\varphi)} F_{p+1} \wedge \cdots \wedge F_{p+1}$$

$$\frac{N(-1)^D}{2\pi} dH_{D-1} + \lambda M \cos{(M\varphi)} F_{p+1} \wedge \cdots \wedge F_{p+1} = 0$$

$\mathbb{Z}_q p$-form symmetry: $\frac{N(-1)^{D-p-1}}{2\pi} dB_{D-p-1} + \lambda d \sin{(M\varphi)} \wedge F_{p+1} \wedge \cdots \wedge F_{p+1} = 0$

$\mathbb{Z}_N (D-p-1)$-form symmetry: $dA_p = 0$

$\mathbb{Z}_N (D-1)$-form symmetry: $d\varphi = 0$

$$d \star J_{n+1} = 0$$

$$Q_n := \int_{C_{D-n-1}} \star J_{n+1}$$

$$S_{\text{gauged}} = -\mathcal{N} \int [dC_p] \left[\frac{1}{\text{Vol}[C_p]^2} \left(D_{\text{CM}}\phi[C_p]\right)^* \wedge\star D_{\text{CM}}\phi[C_p] \right.$$

$$+ \frac{1}{\text{Vol}[C_p]} \int_{S^p} d^p\xi \sqrt{-h(\xi)} \left(D_\sigma \phi[C_p]\right)^* \wedge\star D_\sigma\phi[C_p] + V(\phi[C_p]\phi^*[C_p])]$$

$$- \frac{1}{2g^2}\int_{\Sigma_D} F_2 \wedge\star F_2 - \frac{1}{2\tilde{g}^2}\int_{\Sigma_D} F_{p+2} \wedge\star F_{p+2}$$

$$D_{\text{CM}}\phi[C_p] = \left(d - iq_0 A_1(x_{\text{CM}})\right)\phi[C_p]$$

$$D_\sigma \phi[C_p] = \frac{1}{(p+1)!}\left(\frac{\delta}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)} - iq_p A_{\mu_1\cdots\mu_{p+1}}(X(\xi))\right)\phi[C_p] dX^{\mu_1} \wedge \cdots \wedge dX^{\mu_{p+1}}$$

$$F_2 = dA_1, F_{p+2} = dA_{p+1}$$

$$\phi[C_p] \to e^{iq_0\Lambda(x_{\text{CM}})}\phi[C_p], A_1(x_{\text{CM}}) \to A_1(x_{\text{CM}}) + d\Lambda(x_{\text{CM}})$$

$$\phi[C_p] \to e^{iq_p\int_{C_p}\Lambda_p}\phi[C_p], A_{p+1}(X) \to A_{p+1}(X) + d\Lambda_p(X)$$

$$\Lambda(x_{\text{CM}})(\Lambda_p(X))$$

$$\frac{1}{g^2} d\star F_2 = q_0 \star J_1, \frac{(-1)^p}{\tilde{g}^2} d\star F_{p+2} = q_p \star J_{p+1}$$

$$d\star J_1 = 0, d\star J_{p+1} = 0$$

$$Q_0 = \int_{\Sigma_{D-1}} \star J_1 = \frac{1}{g^2 q_0}\int_{C_{D-2}} \star F_2 \in \mathbb{Z},$$

$$Q_p = \int_{\Sigma_{D-p-1}} \star J_{p+1} = \frac{1}{\tilde{g}^2 q_p}\int_{C_{D-p-2}} \star F_{p+2} \in \mathbb{Z},$$

$$\Sigma_{D-1}(\Sigma_{D-p-1})(D-1)((D-p-1))$$

$$\partial\Sigma_{D-1} = C_{D-2}(\partial\Sigma_{D-p-1} = C_{D-p-2})$$

$$A_1 \ \rightarrow \ A_1 + \frac{1}{q_0}\Lambda_1, d\Lambda_1 = 0, \int_{C_1} \ \Lambda_1 \in 2\pi\mathbb{Z}$$

$$A_{p+1} \ \rightarrow \ A_{p+1} + \frac{1}{q_p}\Lambda_{p+1}, d\Lambda_{p+1} = 0, \int_{C_{p+1}} \ \Lambda_{p+1} \in 2\pi\mathbb{Z}$$

$$dF_2 = 0, dF_{p+2} = 0$$

$$\langle\phi[C_p]\rangle \sim \exp\left(-T_p \mathrm{Vol}[M_{p+1}]\right)$$

$$\langle\phi[C_p]\rangle = v/\sqrt{2} \neq 0$$

$$J_1(x) \propto v^2 d\varphi(x), J_{p+1}(x) \propto v^2 dA_p(x)$$

$$dJ_1 = dJ_{p+1} = 0$$

$$\mathbb{Z}_{q_0}(D-2) \text{ - and } \mathbb{Z}_{q_p}(D-p-2)$$

$$S_{\mathrm{eff}} = \frac{q_0}{2\pi}\int_{\Sigma_D} \ B_{D-2} \wedge dA_1 + \frac{q_p}{2\pi}\int_{\Sigma_D} \ B_{D-p-2} \wedge dA_{p+1}$$

$$B_{D-2}(X)\big(B_{D-p-2}(X)\big)\varphi(X)\big(A_p(X)\big)$$

$$V\big(\phi[C_p], \phi^*[C_p]\big) = T_p^2 \phi^*[C_p]\phi[C_p]$$

$$G[C_p, C_p'] = \langle T\{\phi[C_p]\phi^\dagger[C_p']\}\rangle := \frac{1}{Z}\int \ \mathcal{D}\phi^*\mathcal{D}\phi\phi[C_p]\phi^*[C_p']e^{iS[\phi]}$$

$$= -\frac{i}{2}\langle C_p|(\hat{H} - i\varepsilon/2)^{-1}|C_p'\rangle = \frac{1}{2}\int_0^\infty \ dA\langle C_p|e^{-i\left(\hat{H}-i\frac{\varepsilon}{2}\right)A}|C_p'\rangle$$

$$\hat{H} = \frac{1}{2}\left[-\frac{1}{\mathrm{Vol}[C_p]^2}\frac{\partial^2}{\partial x_{\mathrm{CM}}^\mu \partial x_{\mathrm{CM}\mu}} - \int_{S^p} \ d^p\xi \frac{\delta}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\frac{\sqrt{h(\xi)}}{\mathrm{Vol}[C_p]}\frac{\delta}{\delta\sigma_{\mu_1\cdots\mu_{p+1}}(\xi)} + T_p^2\right]$$

$$\langle x_{\mathrm{CM}} \mid k_{\mathrm{CM}}\rangle = \frac{1}{(2\pi)^{D/2}}e^{ik_{\mathrm{CM}}\cdot x_{\mathrm{CM}}}$$

$$\exp\left(i\int_{C_p} \ K_p\right) := \exp\left(\frac{i}{(p+1)!}\int_{C_p} \ K_{\mu_1\cdots\mu_{p+1}}(\xi)Y^{[\mu_1}(\xi)dY^{\mu_2} \wedge \cdots \wedge dY^{\mu_{p+1}]}\right)$$

$$-i\frac{\delta}{\delta\sigma^{\mu_1\cdots\mu_{p+1}}(\xi)}\exp\left(i\int_{C_p} \ K_p\right) = \left(dK_p\right)_{\mu_1\cdots\mu_{p+1}}(\xi)\exp\left(i\int_{C_p} \ K_p\right)$$

$$= K_{\mu_1\cdots\mu_{p+1}}(\xi)\exp\left(i\int_{C_p} \ K_p\right)$$

$$\left(K_p^{\mathrm{Vol}}\right)_{\mu_1\cdots\mu_{p+1}} := -\big(dE_p(\xi)\big)_{\mu_1\cdots\mu_{p+1}} \times k_{\mathrm{Vol}}, k_{\mathrm{Vol}} \in \mathbb{R}$$

$$e^{i\int_{C_p} K_p^{\mathrm{Vol}}} = e^{ik_{\mathrm{Vol}}\mathrm{Vol}[C_p]}$$

$$K_p \cdot dE_p := \frac{1}{(p+1)!}K_{\mu_1\cdots\mu_{p+1}}\left(dE_p\right)^{\mu_1\cdots\mu_{p+1}} = 0$$

$$1 = \int \frac{d^D k_{\text{CM}}}{(2\pi)^D} \int \frac{dk_{\text{Vol}}}{2\pi} \int [dK_p] \big(|k_{\text{CM}}\rangle \otimes |k_{\text{Vol}}\rangle \otimes |K_p\rangle\big)\big(\langle K_p| \otimes \langle k_{\text{Vol}}| \otimes \langle k_{\text{CM}}|\big)$$

$$[dK_p]\,[dC_p]|k_{\text{CM}}\rangle \otimes |k_{\text{Vol}}\rangle \otimes |K_p\rangle$$

$$\{X^\mu(\xi)\} h(\xi) \text{Vol}[C_p]$$

$$\langle C_p | e^{-i(\hat{H} - i\varepsilon)A} | C'_p \rangle = \int_{t=0, C'_p}^{t=A, C_p} \mathcal{D}X \int \mathcal{D}k_{\text{CM}} \int \mathcal{D}k_{\text{Vol}} \int \mathcal{D}K e^{iS_p}$$

$$S_p = \int_0^A dt \big(k_{\text{CM}\mu}(t) \dot{x}^\mu_{\text{CM}}(t) + k_{\text{Vol}}(t) \dot{\text{Vol}}[C_p(t)] - (H(t) - i\varepsilon)\big) + \int_{M_{p+1}} K_{p+1}$$

$$H(t) = \frac{1}{2}\left(\frac{k^2}{\text{Vol}[C_p(t)]^2} + D[C_p(t)] k_{\text{Vol}}(t)^2 + K_p(t)^2 + T_p^2 \right)$$

$$D[C_p(t)] = \frac{1}{\text{Vol}[C_p(t)]} \int_{S^p} d^p \xi \sqrt{h(t, \xi)} (dE_p) \cdot (dE_p)$$

$$K_p(t)^2 = \frac{1}{\text{Vol}[C_p(t)]} \int_{S^p} d^p \xi \sqrt{h(t, \xi)} K_p \cdot K_p$$

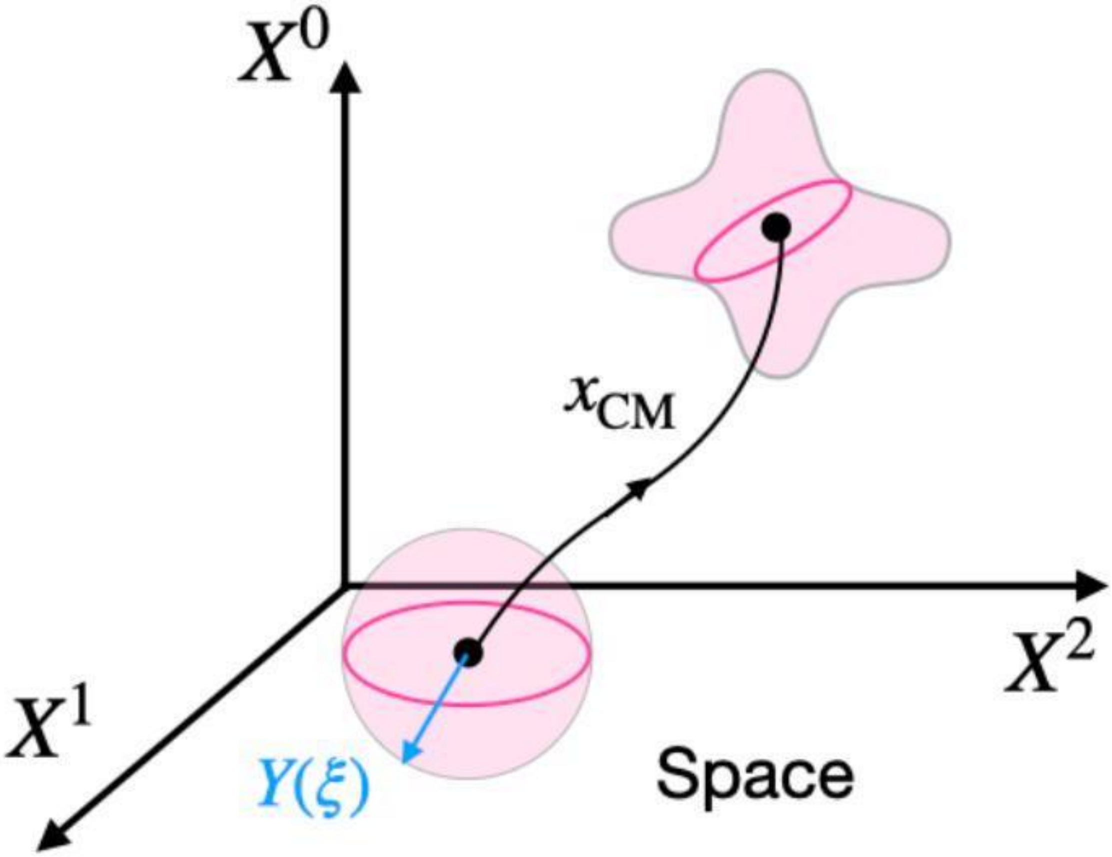
$$\int_{M_{p+1}} K_{p+1} = \frac{1}{(p+1)!} \int_{M_{p+1}} K_{\mu_1 \cdots \mu_{p+1}}(t, \xi) dY^{\mu_1} \wedge \cdots \wedge dY^{\mu_{p+1}}$$

$$\partial M_{p+1} = C_p - C'_p \{x^\mu_{\text{CM}}(t)\}$$

$$\dot{k}_{\text{CM}\mu}(t) = 0 \;\therefore\; k_{\text{CM}\mu}(t) = k_\mu = \text{ constant}$$

$$\langle C_p | e^{-i(\hat{H} - i\varepsilon)A} | C'_p \rangle = \int \frac{d^D k}{(2\pi)^D} e^{ik \cdot (x_{\text{CM}} - x'_{\text{CM}})} \int_{t=0, \{Y'(\xi)\}}^{t=A, \{Y(\xi)\}} \mathcal{D}Y \int \mathcal{D}k_{\text{Vol}} \int \mathcal{D}K e^{i \int_{M_{p+1}} K_{p+1} - i \int_0^A dt (H(t) - i\varepsilon)}$$

$$C_p = \big(\{x^\mu_{\text{CM}}\}, \{Y^\mu(\xi)\}\big), C'_p = \big(\{x'^\mu_{\text{CM}}\}, \{Y'^\mu(\xi)\}\big)$$



$$\text{Vol}[C_p] = V_p \;\leftrightarrow\; M_p[C_p] := T_p\text{Vol}[C_p] = T_pV_p = M_p\dot{\text{V}}\text{ol}[C_p(t)]$$

$$\langle C_p|e^{-i(\hat{H}-i\varepsilon)A}|C_p'\rangle\big|_{\text{CM}} = \int \frac{d^Dk_{\text{CM}}}{(2\pi)^D} e^{ik_{\text{CM}}\cdot(x_{\text{CM}}-x'_{\text{CM}})-i\frac{AT_p^2}{2}\left(\frac{k_{\text{CM}}^2}{M_p^2}-i\varepsilon\right)}$$

$$\int_{M_{p+1}} K_{p+1} = \frac{1}{(p+1)!}\int_{M_{p+1}} \left[d\left(K_{\mu_1\cdots\mu_{p+1}}(t,\xi)Y^{\mu_1}\right)\wedge\cdots\wedge dY^{\mu_{p+1}}\right.$$
$$\left.-\left(dK_{\mu_1\cdots\mu_{p+1}}(t,\xi)\right)Y^{[\mu_1}dY^{\mu_2}\wedge\cdots\wedge dY^{\mu_{p+1}]}\right]$$
$$= \int_{C_p} K_p(A) - \int_{C_p'} K_p(0) - \frac{1}{(p+1)!}\int_{M_{p+1}} \left(dK_{\mu_1\cdots\mu_{p+1}}(t,\xi)\right)Y^{[\mu_1}dY^{\mu_2}\wedge\cdots\wedge dY^{\mu_{p+1}]}$$

$$dK_{\mu_1\cdots\mu_{p+1}}(t,\xi) = 0 \;\therefore\; K_{\mu_1\cdots\mu_{p+1}}(t,\xi) = k_{\mu_1\cdots\mu_{p+1}} = \text{ constant}$$

$$K_p(t)^2 = k\cdot k := \frac{1}{(p+1)!}k_{\mu_1\cdots\mu_{p+1}}k^{\mu_1\cdots\mu_{p+1}}$$

$$\langle C_p|e^{-i\hat{H}A}|C_p'\rangle\big|_{\text{BO}}$$
$$\approx \int \frac{d^Dk_{\text{CM}}}{(2\pi)^D}\int \frac{d^{D'}k}{(2\pi)^{D'}}\exp\left(ik_{\text{CM}}\cdot(x_{\text{CM}}-x'_{\text{CM}}) + ik\cdot(\sigma[C_p]-\sigma[C_p']) - i\frac{AT_p^2}{2}\left(\frac{k_{\text{CM}}^2}{M_p^2}+\frac{k\cdot k}{T_p^2}+1-i\varepsilon\right)\right),$$

$$k\cdot\sigma[C_p] := \frac{1}{(p+1)!}k_{\mu_1\cdots\mu_{p+1}}\sigma^{\mu_1\cdots\mu_{p+1}}[C_p]$$

$$T_p \to \infty \text{ with } M_p = \text{ fixed } (\text{Point-particle limit})$$

$$\langle C_p | e^{-i\hat{H}A} | C_p' \rangle \big|_{\text{BO}} \approx \delta^{(D')}(\sigma[C_p] - \sigma[C_p']) \int \frac{d^D k_{\text{CM}}}{(2\pi)^D} e^{ik_{\text{CM}}\cdot(x_{\text{CM}} - x_{\text{CM}}') - i\frac{AT_p^2}{2}\left(\frac{k_{\text{CM}}^2}{M_p^2} + 1 - i\varepsilon\right)}$$

$$V_p \to \infty \text{ with } T_p = \text{ fixed } (\text{Large-brane limit})$$

$$\langle C_p | e^{-i\hat{H}A} | C_p' \rangle \big|_{\text{BO}} \approx \delta^{(D)}(x_{\text{CM}} - x_{\text{CM}}') \int \frac{d^{D'} k}{(2\pi)^{D'}} e^{ik\cdot(\sigma[C_p] - \sigma[C_p']) - i\frac{A}{2}(k\cdot k + T_p^2 - i\varepsilon)}$$

$$S_{\text{eff}} = \int_0^A dt \left[k_{\text{Vol}}(t) \dot{\text{Vol}}[C_p(t)] - \frac{1}{2}\left(\frac{k^2}{M_p(t)^2} + D[C_p(t)] k_{\text{Vol}}(t)^2 \right) \right], M_p(t) = T_p \text{Vol}[C_p(t)]$$

$$k^2/M_p(t)^2 \text{Vol}[C_p] = V_p$$

$$\tau_{\text{Vol}} \sim T_p \left(\left| D[V_p] \frac{(k^2/M_p^2)''}{k^2/M_p^2} \right| \right)^{-\frac{1}{2}} \sim T_p \sqrt{\frac{V_p^2}{D[V_p]}} \sim T_p V_p^{\frac{p+1}{p}}$$

$$D[V_p] \sim V_p^{-2/p}$$

$$\tau_{\text{CM}} \sim \tau_{\text{AE}} \sim AT_p^2$$

$$s := \frac{AT_p}{V_p} \ll L_p := V_p^{\frac{1}{p}},$$

$$n_\chi(C_p, C_p'; A),$$

$$N_\chi(C_p'; A) := \sum_{C_p} n_\chi(C_p, C_p'; A),$$

$$P_\chi(C_p, C_p'; A) := \frac{n_\chi(C_p, C_p'; A)}{N_\chi(C_p'; A)},$$

$$\langle X^2 \rangle_A := \sum_{C_p} P_\chi(C_p, 0; A) \left(x_{\text{CM}}^\mu x_{\text{CM}\mu} + (\sigma[C_p] \cdot \sigma[C_p])^{\frac{1}{p+1}} \right),$$

$$\langle X^2 \rangle_A \sim A^{\frac{2}{D_{\text{H}}}} \leftrightarrow A \sim \left(\sqrt{\langle X^2 \rangle_A} \right)^{D_{\text{H}}}$$

$$P_\chi(C_p, C_p'; A) = \langle C_p | e^{-\hat{H}A} | C_p' \rangle,$$

$$\langle X^2 \rangle_A \propto \begin{cases} A & \text{(Point-particle limit)} \\ A^{\frac{1}{p+1}} & \text{(Large-brane limit)} \end{cases}$$

$$D_{\text{H}} \approx \begin{cases} 2 & \text{(Point-particle limit)} \\ 2(p+1) & \text{(Large-brane limit)} \end{cases}$$

$$\frac{\delta F[\phi]}{\delta\phi(X)} = \lim_{\varepsilon\to 0}\frac{F\left[\phi(Y)+\varepsilon\delta^{(d)}(Y-X)\right]-F[\phi]}{\varepsilon}$$

$$\frac{\delta_c F[\phi]}{\delta\phi(X)} = \lim_{\varepsilon\to 0}\frac{F\left[\phi(Y)+\varepsilon\delta_c^{(d)}(Y-X)\right]-F[\phi]}{\varepsilon}$$

$$\delta_c^{(d)}(Y-X) := \frac{1}{\sqrt{-g(X)}}\delta^{(d)}(Y-X)$$

$$\frac{\delta_c\phi(X)}{\delta\phi(Y)} = \delta_c^{(d)}(X-Y)$$

$$\frac{\delta_c F[\phi]}{\delta\phi(X)} = \int d^dY\frac{\delta_c\phi(Y)}{\delta\phi(X)}\frac{\delta_c F[\phi]}{\delta_c\phi(Y)} = \frac{1}{\sqrt{-g(X)}}\frac{\delta F[\phi]}{\delta\phi(X)}$$

$$\begin{aligned} F[\phi+\delta\phi] &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\prod_{i=1}^{n}\int d^dX_i\sqrt{-g(X)}\delta\phi(X_i)\right)\frac{\delta_c^n F[\phi]}{\delta\phi(X_1)\cdots\delta\phi(X_n)} \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\prod_{i=1}^{n}\int d^dX_i\delta\phi(X_i)\right)\frac{\delta^n F[\phi]}{\delta\phi(X_1)\cdots\delta\phi(X_n)} \end{aligned}$$

$$\sqrt{h(\xi)}\delta/\delta X^{\mu}(\xi)$$

$$\frac{N}{8\pi^2}\int_{\Sigma_4}\varphi F_2\wedge F_2$$

$$\sum_{C_p} P_\chi(C_p,0;A)\frac{1}{\mathrm{Vol}[C_p]}\int_{S^p} d^p\xi\sqrt{h(\xi)}X^{\mu}(\xi)X_{\mu}(\xi)$$

$$\langle X^{\mu}(\xi)X^{\nu}(\xi')\rangle$$

$$e^+e^-\to K^+D_s^-D^{*0}$$

$$K^+D_s^{*-}D^0$$

$$B^+\to J/\psi\phi K^+$$

$$\begin{aligned}\mathcal{H} = \sum_{i=1}^{4}\left(\frac{p_i^2}{2m_i}\right) + V(\boldsymbol{x}_{A,B}) \\ + V_I(\boldsymbol{x}_{A,B},\boldsymbol{x}_{1,2}) + V_{\mathrm{conf}}\end{aligned}$$

$$\sum_{i=1}^{4}\left(\frac{p_i^2}{2m_i}\right)V(\boldsymbol{x}_{A,B})V_I(\boldsymbol{x}_{A,B},\boldsymbol{x}_{1,2})$$

$$H = \sum_{i=1}^{4} m_i + E + H_{ss}$$

$$H_{ss} = \sum_{i<j} 2\kappa_{ij}(s_i \cdot s_j),$$

$$\left[\left(\sum_{\text{light}} \frac{p_i^2}{2m}\right) + V_I(\boldsymbol{x}_{A,B}, \boldsymbol{x}_{1,2})\right] f = \mathcal{E}(\boldsymbol{x}_{A,B}) f,$$

$$f = f(\boldsymbol{x}_{A,B}, \boldsymbol{x}_{1,2})$$

$$\Psi = \psi(\boldsymbol{x}_{A,B}) f(\boldsymbol{x}_{A,B}, \boldsymbol{x}_{1,2}),$$

$$\nabla_i^2 \Psi \approx \left(f \nabla_i^2 \psi + \psi \nabla_i^2 f\right).$$

$$\left(\sum_{\text{heavy}} \frac{p_i^2}{2M} + V_{\text{BO}}(\boldsymbol{x}_{A,B})\right) \psi = E\psi,$$

$$V_{\text{BO}}(\boldsymbol{x}_{A,B}) = V(\boldsymbol{x}_{A,B}) + \mathcal{E}(\boldsymbol{x}_{A,B}) + V_{\text{conf}}.$$

$$V(r) = \lambda_{q_1 q_2}(\boldsymbol{R}) \frac{\alpha_s}{r},$$

$$\lambda_{q_1 q_2}(\boldsymbol{R}) = \frac{1}{2}[C(\boldsymbol{R}) - C(q_1) - C(q_2)],$$

$C(3) = 4/3, C(6) = 10/3, C(1) = 0, C(8) = 3, C(\bar{q}) = C(q)$, and $C(\overline{\boldsymbol{R}}) = C(\boldsymbol{R})$

$$V_{\bar{Q}q}(r) = -\frac{4}{3}\frac{\alpha_s}{r} + \sigma r + V_0$$

$$V_{Qq}(r) = -\frac{1}{3}\frac{\alpha_s}{r} + \frac{1}{4}\sigma r + V_0$$

$$R(r) = \frac{A^{3/2}}{\sqrt{4\pi}} e^{-Ar}$$

$$f = \zeta(\boldsymbol{\rho})\xi(\boldsymbol{\eta}) = R(|\boldsymbol{x}_1 - \boldsymbol{x}_A|) R(|\boldsymbol{x}_2 - \boldsymbol{x}_B|)$$

$$E_{Qq \leftrightarrow \bar{Q}\bar{q}} = 2\langle H \rangle_{\min}.$$

$$H_p = -\frac{7}{6}\alpha_s \left(\frac{1}{|\boldsymbol{x}_1 - \boldsymbol{x}_B|} + \frac{1}{|\boldsymbol{x}_2 - \boldsymbol{x}_A|}\right) + \frac{1}{6}\alpha_s \frac{1}{|\boldsymbol{x}_1 - \boldsymbol{x}_2|}$$

$$\Delta E = \langle f | H_p | f \rangle,$$

$$\Delta E = -\frac{7}{6}\alpha_s 2 I_1(r_{AB}) + \frac{1}{6}\alpha_s I_2(r_{AB})$$

$$r_{AB} = |\boldsymbol{x}_B - \boldsymbol{x}_A|$$

$$I_1(r_{AB}) = \int \mathrm{d}^3\rho|\psi(\rho)|^2 \frac{1}{|\boldsymbol{\rho} - \boldsymbol{r}_{AB}|}$$

$$I_2(r_{AB}) = \int \mathrm{d}^3\rho\, \mathrm{d}^3\eta|\psi(\rho)|^2|\phi(\eta)|^2 \frac{1}{|\boldsymbol{\rho} - \boldsymbol{\eta}|}$$

$$\mathcal{E}(\boldsymbol{x}_{A,B}) = E_{Qq\leftrightarrow\bar{Q}\bar{q}} + \Delta E$$

$$V_{\text{conf}} = \sigma \times (r - R_0) \times \theta(r - R_0)$$

$$V_{\text{BO}}(r_{AB}) = \frac{1}{6}\alpha_S\frac{1}{r_{AB}} + E_{Qq\leftrightarrow\bar{Q}\bar{q}} + \Delta E \\ +\sigma \times (r_{AB} - R_0) \times \theta(r_{AB} - R_0).$$

$$|(Q\bar{Q})(q\bar{q})\rangle|(Q\bar{q})(q\bar{Q})\rangle$$

$$|(Qq)(\bar{Q}\bar{q})\rangle$$

$$|0^{+(+)}\rangle_1 = |0_{Qq}, 0_{\bar{Q}\bar{q}}; J = 0\rangle,$$
$$|0^{+(+)}\rangle_2 = |1_{Qq}, 1_{\bar{Q}\bar{q}}; J = 0\rangle.$$

$$|A\rangle = |0_{Qq}, 1_{\bar{Q}\bar{q}}; J = 1\rangle$$
$$|B\rangle = |1_{Qq}, 0_{\bar{Q}\bar{q}}; J = 1\rangle$$
$$|C\rangle = |1_{Qq}, 1_{\bar{Q}\bar{q}}; J = 1\rangle$$

$$|1^{+(+)}\rangle = \frac{1}{\sqrt{2}}(|A\rangle + |B\rangle)$$
$$|1^{+(-)}\rangle_1 = \frac{1}{\sqrt{2}}(|A\rangle - |B\rangle)$$
$$|1^{+(-)}\rangle_2 = |C\rangle$$

$$|2^{+(+)}\rangle = |1_{Qq}, 1_{\bar{Q}\bar{q}}; J = 2\rangle$$

$$M(T) = 2(m_c + m_q) + E + H_{ss},$$

$$i\partial_\eta|\alpha_{\mathrm{B}}\rangle = \hat{H}^{(0)}|\alpha_{\mathrm{B}}\rangle,$$

$$\eta \mapsto |\alpha_{\mathrm{B}}(\eta)\rangle,$$

$$\int \mathrm{d}\alpha|\alpha\rangle\langle\alpha| = \mathbb{1}$$

$$\langle\alpha_{\mathrm{B}}(\eta)|\hat{\mathcal{O}}|\alpha_{\mathrm{B}}(\eta)\rangle$$

$$\langle\alpha_{\mathrm{B}}|\hat{\mathcal{O}}^2|\alpha_{\mathrm{B}}\rangle$$

$$\langle\alpha_{\mathrm{B}}|\hat{\mathcal{O}}^2|\alpha_{\mathrm{B}}\rangle = \int \mathrm{d}\alpha\langle\alpha_{\mathrm{B}}|\hat{\mathcal{O}}|\alpha\rangle\langle\alpha|\hat{\mathcal{O}}|\alpha_{\mathrm{B}}\rangle.$$

$$\left(\langle\alpha_{\mathrm{B}}|\hat{\mathcal{O}}|\alpha_{\mathrm{B}}\rangle\right)^2$$

$$\langle\alpha_{\mathrm{B}}|\hat{\mathcal{O}}^2|\alpha_{\mathrm{B}}\rangle = \lambda\left(\langle\alpha_{\mathrm{B}}|\hat{\mathcal{O}}|\alpha_{\mathrm{B}}\rangle\right)^2,$$

$$H(q,p,v,\pi) = H^{(0)}(q,p) + \sum_{\boldsymbol{k}=\boldsymbol{k}_{\min}}^{\boldsymbol{k}_{\max}} H_{\boldsymbol{k}}^{(2)}(q,p,v_{\boldsymbol{k}},\pi_{\boldsymbol{k}})$$

$$H_{\boldsymbol{k}}^{(2)} = |\pi_{\boldsymbol{k}}|^2 + [\boldsymbol{k}^2 - V_{\mathrm{B}}(q,p)]|v_{\boldsymbol{k}}|^2$$

$$|v_{\boldsymbol{k}}|^2 = v_{\boldsymbol{k}}v_{\boldsymbol{k}}^* = v_{\boldsymbol{k}}v_{-\boldsymbol{k}}$$

$$\boldsymbol{k} \in [\boldsymbol{k}_{\min}, \boldsymbol{k}_{\max}]^2$$

$$H^{(0)}(q,p) \mapsto H^{(0)}(q,p) - V_{\mathrm{B}}(q,p) \sum_{\boldsymbol{k}=\boldsymbol{k}_{\min}}^{\boldsymbol{k}_{\max}} |v_{\boldsymbol{k}}|^2$$

$$V_{\mathrm{B}}(q,p) \sum_{k} |v_{\boldsymbol{k}}|^2 \ll 1$$

$$H^{(2)}(q_\eta, p_\eta, v_k, \pi_k)$$

$$\mathcal{H} = \mathcal{H}_{\mathrm{B}} \otimes \mathcal{H}_{\mathrm{P}}$$

$$i\partial_\eta|\psi_{\mathrm{P}}(\eta)\rangle = \tilde{H}^{(2)}|\psi_{\mathrm{P}}(\eta)\rangle$$

$$\tilde{H}^{(2)} = \langle\alpha_{\mathrm{B}}(\eta)|\hat{H}^{(2)}|\alpha_{\mathrm{B}}(\eta)\rangle,$$

$$|\alpha_{\mathrm{B}}(\eta)\rangle \otimes |\psi_{\mathrm{P}}(\eta)\rangle$$

$$\hat{H} = \hat{H}^{(0)} + \hat{H}^{(2)},$$

$$i\partial_\eta|\Phi(\eta)\rangle = \hat{H}|\Phi(\eta)\rangle$$

$$|\Phi(\eta_0)\rangle = |\alpha_{\mathrm{B}}(\eta_0)\rangle \otimes |\psi_{\mathrm{P}}(\eta_0)\rangle$$

$$|\Phi(0)\rangle = |\alpha_{\mathrm{B}}(0)\rangle \otimes |\psi_{\mathrm{P}}(0)\rangle$$

$$|\psi_{\mathrm{P}}(\eta)\rangle \overset{\mathrm{def}}{=} \frac{1}{Z_\eta} \langle\alpha_{\mathrm{B}}(\eta) \mid \Phi(\eta)\rangle\Big\rangle_{\mathcal{H}_{\mathrm{P}}},$$

$$\psi_{\mathrm{P}}(v_k,\eta) \overset{\mathrm{def}}{=} \frac{1}{Z_\eta} \int \mathrm{d}\alpha \langle\alpha_{\mathrm{B}}(\eta) \mid \alpha\rangle \Phi(\alpha, v_k, \eta)$$

$$|\Phi(\eta)\rangle = \left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle = |\alpha_{\mathrm{B}}(\eta)\rangle \otimes \left|\psi_{\mathrm{P}}^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\left\langle\alpha_{\mathrm{B}}(\eta) \mid \Phi^{(\mathrm{BO})}(\eta)\right\rangle\Big\rangle_{\mathcal{H}_{\mathrm{P}}} = \left|\psi_{\mathrm{P}}^{(\mathrm{BO})}(\eta)\right\rangle$$

$$|\Phi(\eta_0)\rangle = |\alpha_{\mathrm{B}}(\eta_0)\rangle \otimes |\psi_{\mathrm{P}}(\eta_0)\rangle$$

$$|\alpha_{\mathrm{B}}(\eta)\rangle \otimes |\psi_{\mathrm{P}}(\eta)\rangle$$

$$\hat{\Pi}_{\alpha_{\mathrm{B}}}: \mathcal{H} \mapsto \mathcal{H}_{\mathrm{P}}\mathcal{H} = \mathcal{H}_{\mathrm{B}} \otimes \mathcal{H}_{\mathrm{P}}$$

$$\hat{\Pi}_{\alpha_B} \stackrel{\text{def}}{=} \sum_{n_P} |n_P\rangle(\langle\alpha_B| \otimes \langle n_P|),$$

$$|\psi_P\rangle = \hat{\Pi}_{\alpha_B}|\Phi\rangle$$

$$|\Phi\rangle \in \mathcal{H}_B \otimes \mathcal{H}_p$$

$$\hat{\Pi}^{\dagger}_{\alpha_B}: \mathcal{H}_P \mapsto \mathcal{H}$$

$$\hat{\Pi}^{\dagger}_{\alpha_B} = \sum_{n_P} (|\alpha_B\rangle \otimes |n_P\rangle)\langle n_P|,$$

$$\hat{\Pi}_{\alpha_B}\hat{\Pi}^{\dagger}_{\alpha_B}$$

$$\hat{\Pi}^{\dagger}_{\alpha_B}\hat{\Pi}_{\alpha_B} = (|\alpha_B\rangle\langle\alpha_B|) \otimes \mathbb{I}_{\mathcal{H}_P},$$
$$\hat{\Pi}_{\alpha_B}\hat{\Pi}^{\dagger}_{\alpha_B} = \mathbb{I}_{\mathcal{H}_P}.$$

$$\hat{\Pi}^{\dagger}_{\alpha'_B}\hat{X}_P\hat{\Pi}_{\alpha_B} = (|\alpha'_B\rangle\langle\alpha_B|) \otimes \hat{X}_P$$
$$\hat{\Pi}_{\alpha_B}(\hat{W}_B \otimes \hat{X}_P)\hat{\Pi}^{\dagger}_{\alpha'_B} = \langle\alpha_B|\hat{W}_B|\alpha'_B\rangle\hat{X}_P$$

$$\sum_{n_B} \hat{\Pi}^{\dagger}_{n_B}\hat{\Pi}_{n_B} = \left(\sum_{n_B} |n_B\rangle\langle n_B|\right) \otimes \mathbb{I}_{\mathcal{H}_P} = \mathbb{I}_{\mathcal{H}_B} \otimes \mathbb{I}_{\mathcal{H}_P} = \mathbb{I}_{\mathcal{H}}.$$

$$P(\alpha_B) = \langle\Phi|\hat{\Pi}^{\dagger}_{\alpha_B}\hat{\Pi}_{\alpha_B}|\Phi\rangle = \langle\Phi|(|\alpha_B\rangle\langle\alpha_B|) \otimes \mathbb{I}_{\mathcal{H}_P}|\Phi\rangle$$

$$\sum_{n_B} P(n_B) = \langle\Phi \mid \Phi\rangle = 1$$

$$|\psi_P\rangle = \frac{1}{\sqrt{P(\alpha_B)}}\hat{\Pi}_{\alpha_B}|\Phi\rangle,$$

$$|\Phi'\rangle = |\alpha_B\rangle \otimes |\psi_P\rangle = \frac{1}{\sqrt{P(\alpha_B)}}\hat{\Pi}^{\dagger}_{\alpha_B}\hat{\Pi}_{\alpha_B}|\Phi\rangle.$$

$$\tilde{H}^{(2)}_{\alpha,\beta} \stackrel{\text{def}}{=} \hat{\Pi}_{\alpha}\hat{H}^{(2)}\hat{\Pi}^{\dagger}_{\beta} \equiv \langle\alpha|\hat{H}^{(2)}|\beta\rangle,$$

$$\tilde{H}^{(2)}_{\alpha} \stackrel{\text{def}}{=} \tilde{H}^{(2)}_{\alpha,\alpha}$$

$$i\partial_\eta|\alpha_B(\eta)\rangle = \hat{H}^{(0)}|\alpha_B(\eta)\rangle,$$

$$|\alpha_B(\eta)\rangle = e^{-i\hat{H}^{(0)}(\eta-\eta_0)}|\alpha_B(\eta_0)\rangle.$$

$$\left|\psi^{(\mathrm{Bo})}_P(\eta)\right\rangle$$

$$i\partial_\eta\left|\psi^{(\mathrm{BO})}_P(\eta)\right\rangle = \tilde{H}^{(2)}_{\alpha_B(\eta)}\left|\psi^{(\mathrm{BO})}_P(\eta)\right\rangle,$$

$$\left|\psi_{\mathrm{P}}^{(\mathrm{so})}(\eta)\right\rangle = T\left\{\exp\left[-i\int_{\eta_0}^{\eta}\tilde{H}_{\alpha_{\mathrm{B}}(\tau)}^{(2)}\mathrm{d}\tau\right]\right\}\left|\psi_{\mathrm{P}}^{(\mathrm{so})}(\eta_0)\right\rangle,$$

$$\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle = |\alpha_{\mathrm{B}}(\eta)\rangle \otimes \left|\psi_{\mathrm{P}}^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\begin{aligned}\tilde{H}_{\alpha_{\mathrm{B}}(\tau)}^{(2)} &= \hat{\Pi}_{\alpha_{\mathrm{B}}(0)} e^{i\hat{H}^{(0)}\tau}\hat{H}^{(2)}e^{-i\hat{H}^{(0)}\tau}\hat{\Pi}_{\alpha_{\mathrm{B}}(0)}^{\dagger}\\ &= \hat{\Pi}_{\alpha_{\mathrm{B}}(0)}\hat{H}_{\mathrm{I}}^{(2)}(\tau)\hat{\Pi}_{\alpha_{\mathrm{B}}(0)}^{\dagger}\end{aligned}$$

$$\hat{H}_{\mathrm{I}}^{(2)}(\eta) = e^{i\hat{H}^{(0)}\eta}\hat{H}^{(2)}e^{-i\hat{H}^{(0)}\eta}$$

$$\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle = \hat{U}^{(\mathrm{BO})}(\eta,\eta_0)\left|\Phi^{(\mathrm{BO})}(\eta_0)\right\rangle,$$

$$\hat{U}^{(\mathrm{BO})}(\eta,\eta_0) = T\left(\exp\left\{-i\int_{\eta_0}^{\eta}\left[\hat{H}^{(0)} + \tilde{H}_{\alpha_{\mathrm{B}}(\tau)}^{(2)}\right]\mathrm{d}\tau\right\}\right),$$

$$\hat{H}^{(0)}\tilde{H}_{\alpha_{\mathrm{B}}(\tau)}^{(2)}\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle\hat{U}^{(\mathrm{BO})}(\eta,\eta_0)|\alpha_{\mathrm{P}}(\eta)\rangle\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle$$

$$i\partial_\eta\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle = \left[\hat{H}^{(0)} + \tilde{H}_{\alpha_{\mathrm{B}}(\eta)}^{(2)}\right]\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle\tilde{H}_{\alpha_{\mathrm{B}}(\eta)}^{(2)}$$

$$i\partial_\eta|\Phi(\eta)\rangle = \left[\hat{H}^{(0)} + \hat{H}^{(2)}\right]|\Phi(\eta)\rangle,$$

$$|\Phi(\eta)\rangle = \hat{U}_{\mathrm{tot}}(\eta,\eta_0)|\Phi(\eta_0)\rangle,$$

$$\hat{U}_{\mathrm{tot}}(\eta,\eta_0) = e^{-i\left[\hat{H}^{(0)}+\hat{H}^{(2)}\right](\eta-\eta_0)},$$

$$\hat{U}_{\mathrm{tot}}(\eta,\eta_0) = e^{-i\hat{H}^{(0)}\eta}\hat{S}(\eta,\eta_0)e^{i\hat{H}^{(0)}\eta_0}$$

$$\hat{S}(\eta,\eta_0) = T\left\{\exp\left[-i\int_{\eta_0}^{\eta}\hat{H}_{\mathrm{I}}^{(2)}(\tau)\mathrm{d}\tau\right]\right\},$$

$$\hat{H}_{\mathrm{I}}^{(2)}(\tau) = e^{i\hat{H}^{(0)}\tau}\hat{H}^{(2)}e^{-i\hat{H}^{(0)}\tau}$$

$$|\Phi(\eta_0)\rangle = |\alpha_{\mathrm{B}}(\eta_0)\rangle \otimes |\psi_{\mathrm{P}}(\eta_0)\rangle$$

$$|\alpha_{\mathrm{B}}(\eta_0)\rangle\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle|\Phi(\eta_0)\rangle = |\alpha_{\mathrm{B}}(\eta_0)\rangle \otimes |\psi_{\mathrm{P}}(\eta_0)\rangle$$

$$|\Phi(\eta_0)\rangle = \left[\hat{U}^{(\mathrm{BO})}(\eta,\eta_0)\right]^{\dagger}\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle.$$

$$|\Phi(\eta)\rangle = \hat{V}(\eta,\eta_0)\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle,$$

$$\hat{V}(\eta,\eta_0) = \hat{U}_{\mathrm{tot}}(\eta,\eta_0)\left[\hat{U}^{(\mathrm{BO})}(\eta,\eta_0)\right]^{\dagger}.$$

$$\hat{V}(\eta_0,\eta_0) = \mathbb{1} \text{ and } |\Phi(\eta_0)\rangle = \left|\Phi^{(\mathrm{BO})}(\eta_0)\right\rangle = |\alpha_{\mathrm{B}}(\eta_0)\rangle \otimes |\psi_{\mathrm{P}}(\eta_0)\rangle$$

$$\hat{V}(\eta,\eta_0) = e^{-i\hat{H}^{(0)}\eta}T\left[e^{-i\int_{\eta_0}^{\eta}\hat{H}_{\mathrm{I}}^{(2)}(\tau)\mathrm{d}\tau}\right]e^{i\hat{H}^{(0)}\eta_0}e^{i\hat{H}^{(0)}(\eta-\eta_0)}T\left[e^{i\int_{\eta_0}^{\eta}\tilde{H}_{\alpha_{\mathrm{B}}(\tau)}^{(2)}\mathrm{d}\tau}\right]$$

$$\hat{V}(\eta,\eta_0) = e^{-i\hat{H}^{(0)}\eta} T\left[e^{-i\int_{\eta_0}^{\eta}\hat{H}_1^{(2)}(\tau)\mathrm{d}\tau}\right] T\left[e^{i\int_{\eta_0}^{\eta}\tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau)}\mathrm{d}\tau}\right] e^{i\hat{H}^{(0)}\eta}\tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau)}$$

$$\tilde{H}^{(2)}_{\alpha(\tau),\beta(\tau)}\tilde{H}^{(2)}_{\alpha(\tau)}$$

$$\hat{V}(\eta,\eta_0) \simeq e^{-i\hat{H}^{(0)}\eta}\left(\mathbb{I} + \hat{C}_1 + \hat{C}_2' + \hat{C}_2''\right)e^{i\hat{H}^{(0)}\eta}$$

$$\hat{C}_1 = -i\int_{\eta_0}^{\eta}\left[\hat{H}_\mathrm{I}^{(2)}(\tau) - \tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau)}\right]\mathrm{d}\tau$$

$$\hat{C}_2' = \int_{\eta_0}^{\eta}\mathrm{d}\tau_1\int_{\eta_0}^{\eta}\mathrm{d}\tau_2\hat{H}_\mathrm{I}^{(2)}(\tau_1)\tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau_2)}$$

$$\hat{C}_2'' = -\frac{1}{2}\int_{\eta_0}^{\eta}\mathrm{d}\tau_1\int_{\eta_0}^{\eta}\mathrm{d}\tau_2 T\left[\hat{H}_\mathrm{I}^{(2)}(\tau_1)\hat{H}_\mathrm{I}^{(2)}(\tau_2) + \tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau_1)}\tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau_2)}\right]$$

$$\hat{C}_2 = \hat{C}_2' + \hat{C}_2'' = -\frac{1}{2}\int_{\eta_0}^{\eta}\mathrm{d}\tau_1\int_{\eta_0}^{\eta}\mathrm{d}\tau_2 T\left\{\left[\hat{H}_\mathrm{I}^{(2)}(\tau_1) - \tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau_1)}\right]\left[\hat{H}_\mathrm{I}^{(2)}(\tau_2) - \tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau_2)}\right]\right\}$$

$$\left|\psi_\mathrm{P}^{(\mathrm{BBO})}(\eta)\right\rangle \left|\psi_\mathrm{P}^{(\mathrm{BBO})}(\eta)\right\rangle \stackrel{\mathrm{def}}{=} \hat{\Pi}_{\alpha_\mathrm{B}(\eta)}|\Phi(\eta)\rangle = \hat{\Pi}_{\alpha_\mathrm{B}(\eta)}\hat{V}(\eta,\eta_0)\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\left|\psi_\mathrm{P}^{(\mathrm{BBO})}(\eta)\right\rangle = \hat{\Pi}_{\alpha_\mathrm{B}(\eta)}\hat{V}(\eta,\eta_0)\hat{\Pi}^\dagger_{\alpha_\mathrm{B}(\eta)}\left|\psi_\mathrm{P}^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\left|\psi_\mathrm{P}^{(\mathrm{BO})}(\eta)\right\rangle\left|\psi_\mathrm{P}^{(\mathrm{BBO})}(\eta)\right\rangle$$

$$\hat{\Pi}_{\alpha_\mathrm{B}(\eta)}\hat{V}(\eta,\eta_0)\hat{\Pi}^\dagger_{\alpha_\mathrm{B}(\eta)} \equiv \langle\alpha_\mathrm{B}(\eta)|\hat{V}(\eta,\eta_0)|\alpha_\mathrm{B}(\eta)\rangle$$

$$\left|\psi_\mathrm{P}^{(\mathrm{BBO})}(\eta)\right\rangle \simeq \left[\mathbb{1} + \hat{\Pi}_{\alpha_\mathrm{B}(0)}\left(\hat{C}_1 + \hat{C}_2\right)\hat{\Pi}^\dagger_{\alpha_\mathrm{B}(0)}\right]\left|\psi_\mathrm{P}^{(\mathrm{BO})}(\eta)\right\rangle,$$

$$\hat{\Pi}_{\alpha_\mathrm{B}}\hat{\Pi}^\dagger_{\alpha_\mathrm{B}} = \mathbb{1}_{\mathcal{H}_\mathrm{P}}, |\alpha_\mathrm{B}(\eta)\rangle = e^{-i\hat{H}^{(0)}\eta}|\alpha_\mathrm{B}(0)\rangle \text{ and } \hat{\Pi}_{\alpha_\mathrm{B}(\eta)} = \hat{\Pi}_{\alpha_\mathrm{B}(0)}e^{i\hat{H}^{(0)}\eta}$$

$$\hat{\Pi}_{\alpha_\mathrm{B}(0)}\hat{C}_1\hat{\Pi}^\dagger_{\alpha_\mathrm{B}(0)}$$

$$\hat{\Pi}_{\alpha_\mathrm{B}(0)}\tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau)}\hat{\Pi}^\dagger_{\alpha_\mathrm{B}(0)} = \tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau)}$$

$$\hat{\Pi}_{\alpha_\mathrm{B}(0)}\hat{H}_\mathrm{I}^{(2)}(\tau)\hat{\Pi}^\dagger_{\alpha_\mathrm{B}(0)} = \hat{\Pi}_{\alpha_\mathrm{B}(\tau)}\hat{H}^{(2)}\hat{\Pi}^\dagger_{\alpha_\mathrm{B}(\tau)} = \tilde{H}^{(2)}_{\alpha_\mathrm{B}(\tau)}$$

$$\hat{H}^{(2)} = \sum_{\boldsymbol{k}}\hat{H}^{(2)}_{\boldsymbol{k}}$$

$$\tilde{H}^{(2)}_{\alpha_\mathrm{B}(\eta)} = \sum_{\boldsymbol{k}}\left\{\hat{\pi}_{\boldsymbol{k}}\hat{\pi}_{-\boldsymbol{k}} + [k^2 - V_\mathrm{B}(\eta)]\hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right\}$$

$$\hat{H}_\mathrm{I}^{(2)}(\eta) = \sum_{\boldsymbol{k}}\left\{\hat{\pi}_{\boldsymbol{k}}\hat{\pi}_{-\boldsymbol{k}} + \left[k^2 - \hat{V}_\mathrm{B}^{(\mathrm{I})}(\eta)\right]\hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right\}$$

$$V_\mathrm{B}(\eta) = \langle\alpha_\mathrm{B}(\eta)|\hat{V}_\mathrm{B}|\alpha_\mathrm{B}(\eta)\rangle$$

$$\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\eta) = e^{i\hat{H}^{(0)}\eta}\hat{V}_{\mathrm{B}}e^{-i\hat{H}^{(0)}\eta}$$

$$\hat{C}_2 = -\frac{1}{2}\left(\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right)^2 \int_{\eta_0}^{\eta} \mathrm{d}\tau_1 \int_{\eta_0}^{\eta} \mathrm{d}\tau_2 T\left\{\left[\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_1) - V_{\mathrm{B}}(\tau_1)\right]\left[\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_2) - V_{\mathrm{B}}(\tau_2)\right]\right\}$$

$$\hat{C}_2 = -\frac{1}{2}\left(\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right)^2 \int_{\eta_0}^{\eta} \mathrm{d}\tau_1 \int_{\eta_0}^{\eta} \mathrm{d}\tau_2 \left\{T\left[\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_1)\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_2)\right] - V_{\mathrm{B}}(\tau_1)V_{\mathrm{B}}(\tau_2)\right\}.$$

$$\hat{C}_2 = -\left(\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right)^2 \left\{\left[\int_{\eta_0}^{\eta} \mathrm{d}\tau_1 \int_{\eta_0}^{\tau_1} \mathrm{d}\tau_2 \hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_1)\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_2)\right] - \frac{1}{2}\left[\int_{\eta_0}^{\eta} V_{\mathrm{B}}(\tau)\mathrm{d}\tau\right]^2\right\}$$

$$\left(\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right)^2 K_{\eta,\eta_0} = -\hat{\Pi}_{\alpha_{\mathrm{B}}(0)}\hat{C}_2\hat{\Pi}^{\dagger}_{\alpha_{\mathrm{B}}(0)}$$

$$K_{\eta,\eta_0} = \int_{\eta_0}^{\eta} \mathrm{d}\tau_1 \int_{\eta_0}^{\tau_1} \mathrm{d}\tau_2 \langle\alpha_{\mathrm{B}}(0)|\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_1)\hat{V}_{\mathrm{B}}^{(\mathrm{I})}(\tau_2)|\alpha_{\mathrm{B}}(0)\rangle - \frac{1}{2}\left[\int_{\eta_0}^{\eta} V_{\mathrm{B}}(\tau_1)d\tau_1\right]^2$$

$$\left|\psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta)\right\rangle \simeq \left[\mathbb{1} - K_{\eta,\eta_0}\left(\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right)^2\right]\left|\psi_{\mathrm{P}}^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\left\langle\psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \mid \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta)\right\rangle \simeq 1$$

$$\left|\Re\mathrm{e}K_{\eta,\eta_0}\right|\left\langle\left(\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right)^2\right\rangle_{\eta}^{(\mathrm{sO})} \ll 1,$$

$$\rangle_{\eta}^{(\mathrm{BO})} := \left|\psi_{\mathrm{P}}^{(\mathrm{BO})}(\eta)\right\rangle$$

$$\left\langle\left(\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right)^2\right\rangle_{\eta}^{(\mathrm{BO})} = \left[\left\langle\sum_{\boldsymbol{k}} \hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\right\rangle_{\eta}^{(\mathrm{BO})}\right]^2$$

$$+2\sum_{\boldsymbol{k}} \left[\langle\hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\rangle_{\eta}^{(\mathrm{BO})}\right]^2.$$

$$\langle\hat{v}_{\boldsymbol{k}}\hat{v}_{\boldsymbol{\ell}}\rangle_{\eta} = \delta_{\boldsymbol{k}+\boldsymbol{\ell}} f(\eta)P_{\eta}(k)$$

$$P_{\eta}(k) \to P(k) \propto k^{n_{\mathrm{s}}-4}$$

$$\delta_{\boldsymbol{v}+\boldsymbol{w}} \to (2\pi)^3\delta^{(3)}(\boldsymbol{v}+\boldsymbol{w})$$

$$\sum_{\boldsymbol{v}} \to \frac{1}{(2\pi)^3}\int \mathrm{d}^3\boldsymbol{v}$$

$$S_{\mathrm{R}} = \left\langle \sum_{\boldsymbol{p}} \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \right\rangle_{\eta}^{(\mathrm{BO})},$$

$$\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{BBO})} = \frac{\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \middle| \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \middle| \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle}{\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \mid \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle},$$

$$\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \middle| \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \middle| \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle \simeq \langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{BO})} - 2\Re\mathrm{e}(K_{\eta,\eta_0}) \left\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \left(\sum_{\boldsymbol{p}} \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \right)^2 \right\rangle_{\eta}^{(\mathrm{BO})}$$

$$\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \mid \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle \simeq 1 - 2\Re\mathrm{e}(K_{\eta,\eta_0}) \left\langle \left(\sum_{\boldsymbol{p}} \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \right)^2 \right\rangle_{\eta}^{(\mathrm{BO})}$$

$$\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{B[illegible])}} \simeq \langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{BO})} - 2\Re\mathrm{e}(K_{\eta,\eta_0}) \left[\left\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \left(\sum_{\boldsymbol{p}} \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \right)^2 \right\rangle_{\eta}^{(\mathrm{BO})} - \langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{BO})} \left\langle \left(\sum_{\boldsymbol{p}} \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \right)^2 \right\rangle_{\eta}^{(\mathrm{BO})} \right]$$

$$4 \sum_{\boldsymbol{p},\boldsymbol{q}} \left[\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{q}} \rangle_{\eta}^{(\mathrm{BO})} \langle \hat{v}_{\boldsymbol{\ell}} \hat{v}_{-\boldsymbol{q}} \rangle_{\eta}^{(\mathrm{BO})} \langle \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \rangle_{\eta}^{(\mathrm{BO})} + 2 \langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{p}} \rangle_{\eta}^{(\mathrm{BO})} \langle \hat{v}_{\boldsymbol{\ell}} \hat{v}_{-\boldsymbol{q}} \rangle_{\eta}^{(\mathrm{BO})} \langle \hat{v}_{-\boldsymbol{p}} \hat{v}_{\boldsymbol{q}} \rangle_{\eta}^{(\mathrm{BO})} \right]$$

$$P_{\eta}^{(\mathrm{BBO})}(k) = P_{\eta}^{(\mathrm{BO})}(k) \left[1 - 8\Re\mathrm{e}(K_{\eta,\eta_0}) S_{\mathrm{R}} P_{\eta}^{(\mathrm{BO})}(k) \right],$$

$$\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \rangle_{\eta}^{(\mathrm{BBO})} = \frac{\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \middle| \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \middle| \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle}{\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \mid \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle}$$

$$\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \hat{v}_{\boldsymbol{n}} \rangle_{\eta}^{(\mathrm{BBO})} = \frac{\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \middle| \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \hat{v}_{\boldsymbol{n}} \middle| \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle}{\left\langle \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \mid \psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta) \right\rangle}$$

$$\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \hat{v}_{\boldsymbol{n}} \rangle_{\eta}^{(\mathrm{BBO})} \simeq \langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \hat{v}_{\boldsymbol{n}} \rangle_{\eta}^{(\mathrm{BO})} + T(\boldsymbol{k}, \boldsymbol{\ell}, \boldsymbol{m}, \boldsymbol{n}),$$

$$T(\boldsymbol{k}, \boldsymbol{\ell}, \boldsymbol{m}, \boldsymbol{n}) = -2\Re\mathrm{e}(K_{\eta,\eta_0}) \left[\left\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \hat{v}_{\boldsymbol{n}} \left(\sum_{\boldsymbol{p}} \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \right)^2 \right\rangle_{\eta}^{(\mathrm{BO})} - \langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \hat{v}_{\boldsymbol{m}} \hat{v}_{\boldsymbol{n}} \rangle_{\eta}^{(\mathrm{BO})} \left\langle \left(\sum_{\boldsymbol{p}} \hat{v}_{\boldsymbol{p}} \hat{v}_{-\boldsymbol{p}} \right)^2 \right\rangle_{\eta}^{(\mathrm{BO})} \right],$$

$$T \sim T_9 S_{\mathrm{R}}^2 + T_{24} S_{\mathrm{R}} + T_{72}$$

$$\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{BO})} \propto \delta_{\boldsymbol{k}+\boldsymbol{\ell}}$$

$$T(\boldsymbol{k}, \boldsymbol{\ell}, \boldsymbol{m}, \boldsymbol{n}) = -4\Re\mathrm{e}(K_{\eta,\eta_0}) S_{\mathrm{R}} \delta_{\boldsymbol{k}+\boldsymbol{\ell}+\boldsymbol{m}+\boldsymbol{n}} \Big\{ \langle \hat{v}_{\boldsymbol{k}} \hat{v}_{-\boldsymbol{k}} \rangle_{\eta}^{(\mathrm{BO})} \left[\langle \hat{v}_{\boldsymbol{m}} \hat{v}_{-\boldsymbol{m}} \rangle_{\eta}^{(\mathrm{BO})} \right]^2 (\delta_{\boldsymbol{k}+\boldsymbol{\ell}} + \delta_{\boldsymbol{k}+\boldsymbol{n}})$$
$$+ \langle \hat{v}_{\boldsymbol{\ell}} \hat{v}_{-\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{BO})} \left[\langle \hat{v}_{\boldsymbol{k}} \hat{v}_{-\boldsymbol{k}} \rangle_{\eta}^{(\mathrm{BO})} \right]^2 (\delta_{\boldsymbol{\ell}+\boldsymbol{m}} + \delta_{\boldsymbol{\ell}+\boldsymbol{n}}) + \langle \hat{v}_{\boldsymbol{n}} \hat{v}_{-\boldsymbol{n}} \rangle_{\eta}^{(\mathrm{BO})} \left[\langle \hat{v}_{\boldsymbol{\ell}} \hat{v}_{-\boldsymbol{\ell}} \rangle_{\eta}^{(\mathrm{BO})} \right]^2 (\delta_{\boldsymbol{n}+\boldsymbol{m}} + \delta_{\boldsymbol{n}+\boldsymbol{k}}) \Big\}.$$

$$g_{\mathrm{NL}}^{\mathrm{BBO}} = -4\Re\mathrm{e}\left(K_{\eta,\eta_0}\right)S_{\mathrm{R}}$$

$$t(\boldsymbol{k},\boldsymbol{\ell},\boldsymbol{m},\boldsymbol{n}) := T(\boldsymbol{k},\boldsymbol{\ell},\boldsymbol{m},\boldsymbol{n})/g_{\mathrm{NL}}^{\mathrm{BBO}}$$

$$t(\boldsymbol{k},-\boldsymbol{k},\boldsymbol{m},-\boldsymbol{m}) = \delta_{\boldsymbol{k}+\boldsymbol{\ell}+\boldsymbol{m}+\boldsymbol{n}}\delta_{\boldsymbol{k}+\boldsymbol{\ell}}\left\{\langle\hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\rangle_\eta^{(\mathrm{BO})}\left[\langle\hat{v}_{\boldsymbol{m}}\hat{v}_{-\boldsymbol{m}}\rangle_\eta^{(\mathrm{BO})}\right]^2 + \langle\hat{v}_{\boldsymbol{m}}\hat{v}_{-\boldsymbol{m}}\rangle_\eta^{(\mathrm{BO})}\left[\langle\hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\rangle_\eta^{(\mathrm{BO})}\right]^2\right\}$$

$$\delta_{\boldsymbol{k}+\boldsymbol{\ell}}t^{\mathrm{local}}(\boldsymbol{k},\boldsymbol{\ell},\boldsymbol{m},\boldsymbol{n})$$

$$t^{\mathrm{local}}(\boldsymbol{k},\boldsymbol{\ell},\boldsymbol{m},\boldsymbol{n}) = \delta_{\boldsymbol{k}+\boldsymbol{\ell}+\boldsymbol{m}+\boldsymbol{n}}\left[\langle\hat{v}_{\boldsymbol{k}}\hat{v}_{-\boldsymbol{k}}\rangle_\eta^{(\mathrm{BO})}\langle\hat{v}_{\boldsymbol{\ell}}\hat{v}_{-\boldsymbol{\ell}}\rangle_\eta^{(\mathrm{BO})}\langle\hat{v}_{\boldsymbol{m}}\hat{v}_{-\boldsymbol{m}}\rangle_\eta^{(\mathrm{BO})} + 3\text{ perms}\right]$$

$$t(\boldsymbol{k},-\boldsymbol{k},\boldsymbol{\ell},-\boldsymbol{\ell}) \propto \frac{1}{k^{4-n_s}}\left(\frac{1}{\ell^{4-n_s}}\right)^2 + \frac{1}{\ell^{4-n_s}}\left(\frac{1}{k^{4-n_s}}\right)^2 \propto [P(k)]^3\left[\left(\frac{k}{\ell}\right)^{2(4-n_s)} + \left(\frac{k}{\ell}\right)^{4-n_s}\right]$$

$$\left|\psi_{\mathrm{P}}^{(\mathrm{BBO})}(\eta)\right\rangle = \hat{\Pi}_{\alpha_{\mathrm{B}}(\eta)}\hat{V}(\eta,\eta_0)\left|\Phi^{(\mathrm{BO})}(\eta)\right\rangle$$

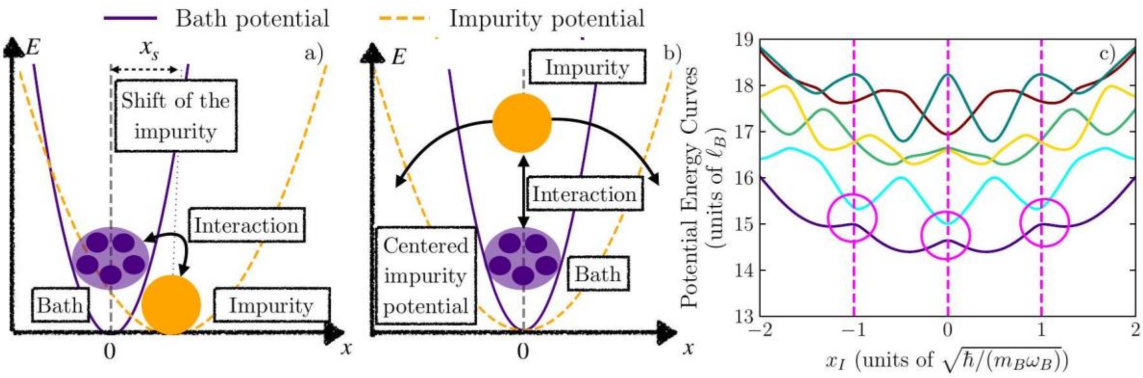
$$\hat{v}_k^{(\mathrm{BBO})} = \hat{V}(\eta,\eta_0)^\dagger\hat{\Pi}_{\alpha_{\mathrm{B}}(\eta)}^\dagger\hat{v}_k\hat{\Pi}_{\alpha_{\mathrm{B}}(\eta)}\hat{V}(\eta,\eta_0)$$

$$\hat{v}_k^{(\mathrm{BBO})} = \left[\hat{v}_k - 2\Re\mathrm{e}\left(K_{\eta,\eta_0}\right)\left(\sum_{\boldsymbol{p}}\hat{v}_{\boldsymbol{p}}\hat{v}_{-\boldsymbol{p}}\right)^2\hat{v}_k\right],$$

$$\hat{v}^{(\mathrm{BBO})}(x) = \hat{v}(x) - 2\Re\mathrm{e}\left(K_{\eta,\eta_0}\right)\left[\int \hat{v}^2(y)\mathrm{d}^3y\right]^2\hat{v}(x),$$

$$|\alpha_{\mathrm{B}}\rangle = |q,p\rangle$$

$$|\alpha_{\mathrm{B}}(\eta)\rangle = |q_\eta,p_\eta\rangle$$



$$\hat{H} = \hat{H}_B + \hat{H}_I + \hat{H}_{BI}$$

$$\hat{H}_B = \sum_{j=1}^{N_B}\left[-\frac{\hbar^2}{2m_B}\left(\frac{\partial}{\partial x_j^B}\right)^2 + \frac{1}{2}m_B\omega_B^2\left(x_j^B\right)^2\right]$$

$$\hat{H}_I = \sum_{j=1}^{N_I}\left[-\frac{\hbar^2}{2m_I}\left(\frac{\partial}{\partial x_j^I}\right)^2 + \frac{1}{2}m_I\omega_I^2\left(x_j^I - x_s\right)^2\right]$$

$$\hat{H}_{BI} = \sum_{k=1}^{N_B}\sum_{j=1}^{N_I} g\delta\left(x_k^B - x_j^I\right)$$

$$\ell_B = \sqrt{\frac{\hbar}{m_B \omega_B}},$$

$$\ell_I = \sqrt{\frac{m_B \omega_B}{m_I \omega_I}} \ell_B$$

$$\sigma_B \approx \ell_B \sqrt{N_B + \frac{1}{2}}$$

$$\ell_I \approx \sqrt{N_B} \ell_B$$

$$|\Psi(t)\rangle = \sum_{k=1}^{D} \sqrt{\lambda_k(t)} \left|\tilde{\Psi}_k^B(t)\right\rangle \left|\tilde{\Psi}_k^I(t)\right\rangle$$

$$\Psi\left(x_1^B, \dots, x_{N_B}^B, x_I; t\right) = \sum_{j=1}^{M} \Psi_{j,I}(x_I; t) \underbrace{\Psi_{j,B}\left(x_1^B, \dots, x_{N_B}^B; x_I\right)}_{\equiv \left\langle x_1^B, \dots, x_{N_B}^B | \Psi_{j,B}(x_I) \right\rangle}.$$

$$\left|\Psi_{j,B}(x_I)\right\rangle \Psi_{j,I}(x_I; t) \sum_{j=1}^{M} \int \mathrm{d}x_I \left|\Psi_{j,I}(x_I; t)\right|^2 = 1$$

$$\langle \delta\Psi | \hat{H} - i\hbar \frac{\partial}{\partial t} | \Psi \rangle = 0$$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \Psi_{k,I}(x_I, t) = -\frac{\hbar^2}{2m_I} \sum_{j,l=1}^{M} \left(\delta_{kj} \frac{\mathrm{d}}{\mathrm{d}x_I} - iA_{kj}(x_I) \right) \times \left(\delta_{jl} \frac{\mathrm{d}}{\mathrm{d}x_I} - iA_{jl}(x_I) \right) \Psi_{l,I}(x_I) + \sum_{l=1}^{M} \left(\delta_{kl} \varepsilon_k(x_I) + \delta_{kl} \frac{1}{2} m_B \omega_I^2 x_I^2 + V_{kl}^{\mathrm{ren}}(x_I) \right) \Psi_{l,I}(x_I, t)$$

$$\left|\Psi_{k,B}(x_I)\right\rangle$$

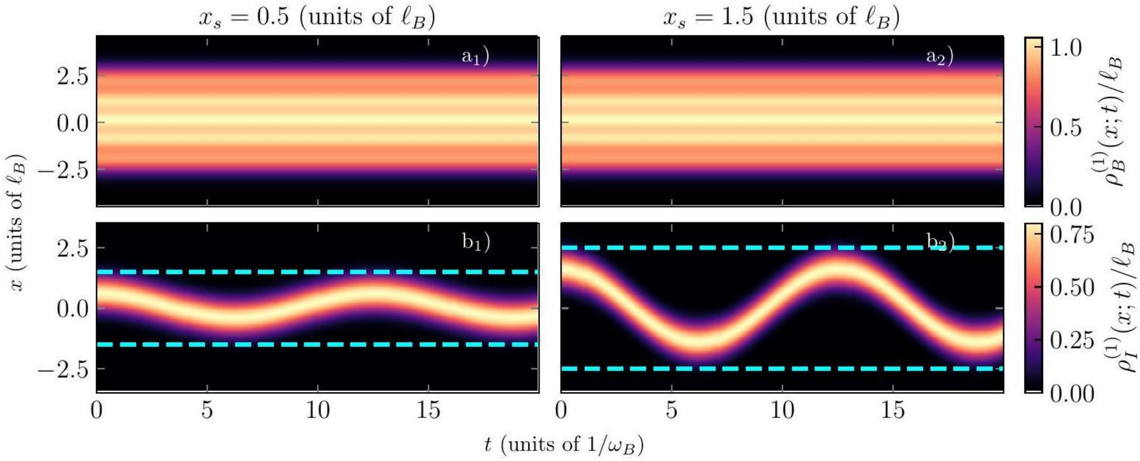
$$\hat{H}_B + \hat{H}_{BI}$$

$$\left\langle \Psi_{k,B}(x_I) \middle| \hat{H}_B + \hat{H}_{BI} \middle| \Psi_{l,B}(x_I) \right\rangle = \delta_{kl} \varepsilon_k(x_I),$$

$$A_{kj}(x_I) = i \left\langle \Psi_{k,B}(x_I) \middle| \frac{\partial \Psi_{j,B}}{\partial x_I}(x_I) \right\rangle$$

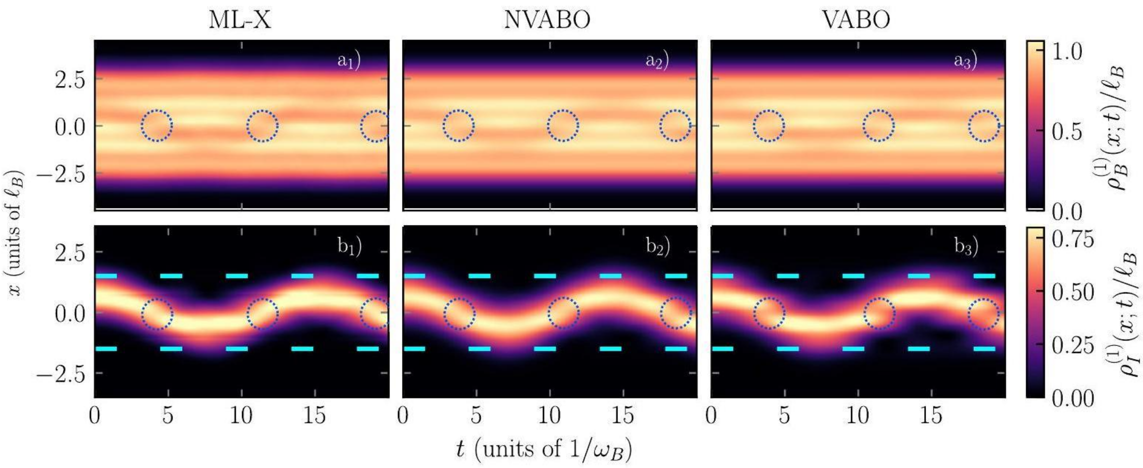
$$V_{kl}^{\mathrm{ren}}(x_I) = \frac{\hbar^2}{2m_I} \left\langle \frac{\mathrm{d}\Psi_{k,B}}{\mathrm{d}x_I}(x_I) \middle| 1 - \hat{\mathcal{P}}_M \middle| \frac{\mathrm{d}\Psi_{l,B}}{\mathrm{d}x_I}(x_I) \right\rangle$$

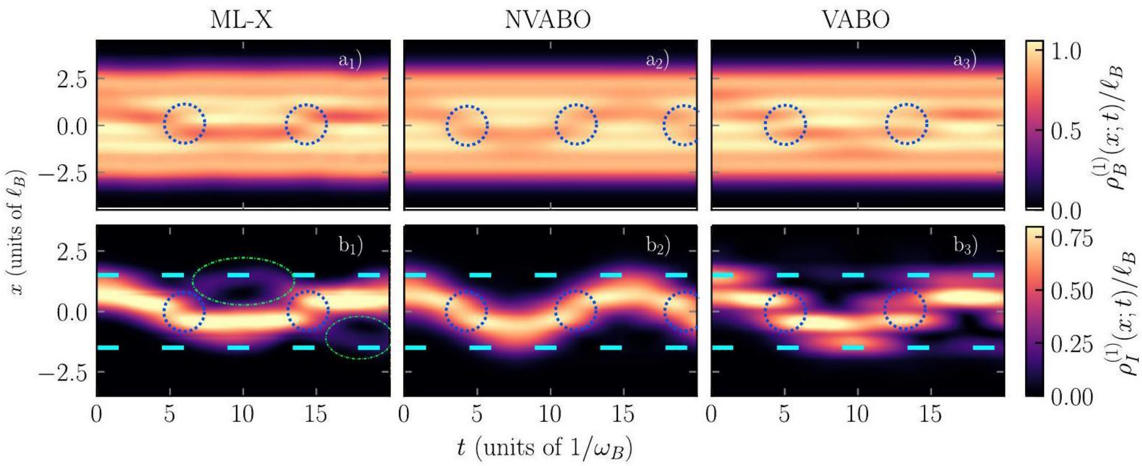
$$\hat{\mathcal{P}}_M = \sum_{j=1}^{M} \left|\Psi_{j,B}(x_I)\right\rangle\left\langle\Psi_{j,B}(x_I)\right|$$

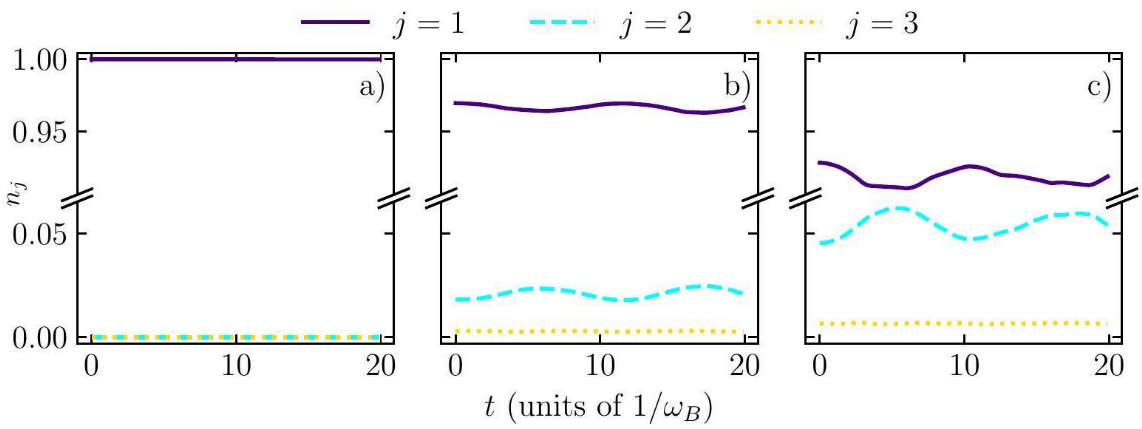


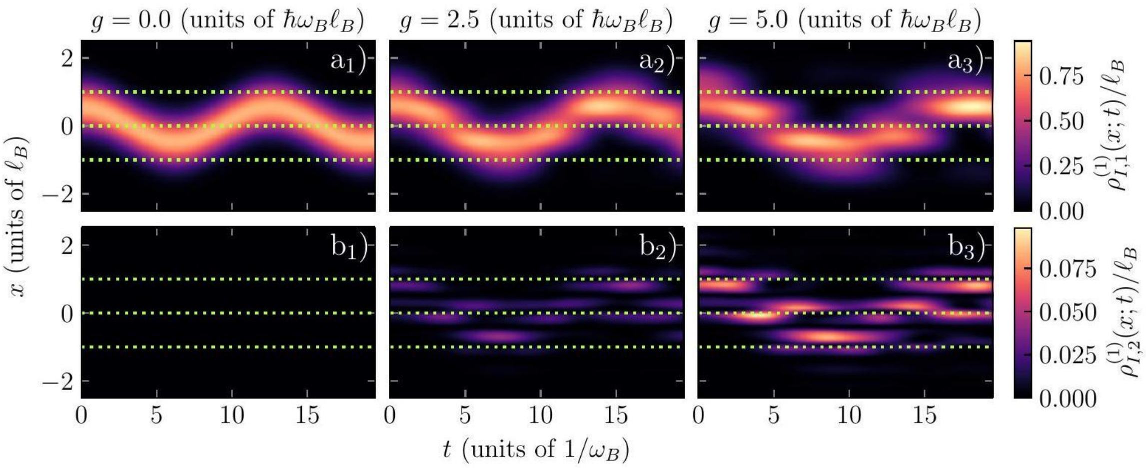
$$\left(\rho_B^{(1)}(x;t)\right)\left(\rho_I^{(1)}(x;t)\right)$$

$$\rho_\sigma^{(1)}(x;t) = \langle\Psi(t)|\hat{\Psi}_\sigma^\dagger(x)\hat{\Psi}_\sigma(x)|\Psi(t)\rangle|\Psi(t)\rangle\hat{\Psi}_\sigma^\dagger(x)\hat{\Psi}(x)$$

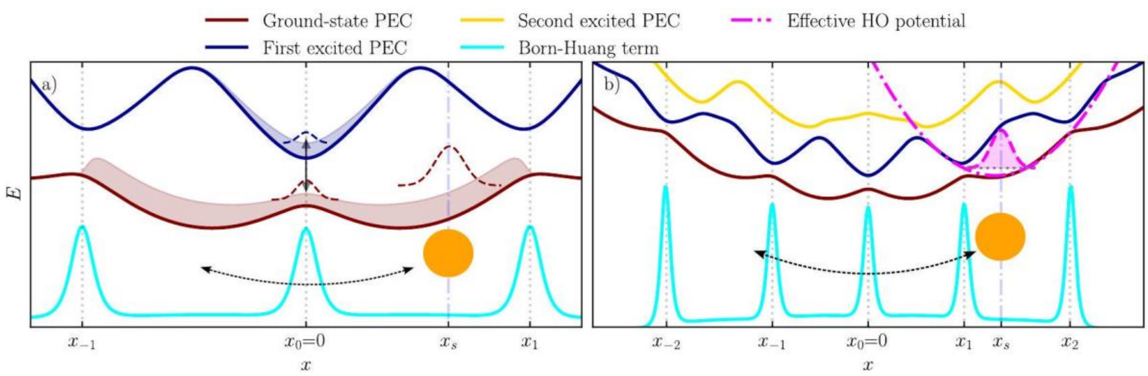




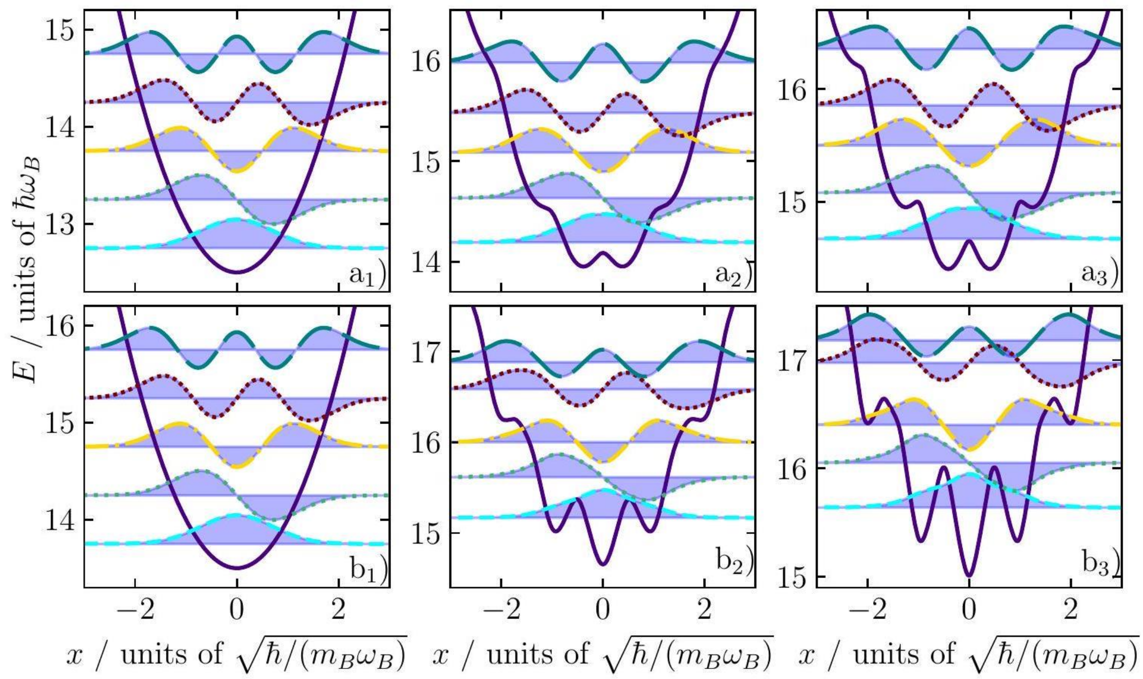




$$n_j(t) \equiv \langle \Psi(t)|\hat{\mathcal{P}}_j|\Psi(t)\rangle = \int \mathrm{d}x_I \left|\Psi_{j,I}(x_I;t)\right|^2.$$



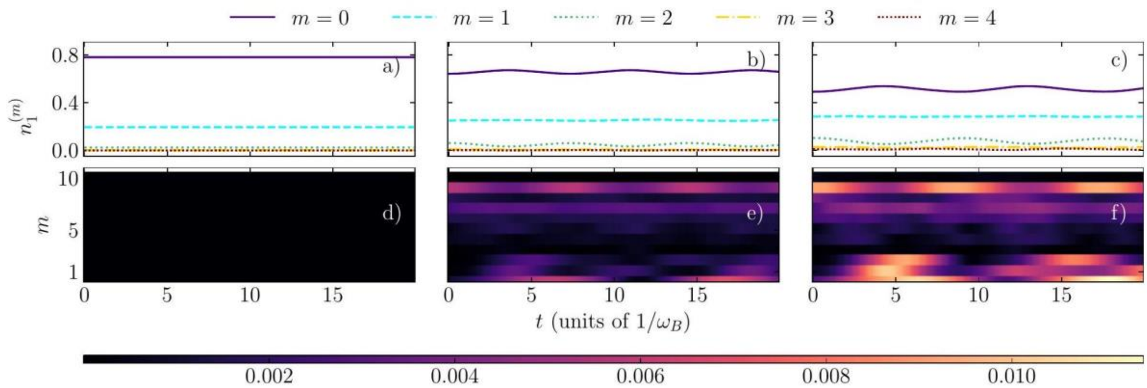
$$\rho_I^{(1)}(x_I;t) = \sum_{j=1}^{M} \rho_{I,j}^{(1)}(x_I;t) = \sum_{j=1}^{M} \left|\Psi_{j,I}(x_I;t)\right|^2.$$



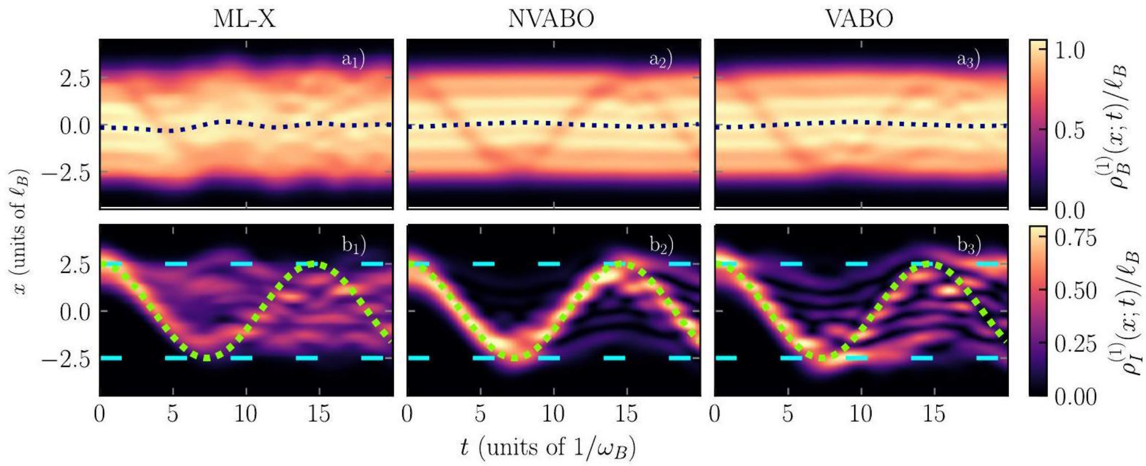
$$2\psi_j^{(m)}(x) + E_j^{(m)}$$

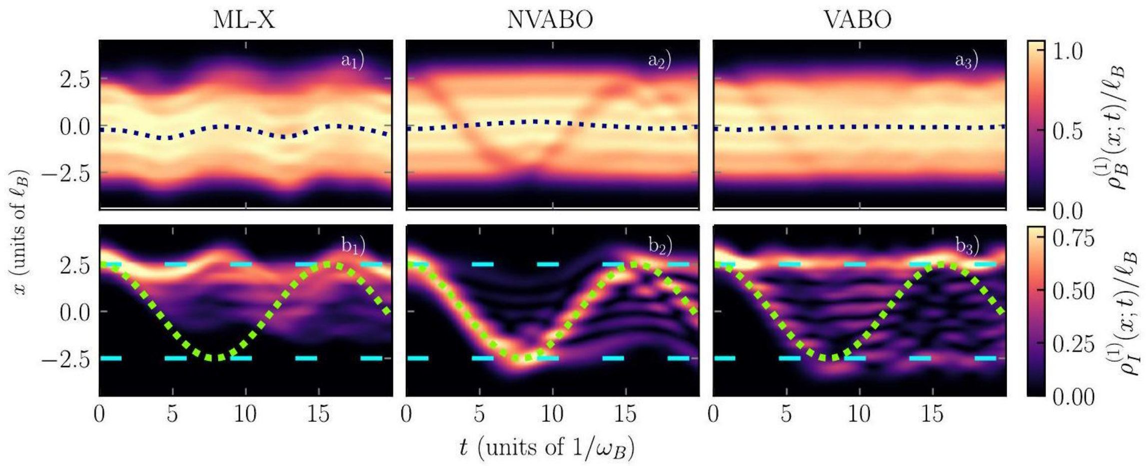
$$\hat{H}_{\mathrm{PEC}}^{j} = -\frac{\hbar^2}{2m_I}\left(\frac{\partial}{\partial x_I}\right)^2 + \frac{1}{2}m_B\omega_I^2 x_I^2 + \varepsilon_j(x_I).$$

$$\hat{H}_{\mathrm{PEC}}^{j}\phi_{j,m}(x) = E_{j,m}\phi_{j,m}(x),$$

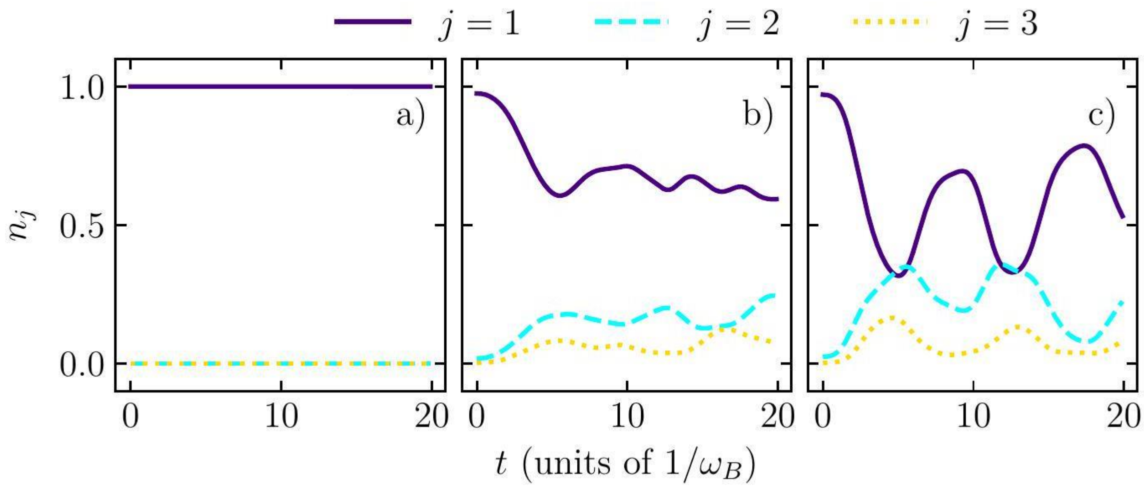


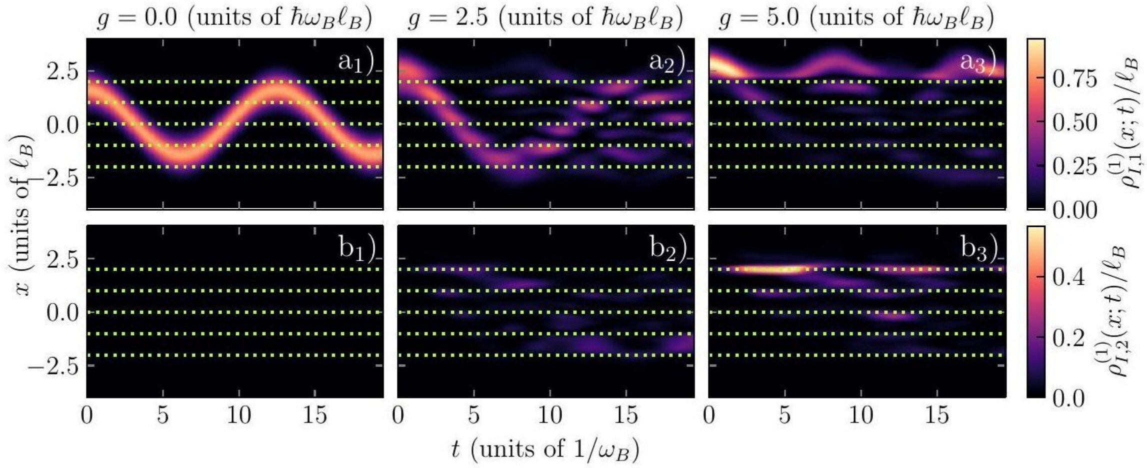
$$n_j^{(m)} = \left|\int \mathrm{d}x_I \Psi_{j,I}^{*}(x_I)\phi_{m,j}(x_I)\right|^2,$$

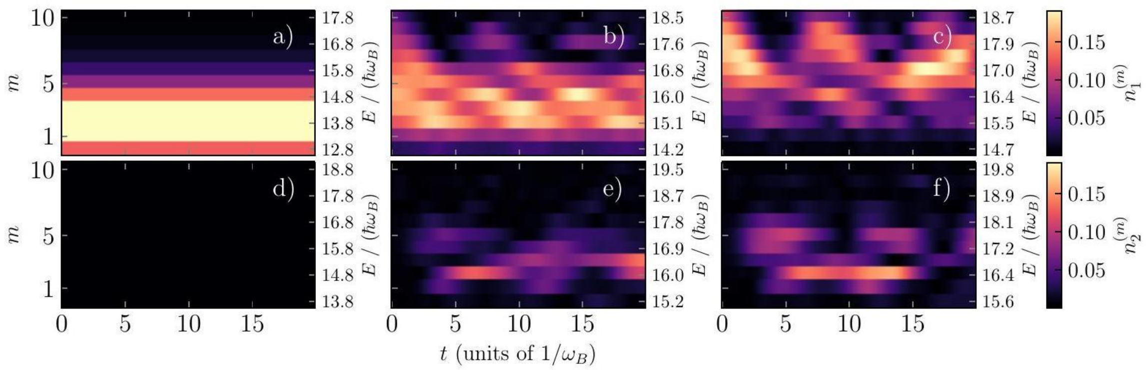


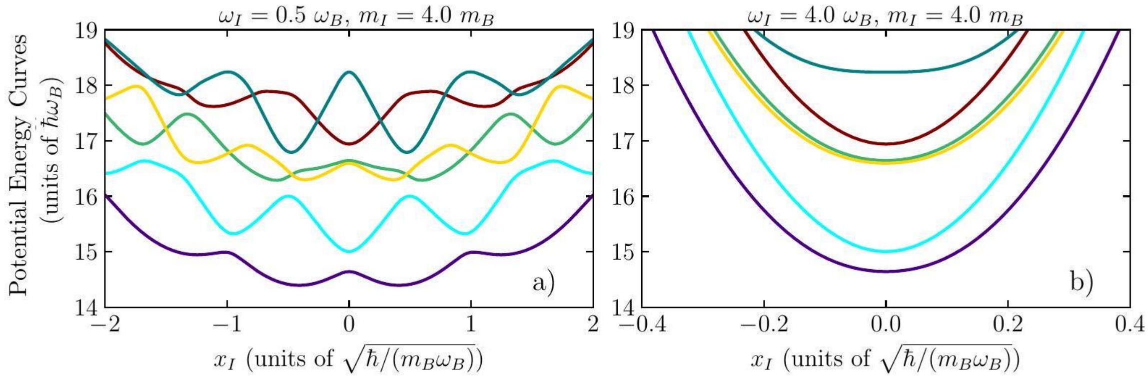


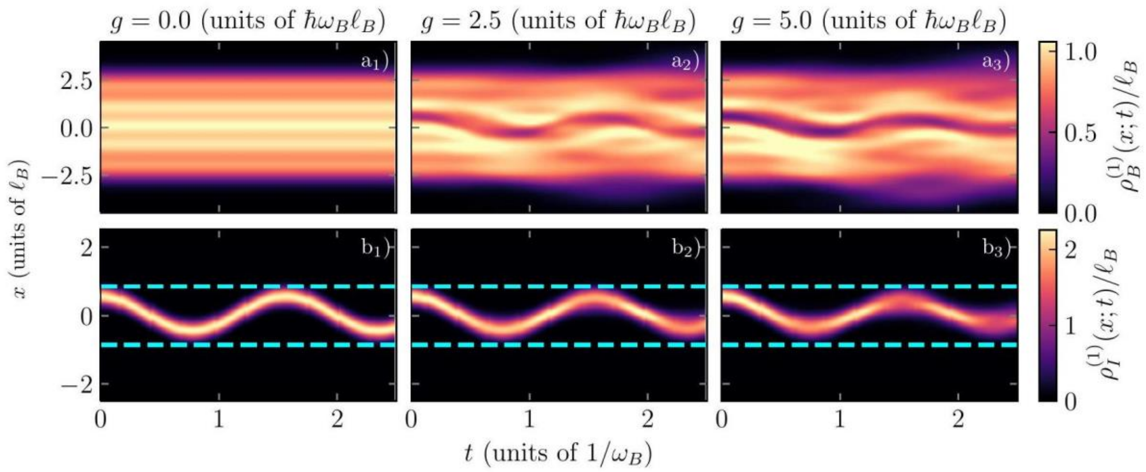
$$\langle x_B(t)\rangle = \int \mathrm{d}x x \rho_B^{(1)}(x,t) / \int \mathrm{d}x \rho_B^{(1)}(x,t)$$











$$Z = \sqrt{\left|\langle \psi_{g=0} \mid \psi_{g\neq 0}\rangle\right|^2} \propto N^{-\alpha}$$

$$|\Psi(t)\rangle = \sum_{j_B,j_I=1}^{D} A_{j_B,j_I}(t)|\Psi_{j_B}^B(t)\rangle|\Psi_{j_I}^I(t)\rangle$$

$$|\Psi_j^\sigma(t)\rangle(\sigma = B, I)A_{j_B,j_I}(t)$$

$$|\Psi(t)\rangle = \sum_{k=1}^{D} \sqrt{\lambda_k(t)}|\tilde{\Psi}_k^B(t)\rangle|\tilde{\Psi}_k^I(t)\rangle$$

$$\rho_\sigma^{(N_\sigma)}(t)|\tilde{\Psi}_k^\sigma(t)\rangle$$

$$\rho_\sigma^{(N_\sigma)}(x_1, \dots, x_{N_\sigma}, x_1', \dots, x_{N_\sigma}', t) = \int \prod_{j=1}^{N_{\bar{\sigma}}} \mathrm{d}x_j^{\bar{\sigma}}$$
$$\times \Psi^*(x_1^\sigma = x_1', \dots, x_{N_\sigma}^\sigma = x_{N_\sigma}', x_1^{\bar{\sigma}}, \dots, x_{N_{\bar{\sigma}}}^{\bar{\sigma}}, t)$$
$$\times \Psi(x_1^\sigma = x_1, \dots, x_{N_\sigma}^\sigma = x_{N_\sigma}, x_1^{\bar{\sigma}}, \dots, x_{N_{\bar{\sigma}}}^{\bar{\sigma}}, t)$$

$$\rho_\sigma^{(N_\sigma)}(x_1, \dots, x_{N_\sigma}, x_1', \dots, x_{N_\sigma}', t) = \langle x_1, \dots, x_{N_\sigma}|\hat{\rho}_\sigma^{(N_\sigma)}(t)|x_1', \dots, x_{N_\sigma}'\rangle$$

$$\hat{\rho}_\sigma^{(N_\sigma)}(t) = \sum_{\substack{j_\sigma,j_\sigma'=1 \\ j_\sigma=1}}^{D} \left[\hat{\rho}_\sigma^{(N_\sigma)}(t)\right]_{j_\sigma,j_\sigma'} |\Psi_{j_\sigma}^\sigma(t)\rangle \langle\Psi_{j_\sigma'}^\sigma(t)|$$

$$A_{j_\sigma,j_{\bar{\sigma}}}^*(t)A_{j_{\bar{\sigma}},j_\sigma'}(t) \equiv \left[\hat{\rho}_\sigma^{(N_\sigma)}(t)\right]_{j_\sigma,j_\sigma'}$$

$\left[\hat{\rho}_\sigma^{(N_\sigma)}(t)\right]_{j_\sigma,j_\sigma'}$ for $j_\sigma, j_\sigma' = 1, \cdots, D$ yields $\lambda_k(t)$ and $|\tilde{\Psi}_k^\sigma(t)\rangle$

$$|\Psi_j^\sigma(t)\rangle = \sum_{\vec{n}} B_{j,\vec{n}}^\sigma(t)|\vec{n}(t)\rangle^\sigma$$

$$B_{j,\vec{n}}^\sigma(t)|\vec{n}(t)\rangle^\sigma$$

$$|\phi_j^\sigma(t)\rangle = \sum_{k=1}^{\mathcal{M}} C_{jk}^\sigma(t)|k\rangle$$

$$\langle\delta\Psi(t)|i\hbar\frac{\partial}{\partial t} - H|\Psi(t)\rangle = 0$$

$$A_{j_B,j_I}(t)B_{j,\vec{n}}^\sigma(t)C_{j,k}^\sigma(t)$$

$$|\Psi(t)\rangle = \int \mathrm{d}x_I \Psi_{j,I}(x_I; t)\hat{\Psi}_I^\dagger(x_I)|0_I\rangle \otimes |\Psi_{j,B}(x_I)\rangle$$

$$\Psi_{j,I}(x_I; t)|\Psi_{j,B}(x_I)\rangle\hat{H}_B + \hat{H}_{BI}\hat{\Psi}_I^\dagger(x_I)\{\hat{\Psi}_I(x_1), \hat{\Psi}_I^\dagger(x_2)\} = \delta(x_1 - x_2)\hat{\Psi}_I(x_I)$$

$$\rho_I^{(1)}(x_1, x_2; t) = \langle\Psi(t)|\hat{\Psi}_I^\dagger(x_1)\hat{\Psi}_I(x_2)|\Psi(t)\rangle$$

$$\rho_I^{(1)}(x_1, x_2; t) = \sum_{j,k=1}^{M} \Psi_{j,I}^*(x_1; t)\Psi_{k,I}(x_2; t)$$
$$\times \langle \Psi_{j,B}(x_1) \mid \Psi_{k,B}(x_2) \rangle.$$

$$\langle \Psi_{j,B}(x_1) \mid \Psi_{k,B}(x_2) \rangle$$

$$\rho_I^{(1)}(x_I; t) = \rho^{(1)}(x_I, x_I; t)$$

$$\rho_I^{(1)}(x_I; t) = \sum_{j=1}^{M} \underbrace{\left|\Psi_{j,I}(x_I; t)\right|^2}_{\equiv \rho_{I,j}^{(1)}(x_I;t)}$$

$$\rho_{j,I}^{(1)}(x_I; t)\langle \Psi_{j,B}(x_I) \mid \Psi_{k,B}(x_I) \rangle = \delta_{j,k}$$

$$\hat{\mathcal{P}}_j = \int \mathrm{d}x_I \left|\Psi_j(x_I)\right\rangle \left\langle \Psi_j(x_I)\right|$$

$$\left|\Psi_j(x_I)\right\rangle = \hat{\Psi}_I^\dagger(x_I)|0_I\rangle \otimes \left|\Psi_{j,B}(x_I)\right\rangle.$$

$$\left|\Psi_j(x_I)\right\rangle \hat{\mathcal{P}}_j \hat{\mathcal{P}}_k = \delta_{j,k}\hat{\mathcal{P}}_j \sum_{j=1}^{M} \hat{\mathcal{P}}_j = \hat{I}_M$$

$$\langle \Psi_j(x_1) \mid \Psi_k(x_2) \rangle = \delta_{j,k}\delta(x_1 - x_2)$$

$$\langle \Psi_{j,B}(x_I) \mid \Psi_{k,B}(x_I) \rangle = \delta_{j,k}$$

$$\langle \Psi(t)|\hat{\mathcal{P}}_j|\Psi(t)\rangle = \int \mathrm{d}x_I \left|\Psi_{j,I}(x_I; t)\right|^2$$
$$= \int \mathrm{d}x_I \rho_{I,j}^{(1)}(x_I; t)$$

$$\langle \Psi_{j,B}(x_I) \mid \Psi_{k,B}(x_I) \rangle = \delta_{j,k}$$

$$\hat{\mathcal{P}}_{m,j} = \left|\Psi_{m,j}\right\rangle \left\langle \Psi_{m,j}\right|.$$

$$\left|\Psi_{m,j}\right\rangle = \int \mathrm{d}x_I \phi_{m,j}(x_I)\hat{\Psi}_I^\dagger(x_I)|0_I\rangle \otimes \left|\Psi_{j,B}(x_I)\right\rangle$$

$$\hat{\mathcal{P}}_{m,j}^2 = \hat{\mathcal{P}}_{m,j} \int \mathrm{d}x_I \left|\phi_{m,j}(x_I)\right|^2 = 1$$

$$\langle \Psi(t)|\hat{\mathcal{P}}_{m,j}|\Psi(t)\rangle = \left|\int \mathrm{d}x_I \Psi_{I,j}^*(x_I; t)\phi_{m,j}(x_I)\right|^2$$

$$\langle \Psi_{j,B}(x_I) \mid \Psi_{k,B}(x_I) \rangle = \delta_{j,k}$$

$$\hat{H}(t) = \sum_{i=1}^{n} \left(-\frac{1}{2\mu_i}\nabla_{\mathbf{r}_i}^2 + \frac{q_0 q_i}{r_i}\right) + \sum_{i<j}^{n} \left(\frac{q_i q_j}{r_{ij}} + \frac{1}{M_1}\nabla'_{\mathbf{r}_i}\nabla_{\mathbf{r}_j}\right) - \mathcal{F}(t)\sum_{i=1}^{n} q_i x_i$$

$$q_i = Q_{i+1}(i = 0, \ldots, n), \mu_i = M_1 M_{i+1}/(M_1 + M_{i+1})$$

$$(i = 1, \dots, N), r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = |\mathbf{R}_{i+1} - \mathbf{R}_{j+1}|, r_i = |\mathbf{r}_i|$$

$$\hat{H}(t) = -\frac{1}{2\mu}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y) - qx\mathcal{F}(t)$$

$$V(x,y) = -(x^2 + y^2 + 1/2)^{-1/2}$$

$$V(x,y) = D_e\left[1 - \exp\left(-\alpha\left((x^2 + y^2)^{1/2} - r_e\right)\right)\right]^2$$

$$\mathcal{F}(t) = \mathcal{E}_0 \sin^2\left(\pi\frac{t - t_0}{t_1 - t_0}\right)\cos\left(\omega(t - \bar{t})\right), \bar{t} = \frac{t_0 + t_1}{2}$$

$$\phi(\mathbf{r};\mathbf{x}) = \exp\left[-(a + \mathrm{i}b)\|\mathbf{r} - \mathbf{q}\|^2 + \mathrm{i}\mathbf{p}\cdot(\mathbf{r} - \mathbf{q})\right]$$

$$\frac{\phi(-b) - \phi(+b)}{2\mathrm{i}} = \exp\{-a(x^2 + y^2)\sin[b(x^2 + y^2)]\} = \exp(-ar^2)\sin(br^2)$$

$$\Psi(\mathbf{C},\mathbf{x}) = \sum_i \phi_i(\mathbf{x}_i)c_i \equiv \phi(\mathbf{x})\mathbf{C}$$

$$\mathrm{i}\Psi^{n+1} - \mathrm{i}\Psi^n - \frac{1}{2}\left(\hat{H}\left(t + \frac{1}{2}\Delta t\right)\Psi^{n+1} + \hat{H}\left(t + \frac{1}{2}\Delta t\right)\Psi^n\right)\Delta t = 0$$

$$\left\|A\Psi(\mathbf{x}^{n+1}, \mathbf{C}^{n+1}) - A^\dagger\Psi(\mathbf{x}^n, \mathbf{C}^n)\right\| < \epsilon$$

$$A = I + \frac{\mathrm{i}\Delta t}{2}\hat{H}(t + \Delta t/2)$$

$$\mathbf{C}^{n+1} = \mathbf{S}_A^{-1}\phi^\dagger A^\dagger\Psi^n$$

$$(S_A)_{ij} = \langle\phi_i|A^\dagger A|\phi_j\rangle.$$

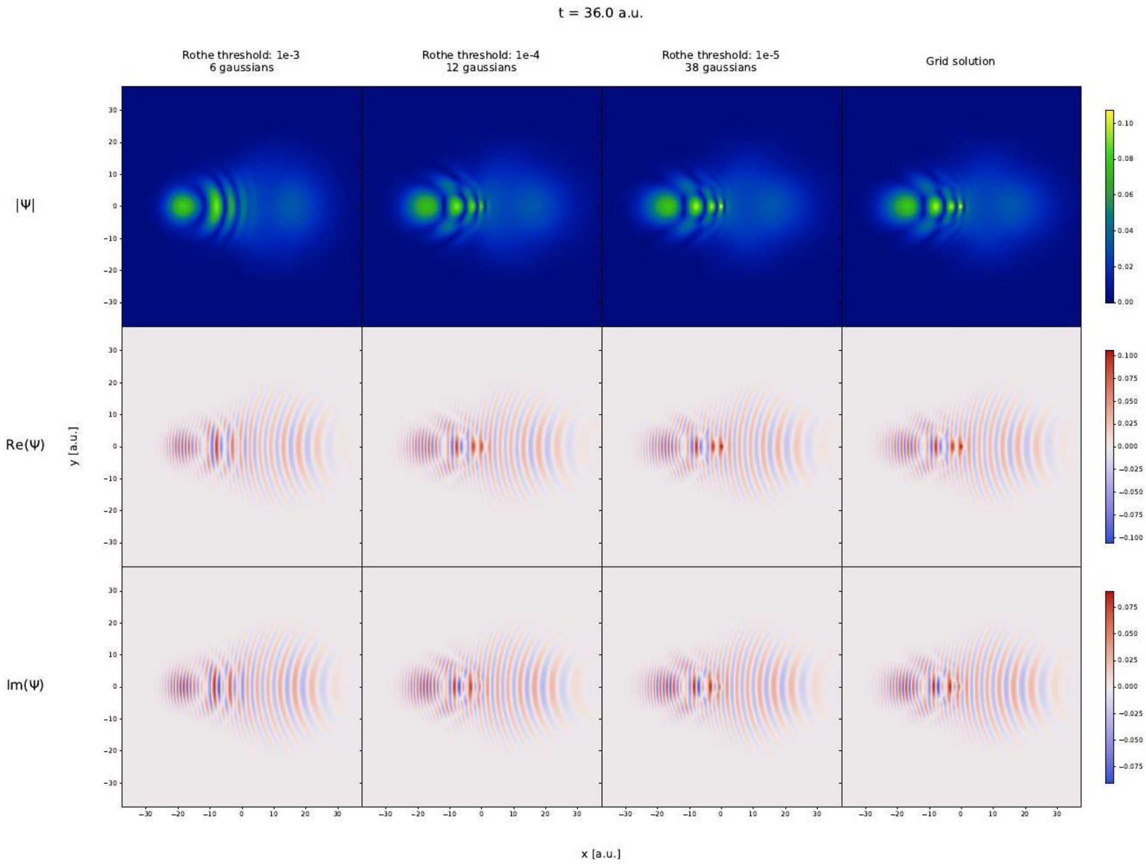
$$P_A = (A\phi)\mathbf{S}_A^{-1}(A\phi)^\dagger = \sum_{ij} A|\phi_i\rangle(S_A^{-1})_{ij}\langle\phi_j|A^\dagger$$

$$F(\mathbf{x}^{n+1}) \equiv \|(P_A(\mathbf{x}^{n+1}) - I)A\Psi^n\| < \epsilon$$

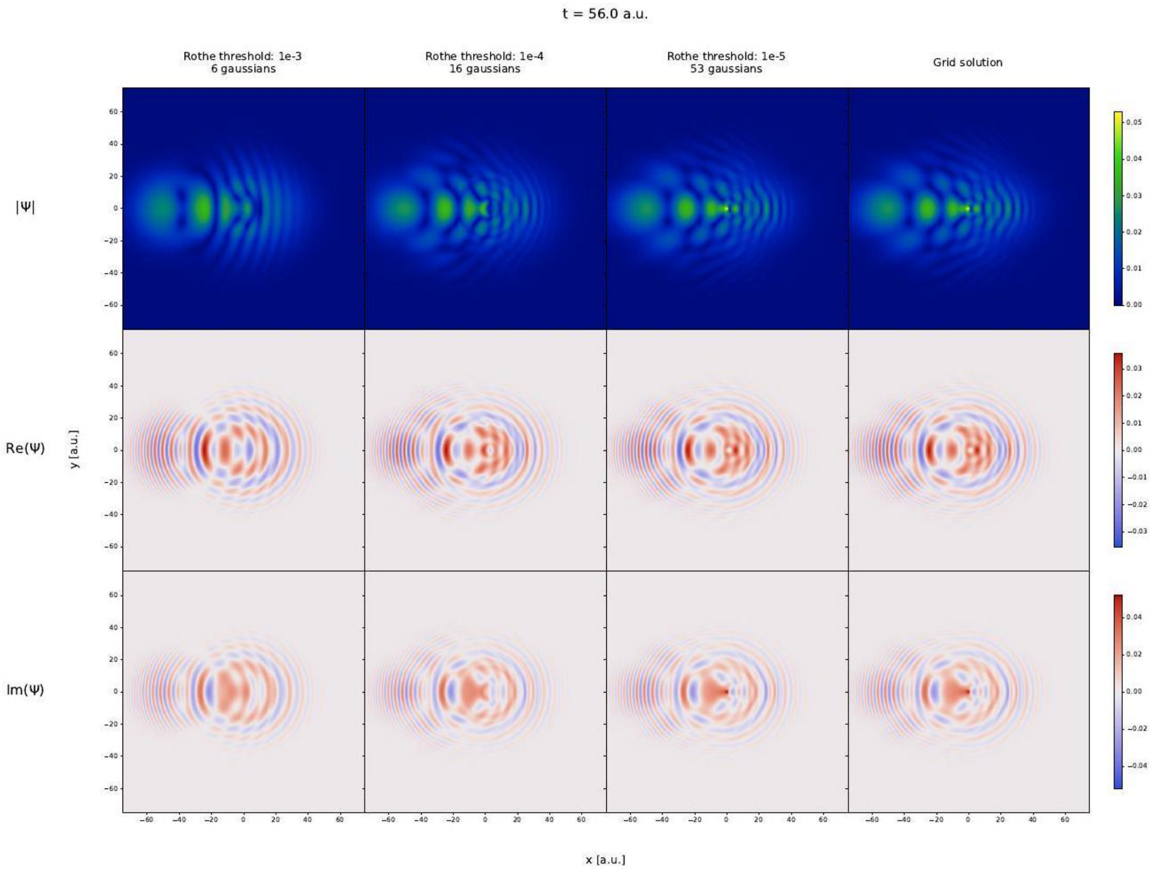
$$\left\|\hat{H}_0\Psi(\mathbf{x}^0, \mathbf{C}^0) - E_0\Psi(\mathbf{x}^0, \mathbf{C}^0)\right\| = \min!$$

$$\phi\left(a' = \frac{\sum_i c_i a_i}{\sum_i c_i}, b' = \frac{\sum_i c_i b_i}{\sum_i c_i}, p_x = \frac{\sum_i c_i p_{x,i}}{\sum_i c_i}, p_y = \frac{\sum_i c_i p_{y,i}}{\sum_i c_i}, q_x = \frac{\sum_i c_i q_{x,i}}{\sum_i c_i}, q_y = \frac{\sum_i c_i q_{y,i}}{\sum_i c_i}\right).$$

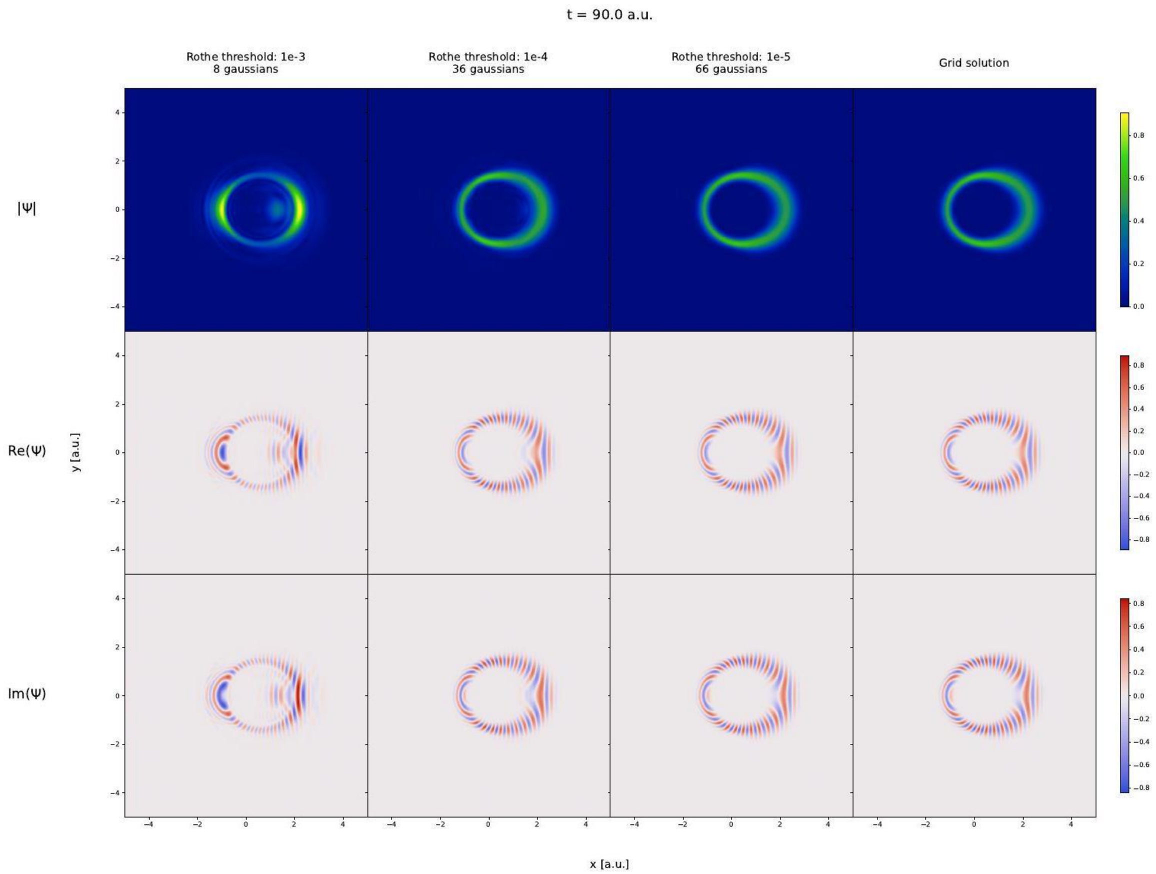
$$\phi\left(a' = \frac{\sum_i c_i a_i}{\sum_i c_i}, b' = \frac{\sum_{i,b_i>0} c_i b_i}{\sum_{i,b_i>0} c_i}, p_x = \frac{\sum_i c_i p_{x,i}}{\sum_i c_i}, p_y = \frac{\sum_i c_i p_{y,i}}{\sum_i c_i}, q_x = \frac{\sum_i c_i q_{x,i}}{\sum_i c_i}, q_y = \frac{\sum_i c_i q_{y,i}}{\sum_i c_i}\right),$$
$$\phi\left(a' = \frac{\sum_i c_i a_i}{\sum_i c_i}, b' = \frac{\sum_{i,b_i<0} c_i b_i}{\sum_{i,b_i<0} c_i}, p_x = \frac{\sum_i c_i p_{x,i}}{\sum_i c_i}, p_y = \frac{\sum_i c_i p_{y,i}}{\sum_i c_i}, q_x = \frac{\sum_i c_i q_{x,i}}{\sum_i c_i}, q_y = \frac{\sum_i c_i q_{y,i}}{\sum_i c_i}\right).$$

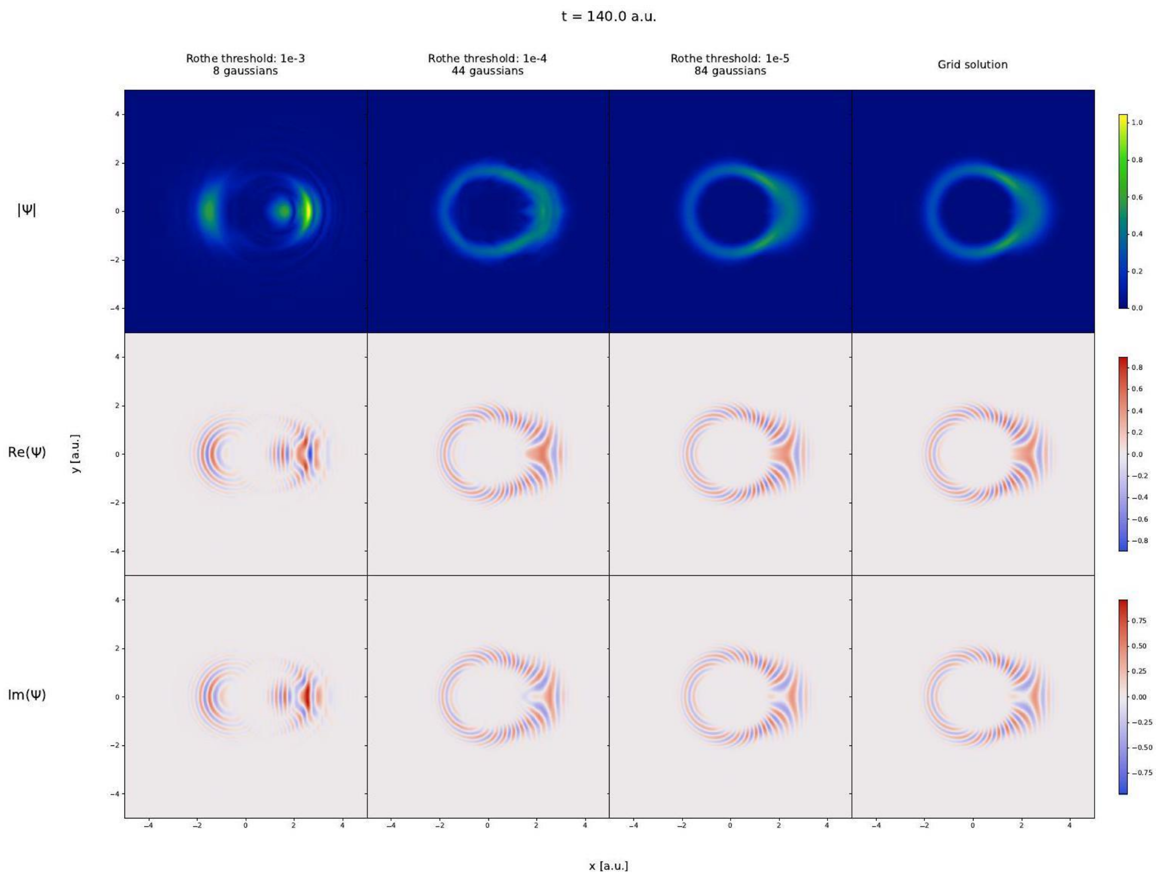


t = 36.0 a.u.
Rothe threshold: 1e-3
6 gaussians
Rothe threshold: 1e-4
12 gaussians
Rothe threshold: 1e-5
38 gaussians
Grid solution
|Ψ|
Re(Ψ)
Im(Ψ)
y [a.u.]
x [a.u.]



t = 56.0 a.u.
Rothe threshold: 1e-3
6 gaussians
Rothe threshold: 1e-4
16 gaussians
Rothe threshold: 1e-5
53 gaussians
Grid solution
|Ψ|
Re(Ψ)
Im(Ψ)
y [a.u.]
x [a.u.]





$$H = T_e + T_n + V_{ee} + V_{en} + V_{nn}$$

$$H\Psi(\mathbf{r}, \mathbf{R}) = E\Psi(\mathbf{r}, \mathbf{R})$$

$$H_{BO}\Phi_{\mathbf{R}}(\mathbf{r}) = \mathcal{E}_{BO}(\mathbf{R})\Phi_{\mathbf{R}}(\mathbf{r})$$
$$H_n\chi(\mathbf{R}) = E\chi(\mathbf{R})$$

$$H = T_{cm} + H'$$

$$\int d\mathbf{r}|\Phi_{\mathbf{R}}(\mathbf{r})|^2 = 1$$

$$\chi_s(q_s) = (\omega_s/\pi)^{1/4}\exp\left[-\omega_s q_s^2\right]$$

$$\hat{H}_{BO} = \hat{T}_e + \hat{V}_{ee} + \hat{V}_{en} + V_{nn}$$

$$\hat{T}_e = -\frac{1}{2m_e}\int d\mathbf{y}\hat{\psi}^\dagger(\mathbf{y})\nabla_{\mathbf{y}}^2\hat{\psi}(\mathbf{y})$$
$$\hat{V}_{en} = \int d\mathbf{y}\int d\mathbf{y}' v(\mathbf{y},\mathbf{y}')n_n(\mathbf{y}')\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})$$
$$\hat{V}_{ee} = \frac{1}{2}\int d\mathbf{y}\int d\mathbf{y}' v(\mathbf{y},\mathbf{y}')\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{y}')\hat{\psi}(\mathbf{y}')\hat{\psi}(\mathbf{y})$$
$$V_{nn} = \frac{1}{2}\sum_{k,k'=1}^{N_n}\frac{Z_k Z_{k'}\varsigma}{|\mathbf{R}_k - \mathbf{R}_{k'}|}$$

$$n_n(\mathbf{y}) = -\sum_k Z_k\delta(\mathbf{y}-\mathbf{R}_k), v(\mathbf{y},\mathbf{y}') = \varsigma/|\mathbf{y}-\mathbf{y}'| \text{ and } \varsigma = e^2/(4\pi\epsilon_0)$$

$$\left[\hat{\psi}(\mathbf{y}),\hat{\psi}^\dagger(\mathbf{y}')\right]_+ = \delta(\mathbf{y}-\mathbf{y}')$$

$$G_{\mathbf{R}}^{BO}(\mathbf{y}t,\mathbf{y}'t') \equiv \frac{1}{i}\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}_{BO}^M}\mathcal{T}\{\hat{\psi}(\mathbf{y}t)\hat{\psi}^\dagger(\mathbf{y}'t')\}\right]_{\Phi_{\mathbf{R}}}}{\mathrm{Tr}\left[e^{-\beta\hat{H}_{BO}^M}\right]_{\Phi_{\mathbf{R}}}}$$

$$\hat{\psi}(\mathbf{y}t) \equiv \hat{U}_{BO}^\dagger(t)\hat{\psi}(\mathbf{y})\hat{U}_{BO}(t)$$

$$\hat{U}_{BO}(t)\beta = k_B^{-1}T^{-1}$$

$$\hat{H}_{BO}^M \equiv \hat{H}_{BO} - \mu_e\hat{N}_e$$

$$\mathrm{Tr}[\hat{o}]_{\Phi_{\mathbf{R}}} = \sum_m \left\langle \Phi_{\mathbf{R}}^{(m)} \middle| \hat{o} \middle| \Phi_{\mathbf{R}}^{(m)} \right\rangle$$

$$D_{\alpha_{\bar{n}}}^{BO}(k_{\bar{n}}t_{\bar{n}}) \equiv \frac{1}{i^{n-1}}\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}_n}\mathcal{T}\{\hat{R}_{\alpha_{\bar{n}}}(k_{\bar{n}}t_{\bar{n}})\}\right]_\chi}{\mathrm{Tr}\left[e^{-\beta\hat{H}_n}\right]_\chi}$$

$$\alpha_{\bar{n}} \equiv \alpha_1\cdots\alpha_n, k_{\bar{n}}t_{\bar{n}} \equiv k_1t_1,\ldots,k_nt_n$$

$$\hat{R}_{\alpha_{\bar{n}}}(k_{\bar{n}}t_{\bar{n}}) \equiv \hat{R}_{\alpha_1}(k_1t_1)\cdots\hat{R}_{\alpha_n}(k_nt_n)$$

$$\hat{R}_\alpha(kt) = \hat{U}_n^\dagger(t)\hat{R}_\alpha(k)\hat{U}_n(t)$$

$$\left[\hat{R}_\alpha(kt),\hat{P}_\beta(k't)\right]_- = i\delta_{\alpha\beta}\delta_{kk'}$$

$$\mathbf{r}_i' = \mathcal{R}(\boldsymbol{\theta})(\mathbf{r}_i - \mathbf{R}_{cmn}), \mathbf{R}_k' = \mathbf{R}_k - \mathbf{R}_{cmn}, \mathbf{R}_{N_n}' = \mathbf{R}_{cm}$$

$$\mathbf{R}_{cmn} = \frac{1}{M_{nuc}} \sum_k M_k \mathbf{R}_k$$

$$M_{nuc} \equiv \sum_k M_k \mathbf{R}_{cm}$$

$$G(\mathbf{y}t, \mathbf{y}'t') \equiv \frac{1}{i} \frac{\mathrm{Tr}\left[e^{-\beta \hat{H}'^M} \mathcal{T}\{\hat{\psi}(\mathbf{y}t)\hat{\psi}^\dagger(\mathbf{y}'t')\}\right]_{\Psi'}}{\mathrm{Tr}\left[e^{-\beta \hat{H}'^M}\right]_{\Psi'}}$$

$$D_{\alpha_{\bar{n}}}(k_{\bar{n}} t_{\bar{n}}) \equiv \frac{1}{i^{n-1}} \frac{\mathrm{Tr}\left[e^{-\beta \hat{H}'^M} \mathcal{T}\{\hat{R}_{\alpha_{\bar{n}}}(k_{\bar{n}} t_{\bar{n}})\}\right]_{\Psi'}}{\mathrm{Tr}\left[e^{-\beta \hat{H}'^M}\right]_{\Psi'}}$$

$$\delta(t-t')\delta(\mathbf{y}-\mathbf{y}') = \left[i\frac{\partial}{\partial t} + \frac{\nabla_{\mathbf{y}}^2}{2m_e} - V_{tot}(\mathbf{y}t)\right] G(\mathbf{y}t, \mathbf{y}'t') - \int d\mathbf{y}'' \int dt'' \Sigma(\mathbf{y}t, \mathbf{y}''t'') G(\mathbf{y}''t'', \mathbf{y}'t')$$

$$M_k \frac{\partial^2}{\partial t^2} D_{\alpha\beta}(kt, k't') = -\sum_{k'', \alpha'} \int dt'' \Pi_{\alpha\alpha'}(kt, k''t'') D_{\alpha'\beta}(k''t'', k't') - \delta_{\alpha\beta}\delta_{kk'}\delta(t-t')$$

$$\Psi(\mathbf{r}, \mathbf{R}) = \Phi_{\mathbf{R}}(\mathbf{r})\chi(\mathbf{R})$$

$$H_n \chi(\mathbf{R}) = E\chi(\mathbf{R}), H_e \Phi_{\mathbf{R}}(\mathbf{r}) = \epsilon(\mathbf{R})\Phi_{\mathbf{R}}(\mathbf{r})$$

$$H_n = \sum_k \frac{1}{2M_k}\left[-i\nabla_{\mathbf{R}_k} + \mathbf{A}_k(\mathbf{R})\right]^2 + \epsilon(\mathbf{R}), H_e = H_{BO}(\mathbf{r}, \mathbf{R}) + U_{en}(\mathbf{R})$$

$$\epsilon(\mathbf{R}) = \int d\mathbf{r} \Phi_{\mathbf{R}}^*(\mathbf{r}) H_e \Phi_{\mathbf{R}}(\mathbf{r})$$

$$\mathbf{A}_k(\mathbf{R}) = -i \int d\mathbf{r} \Phi_{\mathbf{R}}^*(\mathbf{r}) \nabla_{\mathbf{R}_k} \Phi_{\mathbf{R}}(\mathbf{r})$$

$$U_{en}(\mathbf{R}) = \sum_k \frac{1}{2M_k}\left[\left(-i\nabla_{\mathbf{R}_k} - \mathbf{A}_k\right)^2 + 2(\mathbf{D}_k + \mathbf{A}_k) \cdot \left(-i\nabla_{\mathbf{R}_k} - \mathbf{A}_k\right)\right]$$

$$\mathbf{D}_k(\mathbf{R}) = -i\chi^{-1}(\mathbf{R})\nabla_{\mathbf{R}_k}\chi(\mathbf{R})$$

$$\int d\mathbf{R}|\chi(\mathbf{R})|^2 = \int d\mathbf{r}|\Phi_{\mathbf{R}}(\mathbf{r})|^2 = 1$$

$$L = \sum_{s=1}^{N_s} \int d\mathbf{y} \psi_s^\dagger(\mathbf{y}) \tilde{D}_s(\mathbf{y}) \psi_s(\mathbf{y}) - \frac{1}{2} \sum_{s=1}^{N_s} \int d\mathbf{y} \int d\mathbf{y}' v_{ss}(\mathbf{y}, \mathbf{y}') \psi_s^\dagger(\mathbf{y}) \psi_s^\dagger(\mathbf{y}') \psi_s(\mathbf{y}'t) \psi_s(\mathbf{y})$$
$$-\frac{1}{2} \sum_{s,s'=1}^{N_s} \int d\mathbf{y} \int d\mathbf{y}' v_{ss'}(\mathbf{y}, \mathbf{y}') n_s(\mathbf{y}) n_{s'}(\mathbf{y}')$$

$$n_s(\mathbf{y}) \equiv \psi_s^\dagger(\mathbf{y})\psi_s(\mathbf{y}), \tilde{D}_s(\mathbf{y}t) \equiv i\frac{\partial}{\partial t} + \frac{1}{2m_s}\nabla_s^2$$

$$v_{ss'}(\mathbf{y}, \mathbf{y}') \equiv Z_s Z_{s'} \chi_{ss'} v(\mathbf{y}, \mathbf{y}')$$

$$\psi_s(\mathbf{y}), \psi_s^\dagger(\mathbf{y})$$

$$[\hat{\psi}_s(\mathbf{y}t), \hat{\psi}_s^\dagger(\mathbf{y}'t)]_\pm = \delta(\mathbf{y}-\mathbf{y}')$$

$$G_s(\mathbf{y}t, \mathbf{y}'t') \equiv \frac{1}{i}\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\mathcal{T}\{\hat{\psi}_s(\mathbf{y}t)\hat{\psi}_s^\dagger(\mathbf{y}'t')\}\right]_\Psi}{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\right]_\Psi}$$

$$\delta(1-2) = \left[i\hbar\frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m_s}\nabla_s^2 - V_{tot}(1,s)\right]G_s - \int d\mathfrak{R}\Sigma_s G_s$$

$$\Sigma_s = i\hbar\int d\mathfrak{H}\int d5 W_s G_s \Gamma_s$$

$$\Gamma_s = \delta(1-2)\delta(1-3) + \int d\delta\int d\zeta\int d\xi\int d\lambda\frac{\delta\Sigma_s}{\delta G_s}G_s G_s \Gamma_s$$

$$W_s = Z_s^2 v + Z_s^2\int d\triangle\int dv\sum_{s'} P_{s'}W_{s'}$$

$$P_s = -i\hbar\int d\Vdash\int d\,\mho\, G_s G_s \Gamma_s$$

$$1 = \mathbf{y}t, \delta(1-2) = \delta(t-t')\delta(\mathbf{y}-\mathbf{y}')$$

$$m_{\chi_{c1}(3872)} - m_{D^0} - m_{D^{*0}} = -0.05 \pm 0.09\mathrm{MeV}$$

$$H = K_{\mathrm{heavy}} + H_{\mathrm{light}} = \frac{\mathbf{p}^2}{2\mu_{\mathrm{heavy}}} + H_{\mathrm{light}}$$

$$|\psi\rangle = \sum_i\int d\mathbf{r}\tilde{\psi}_i(\mathbf{r})|\mathbf{r}\rangle|\xi_i(\mathbf{r})\rangle$$

$$\sum_i\left(-\frac{\hbar^2}{2\mu_i}[\nabla + \tau(\mathbf{r})]_{ji}^2 + [V_j(\mathbf{r}) - E]\delta_{ji}\right)\tilde{\psi}_i(\mathbf{r}) = 0$$

$$\tau_{ji}(\mathbf{r}) \equiv \langle\xi_j(\mathbf{r}) \mid \nabla\xi_i(\mathbf{r})\rangle$$

$$\tau_{ji}(\mathbf{r}) = \langle\xi_j(\mathbf{r}) \mid \nabla\xi_i(\mathbf{r})\rangle \simeq 0.$$

$$|\psi\rangle = \sum_i\int d\mathbf{r}'\tilde{\psi}_i(\mathbf{r}', \mathbf{r}_0)|\mathbf{r}'\rangle|\xi_i(\mathbf{r}_0)\rangle$$

$$\sum_i\left[-\frac{\hbar^2}{2\mu_i}\delta_{ij}\nabla^2 + V_{ji}(\mathbf{r}, \mathbf{r_0}) - E\delta_{ji}\right]\tilde{\psi}_i(\mathbf{r}, \mathbf{r_0}) = 0$$

$$V_{ji}(\mathbf{r}, \mathbf{r_0}) \equiv \langle\xi_j(\mathbf{r}_0)|H_{\mathrm{light}}|\xi_i(\mathbf{r}_0)\rangle.$$

$$\mathrm{V} = \begin{pmatrix} V_{\delta\bar{\delta}}(\mathbf{r}) & V_{\mathrm{mix}}^{(1)}(\mathbf{r}) & \cdots & V_{\mathrm{mix}}^{(N)}(\mathbf{r}) \\ V_{\mathrm{mix}}^{(1)}(\mathbf{r}) & V_{M_1\bar{M}_2}^{(1)}(\mathbf{r}) & & \\ \vdots & & \ddots & \\ V_{\mathrm{mix}}^{(N)}(\mathbf{r}) & & & V_{M_1\bar{M}_2}^{(N)}(\mathbf{r}) \end{pmatrix},$$

$$V_{M_1\bar{M}_2}^{(i)}(\mathbf{r}) \to T_{M_1\bar{M}_2} \equiv M_1 + M_2$$

$$V_{M_1\bar{M}_2}^{(i)}(\mathbf{r}) = \begin{cases} T_{M_1\bar{M}_2} - V_0, & r \le r_c \\ T_{M_1\bar{M}_2}, & r > r_c \end{cases}$$

$$V_{M_1\bar{M}_2}^{(i)}(\mathbf{r}) = \begin{cases} T_{M_1\bar{M}_2} + \frac{1}{2}k_{M\bar{M}}(r^2 - r_c^2), & r \leq r_c \\ T_{M_1\bar{M}_2}, & r > r_c \end{cases}$$

$$V_{\delta\bar{\delta}}(r) = -\frac{\alpha}{r} + \sigma r + \bar{V}_0 + m_\delta + m_{\bar{\delta}}$$

$$\left|V_{\text{mix}}^{(i)}(r)\right| = \frac{\Delta}{2}\exp\left\{-\frac{1}{2}\frac{\left[V_{\delta\bar{\delta}}(r) - T_{M_1}^{(i)}\bar{M}_2\right]^2}{(\sigma\rho)^2}\right\}$$

$$V_{M_1\bar{M}_2}^{(i)}(\mathbf{r} = 0) \equiv -V_0 = -\frac{1}{2}k_{M\bar{M}}r_c^2$$

$$V_{M_1\bar{M}_2}^{(i)}(\mathbf{r} = 0) \gtrsim -20\text{MeV}$$

$$k \equiv 2V_0/r_c^2(m_{\delta(\bar{\delta})}, V_0, r_c)(m_{\delta(\bar{\delta})}, k, r_c)$$

$$m_{\delta=(cq)} = ak^2 + bk + c$$

$$a = Ae^{Br_c},$$

$$f_{\delta\bar{\delta}} = \alpha k^2 + \beta k + \gamma,$$

$$k_{\text{crit}}^{\text{SHO}} = 0.177 \cdot r_c^{-3.743},$$

$$k_{\text{crit}}^{\text{square}}/k_{\text{crit}}^{\text{SHO}} \simeq 0.58$$

$$k_{\text{crit}}^{\text{square}} = 0.096 \cdot r_c^{-3.576}.$$

$$k_{\text{crit}}^{\text{SHO}} = 0.335 \cdot r_c^{-3.312},$$

$$k_{\text{crit}}^{\text{square}} = 0.179 \cdot r_c^{-3.149}.$$

$$R \simeq (2\mu E)^{-1/2}.$$

$$k_{\text{crit}}^{\text{SHO}} = 9.72 \cdot 10^{-6} r_c^{-0.286},$$

$$qq = \frac{1}{\sqrt{2}}(ud - du)$$

$$qq = \left(uu, dd, \frac{ud + du}{\sqrt{2}}\right)$$

$$qq = \frac{1}{\sqrt{2}}(ud - du), \{I = 0, j_l = 0, j_b = 1 \text{ and } J = 1\}$$

$$\Longrightarrow I(J^P) = \{0(1^+)\}$$

$$qq = \left(uu, dd, \frac{ud+du}{\sqrt{2}}\right), \{I = 1, j_l = 1, j_b = 1 \text{ and } J = 0,1,2\}$$

$$\Longrightarrow I(J^P) = \{1(0^+), 1(1^+), 1(2^+)\}$$

$$1 = (-1)^{I+j_b+j_l+1}$$

$$\mathcal{L}_{\mathrm{LO}} = -i\mathrm{Tr}\left[\bar{H}_a v_\mu D^\mu_{ba} H_b\right] + g_\pi \mathrm{Tr}[\bar{H}_a H_b \gamma_\nu \gamma_5] u^\nu_{ba} + \frac{\lambda}{m_Q}\mathrm{Tr}\left[\bar{H}_a \sigma_{\mu\nu} H_a \sigma^{\mu\nu}\right]$$

$$H = \frac{1+\psi}{2}[Y + iP\gamma_5], \bar{H} = \gamma^0 H^\dagger \gamma^0$$

$$v_\mu = (1, \vec{0}) + O(\vec{p}/M)$$

$$D_\mu = \partial_\mu + \Gamma_\mu, \Gamma_\mu = \frac{1}{2}\left(u^\dagger \partial_\mu u + u \partial_\mu u^\dagger\right)$$

$$U = \exp\left(\sqrt{2} i\phi/F\right), u^2 = U$$

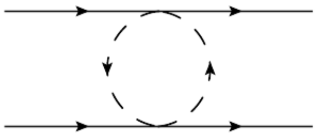
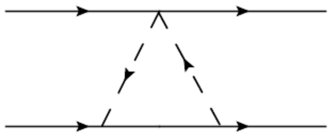
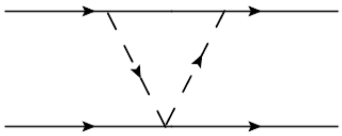
$$\phi = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta & \pi^+ & K^+ \\ \pi^- & -\frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta & K^0 \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}}\eta \end{pmatrix}.$$

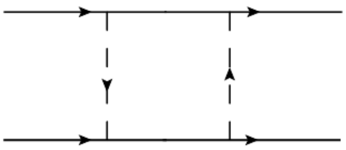
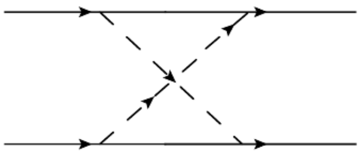
$$\mathcal{L}_{H\pi} = -\frac{g_\pi}{2}\left\langle H^\dagger_a H_b \sigma \cdot \boldsymbol{u}_{ab}\right\rangle$$

$$\boldsymbol{u} = -\sqrt{2}\boldsymbol{\nabla}\phi/F_\pi$$

$$V_\pi(q) = (I_1 \cdot I_2)\frac{g_\pi^2}{F_\pi^2}\frac{(q\cdot\epsilon_2)(q\cdot\epsilon_4^*)}{q^2 - m_\pi^2}$$

$$V_\pi(r) = (I_1 \cdot I_2)\frac{g_\pi^2}{3F_\pi^2}\left(m_\pi^2 \frac{e^{-m_\pi r}}{4\pi r} - \delta(r)\right),$$

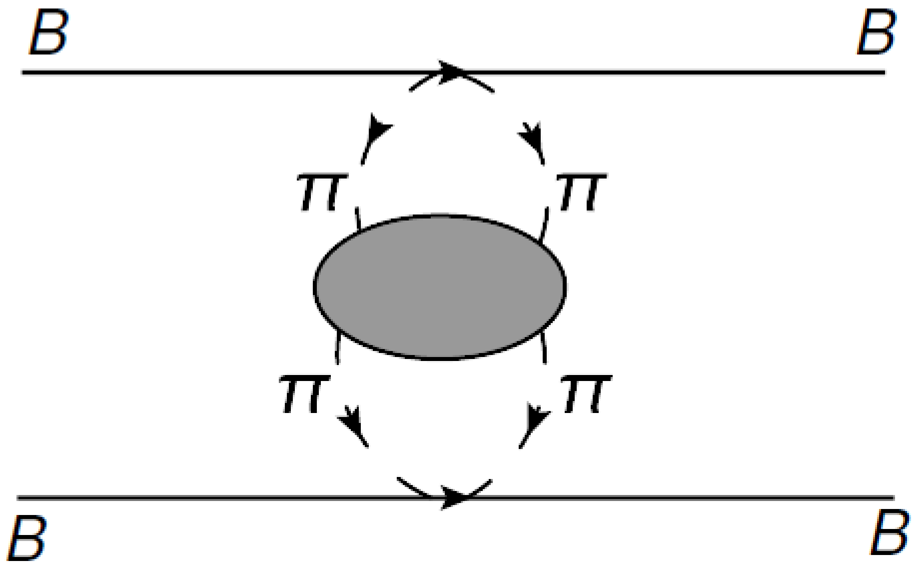




$$\mathcal{M}(s,t) = \frac{1}{\pi}\int_{4m_\pi^2}^{\infty} dz \frac{\mathrm{Im}\mathcal{M}(z,t)}{z - s - i\epsilon}$$

$$\Gamma_{\mathrm{out}} = 1 + T_{\pi\pi} G$$

$$\mathrm{disc}\Gamma_{\mathrm{out}} = 2i\sigma T^* \Gamma_{\mathrm{out}}$$



$$\sigma = \frac{\sqrt{1 - 4m_\pi^2/s}}{16\pi}$$

$$\mathcal{M}_{\pi\pi} = G\Gamma_{\text{out}} a^2$$

$$\text{Im}\mathcal{M}_{\pi\pi} = 2i\sigma a^2 |\Gamma_{\text{out}}|^2$$

$$\Gamma_{\text{out}} = \Omega^{L=0}(s) = \exp\left[\frac{s}{\pi}\int_{4m_\pi^2}^{\infty} dz \frac{\delta^0(z)}{z(z - s - i\epsilon)}\right]$$

$$(a^0)^2 = \sum_{\alpha,\beta} a^{(+)2}\delta_{\alpha\beta}\delta_{\alpha\beta} = 3T^{(+)2}$$

$$T_{\alpha\beta} = T^{(+)}\delta_{\alpha\beta} - T^{(-)}\frac{1}{2}[\tau_\alpha, \tau_\beta]$$

$$T^{(+)} = \frac{1}{3}\left(T^{\frac{1}{2}} + 2T^{\frac{3}{2}}\right)$$

$$T^{(-)} = \frac{1}{3}\left(-T^{\frac{1}{2}} + T^{\frac{3}{2}}\right)$$

$$\text{Im}\mathcal{M}_{\pi\pi}^{I=0} = -\frac{3}{2}i\pi\left(a^{(+)}\right)^2\sqrt{1 - \frac{4m_\pi^2}{s}}|\Omega^0(s)|^2\Theta(s - 4m_\pi^2)$$

$$V(s,t,u) = \frac{1}{F_\pi^2}\left[\frac{C_{\text{LO}}}{4}(s-u) - 4C_0h_0 + 2C_1h_1 - 2C_{24}H_{24}(s,t,u) + 2C_{35}H_{35}(s,t,u)\right]$$

$$V_{\text{thr}}^{H\pi} = \frac{m_\pi^2}{f_\pi^2}\left[C_{\text{LO}}\frac{M_H}{m_\pi} - 4h_0 - 2h_1 - 4(h_2 + h_4M_H^2) + 2(h_3 + 2h_5M_H^2)\right].$$

$$h_{0,1,24,35}^{Q} = h_{0,1,24,35}^{c}\frac{M_H}{M_D}.$$

$$V_{\text{thr}}^{H\pi,I} = \frac{m_\pi^2 M_H}{f_\pi^2}\left[\frac{C_{\text{LO}}^I}{m_\pi} - \frac{2}{M_D}\left(2h_0^c + h_1^c + 2h_{24}^c - h_{35}^c\right)\right]$$

$$G_{\text{thr}}^{\Lambda} = \frac{1}{16\pi^2(M_H + m_\pi)}\left[M_H \log\left(\frac{M_H^2}{\left(\sqrt{M_H^2+\Lambda^2}+\Lambda^2\right)^2}\right) + m_\pi \log\left(\frac{m_\pi^2}{\left(\sqrt{m_\pi^2+\Lambda^2}+\Lambda^2\right)^2}\right)\right]$$

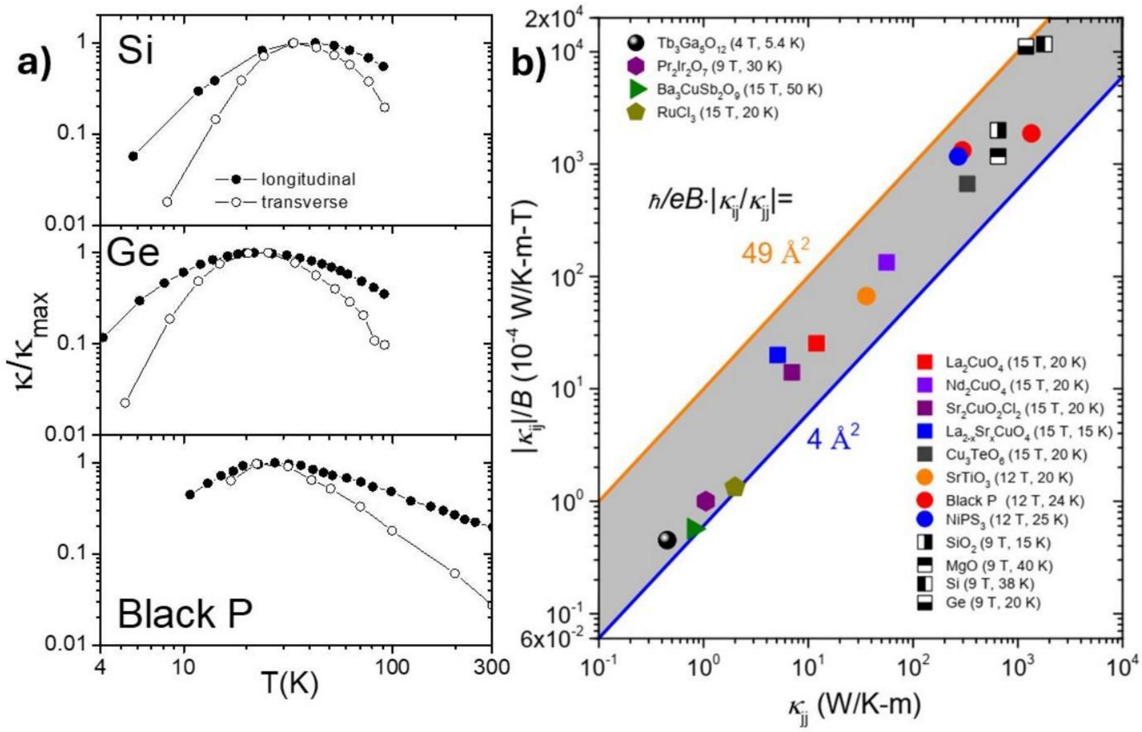
$$a_0^I = -\frac{M_H T_{\text{thr,NR}}^I}{4\pi(M_H + m\pi)} \text{ with } T_{\text{thr}}^I = \frac{V_{\text{thr}}^{H\pi,I}}{\left[1 - V_{\text{thr}}^{H\pi,I} G_{\text{thr}}^{\Lambda}\right]}$$

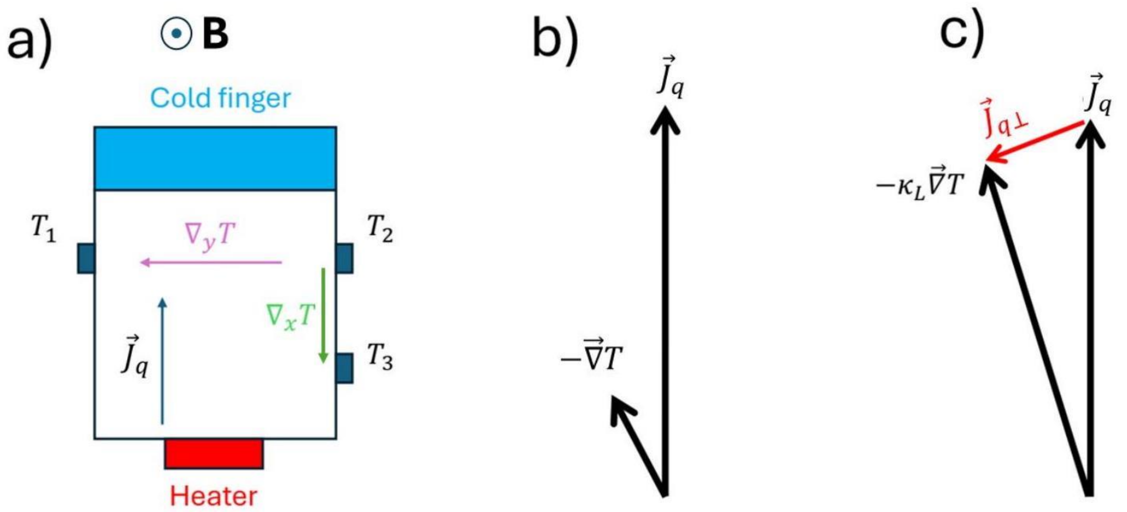
$$T_{\text{thr,Rel}}^I = 2M_H T_{\text{thr,NR}}^I$$

$$V_\sigma(q^2) = \frac{2}{\pi}\int_{2m_\pi}^{\infty} d\mu\mu \frac{\text{Im}\mathcal{M}(s,\mu^2)}{\mu^2+q^2}$$

$$V_\sigma(r) = \frac{1}{2\pi^2 r}\int_{2m_\pi}^{\infty} d\mu\mu e^{-\mu r}\text{Im}\mathcal{M}(s,\mu^2)$$

$$V_\sigma(r) = -\frac{3}{4\pi r}\left(a^{(+)}\right)^2\int_{2m_\pi}^{\infty} d\mu\sqrt{\mu^2-4m_\pi^2}e^{-\mu r}|\Omega^0(\mu^2)|^2$$





$$\vec{J_s} = \frac{\vec{J_q}}{T}$$

$$\sigma^s = \vec{\nabla} \cdot \vec{J_s}$$

$$\sigma^s = \vec{J_q} \cdot \vec{\nabla}\frac{1}{T} + \Sigma_\alpha J_\alpha X_\alpha \cdot s$$

$$\sigma^s = \frac{1}{T^2}\vec{J_q} \cdot \vec{\nabla}T$$

$$\eta = J_{q\perp}/J_q$$

$$\mathbf{tan}\Theta_H = \frac{\nabla_y T}{\nabla_x T}$$

$$\tan\ \Theta_H = \frac{\eta}{\sqrt{1-\eta^2}}\left(\gamma_i = \frac{V\partial\omega_i}{\omega_i\partial V}\right)$$

$$A = \mathrm{Re}\left[e^{i(\vec{q_1}\cdot\vec{r}-\omega_1 t)}\right]$$

$$A = \mathrm{Re}\left[e^{i[\vec{q_1}\cdot\vec{r}-\omega_1 t + C\cos(\vec{q_2}\cdot\vec{r}-\omega_2 t)]}\right]$$

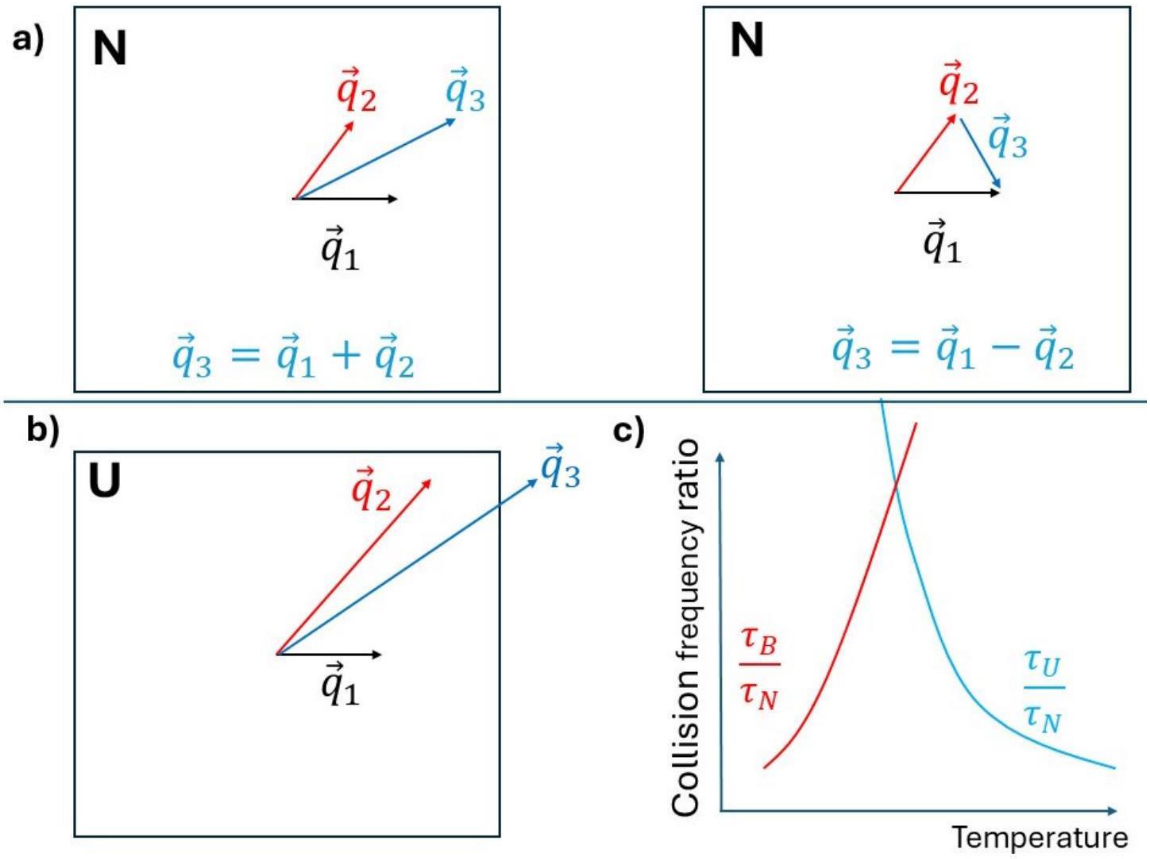
$$A = \mathrm{Re}\left[e^{[i(\vec{q_1}\cdot\vec{r}-\omega_1 t)}[1 + iC\cos(\vec{q_2}\cdot\vec{r}-\omega_2 t) + \cdots]\right]$$

$$A \simeq \mathrm{Re}\left[e^{i(\vec{q_1}\cdot\vec{r}-\omega_1 t)} + \frac{1}{2}Cie^{i[(\vec{q_1}+\vec{q_2})\cdot\vec{r}-(\omega_1+\omega_2)t]} + \frac{1}{2}Cie^{i[(\vec{q_1}-\vec{q_2})\cdot\vec{r}-(\omega_1-\omega_2)t]}\right]$$

$$A \simeq \cos(\vec{q_1}\cdot\vec{r}-\omega_1 t) - \frac{1}{2}C[\sin[(\vec{q_1}+\vec{q_2})\cdot\vec{r}-(\omega_1+\omega_2)t] - \sin[(\vec{q_1}-\vec{q_2})\cdot\vec{r}-(\omega_1-\omega_2)t]]$$

$$\vec{q_3} = \vec{q_1} + \vec{q_2};\ \omega_3 = \omega_1 + \omega_2$$

$$\overrightarrow{q_3} = \overrightarrow{q_1} - \overrightarrow{q_2}; \omega_3 = \omega_1 - \omega_2$$

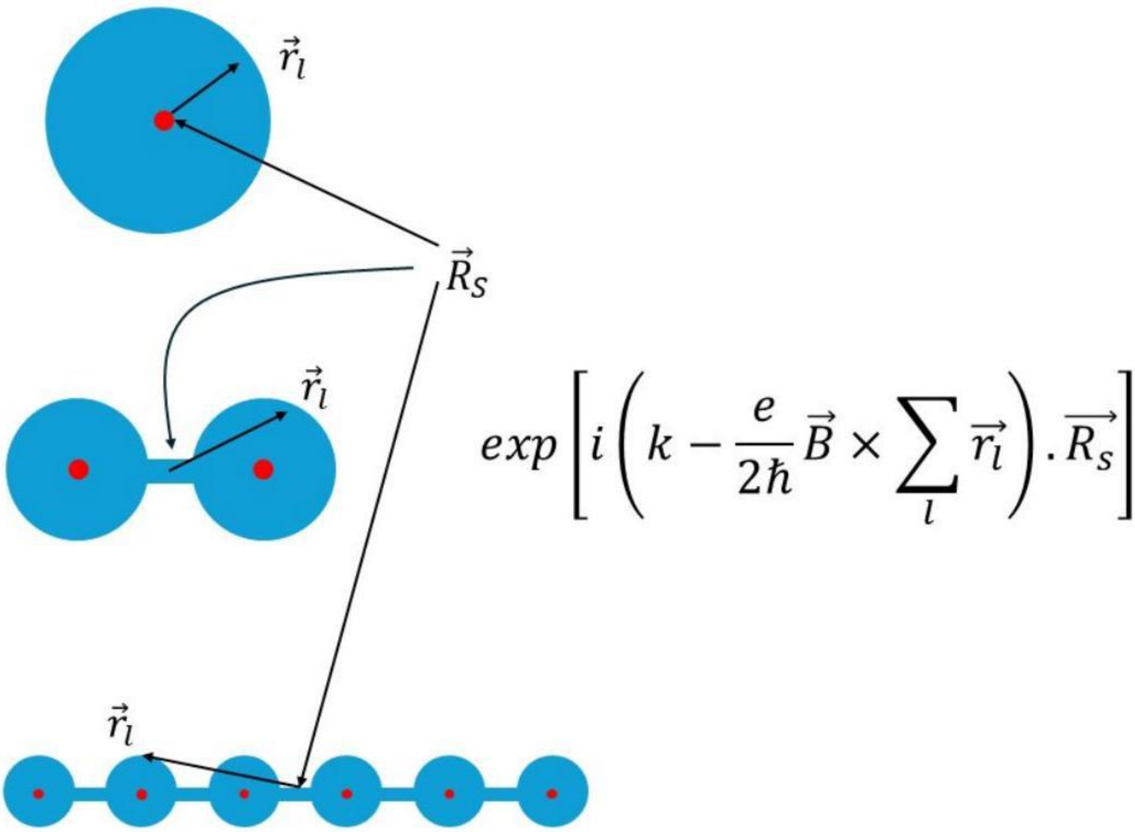


$$|\Psi(R)\rangle \approx |\chi(R)\rangle \psi(R)$$

$$\widehat{\boldsymbol{P}} = -\boldsymbol{i}\hbar\nabla_R$$

$$\widehat{\Pi}\psi(R) = \langle\chi(R)|\widehat{P}|\Psi(R)\rangle$$

$$\langle\chi(R)|(-i\hbar\nabla_R)|\Psi(R)\rangle = -i\hbar[\nabla_R\Psi(R) + \langle\chi(R) \mid \nabla_R\chi(R)\rangle]$$



$$\mathbf{A}(\mathbf{r}) = \frac{\mathbf{1}}{\mathbf{2}}\mathbf{B}\times\mathbf{r}$$

$$\exp\left\{\left[+i\left[\vec{k}-\frac{e}{2\hbar}\left(\vec{B}\times\sum_l \vec{r_l}\right)\right]\cdot\overrightarrow{R_S}\right]\right\}$$

$$\sum_l r_l \cdot R_S \ell_B^2 = \sqrt{\frac{\hbar}{eB}}$$

$$\delta\phi_B \approx q_e \frac{\lambda_{ph}\delta u_m}{\ell_B^2}$$

$$H = \frac{1}{2M}\sum_l P_l P_l + \frac{1}{2}k\sum_l (\eta_l\eta_l - \eta_l\eta_{l+1} - \eta_l\eta_{l-1})$$

$$H = \frac{1}{2}\sum_q \left[\frac{1}{M}\Pi_q\Pi_q^\star + 2k(1-\cos\ q)\xi_q\xi_q^\star\right]$$

$$\xi_q = \frac{1}{\sqrt{N}}\sum_l \eta_l s^{iql}$$

$$\Pi_q = \frac{1}{\sqrt{N}}\sum_l P_l s^{-iql}$$

$$|\boldsymbol{n_q}\rangle \equiv |\boldsymbol{n_{q+2n\pi}}\rangle$$

$$\langle \boldsymbol{x} \mid \boldsymbol{n}_q \rangle = e^{-i(qx-\omega t)}$$

$$\left(\phi(x) = \frac{x\delta u}{\ell_B^2}\right)\langle x \mid n_q \rangle = e^{-i[(qx-\omega t)+\phi(x)]}$$

$$i\langle n_q \mid \nabla n_q \rangle = \frac{\delta u}{\ell_B^2}$$

$$\delta\phi_B = \lambda \frac{\overline{\delta u}}{\ell_B^2}$$

$$\propto \frac{\delta u_m \lambda_{ph}}{\ell_B^2} \gamma_i = \frac{\mathrm{dln}\ \omega_i}{\mathrm{dln}\ V}$$

$$\rho_0 E(\eta) = \rho_0 E(0) + \frac{1}{2!}\sum_{i,j=1}^{6} C_{ij}\eta_i\eta_j + \frac{1}{3!}\sum_{i,j,k=1}^{6} C_{ijk}\eta_i\eta_j\eta_k$$

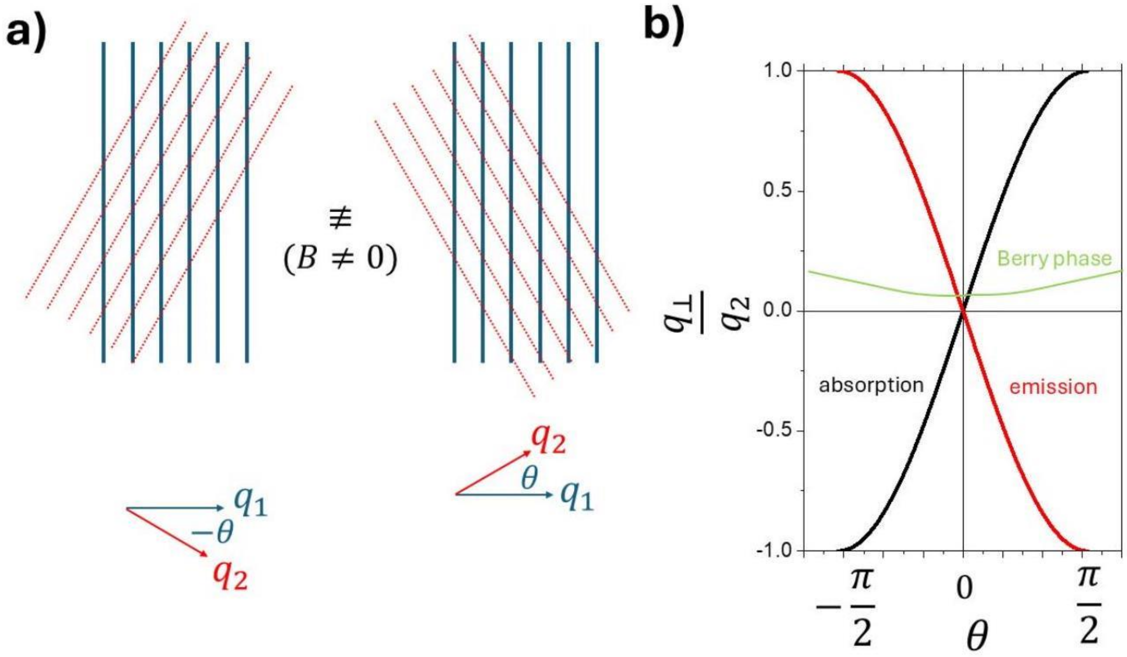
$$\left|\frac{\overline{\eta_{\text{crest}}} - \overline{\eta_{\text{trough}}}}{\bar{\eta}}\right| \simeq \frac{1}{3}\left|\frac{\overline{C_{ijk}}}{\overline{C_{ij}}}\right|$$

$$\boldsymbol{\frac{1}{3}\frac{\overline{C_{ijk}}}{\approx} - q_e \approx 1}$$

$$\frac{1}{3}\frac{\overline{C_{ijk}}}{\approx} - \left(\frac{d^3V}{dr^3}\right)$$

$$A = e^{i[\overrightarrow{q_1}\cdot\vec{r} - \omega_1 t + C\cos(\overrightarrow{q_2}\cdot\vec{r} - \omega_2 t + \delta\phi_B)]}$$

$$A \simeq e^{i(\overrightarrow{q_1}\cdot\vec{r} - \omega_1 t)}$$
$$+\frac{1}{2}Cie^{i[(\overrightarrow{q_1}+\overrightarrow{q_2})\cdot\vec{r} - (\omega_1+\omega_2)t + \delta\phi_B]}$$
$$+\frac{1}{2}Cie^{i[(\overrightarrow{q_1}-\overrightarrow{q_2})\cdot\vec{r} - (\omega_1-\omega_2)t] - \delta\phi_B]}$$



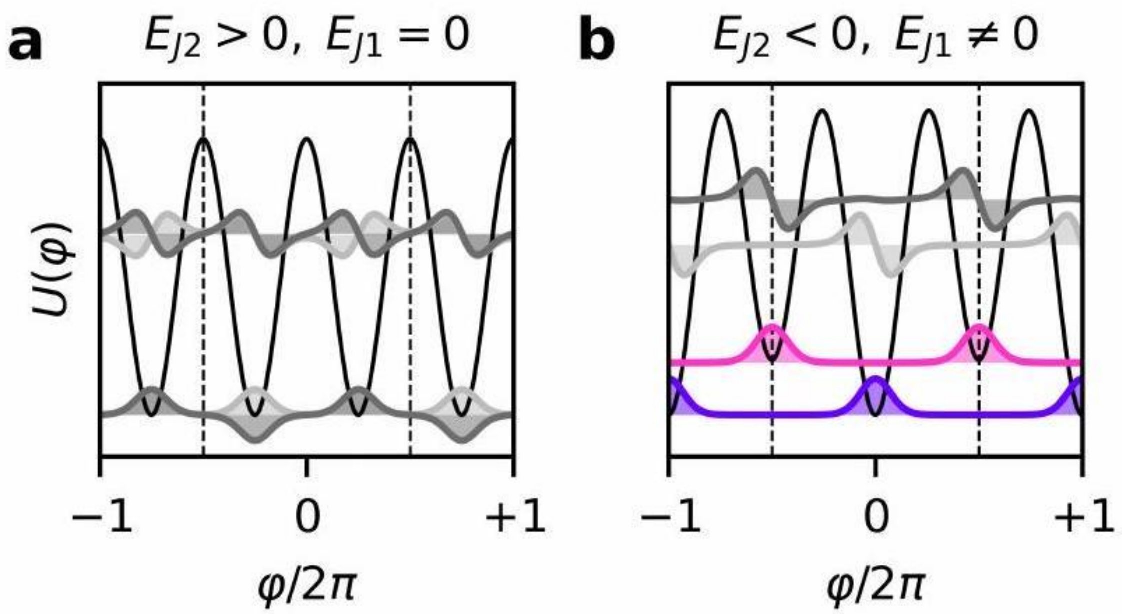
$$\boldsymbol{v_{ph}} = \boldsymbol{\omega}/\boldsymbol{q} = \frac{2\pi}{\lambda_{ph}}$$

$$\lambda_{ph}(T_{\max}) \approx \frac{h v_{ph}}{k_B T_{\max}}$$

$$\boldsymbol{M\delta u_m^2 \omega_{ph}^2 = k_B T_{\max}}$$

$$\hbar\omega_{ph}(T_{\max}) = \boldsymbol{k}_B \boldsymbol{T}_{\max}$$

$$\delta u_m(T_{\max}) \approx \frac{\hbar}{\sqrt{M k_B T_{\max}}}$$



$$\cos\ 2\hat{\varphi} = \frac{1}{2}\sum_{n} |n\rangle\langle n+2| + \text{ h.c.}$$

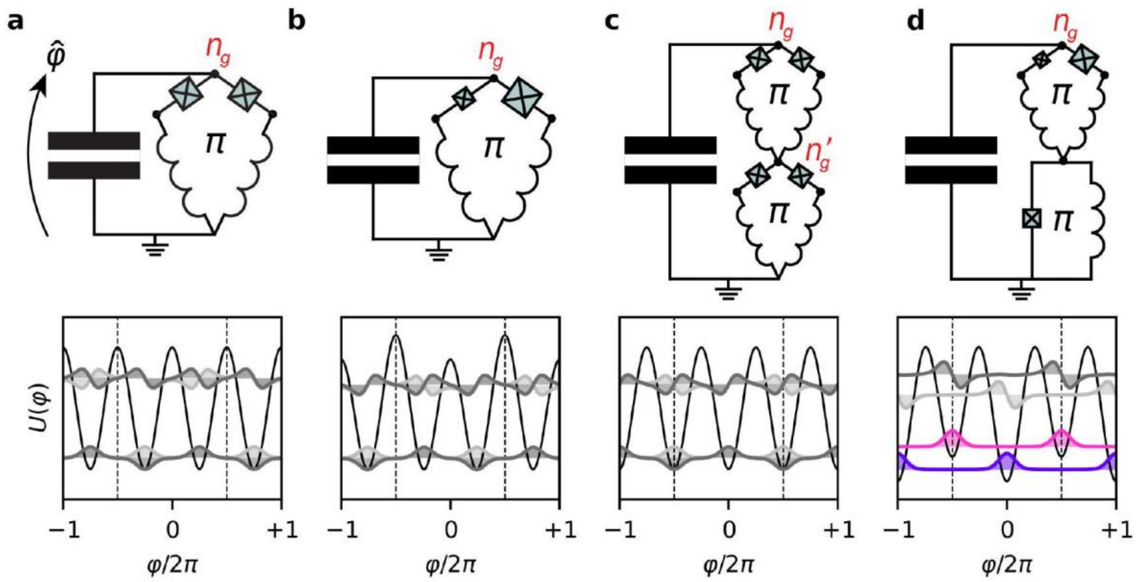
$$\langle e|\hat{n}|g\rangle = \langle e|e^{i\hat{\varphi}}|g\rangle \neq 0$$

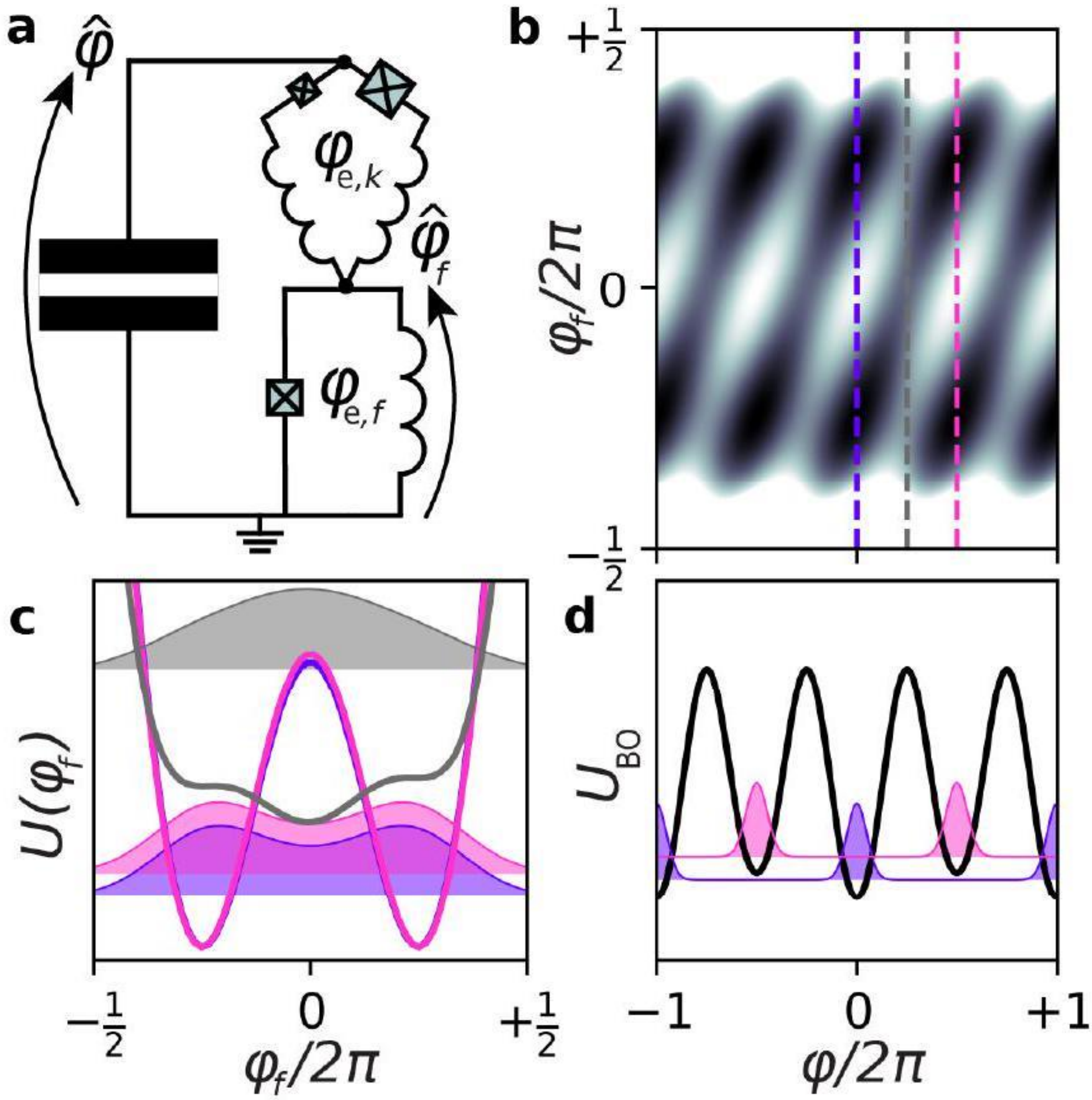
$$U = E_{J1}\cos\ \hat{\varphi} + E_{J2}\cos\ 2\hat{\varphi}.\ \text{If}\ |E_{J1}| \ll |E_{J2}|$$

$$\langle e|\hat{\varphi}|g\rangle\langle e|\hat{n}|g\rangle = -i\langle e|\frac{\partial}{\partial\hat{\varphi}}|g\rangle$$

$$\varphi_{\mathrm{e}}/2 = +\pi/2$$

$$(\varphi_{\mathrm{e}} - 1)/2 = -\pi/2$$





$$\varphi_{e,f} = \varphi_{e,k} = \pi$$

$$H = +4E_C(\hat{n} - n_g)^2 + 4E_{C,f}\hat{n}_f^2 + \frac{E_L}{2}\hat{\varphi}_f^2 + E_J\cos\,\hat{\varphi}_f$$
$$+E_{J2,k}\cos\,2(\hat{\varphi} - \hat{\varphi}_f) - E_{J1,k}\cos\,(\hat{\varphi} - \hat{\varphi}_f)$$

$$H_{\text{fast}}(\varphi) = +4E_{C,f}\hat{n}_f^2 + \frac{E_L}{2}\hat{\varphi}_f^2 + E_J\cos\,\hat{\varphi}_f$$
$$+E_{J2,k}\cos\,2(\varphi - \hat{\varphi}_f) + E_{J1,k}\cos\,(\varphi - \hat{\varphi}_f)$$

$$\epsilon_{g,\,\text{fast}}\,(\varphi)H_{\text{fast}}\,(\varphi)$$

$$\epsilon_{g,\,\text{fast}}\,(\varphi) = U_{\text{BO}}(\varphi)$$

$$H_{\text{slow}} = 4E_C(\hat{n} - n_g)^2 + U_{\text{BO}}(\hat{\varphi})$$

$$-E_{J1,k}\cos\,(\hat{\varphi} - \hat{\varphi}_f)$$

$$\epsilon_{g,\,\text{fast}}\,(\varphi = 0)\epsilon_{g,\,\text{fast}}\,(\varphi = \pi)\epsilon_{g,\,\text{fast}}\,(\varphi = \pi/2)$$

$$U_{\mathrm{BO}}(\varphi) = \epsilon_{g,\,\mathrm{fast}}\,(\varphi)$$

$$H_{\mathrm{fast}}\,(\varphi = 0)H_{\mathrm{fast}}\,(\varphi = \pi)$$

$$\omega_q = \epsilon_{\mathrm{fast}}\,(\varphi = \pi) - \epsilon_{\mathrm{fast}}\,(\varphi = 0)$$

$$\begin{aligned} H_{\mathrm{fast}}\,(\varphi = 0, \pi) = &+4E_{C,f}\hat{n}_f^2 + \frac{E_L}{2}\hat{\varphi}_f^2 \\ &-E_J\cos\left(\varphi_{\mathrm{e},f} - \hat{\varphi}_f\right) \\ &+E_{J2,k}\cos\,2\hat{\varphi}_f \mp E_{k,\Phi}\left(\pi - \varphi_{\mathrm{e},k}\right)\sin\,\hat{\varphi}_f \end{aligned}$$

$$H_{\mathrm{fast}}\,(\varphi = 0)H_{\mathrm{fast}}\,(\varphi = \pi)H_{\mathrm{fast}}\,(\varphi = 0)H_{\mathrm{fast}}\,(\varphi = \pi)\varphi_{\mathrm{e},k}\text{-}\omega_q\varphi_{\mathrm{e},f}\varphi_{\mathrm{e},k} = \pi$$

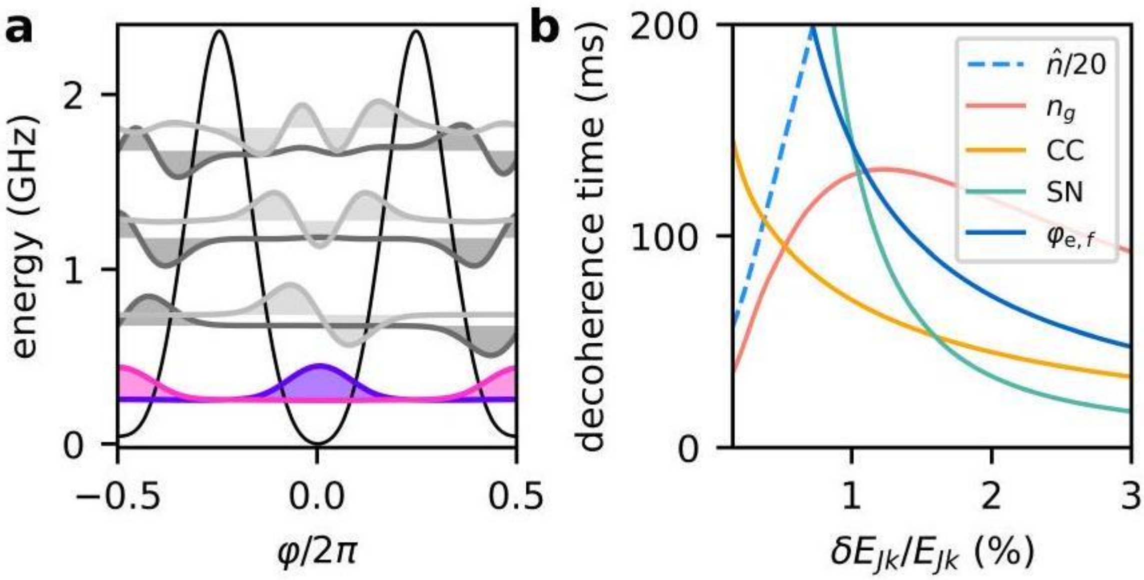
$$H_{\mathrm{fast}}\,(\varphi = 0) = H_{\mathrm{fast}}\,(\varphi = \pi)\omega_q = \epsilon_{\mathrm{fast}}\,(\varphi = \pi) - \epsilon_{\mathrm{fast}}\,(\varphi = 0) = 0$$

$$\varphi_{\mathrm{e},f}\varphi_{\mathrm{e},k}\varphi_{\mathrm{e},f} = \pi\varphi = \hat{\varphi}_f \rightarrow -\hat{\varphi}_f H_{\mathrm{fast}}\,(\varphi = \pi)$$

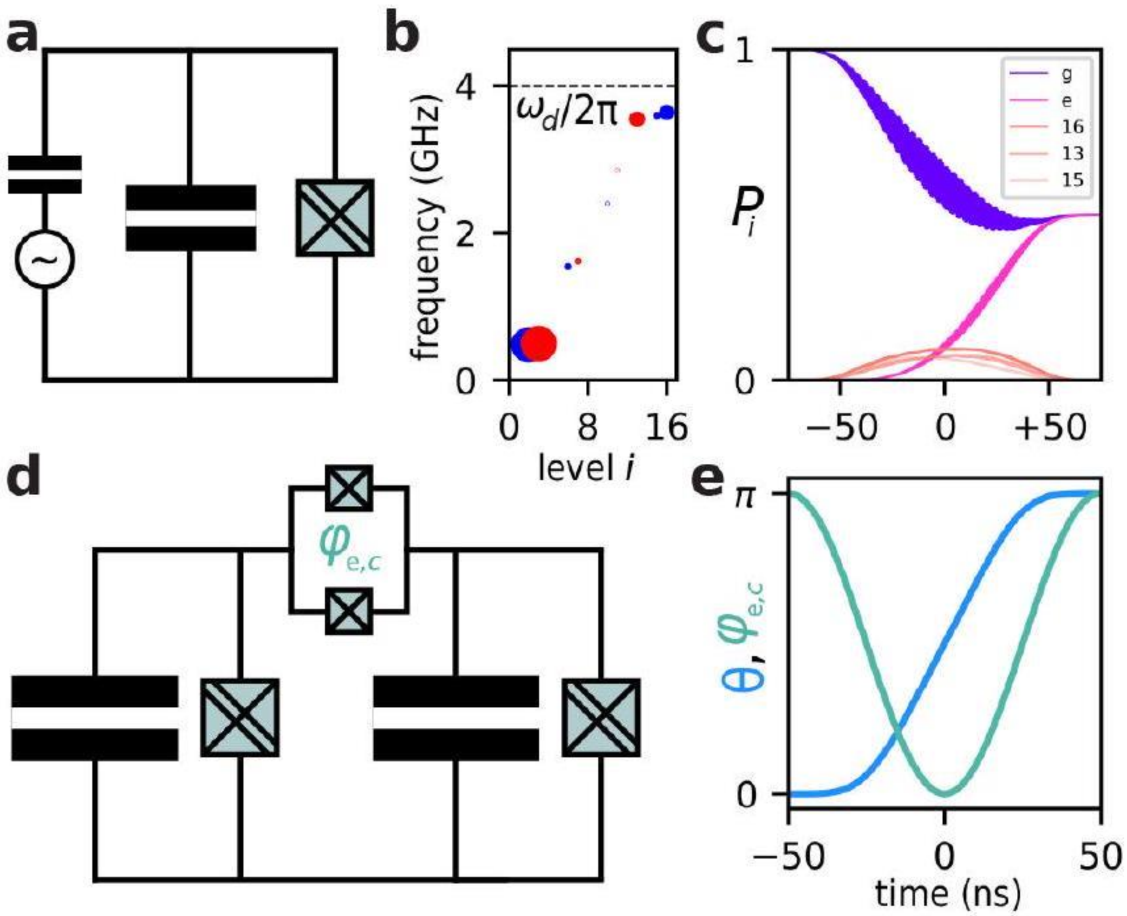
$$H_{\mathrm{fast}}\,(\varphi = 0) = H_{\mathrm{fast}}\,(\varphi = \pi)$$

$$\varphi_{\mathrm{e},f} = \varphi_{\mathrm{e},k} = \pi$$

$$e^{-\hbar\omega/k_BT}C_i \sim \epsilon L\frac{E_J}{C_J} = \frac{\Phi_0}{2\pi}\frac{j_c}{C_s}$$



$$\Delta E_{Jk}/E_{Jk} = C_{Jk}, C_{Jf}\,\frac{E_J}{C_J} = \frac{\Phi_0}{2\pi}\frac{j_c}{C_s}$$



$$\langle e|\hat{n}|i\rangle\langle i|\hat{n}|g\rangle$$

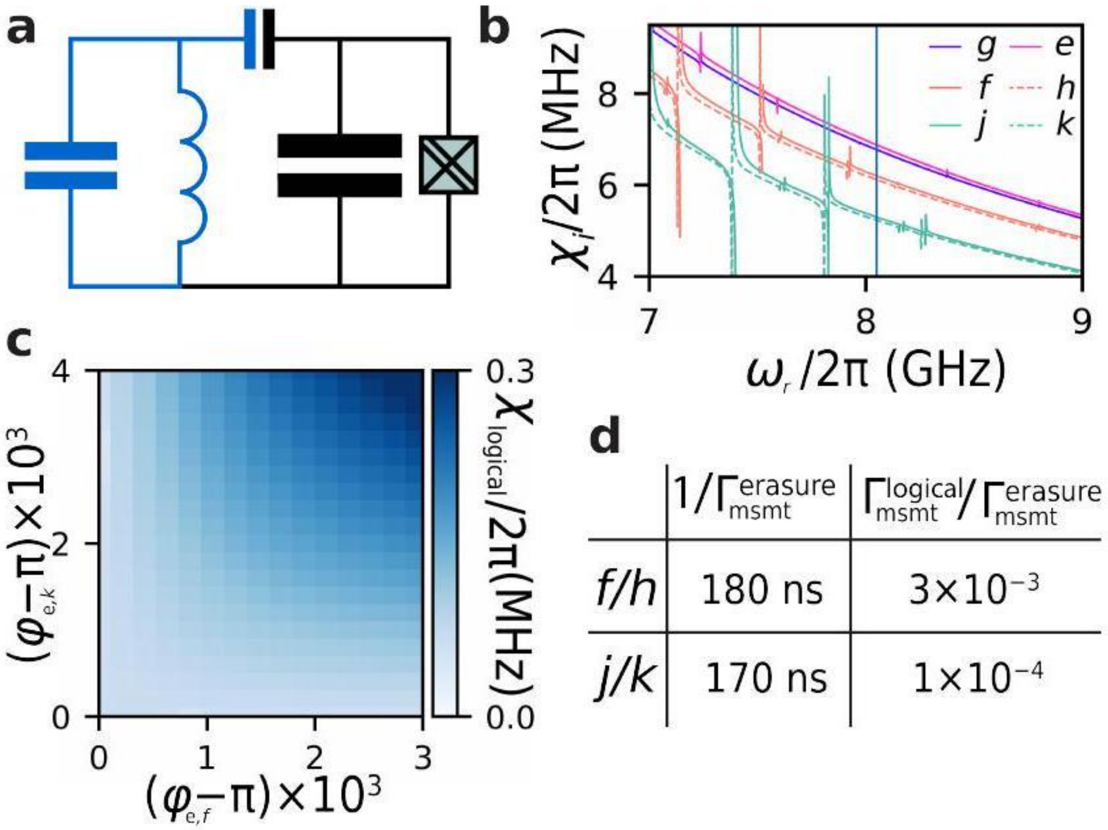
$$\omega_{eg}|e\rangle\langle e| + \Delta|i\rangle\langle i| + \frac{\Omega_{ig}}{2}|i\rangle\langle g| + \frac{\Omega_{ie}}{2}|i\rangle\langle e| + h.c.$$

$$\frac{\delta_{\text{eff}}}{2}\sigma_z + \frac{\Omega_{\text{eff}}}{2}\sigma_x$$

$$\Omega_{\text{eff}} = -\frac{\Omega_{ig}\Omega_{ie}}{2\Delta}$$

$$\delta_{\text{eff}} = \omega_{ge} + \frac{\Omega_{ig}^2}{4\Delta} - \frac{\Omega_{ie}^2}{4\Delta}$$

$$\begin{aligned} U_c &= -E_{Jc}\cos\left(\varphi_{e,c} - (\hat{\varphi}_1 - \hat{\varphi}_2)\right) - E_{Jc}\cos(\hat{\varphi}_1 - \hat{\varphi}_2) \\ &\approx -E_{Jc}\left(1 + \cos\ \varphi_{e,c}\right)\cos\ \hat{\varphi}_1 \cos\ \hat{\varphi}_2 \\ &\approx -E_{Jc}\left(1 + \cos\ \varphi_{e,c}\right)\sigma_{z1}\sigma_{z2} \end{aligned}$$



$$\chi_i = g_r^2 \sum_{j\neq i} |n_{ij}|^2 \frac{2\omega_{ij}}{\omega_{ij}^2 - \omega_r^2}$$

$$\omega_{ij} = \epsilon_i - \epsilon_j$$

$$n_{ij} = \langle j|\hat{n}|i\rangle$$

$$\chi_{\text{logical}} = (\chi_e - \chi_g)/2 \sim \kappa$$

$$\varphi_{e,k} = \varphi_{e,f} = \pi$$

$$\chi_e \approx \chi_g \to \chi_{\text{logical}} \approx 0$$

$$\varphi_{e,k}, \varphi_{e,f} \neq \pi$$

$$\varphi_{e,k}, \varphi_{e,f} = \pi$$

$$|g\rangle \to |f\rangle$$

$$\chi_{\text{erasure}} = (\chi_f - \chi_g)/2 \approx (\chi_h - \chi_g)/2 \approx (\chi_f - \chi_e)/2 \approx (\chi_h - \chi_e)/2$$

$$\varphi_{e,k} = \varphi_{e,f} = \pi$$

$$\omega_r + \chi_f \approx \omega_r + \chi_h$$

$$\Gamma_{\text{msmt}}^{\text{erasure}} \approx \frac{1}{2}\bar{n}_{\text{erasure}}\,\kappa$$

$$\Gamma_{\text{msmt}}^{\text{logical}}\ \chi_{\text{erasure}}\ \gg \kappa$$

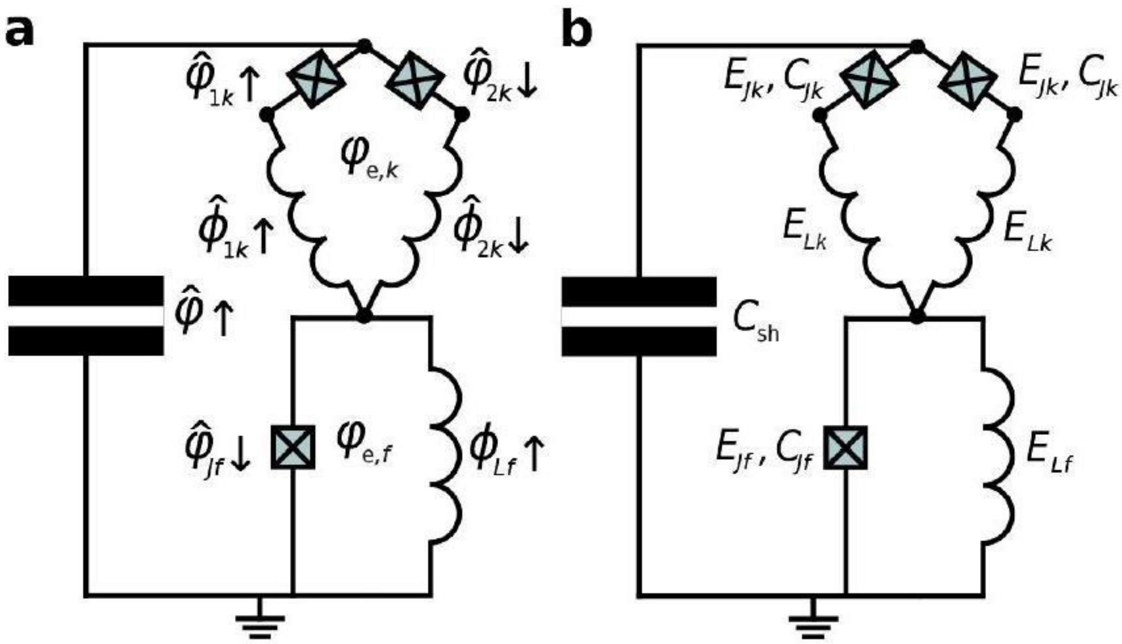
$$p_{\text{err}}\ \approx \frac{\Gamma_{\text{msm}}^{\text{logical}}}{\Gamma_{\text{msmt}}^{\text{resmur}}} \approx \frac{\kappa^2\chi_{\text{logical}}^2}{32\chi_{\text{erasure}}^4}$$

$$\Gamma_\phi^{\text{th}}\ \approx 4\bar{n}_{\text{th}}\,\chi_{\text{logical}}^2/\kappa$$

$$\Delta E_{Jk}/E_{Jk}$$

$$p_{\text{err}}\ \propto \chi_{\text{logical}}^2$$

$$E_{J1}\cos\ \varphi + E_{J2}\cos\ \varphi$$



$$\begin{aligned}
\phi_{Lf} &= +\varphi_f + \delta\varphi_{e,f} \\
\varphi_{Jf} &= -\hat{\varphi}_f + \varphi_{e,f} \\
\phi_{1k} &= +\varphi_{\Sigma k} + \varphi_{\Delta k} \\
\phi_{2k} &= +\varphi_{\Sigma k} - \varphi_{\Delta k} - \delta\varphi_{e,k} \\
\varphi_{1k} &= +\varphi - \hat{\varphi}_f - \varphi_{\Sigma k} - \varphi_{\Delta k} + \varphi_{e,f} \\
\varphi_{2k} &= -\varphi + \hat{\varphi}_f - \varphi_{\Sigma k} + \varphi_{\Delta k} - \varphi_{e,f} - \varphi_{e,k}
\end{aligned}$$

$$\varphi_{e,i} \to \varphi_{e,i} + \delta\varphi_{e,i}$$

$$\vec{\varphi}_B^T = \phi_{Lf}, \varphi_{Jf}, \phi_{1k}, \phi_{2k}, \varphi_{1k}, \varphi_{2k}, \varphi$$

$$\vec{\varphi}_D^T = \left(\varphi, \hat{\varphi}_f, \varphi_{\Sigma k}, \varphi_{\Delta k}\right)$$

$$\overleftrightarrow{M}\vec{\varphi}_B = \overleftrightarrow{M}\vec{\varphi}_D$$

$$\begin{aligned}
U = &+\frac{E_{Lf}}{2}\phi_{Lf}^2 + \frac{E_{Lk}}{2}\phi_{1k}^2 + \frac{E_{Lk}}{2}\phi_{2k}^2 \\
&-E_{Jf}\cos\ \varphi_{Jf} - E_{Jk}\cos\ \varphi_{1k} - E_{Jk}\cos\ \varphi_{2k}
\end{aligned}$$

$$T = +\frac{1}{2}\frac{\Phi_0^2}{(2\pi)^2}\left(C_{\mathrm{sh}}\dot{\varphi}^2 + C_{Jf}\dot{\varphi}_{Jf}^2 + C_{Jk}\dot{\varphi}_{1k}^2 + C_{Jk}\dot{\varphi}_{2k}^2\right)$$

$$+\frac{\Phi_0}{2\pi}C_g V_g \dot{\varphi}$$

$$= +\frac{1}{2}\frac{\Phi_0^2}{(2\pi)^2}\dot{\varphi}_D^T \overleftrightarrow{\mathcal{C}} \vec{\varphi}_D + \frac{\Phi_0}{2\pi}C_g V_g \dot{\varphi}$$

$$\hbar n_i = \frac{\partial L}{\partial \dot{\varphi}_i}$$

$$H = \hbar \sum_i n_i \dot{\varphi}_i - L$$

$$2e\vec{n}_D = \frac{\Phi_0}{2\pi}\overleftrightarrow{\mathcal{M}}\vec{\varphi}_D$$

$$\Gamma_1 = \Gamma_{g\to e} + \Gamma_{e\to g}$$

$$\Gamma_{g,\uparrow} = \sum_{f>e} \Gamma_{g\to f} \Gamma_{e,\uparrow} = \sum_{f>e} \Gamma_{e\to f}$$

$$\Gamma_{i\to f} = \frac{1}{\hbar^2}|\langle f|\mathcal{O}|i\rangle|^2 S_{\varepsilon\varepsilon}[\omega_{if}]$$

$$\omega_{if} = (\epsilon_i - \epsilon_f)/\hbar$$

$$\vec{V}_B = 2e\overleftrightarrow{\mathcal{M}}\overleftrightarrow{\mathcal{C}}\vec{n}_D$$

$$S_{qq}[\omega] = \frac{2\hbar C}{Q}\Theta(\omega)$$

$$\Theta(\omega) \to \Theta(-\omega)n_{\mathrm{BE}}(\omega) + \Theta(+\omega)n_{\mathrm{BE}}(\omega)e^{\hbar\omega/k_B T} \text{ where } n_{\mathrm{BE}}(\omega) = \frac{1}{e^{\hbar|\omega|/k_B T}-1}$$

$$\hat{O} = \frac{dH}{d\delta\Phi_i}$$

$$S_{\Phi\Phi}^{+}[\omega] = \frac{A_\Phi}{\omega}\sqrt{A_\Phi}$$

$$S^{+}[\omega] = (S[+\omega] + S[-\omega]) \diamond \frac{S[\omega]}{S[-\omega]} = e^{\hbar\omega/k_B T}$$

$$S_{\Phi\Phi}[\omega] = \frac{A_\Phi}{|\omega|}\frac{2}{1+e^{-\hbar\omega/k_B T}}$$

$$\Gamma_{\mathrm{qp},i\to f} = +\frac{16E_J}{h}\left|\langle f|\cos\frac{\hat{\varphi}_B}{2}\middle|i\rangle\right|^2 S_{\mathrm{qp},c}[\omega_{fi}]$$

$$+\frac{16E_J}{h}\left|\langle f|\sin\frac{\hat{\varphi}_B}{2}\middle|i\rangle\right|^2 S_{\mathrm{qp},s}[\omega_{fi}]$$

$$\Gamma_{\mathrm{qp},i\to f} = \frac{4E_L}{h}|\langle f|\hat{\varphi}_B|i\rangle|^2 S_{\mathrm{qp},+}[\omega_{fi}]$$

$$\sin\frac{\hat{\varphi}_B}{2}, \cos\frac{\hat{\varphi}_B}{2}$$

$$\left|\frac{d\omega_q}{d\mathcal{E}}\right|\left|\frac{d^2\omega_q}{d\mathcal{E}}\right| S_{\mathcal{E}\mathcal{E}}[\omega] = \frac{A_{\mathcal{E}}}{\omega}$$

$$\Gamma_{\phi,\mathcal{E}} \approx \sqrt{A_{\mathcal{E}}}\left|\frac{d\omega_q}{d\mathcal{E}}\right|$$

$$\Gamma_{\phi,\mathcal{E}} \approx A_{\mathcal{E}}\left|\frac{d^2\omega_q}{d\mathcal{E}^2}\right|$$

$$\varphi_{\mathrm{e},k} = \varphi_{\mathrm{e},f} = \pi\sqrt{A_\Phi}$$

$$\sqrt{A_\Phi} \approx 1\mu\Phi_0$$

$$\sqrt{A_\Phi} = 1\mu\Phi_0$$

$$\omega_q(n_g) = \omega_{ge,0} + \delta\omega_{ge,0}\cos 2\pi n_g$$

$$\frac{d\omega_q}{dn_g} = 2\pi\delta\omega_{ge,0}\sin 2\pi n_g$$

$$\sqrt{A_{E_J}} \propto E_J\sqrt{A_{E_J}}/E_J = 5\times10^{-7}$$

$$\Gamma_\phi = \frac{\sqrt{A_{E_J}}}{E_J}\omega_q/2 \rightarrow \sqrt{A_{E_J}}/E_J = 1.2\times10^{-8}$$

$$\Gamma_\phi^{\mathrm{sn}} = \frac{\bar{n}_{\mathrm{th}}\kappa\chi^2}{\kappa^2/4+\chi^2}$$

$$\epsilon_{\mathrm{ps}} = \frac{4\sqrt{2}}{\pi}\hbar\omega_{\mathrm{p}}\sqrt{\frac{1}{z}}e^{-4/\pi z}$$

$$\hbar\omega_{\mathrm{p}} = \sqrt{8E_{J,\,\mathrm{array}}E_{C,\,\mathrm{array}}}$$

$$z = \sqrt{8E_{C,\,\mathrm{array}}/E_{J,\,\mathrm{array}}/(2\pi)}$$

$$\Gamma_{\phi,\mathrm{AC}} = \pi\sqrt{N_{\mathrm{array}}\epsilon_{\mathrm{ps}}|\mathcal{F}_{ge}|}$$

$$\begin{aligned}F_{ge}^a &= \langle e \mid e, \hat{\varphi}_f \rightarrow \hat{\varphi}_f - 2\pi\rangle - \langle g \mid g, \hat{\varphi}_f \rightarrow \hat{\varphi}_f - 2\pi\rangle \\ F_{ge}^b &= +\langle e \mid e, \hat{\varphi}_{\Sigma k} \rightarrow \hat{\varphi}_{\Sigma k} - \pi, \hat{\varphi}_{\Delta k} \rightarrow \hat{\varphi}_{\Delta k} + \pi\rangle \\ &\quad -\langle g \mid g, \hat{\varphi}_{\Sigma k} \rightarrow \hat{\varphi}_{\Sigma k} - \pi, \hat{\varphi}_{\Delta k} \rightarrow \hat{\varphi}_{\Delta k} + \pi\rangle\end{aligned}$$

$$\hat{\varphi}_D \rightarrow \hat{\varphi}_D + \theta$$

$$E(\mathbf{q}) = \boldsymbol{\chi}^{\mathrm{T}}\mathbf{q} + \frac{1}{2}\mathbf{q}^{\mathrm{T}}\mathbf{C}\mathbf{q}$$

$$\sum_i q_i = Q_{\mathrm{tot}}$$

$$\begin{bmatrix} \mathbf{C} & \mathbf{1} \\ \mathbf{1}^{\mathrm{T}} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{q} \\ \mu \end{bmatrix} = \begin{bmatrix} -\boldsymbol{\chi} \\ Q_{\mathrm{tot}} \end{bmatrix}$$

$$E(\mathbf{q},\mathbf{v}) = \boldsymbol{\chi}^{\mathrm{T}}\mathbf{q} + (\mathbf{q}-\mathbf{q}_0)^{\mathrm{T}}\mathbf{v} + \frac{1}{2}\mathbf{q}^{\mathrm{T}}\mathbf{C}\mathbf{q} + \frac{1}{2}\mathbf{v}^{T}\mathbf{X}\mathbf{v}$$

$$U_{\mathrm{BO}}(\mathbf{R}) = V_{\mathrm{S}}(\mathbf{R}) + \mathrm{stat}_{\mathbf{q},\mathbf{v}}\left\{E(\mathbf{q},\mathbf{v}) \mid \sum_i v_i = V_{\mathrm{tot}}, \sum_i q_i = Q_{\mathrm{tot}}\right\}.$$

$$M_i\ddot{\mathbf{R}}_i = -\nabla_i U_{\mathrm{BO}}(\mathbf{R}),$$

$$\begin{bmatrix} \mathbf{C} & \mathbf{I} & \mathbf{1} & \mathbf{0} \\ \mathbf{I} & \mathbf{X} & \mathbf{0} & \mathbf{1} \\ \mathbf{1}^{\mathrm{T}} & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{1}^{\mathrm{T}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{q} \\ \mathbf{v} \\ \mu \\ \lambda \end{bmatrix} = \begin{bmatrix} -\boldsymbol{\chi} \\ \mathbf{q}_0 \\ Q_{\mathrm{tot}} \\ V_{\mathrm{tot}} \end{bmatrix}.$$

$$C_{ij} = \delta_{ij}\eta_i + (1-\delta_{ij})\Gamma_{ij}$$

$$\Gamma_{ij} = \left(r_{ij}^3 + \gamma_{ij}^{-3}\right)^{-\frac{1}{3}} \text{ with } r_{ij} = \left|\mathbf{r}_i - \mathbf{r}_j\right|$$

$$X_{ij} = \Lambda\left(\frac{r_{ij}}{\sigma_{ij}}\right)^3\left(1-\frac{r_{ij}}{\sigma_{ij}}\right)^6$$

$$\mathcal{E}(\mathbf{q},\mathbf{v},\mathbf{n},\mathbf{u}) = \boldsymbol{\chi}^{\mathrm{T}}\mathbf{q} - \mathbf{q}_0^{\mathrm{T}}\mathbf{v} + \frac{1}{2}[\mathbf{q}^{\mathrm{T}}\mathbf{v}^{\mathrm{T}}]\begin{bmatrix} \mathbf{C}_{\mathrm{S}} & \mathbf{I} \\ \mathbf{I} & \mathbf{X}_{\mathrm{S}} \end{bmatrix}\begin{bmatrix} \mathbf{q} \\ \mathbf{v} \end{bmatrix} + \frac{1}{2}\left(2[\mathbf{q}^{\mathrm{T}}\mathbf{v}^{\mathrm{T}}] - [\mathbf{n}^{\mathrm{T}}\mathbf{u}^{\mathrm{T}}]\right)\begin{bmatrix} \mathbf{C}_{\mathrm{L}} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{X}_{\mathrm{L}} \end{bmatrix}\begin{bmatrix} \mathbf{n} \\ \mathbf{u} \end{bmatrix}$$

$$\mathcal{U}_{\mathrm{BO}}(\mathbf{R},\mathbf{n},\mathbf{u}) = V_{\mathrm{S}}(\mathbf{R}) + \mathrm{stat}_{\mathbf{q},\mathbf{v}}\left\{\mathcal{E}(\mathbf{q},\mathbf{v},\mathbf{n},\mathbf{u}) \mid \sum_i q_i = Q_{\mathrm{tot}}, \sum_i v_i = V_{\mathrm{tot}}\right\}.$$

$$\begin{bmatrix} \mathbf{C}_{\mathrm{S}} & \mathbf{I} & \mathbf{1} & \mathbf{0} \\ \mathbf{I} & \mathbf{X}_{\mathrm{S}} & \mathbf{0} & \mathbf{1} \\ \mathbf{1}^{\mathrm{T}} & \mathbf{0} & 0 & 0 \\ \mathbf{0} & \mathbf{1}^{\mathrm{T}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{q}(\mathbf{n},\mathbf{u}) \\ \mathbf{v}(\mathbf{n},\mathbf{u}) \\ \mu \\ \lambda \end{bmatrix} = \begin{bmatrix} -\chi - \mathbf{C}_{\mathrm{L}}\mathbf{n} \\ \mathbf{q}_0 - \mathbf{X}_{\mathrm{L}}\mathbf{u} \\ Q_{\mathrm{tot}} \\ V_{\mathrm{tot}} \end{bmatrix}$$

$$\mathcal{L}(\mathbf{R},\dot{\mathbf{R}},\mathbf{n},\dot{\mathbf{n}},\mathbf{u},\dot{\mathbf{u}}) = \frac{1}{2}\sum_i M_i\left|\dot{\mathbf{R}}_i\right|^2 - \mathcal{U}_{\mathrm{BO}}(\mathbf{R},\mathbf{n},\mathbf{u}) + \frac{1}{2}m\sum_i \left(\dot{n}_i^2 + \dot{u}_i^2\right)$$
$$-\frac{1}{2}m\omega^2\left([\mathbf{q}^{\mathrm{T}}(\mathbf{n},\mathbf{u})\mathbf{v}^{\mathrm{T}}(\mathbf{n},\mathbf{u})] - [\mathbf{n}^{\mathrm{T}}\mathbf{u}^{\mathrm{T}}]\right)\mathbf{T}\begin{bmatrix} \mathbf{q}(\mathbf{n},\mathbf{u}) - \mathbf{n} \\ \mathbf{v}(\mathbf{n},\mathbf{u}) - \mathbf{u} \end{bmatrix}.$$

$$J_{ij} = \frac{\partial f_i(\mathbf{x})}{\partial x_j} \equiv \frac{\partial(c_i[\mathbf{x}] - x_i)}{\partial x_j}$$

$$M_i\ddot{\mathbf{R}}_i = -\left.\frac{\partial \mathcal{U}_{\mathrm{BO}}(\mathbf{R},\mathbf{n},\mathbf{u})}{\partial \mathbf{R}_i}\right|_{\mathbf{n},\mathbf{u}},$$

$$\begin{bmatrix}\ddot{\mathbf{n}}\\ \ddot{\mathbf{u}}\end{bmatrix} = -\omega^2\mathbf{K}\begin{bmatrix}\mathbf{q}(\mathbf{n},\mathbf{u})-\mathbf{n}\\ \mathbf{v}(\mathbf{n},\mathbf{u})-\mathbf{u}\end{bmatrix}.$$

$$\hat{\mathcal{H}} = \hat{T}_n(\mathbf{R}) + \hat{W}_{nn}(\mathbf{R}) + \hat{T}_e(\mathbf{r}) + \hat{W}_{ee}(\mathbf{r}) + \hat{W}_{en}(\mathbf{R},\mathbf{r}),$$

$$\hat{\mathcal{H}}\Psi(\mathbf{r},\mathbf{R}) = E\Psi(\mathbf{r},\mathbf{R}),$$

$$\Psi^{ad}(\mathbf{r},\mathbf{R}) = \phi_\alpha^{BO}(\mathbf{r}\mid\mathbf{R})\chi_{\alpha\lambda}(\mathbf{R}).$$

$$\hat{H}^{BO}(\mathbf{r},\mathbf{R})\phi_\alpha^{BO}(\mathbf{r}\mid\mathbf{R}) = \varepsilon_\alpha(\mathbf{R})\phi_\alpha^{BO}(\mathbf{r}\mid\mathbf{R})$$

$$\hat{H}^{BO}(\mathbf{r},\mathbf{R}) = \hat{W}_{nn}(\mathbf{R}) + \hat{T}_e(\mathbf{r}) + \hat{W}_{ee}(\mathbf{r}) + \hat{W}_{en}(\mathbf{R},\mathbf{r})$$

$$\left(\hat{T}_n(\mathbf{R}) + \varepsilon_\alpha(\mathbf{R})\right)\chi_{\alpha\lambda}(\mathbf{R}) = \Omega_{\alpha\lambda}\chi_{\alpha\lambda}(\mathbf{R}),$$

$$\hat{T}_n(\mathbf{R}) = -\mu\cdot\sum_\kappa \frac{1}{2M_\kappa}\nabla_{R_\kappa}^2$$

$$\mu = \frac{m}{M}$$

$$e^2 = \hbar = m = 1$$

$$\left[\mu\sum_\kappa \frac{\left(-i\nabla_{R_\kappa} + A_\kappa[\phi_\alpha^{BO}](\mathbf{R})\right)^2}{2M_\kappa} + \varepsilon_\alpha(\mathbf{R}) + \varepsilon^{geo}[\phi_\alpha^{BO}](\mathbf{R})\right] \\ \times\tilde{\chi}_{\alpha\lambda}(\mathbf{R}) = \tilde{\Omega}_{\alpha\lambda}\tilde{\chi}_{\alpha\lambda}(\mathbf{R})$$

$$A_\kappa[\phi_\alpha](\mathbf{R}) = \langle\phi_\alpha| - i\nabla_{R_\kappa}|\phi_\alpha\rangle$$

$$\varepsilon^{geo}[\phi_\alpha](\mathbf{R}) = \\ \mu\sum_\kappa \frac{1}{2M_\kappa}\left[\langle\nabla_{R_\kappa}\phi_\alpha \mid \nabla_{R_\kappa}\phi_\alpha\rangle - A_\kappa[\phi_\alpha](\mathbf{R})^2\right]$$

$$\phi_\alpha = \phi_\alpha^{BO}$$

$$\Psi(\mathbf{r},\mathbf{R}) = \phi(\mathbf{r}\mid\mathbf{R})\chi(\mathbf{R}).$$

$$\int |\phi(\mathbf{r}\mid\mathbf{R})|^2 dr = 1$$

$$E = \langle\Psi|\hat{\mathcal{H}}|\Psi\rangle \\ = \int \chi^*(\mathbf{R})\mu\sum_\kappa \frac{1}{2M_\kappa}\left(-i\nabla_{R_\kappa} + A_\kappa[\phi](\mathbf{R})\right)^2\chi(\mathbf{R}) \\ + \int |\chi(\mathbf{R})|^2\left(\varepsilon^{BO}[\phi](\mathbf{R}) + \varepsilon^{geo}[\phi](\mathbf{R})\right)$$

$$\varepsilon^{BO}[\phi](\mathbf{R}) = \int dr\phi^*(\mathbf{r}\mid\mathbf{R})\hat{H}^{BO}(\mathbf{r},\mathbf{R})\phi(\mathbf{r}\mid\mathbf{R})$$

$$\left[\mu\sum_\kappa \frac{1}{2M_\kappa}\left(-i\nabla_{R_\kappa} + A_\kappa[\phi](\mathbf{R})\right)^2 + \varepsilon^{BO}[\phi](\mathbf{R}) \\ + \varepsilon^{geo}[\phi](\mathbf{R})\right]\chi(\mathbf{R}) = E\chi(\mathbf{R})$$

$$\left[\mu\sum_{\mathbf{q}\lambda}\frac{\hat{P}_{-\mathbf{q}\lambda}\hat{P}_{\mathbf{q}\lambda}}{2}+\varepsilon(U)\right]\chi(U)=\Omega\chi(U)$$

$$\left[\frac{\hat{p}^2}{2m}+\hat{v}_{en}(\mathbf{r},U)+\hat{v}_{hxc}(\mathbf{r},U)+\hat{v}_{geo}(\mathbf{r},U)\right]\psi_{n\mathbf{k}U}(\mathbf{r})=\epsilon_{n\mathbf{k}U}\psi_{n\mathbf{k}U}(\mathbf{r})$$

$$\Omega=E-\varepsilon(\mathbf{R_0})$$

$$\varepsilon(U)=\varepsilon^{BO}(U)+\varepsilon^{geo}(U)$$

$$\langle\psi_{m,\mathbf{k+q}}|\hat{v}_{geo}|\psi_{n\mathbf{k}}\rangle=\left\langle\psi_{m,\mathbf{k+q}}\middle|\frac{\delta\varepsilon^{geo}}{\delta\psi^*_{n\mathbf{k}}}\right\rangle-\frac{1}{|\chi|^2}\sum_{\mathbf{q}\lambda}\left\langle\psi_{m,\mathbf{k+q}}\middle|\frac{\partial}{\partial U^*_{\mathbf{q}\lambda}}\left[|\chi|^2\frac{\delta\varepsilon^{geo}}{\delta(\partial\psi^*_{n\mathbf{k}}/\partial U^*_{\mathbf{q}\lambda})}\right]\right\rangle.$$

$$\hat{\mathcal{H}}=\hat{\mathcal{H}}_s^{(0)}+\hat{\mathcal{H}}'$$

$$\hat{\mathcal{H}}_s^{(0)}=\frac{\hat{p}^2}{2m}+\hat{v}_{en}^{(0)}(\mathbf{r})+\hat{v}_{hxc}^{(0)}(\mathbf{r})\equiv\frac{\hat{p}^2}{2m}+\hat{v}_s^{(0)}(\mathbf{r}).$$

$$\hat{v}_{\text{en}}^{(0)}(\mathbf{r})=\hat{v}_{\text{en}}(r,U)|_{U=0}$$

$$\hat{v}_{hxc}^{(0)}(\mathbf{r})=\hat{v}_{hxc}(r,U)|_{U=0}$$

$$\hat{\mathcal{H}}'=\hat{v}_s'+\hat{v}_{geo}$$

$$\hat{v}_s'=\hat{v}_s^{(1)}+\hat{v}_s^{(2)}$$

$$\hat{v}_{geo}=\hat{v}_{geo}^{(1)}+\hat{v}_{geo}^{(2)}$$

$$\left\langle\psi_2^{(0)}\middle|\hat{v}_s^{(1)}\middle|\psi_1^{(0)}\right\rangle\equiv\sum_\lambda g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})\frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}},$$

$$L_{\mathbf{q}\lambda}=\sqrt{\frac{\hbar}{2M\omega_{\mathbf{q}\lambda}}}g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})$$

$$\left\langle\psi_2^{(0)}\middle|\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle=\sum_\lambda\hbar\omega_{\mathbf{q}\lambda}U_{\mathbf{q}\lambda}\left\langle\psi_2\middle|\frac{\partial\psi_1^{(1)}}{\partial U_{\mathbf{q}\lambda}}\right\rangle=\sum_\lambda g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})\frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}\frac{\hbar\omega_{\mathbf{q}\lambda}}{\epsilon_1^{(0)}-\epsilon_2^{(0)}\pm\hbar\omega_{\mathbf{q}\lambda}},$$

$$\left|\psi_1^{(1)}\right\rangle=\sum_{2\neq1}\frac{\left\langle\psi_2^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle}{\epsilon_1^{(0)}-\epsilon_2^{(0)}}\left|\psi_2^{(0)}\right\rangle=\sum_\lambda\sum_{2\neq1}\frac{g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})}{\epsilon_1^{(0)}-\epsilon_2^{(0)}\pm\hbar\omega_{\mathbf{q}\lambda}}\frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}\left|\psi_2^{(0)}\right\rangle.$$

$$n_U(\mathbf{r}) = \sum_{n\mathbf{k}} f_{n\mathbf{k}U} |\psi_{n\mathbf{k}U}|^2$$

$$n^{(1)}(\mathbf{r}) = 2Re \sum_{\lambda} \sum_{1,2\neq 1} \frac{g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})}{\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}} \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}} \psi_1^{(0)*}(\mathbf{r})\psi_2^{(0)}(\mathbf{r})$$

$$\epsilon_1^{(2)} = \sum_{2\neq 1} \frac{\left|\left\langle \psi_2^{(0)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_1^{(0)} \right\rangle\right|^2}{\epsilon_1^{(0)} - \epsilon_2^{(0)}} + \left\langle \psi_1^{(0)} \middle| \hat{v}_s^{(2)} + \hat{v}_{geo}^{(2)} \middle| \psi_1^{(0)} \right\rangle$$

$$V_{1,1}^{(2)} \equiv \left\langle \psi_1^{(0)} \middle| \hat{v}_s^{(2)} \middle| \psi_1^{(0)} \right\rangle = \sum_{\mathbf{q}\lambda} g_{n_1,n_1;\lambda,\lambda}^{(2)}(\mathbf{k_1},\mathbf{q},\overline{\mathbf{q}}) \frac{|U_{\mathbf{q}\lambda}|^2}{L_{\mathbf{q}\lambda}^2},$$

$$g_{n_1,n_1;\lambda,\lambda}^{(2)}(\mathbf{k_1},\mathbf{q},\overline{\mathbf{q}})$$

$$W_{1,1}^{(2)} \equiv \left\langle \psi_1^{(0)} \middle| \hat{v}_{geo}^{(2)} \middle| \psi_1^{(0)} \right\rangle = \sum_{2}^{\text{unocc}} \sum_{\lambda\lambda'} \frac{g_{n_2,n_1,\lambda'}^{*}(\mathbf{k_1},\mathbf{q}) g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q}) \hbar\omega_{\mathbf{q}\lambda}}{\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\overline{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}\right)} \times \left(\delta_{\lambda\lambda'} - \frac{U_{\overline{\mathbf{q}}\lambda'}}{L_{\overline{\mathbf{q}}\lambda'}} \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}\right) - \sum_{2}^{\text{unocc}} \sum_{\lambda\lambda'} \frac{g_{n_2,n_1,\lambda'}^{*}(\mathbf{k_1},\mathbf{q}) g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q}) \hbar\omega_{\mathbf{q}\lambda}}{\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\overline{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}\right)} \frac{U_{\overline{\mathbf{q}}\lambda'}}{L_{\overline{\mathbf{q}}\lambda'}} \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}},$$

$$\epsilon_1^{(2)} = \sum_{2\neq 1} \sum_{\lambda\lambda'} \left[\frac{|g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})|^2}{\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}} \frac{|U_{\mathbf{q}\lambda}|^2}{L_{\mathbf{q}\lambda}^2} + \frac{g_{n_2,n_1,\lambda'}^{*}(\mathbf{k_1},\mathbf{q}) g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q}) \hbar\omega_{\mathbf{q}\lambda}}{\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\overline{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}\right)} \times \left(\delta_{\lambda\lambda'} - \frac{U_{\overline{\mathbf{q}}\lambda'}}{L_{\overline{\mathbf{q}}\lambda'}} \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}\right)\right] + \sum_{\mathbf{q}\lambda} g_{n_1,n_1;\lambda,\lambda}^{(2)}(\mathbf{k_1},\mathbf{q},\overline{\mathbf{q}}) \frac{|U_{\mathbf{q}\lambda}|^2}{L_{\mathbf{q}\lambda}^2}.$$

$$\bar{\epsilon}_1^{(2)} = \sum_{2\neq 1} \sum_{\lambda} \frac{|g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})|^2}{\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}} + \sum_{\mathbf{q}\lambda} g_{n_1,n_1;\lambda,\lambda}^{(2)}(\mathbf{k_1},\mathbf{q},\overline{\mathbf{q}}).$$

$$|U_{\mathbf{q}\lambda}|^2 / L_{\mathbf{q}\lambda}^2$$

$$V_{2,1}^{(2)} \equiv \left\langle \psi_2^{(0)} \middle| \hat{v}_s^{(2)} \middle| \psi_1^{(0)} \right\rangle = \sum_{\mathbf{q}\lambda\lambda'} g_{n_2,n_1,\lambda,\lambda'}^{(2)}(\mathbf{k_1},\mathbf{q},\mathbf{q}') \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}} \frac{U_{\mathbf{q}'\lambda'}}{L_{\mathbf{q}'\lambda'}}, (30)$$

$$W_{2,1}^{(2)} \equiv \left\langle \psi_2^{(0)} \middle| \hat{v}_{geo}^{(2)} \middle| \psi_1^{(0)} \right\rangle = \sum_{\mathbf{q}\lambda} \hbar\omega_{\mathbf{q}\lambda} U_{\mathbf{q}\lambda} \left\langle \psi_2^{(0)} \middle| \frac{\partial \psi_1^{(2)}}{\partial U_{\mathbf{q}\lambda}} \right\rangle$$

$$-\delta_{\mathbf{k}_2,\mathbf{k}_1} \sum_{\mathbf{q}\lambda} \hbar\omega_{\mathbf{q}\lambda} L_{\mathbf{q}\lambda} L_{\bar{\mathbf{q}}\lambda} \left\langle \psi_2^{(0)} \middle| \frac{\partial^2 \psi_1^{(2)}}{\partial U_{\bar{\mathbf{q}}\lambda} \partial U_{\mathbf{q}\lambda}} \right\rangle$$

$$\left\langle \psi_2^{(0)} \mid \psi_1^{(2)} \right\rangle V_{2,1}^{(2)} W_{2,1}^{(2)}$$

$$W_{2,1}^{(2)} = \sum_{\mathbf{q}\lambda} \hbar\omega_{\mathbf{q}\lambda} U_{\mathbf{q}\lambda} \frac{1}{\epsilon_1^{(0)} - \epsilon_2^{(0)}} \frac{\partial \left(V_{2,1}^{(2)} + W_{2,1}^{(2)} \right)}{\partial U_{\mathbf{q}\lambda}}$$

$$-\delta_{\mathbf{k}_2\mathbf{k}_1} \sum_{\mathbf{q}\lambda} \hbar\omega_{\mathbf{q}\lambda} L_{\mathbf{q}\lambda} L_{\bar{\mathbf{q}}\lambda} \frac{1}{\epsilon_1^{(0)} - \epsilon_2^{(0)}} \frac{\partial^2 \left(V_{2,1}^{(2)} + W_{2,1}^{(2)} \right)}{\partial U_{\bar{\mathbf{q}}\lambda} \partial U_{\mathbf{q}\lambda}}$$

$$W_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)} = \sum_{\mathbf{q}\lambda\lambda'} \frac{\hbar\omega_{\mathbf{q}\lambda}}{\epsilon_{n_1\mathbf{k}_1}^{(0)} - \epsilon_{n_2\mathbf{k}_2}^{(0)}} \left(\frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}} \frac{U_{\mathbf{q}'\lambda'}}{L_{\mathbf{q}'\lambda'}} - \delta_{\mathbf{k}_2\mathbf{k}_1} \delta_{\lambda\lambda'} \right)$$

$$\times \left[g_{n_2,n_1,\lambda,\lambda'}^{(2)}(\mathbf{k_1}, \mathbf{q}, \mathbf{q}') + g_{n_2,n_1,\lambda',\lambda}^{(2)}(\mathbf{k_1}, \mathbf{q}', \mathbf{q}) \right]$$

$$+\sum_{\mathbf{q}\lambda} \frac{\hbar\omega_{\mathbf{q}\lambda}}{\epsilon_{n_1\mathbf{k}_1}^{(0)} - \epsilon_{n_2\mathbf{k}_2}^{(0)}} U_{\mathbf{q}\lambda} \frac{\partial W_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)}}{\partial U_{\mathbf{q}\lambda}}$$

$$-\delta_{\mathbf{k}_2\mathbf{k}_1} \sum_{\mathbf{q}\lambda} \frac{\hbar\omega_{\mathbf{q}\lambda}}{\epsilon_{n_1\mathbf{k}_1}^{(0)} - \epsilon_{n_2\mathbf{k}_2}^{(0)}} L_{\mathbf{q}\lambda} L_{\bar{\mathbf{q}}\lambda} \frac{\partial^2 W_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)}}{\partial U_{\bar{\mathbf{q}}\lambda} \partial U_{\mathbf{q}\lambda}}$$

$$W_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)} = \sum_{\mathbf{q}\lambda\lambda'} \frac{1}{2} \left(g_{n_2,n_1,\lambda,\lambda'}^{(2)}(\mathbf{k_1}, \mathbf{q}, \mathbf{q}') + g_{n_2,n_1,\lambda',\lambda}^{(2)}(\mathbf{k_1}, \mathbf{q}', \mathbf{q}) \right)$$

$$\times \frac{\hbar\omega_{\mathbf{q}\lambda} + \hbar\omega_{\mathbf{q}',\lambda'}}{\epsilon_{n_1\mathbf{k}_1}^{(0)} - \epsilon_{n_2\mathbf{k}_2}^{(0)} - \hbar\omega_{\mathbf{q}\lambda} - \hbar\omega_{\mathbf{q}'\lambda'}}$$

$$\times \left(\frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}} \frac{U_{\mathbf{q}'\lambda'}}{L_{\mathbf{q}'\lambda'}} - \delta_{\mathbf{k}_1\mathbf{k}_2} \delta_{\lambda\lambda'} \right)$$

$$\left| \psi_{1,\parallel}^{(2)} \right\rangle = -\frac{1}{2} \sum_{3\neq 1}^{\text{occ}} \sum_{2\neq 1}^{\text{unocc}} \frac{\left\langle \psi_3^{(0)} \middle| \left(\hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \right) \middle| \psi_2^{(0)} \right\rangle}{\left(\epsilon_3^{(0)} - \epsilon_2^{(0)} \right)}$$

$$\times \frac{\left\langle \psi_2^{(0)} \middle| \left(\hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \right) \middle| \psi_1^{(0)} \right\rangle}{\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} \right)} \left| \psi_3^{(0)} \right\rangle$$

$$-\sum_{3\neq 1}^{\text{unocc}} \frac{\left\langle \psi_3^{(0)} \middle| \hat{v}_s^{(2)} + \hat{v}_{geo}^{(2)} \middle| \psi_1^{(0)} \right\rangle}{\left(\epsilon_3^{(0)} - \epsilon_1^{(0)} \right)} \left| \psi_3^{(0)} \right\rangle$$

$$-\frac{1}{2} \sum_{2\neq 1}^{\text{unocc}} \frac{\left| \left\langle \psi_2^{(0)} \middle| \left(\hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \right) \middle| \psi_1^{(0)} \right\rangle \right|^2}{\left(\epsilon_2^{(0)} - \epsilon_1^{(0)} \right)^2} \left| \psi_1^{(0)} \right\rangle.$$

$$\left|\psi_{1,d}^{(2)}\right\rangle = \left|\psi_{1,\parallel}^{(2)}\right\rangle + \sum_{3}^{occ} \mathcal{U}_{13}^{(1)*} \left|\psi_{3,\parallel}^{(1)}\right\rangle + \sum_{3}^{occ} \mathcal{U}_{13}^{(2)*} \left|\psi_{3}^{(0)}\right\rangle,$$

$$\varepsilon_{geo} = \frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\sum_{1}^{occ}\left\langle\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right|(1-P_v)\left|\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right\rangle,$$

$$(1-P_v) = P_c = \sum_{3}^{unocc} |\psi_3\rangle\langle\psi_3|$$

$$\begin{aligned}
&\langle\psi_2|\hat{v}_{geo}|\psi_1\rangle = \\
&-\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\sum_{3}^{occ}\left\langle\psi_2\left|\frac{\partial\psi_3}{\partial U_{\mathbf{q}\lambda}}\right.\right\rangle\left\langle\left.\frac{\partial\psi_3}{\partial U_{\mathbf{q}\lambda}}\right|\psi_1\right\rangle \\
&-\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\sum_{1}^{occ}\frac{\partial\ln|\chi|^2}{\partial U_{\mathbf{q}\lambda}^{*}}\langle\psi_2|(1-P_v)\left|\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right\rangle \\
&-\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\sum_{1}^{occ}\langle\psi_2|(1-P_v)\left|\frac{\partial^2\psi_1}{\partial U_{\mathbf{q}\lambda}^{*}\partial U_{\mathbf{q}\lambda}}\right\rangle \\
&+\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\left\langle\frac{\partial\psi_2}{\partial U_{\mathbf{q}\lambda}}\right|\left.\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right\rangle \\
&+\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\sum_{3}^{occ}\left\langle\psi_2\left|\frac{\partial\psi_3}{\partial U_{\mathbf{q}\lambda}^{*}}\right.\right\rangle\left\langle\psi_3\left|\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right.\right\rangle
\end{aligned}$$

$$\begin{aligned}
&\langle\psi_2|\hat{v}_{geo}|\psi_1\rangle^{(2)} = \\
&\left\langle\psi_2^{(0)}\right|\hat{v}_{geo}^{(2)}\left|\psi_1^{(0)}\right\rangle + \left\langle\psi_2^{(0)}\right|\hat{v}_{geo}^{(1)}\left|\psi_1^{(1)}\right\rangle + \left\langle\psi_2^{(1)}\right|\hat{v}_{geo}^{(1)}\left|\psi_1^{(0)}\right\rangle.
\end{aligned}$$

$$\left\langle\psi_2^{(0)} \mid \psi_1^{(i)}\right\rangle + \left\langle\psi_2^{(i)} \mid \psi_1^{(0)}\right\rangle = \begin{cases} -\sum_{j=1}^{i-1}\left\langle\psi_2^{(j)} \mid \psi_1^{(i-j)}\right\rangle & i>1 \\ 0 & i=1, \end{cases}$$

$$\left\langle\psi_2^{(0)} \mid \psi_1^{(i)}\right\rangle - \left\langle\psi_2^{(i)} \mid \psi_1^{(0)}\right\rangle = 0.$$

$$\langle\psi_1|\hat{v}_{\mathrm{geo}}|\psi_1\rangle$$

$$(i) = -\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\sum_{3}^{occ}\left\langle\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right|\psi_3\right\rangle\left\langle\psi_3\left|\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right.\right\rangle.$$

$$\left\langle\psi_3\left|\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right.\right\rangle = \left\langle\psi_3^{(0)}\left|\frac{\partial\psi_1^{(0)}}{\partial U_{\mathbf{q}\lambda}}\right.\right\rangle + \left\langle\psi_3^{(0)}\left|\frac{\partial\psi_1^{(1)}}{\partial U_{\mathbf{q}\lambda}}\right.\right\rangle + \mathcal{O}(U^2).$$

$$\left\langle\frac{\partial\psi_2}{\partial U_{\mathbf{q}\lambda}}\right|\psi_3\right\rangle\mathcal{O}(U^2)$$

$$\langle\psi_1|\hat{v}_{geo}|\psi_1\rangle^{(2)} = \frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\left\langle\frac{\partial\psi_1^{(1)}}{\partial U_{\mathbf{q}\lambda}}\middle|\frac{\partial\psi_1^{(1)}}{\partial U_{\mathbf{q}\lambda}}\right\rangle$$

$$= \sum_{\lambda}\sum_{2}^{unocc}\frac{g^*_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})\hbar\omega_{\mathbf{q}\lambda}}{\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}-\hbar\omega_{\mathbf{q}\lambda}\right)^2}.$$

$$2 \equiv n_2, \mathbf{k_2} = n_2, \mathbf{k_1} + \mathbf{q}$$

$$W_{11}^{(2)} \equiv \left\langle\psi_1^{(0)}\middle|\hat{v}_{geo}^{(2)}\middle|\psi_1^{(0)}\right\rangle$$

$$W_{11}^{(2)} = \langle\psi_1|\hat{v}_{geo}|\psi_1\rangle^{(2)} - \left\langle\psi_1^{(0)}\middle|\hat{v}_{geo}^{(1)}\middle|\psi_1^{(1)}\right\rangle - \left\langle\psi_1^{(1)}\middle|\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle$$

$$= \sum_{\lambda}\sum_{2}^{unocc}\frac{g^*_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})\hbar\omega_{\mathbf{q}\lambda}}{\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}-\hbar\omega_{\mathbf{q}\lambda}\right)^2}$$

$$-\sum_{\lambda\lambda'}\sum_{2}^{unocc}\frac{g^*_{n_2,n_1,\lambda'}(\mathbf{k_1},\mathbf{q})g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})\left(\hbar\omega_{\bar{\mathbf{q}}\lambda'}+\hbar\omega_{\mathbf{q}\lambda}\right)}{\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}-\hbar\omega_{\bar{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}-\hbar\omega_{\mathbf{q}\lambda}\right)}$$

$$\times\frac{U_{\bar{\mathbf{q}}\lambda'}}{L_{\bar{\mathbf{q}}\lambda'}}\frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}$$

$$\frac{g^*_{n_2,n_1,\lambda'}(\mathbf{k_1},\mathbf{q})g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q})}{\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}-\hbar\omega_{\bar{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}-\hbar\omega_{\mathbf{q}\lambda}\right)}\frac{U_{\bar{q}\lambda'}}{L_{\bar{\mathbf{q}}\lambda'}}\frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}$$

$$-\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\frac{\partial\ln|\chi|^2}{\partial U^*_{\mathbf{q}\lambda}}\left\langle\psi_2^{(0)}\middle|\frac{\partial\psi_1}{\partial U_{\mathbf{q}\lambda}}\right\rangle$$

$$= \frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\frac{U_{\mathbf{q}\lambda}}{L^2_{\mathbf{q}\lambda}}\frac{\partial\left\langle\psi_2^{(0)}\mid\psi_1^{(2)}\right\rangle}{\partial U_{\mathbf{q}\lambda}}$$

$$= \sum_{\mathbf{q}\lambda}\hbar\omega_{\mathbf{q}\lambda}U_{\mathbf{q}\lambda}\frac{\partial\left\langle\psi_2^{(0)}\mid\psi_1^{(2)}\right\rangle}{\partial U_{\mathbf{q}\lambda}}.$$

$$-\frac{\hbar^2}{2M}\sum_{\mathbf{q}\lambda}\sum_{n_2}^{unocc}\delta_{\mathbf{k}_2,\mathbf{k}_1}\frac{\partial^2\left\langle\psi_2^{(0)}\mid\psi_1^{(2)}\right\rangle}{\partial U^*_{\mathbf{q}\lambda}\partial U_{\mathbf{q}\lambda}}.$$

$$\langle\psi_2|\hat{v}_{\mathrm{geo}}|\psi_1\rangle^{(2)}$$

$$\left\langle\psi_2^{(0)}\middle|\hat{v}_{geo}^{(1)}\middle|\psi_1^{(1)}\right\rangle = \left\langle\psi_2^{(1)}\middle|\hat{v}_{\mathrm{geo}}^{(1)}\middle|\psi_1^{(0)}\right\rangle = 0$$

$$\left\langle\psi_{n_2\mathbf{k}_2}^{(0)}\mid\psi_{n_1\mathbf{k}_1}^{(2)}\right\rangle$$

$$P_c\left(h_s^{(0)}-\epsilon_{n\mathbf{k}}^{(0)}\right)P_c\left|\psi_{n\mathbf{k}}^{(2)}\right\rangle =$$

$$-P_c\left(\hat{v}_s^{(2)}+\hat{v}_{geo}^{(2)}\right)\left|\psi_{n\mathbf{k}}^{(0)}\right\rangle - P_c\left(\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\right)\left|\psi_{n\mathbf{k}}^{(1)}\right\rangle.$$

$$\left\langle \psi_{n_2\mathbf{k}_2}^{(0)} \mid \psi_{n_1\mathbf{k}_1}^{(2)} \right\rangle = \frac{V_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)} + W_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)}}{\epsilon_{n_1\mathbf{k}_1}^{(0)} - \epsilon_{n_2\mathbf{k}_2}^{(0)}}$$

$$V_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)} W_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)}$$

$$\frac{\partial V_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)}}{\partial U_{\mathbf{q}\lambda}} = \sum_{\lambda'} \left[g_{n_2,n_1,\lambda,\lambda'}^{(2)}(\mathbf{k_2}, \mathbf{q}, \mathbf{q}') \frac{U_{\mathbf{q}'\lambda'}}{L_{\mathbf{q}'\lambda'}} \frac{1}{L_{\mathbf{q}\lambda}} + g_{n_2,n_1,\lambda',\lambda}^{(2)}(\mathbf{k_1}, \mathbf{q}', \mathbf{q}) \frac{U_{\mathbf{q}'\lambda'}}{L_{\mathbf{q}'\lambda'}} \frac{1}{L_{\mathbf{q}\lambda}} \right]$$

$$U_{\overline{\mathbf{q}}\lambda} = U_{\mathbf{q}\lambda}^{*} = U_{-\mathbf{q}\lambda}$$

$$\frac{\partial^2 V_{n_2\mathbf{k}_2,n_1\mathbf{k}_1}^{(2)}}{\partial U_{\overline{\mathbf{q}}\lambda} \partial U_{\mathbf{q}\lambda}} = \delta_{\mathbf{k}_1,\mathbf{k}_2} \frac{1}{L_{-\mathbf{q}\lambda}} \frac{1}{L_{\mathbf{q}\lambda}} \times \left(g_{n_2,n_1,\lambda,\lambda}^{(2)}(\mathbf{k_1}, \mathbf{q}, \overline{\mathbf{q}}) + g_{n_2,n_1,\lambda,\lambda}^{(2)}(\mathbf{k_1}, \overline{\mathbf{q}}, \mathbf{q}) \right)$$

$$\epsilon_{\parallel,2,1}^{(1)} = \left\langle \psi_2^{(0)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_1^{(0)} \right\rangle$$

$$\begin{aligned} \epsilon_{\parallel,2,1}^{(2)} = & \left\langle \psi_2^{(0)} \middle| \hat{v}_s^{(2)} + \hat{v}_{geo}^{(2)} \middle| \psi_1^{(0)} \right\rangle \\ & + \left\langle \psi_2^{(1)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_1^{(0)} \right\rangle + \left\langle \psi_2^{(0)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_1^{(1)} \right\rangle \\ & + \left\langle \psi_2^{(1)} \middle| \hat{\mathcal{H}}_s^{(0)} \middle| \psi_1^{(1)} \right\rangle - \frac{1}{2} \left\langle \psi_2^{(1)} \mid \psi_1^{(1)} \right\rangle \left(\epsilon_2^{(0)} + \epsilon_1^{(0)} \right) \end{aligned}$$

$$\epsilon_{d,1}^{(2)} = \epsilon_{\parallel,1,1}^{(2)} - \sum_{3}^{occ} \frac{\left| \epsilon_{\parallel,3,1}^{(1)} \right|^2}{\epsilon_3^{(0)} - \epsilon_1^{(0)}}$$

$$\begin{aligned} \epsilon_{d,1}^{(2)} = & \sum_{2 \neq 1}^{occ} \frac{\left| \left\langle \psi_2^{(0)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_1^{(0)} \right\rangle \right|^2}{\epsilon_1^{(0)} - \epsilon_2^{(0)}} \\ & + \left\langle \psi_1^{(0)} \middle| \hat{v}_s^{(2)} + \hat{v}_{geo}^{(2)} \middle| \psi_1^{(0)} \right\rangle \\ & + \left\langle \psi_1^{(1)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_1^{(0)} \right\rangle \\ & + \left\langle \psi_1^{(0)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_1^{(1)} \right\rangle \\ & + \left\langle \psi_1^{(1)} \middle| \hat{\mathcal{H}}_s^{(0)} \middle| \psi_1^{(1)} \right\rangle \\ & - \frac{1}{2} \left\langle \psi_1^{(1)} \mid \psi_1^{(1)} \right\rangle \left(\epsilon_1^{(0)} + \epsilon_1^{(0)} \right) \end{aligned}$$

$$(c) + (d) + (e) + (f) = \sum_{2 \neq 1}^{unocc} \frac{\left| \left\langle \psi_1^{(0)} \middle| \hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)} \middle| \psi_2^{(0)} \right\rangle \right|^2}{\epsilon_1^{(0)} - \epsilon_2^{(0)}}$$

$$\epsilon_{d,1}^{(2)} = \sum_{2\neq 1}\sum_{\lambda\lambda'} \frac{g^*_{n_2,n_1,\lambda'}(\mathbf{k_1},\mathbf{q}) g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q}) \left(\epsilon_1^{(0)} - \epsilon_2^{(0)}\right)}{\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\overline{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}\right)} \frac{U_{\overline{\mathbf{q}}\lambda'}}{L_{\overline{\mathbf{q}}\lambda'}} \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}$$

$$+ \sum_{\mathbf{q}\lambda} g^{(2)}_{n_1,n_1,\lambda,\lambda}(\mathbf{k}_1,\mathbf{q},\overline{\mathbf{q}}) \frac{\left|U_{\mathbf{q}\lambda}\right|^2}{L^2_{\mathbf{q}\lambda}}$$

$$+ \sum_{2\neq 1}\sum_{\lambda\lambda'} \frac{g^*_{n_2,n_1,\lambda'}(\mathbf{k_1},\mathbf{q}) g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q}) \hbar\omega_{\mathbf{q}\lambda}}{\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\overline{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}\right)} \times \left(\delta_{\lambda\lambda'} - \frac{U_{\overline{\mathbf{q}}\lambda'}}{L_{\overline{\mathbf{q}}\lambda'}} \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}\right)$$

$$- \sum_{2\neq 1}\sum_{\lambda\lambda'} \frac{g^*_{n_2,n_1,\lambda'}(\mathbf{k_1},\mathbf{q}) g_{n_2,n_1,\lambda}(\mathbf{k_1},\mathbf{q}) \hbar\omega_{\mathbf{q}\lambda}}{\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\overline{\mathbf{q}}\lambda'}\right)\left(\epsilon_1^{(0)} - \epsilon_2^{(0)} - \hbar\omega_{\mathbf{q}\lambda}\right)} \frac{U_{\overline{\mathbf{q}}\lambda'}}{L_{\overline{\mathbf{q}}\lambda'}} \frac{U_{\mathbf{q}\lambda}}{L_{\mathbf{q}\lambda}}$$

$$\mathcal{U}_{13}^{(1)*} = \begin{cases} 0 & 1 = 3 \\ -\dfrac{\epsilon^{(1)}_{\|\|\|,31}}{\epsilon_3^{(0)} - \epsilon_1^{(0)}} & 1 \neq 3 \end{cases}$$

$$\mathcal{U}_{13}^{(2)*} = \begin{cases} -\dfrac{1}{2}\displaystyle\sum_{2\neq 3}^{occ} \left|\mathcal{U}_{23}^{(1)}\right|^2 & 1 = 3 \\ -\dfrac{1}{\epsilon_3^{(0)} - \epsilon_1^{(0)}}\left[\left(\displaystyle\sum_{2}^{occ} \mathcal{U}_{12}^{(1)*}\epsilon^{(1)}_{\|,32}\right) + \epsilon^{(2)}_{\|,31} - \epsilon^{(1)}_{d,1}\mathcal{U}_{13}^{(1)*}\right] & 1 \neq 3 \end{cases}$$

$$\sum_{3}^{occ} \mathcal{U}_{13}^{(1)*}\left|\psi_{3,\|}^{(1)}\right\rangle = \sum_{3\neq 1}^{occ}\left[-\frac{\epsilon^{(1)}_{\|,31}}{\epsilon_3^{(0)} - \epsilon_1^{(0)}}\right]\left|\psi_{3,\|}^{(1)}\right\rangle$$

$$= -\sum_{3\neq 1}^{occ}\sum_{2}^{unocc} \frac{\left\langle\psi_2^{(0)}\middle|\hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)}\middle|\psi_3^{(0)}\right\rangle}{\left(\epsilon_3^{(0)} - \epsilon_1^{(0)}\right)} \times \frac{\left\langle\psi_3^{(0)}\middle|\hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle}{\left(\epsilon_3^{(0)} - \epsilon_2^{(0)}\right)}\left|\psi_2^{(0)}\right\rangle$$

$$\mathcal{U}_{11}^{(2)*}\left|\psi_1^{(0)}\right\rangle = \left[-\frac{1}{2}\sum_{4\neq 1}^{occ}\left|\mathcal{U}_{41}^{(1)}\right|^2\right]\left|\psi_1^{(0)}\right\rangle$$

$$= -\frac{1}{2}\sum_{4\neq 1}^{occ}\left|\frac{\left\langle\psi_1^{(0)}\middle|\hat{v}_s^{(1)} + \hat{v}_{geo}^{(1)}\middle|\psi_4^{(0)}\right\rangle}{\epsilon_4^{(0)} - \epsilon_1^{(0)}}\right|^2\left|\psi_1^{(0)}\right\rangle.$$

$$\sum_{3\neq 1}^{occ}\mathcal{U}_{13}^{(2)*}\left|\psi_3^{(0)}\right\rangle =$$

$$\sum_{3\neq 1}^{occ} -\frac{\left(\sum_4^{occ}\mathcal{U}_{14}^{(1)*}\epsilon^{(1)}_{\|,34}\right) + \epsilon^{(2)}_{\|,31} - \epsilon^{(1)}_{d,1}\mathcal{U}_{13}^{(1)*}}{\epsilon_3^{(0)} - \epsilon_1^{(0)}}\left|\psi_3^{(0)}\right\rangle$$

$$\sum_{4}^{occ} \mathcal{U}_{14}^{(1)*}\epsilon_{\parallel,34}^{(1)} =$$

$$\sum_{4}^{occ} \frac{\left\langle\psi_4^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle\left\langle\psi_3^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_4^{(0)}\right\rangle}{\left(\epsilon_4^{(0)}-\epsilon_1^{(0)}\right)} - \frac{1}{2}\sum_{3\neq 1}^{occ}\sum_{2}^{unocc}\frac{\left(V_{21}^{(1)}+W_{21}^{(1)}\right)\left(V_{32}^{(1)}+V_{32}^{(1)}\right)}{\left(\epsilon_2^{(0)}-\epsilon_1^{(0)}\right)\left(\epsilon_3^{(0)}-\epsilon_2^{(0)}\right)}\left|\psi_3^{(0)}\right\rangle$$

$$\begin{aligned}
\epsilon_{\parallel,3,1}^{(2)} &= \left\langle\psi_3^{(0)}\middle|\hat{v}_s^{(2)}+\hat{v}_{geo}^{(2)}\middle|\psi_1^{(0)}\right\rangle \\
&+\frac{1}{2}\sum_{2}^{unocc}\left\langle\psi_3^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_2^{(0)}\right\rangle\left\langle\psi_2^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle \\
&\times\left(\frac{1}{\left(\epsilon_3^{(0)}-\epsilon_2^{(0)}\right)}+\frac{1}{\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}\right)}\right) \\
&-\sum_{3\neq 1}^{occ}\sum_{2}^{unocc}\frac{\left(V_{31}^{(1)}+W_{31}^{(1)}\right)\left(V_{32}^{(1)}+W_{32}^{(1)}\right)}{\left(\epsilon_3^{(0)}-\epsilon_1^{(0)}\right)\left(\epsilon_3^{(0)}-\epsilon_2^{(0)}\right)}\left|\psi_2^{(0)}\right\rangle \\
&+\sum_{3\neq 1}^{occ}\sum_{2\neq 1}^{occ}\frac{\left(V_{21}^{(1)}+W_{21}^{(1)}\right)\left(V_{32}^{(1)}+W_{32}^{(1)}\right)}{\left(\epsilon_2^{(0)}-\epsilon_1^{(0)}\right)\left(\epsilon_3^{(0)}-\epsilon_1^{(0)}\right)}\left|\psi_3^{(0)}\right\rangle \\
&-\frac{1}{2}\sum_{3\neq 1}^{occ}\sum_{2}^{unocc}\frac{\left(V_{21}^{(1)}+W_{21}^{(1)}\right)\left(V_{32}^{(1)}+W_{32}^{(1)}\right)}{\epsilon_3^{(0)}-\epsilon_1^{(0)}} \\
&\times\left(\frac{1}{\left(\epsilon_3^{(0)}-\epsilon_2^{(0)}\right)}+\frac{1}{\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}\right)}\right)\left|\psi_3^{(0)}\right\rangle
\end{aligned}$$

$$\begin{aligned}
&\sum_{3\neq 1}^{occ}\mathcal{U}_{13}^{(2)*}\left|\psi_3^{(0)}\right\rangle \\
&= \sum_{3\neq 1}^{occ}\sum_{2}^{occ}\frac{\left\langle\psi_3^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_2^{(0)}\right\rangle\left\langle\psi_2^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle}{\left(\epsilon_3^{(0)}-\epsilon_1^{(0)}\right)\left(\epsilon_2^{(0)}-\epsilon_1^{(0)}\right)}\Bigg|\psi_3^{(0)}\left(V_{21}^{(1)}\right. \\
&\left.+W_{21}^{(1)}\right)\left\langle\psi_2^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle - \sum_{3\neq 1}^{occ}\frac{\left\langle\psi_3^{(0)}\middle|\hat{v}_s^{(2)}+\hat{v}_{geo}^{(2)}\middle|\psi_1^{(0)}\right\rangle}{\epsilon_3^{(0)}-\epsilon_1^{(0)}}\left|\psi_3^{(0)}\right\rangle \\
&-\frac{1}{2}\sum_{3\neq 1}^{occ}\sum_{2}^{unocc}\frac{\left\langle\psi_3^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_2^{(0)}\right\rangle\left\langle\psi_2^{(0)}\middle|\hat{v}_s^{(1)}+\hat{v}_{geo}^{(1)}\middle|\psi_1^{(0)}\right\rangle}{\epsilon_3^{(0)}-\epsilon_1^{(0)}} \\
&\times\left(\frac{1}{\left(\epsilon_3^{(0)}-\epsilon_2^{(0)}\right)}+\frac{1}{\left(\epsilon_1^{(0)}-\epsilon_2^{(0)}\right)}\right)\left|\psi_3^{(0)}\right\rangle
\end{aligned}$$

$$V_X(r) = -\frac{\alpha_X}{r}e^{-(r/d_X)^2}, X = 5, j$$

$$\left(\begin{pmatrix}2m_B & 0\\ 0 & 2m_{B^*}\end{pmatrix} - \frac{\nabla^2}{2\mu_{bb}} + H_{\text{int},S=0}\right)\vec{\varphi}_{L=1,S=0}(r) = E\vec{\varphi}_{L=1,S=0}(r)$$

$$\nabla^2 = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{L(L+1)}{r^2}\Big|_{L=1} = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{2}{r^2}$$

$$H_{\text{int},S=0} = \frac{1}{4}\begin{pmatrix} V_5(r) + 3V_j(r) & \sqrt{3}\big(V_5(r) - V_j(r)\big) \\ \sqrt{3}\big(V_5(r) - V_j(r)\big) & 3V_5(r) + V_j(r) \end{pmatrix}$$

$$\vec{\varphi}_{L=1,S=0} \equiv \left(BB, \frac{1}{\sqrt{3}}\vec{B}^*\vec{B}^*\right)^T = \left(BB, \frac{1}{\sqrt{3}}\left(B_x^*B_x^* + B_y^*B_y^* + B_z^*B_z^*\right)\right)^T .$$

$$H_0 = M_B \otimes \mathbb{1}_{4\times 4} + \mathbb{1}_{4\times 4} \otimes M_D + \frac{\vec{p}^2}{2\mu_{bc}}$$

$$M_B = \text{diag}(m_B, m_{B^*}, m_{B^*}, m_{B^*})$$

$$M_D = \text{diag}(m_D, m_{D^*}, m_{D^*}, m_{D^*})$$

$$\mu_{bc} = m_b m_c/(m_b + m_c)$$

$$\vec{\Psi} \equiv \big(BD, BD_x^*, BD_y^*, BD_z^*, B_x^*D, B_x^*D_x^*, B_x^*D_y^*, B_x^*D_z^*, B_y^*D, B_y^*D_x^*, B_y^*D_y^*, B_y^*D_z^* \\ B_z^*D, B_z^*D_x^*, B_z^*D_y^*, B_z^*D_z^*\big)^T$$

$$H_{\text{int}} = TV_{\text{diag}}T^{-1}, V_{\text{diag}} = \text{diag}(\underbrace{V_5(r), \dots, V_5(r)}_{4\times}, \underbrace{V_j(r), \dots, V_j(r)}_{12\times}).$$

$$H\vec{\Psi}(\vec{r}) = (H_0 + H_{\text{int}})\vec{\Psi}(\vec{r}) = E\vec{\Psi}(\vec{r})$$

$$\left(\begin{pmatrix} m_B + m_D & 0 \\ 0 & m_{B^*} + m_{D^*} \end{pmatrix} - \frac{1}{2\mu_{bc}}\frac{d^2}{dr^2} + H_{\text{int},S=0}\right)\vec{\varphi}_{L=0,S=0}(r) = E\vec{\varphi}_{L=0,S=0}(r)$$

$$\vec{\varphi}_{L=0,S=0} \equiv \left(BD, \frac{1}{\sqrt{3}}\vec{B}^*\vec{D}^*\right)^T = \left(BD, \frac{1}{\sqrt{3}}\left(B_x^*D_x^* + B_y^*D_y^* + B_z^*D_z^*\right)\right)^T$$

$$\left(\begin{pmatrix} m_{B^*} + m_D & 0 & 0 \\ 0 & m_B + m_{D^*} & 0 \\ 0 & 0 & m_{B^*} + m_{D^*} \end{pmatrix} - \frac{1}{2\mu_{bc}}\frac{d^2}{dr^2} + H_{\text{int},S=1}\right)\vec{\varphi}_{L=0,S=1,S_z}(r) = E\vec{\varphi}_{L=0,S=1,S_z}(r)$$

$$H_{\text{int},S=1} = \frac{1}{4}\begin{pmatrix} V_5(r) + 3V_j(r) & V_j(r) - V_5(r) & \sqrt{2}\big(V_5(r) - V_j(r)\big) \\ V_j(r) - V_5(r) & V_5(r) + 3V_j(r) & \sqrt{2}\big(V_j(r) - V_5(r)\big) \\ \sqrt{2}\big(V_5(r) - V_j(r)\big) & \sqrt{2}\big(V_j(r) - V_5(r)\big) & 2\big(V_5(r) + V_j(r)\big) \end{pmatrix}.$$

$$\vec{\varphi}_{L=0,S=1,S_z} \equiv \left(B_{S_z}^*D, BD_{S_z}^*, T_{1,S_z}\left(\vec{B}^*, \vec{D}^*\right)\right)^T$$

$$\vec{\varphi}_{L=1,S=0}(r) = \begin{pmatrix} A_{BB}j_1(k_{BB}r) + \chi_{BB}(r)/r \\ A_{B^*B^*}j_1(k_{B^*B^*}r) + \chi_{B^*B^*}(r)/r \end{pmatrix},$$

$$k_{BB} = \sqrt{2\mu(E - 2m_B)}$$

$$k_{B^*B^*} = \sqrt{2\mu(E - 2m_{B^*})}$$

$$\chi_{BB}(r)/r \text{ and } \chi_{B^*B^*}(r)/r$$

$$\vec{\varphi}_{L=1,S=0}(r)$$

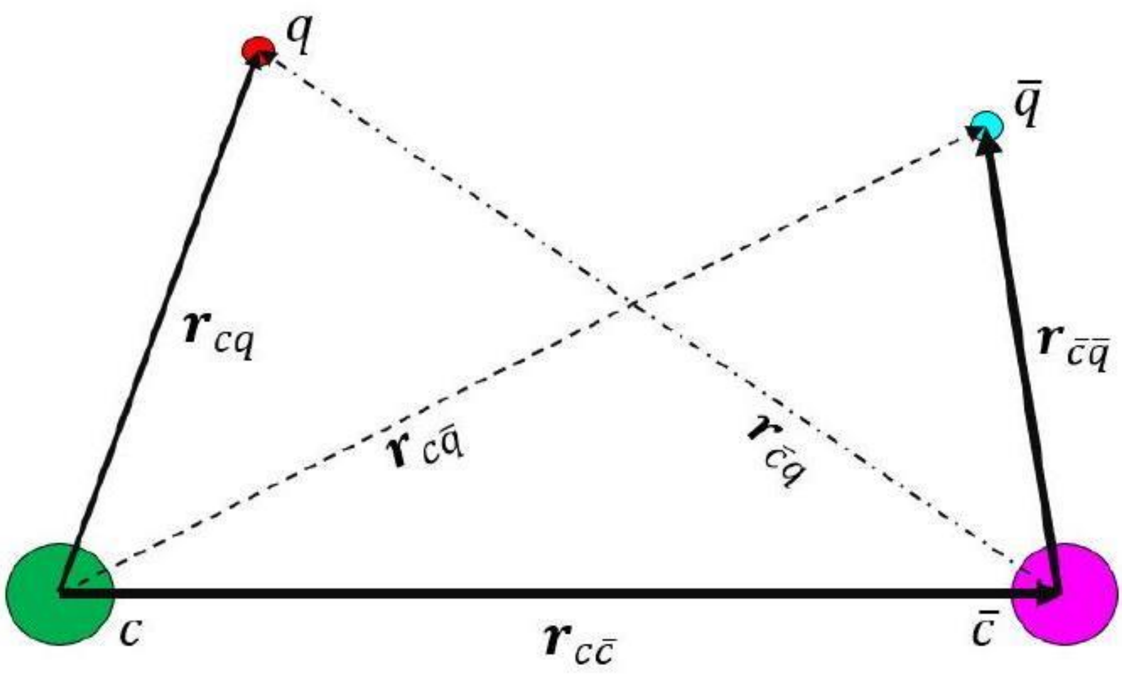
$$\left(\begin{pmatrix} 2m_B & 0 \\ 0 & 2m_{B^*} \end{pmatrix} - \frac{1}{2\mu_{bb}}\left(\frac{d^2}{dr^2} - \frac{2}{r^2}\right) + H_{\text{int},S=0} - E\right)\begin{pmatrix} \chi_{BB}(r) \\ \chi_{B^*B^*}(r) \end{pmatrix} = -H_{\text{int},S=0}\begin{pmatrix} A_{BB} r j_1(k_{BB} r r) \\ A_{B^*B^*} r j_1(k_{B^*B^*} r) \end{pmatrix}$$

$$\chi_\alpha(r) \propto r^{L+1}|_{L=1} = r^2$$

$$\chi_\alpha(r) \propto \text{irt}_{BB;\alpha} h_1^{(1)}(k_\alpha r) \text{ for } r \to \infty \text{ and } (A_{BB}, A_{B^*B^*}) = (1{,}0)$$
$$\chi_\alpha(r) \propto \text{irt}_{B^*B^*;\alpha} h_1^{(1)}(k_\alpha r) \text{ for } r \to \infty \text{ and } (A_{BB}, A_{B^*B^*}) = (0{,}1),$$

$$\mathrm{T} = \begin{pmatrix} t_{BB;BB} & t_{BB;B^*B^*} \\ t_{B^*B^*;BB} & t_{B^*B^*;B^*B^*} \end{pmatrix}$$

$$m_{D^*} - m_D = \frac{m_b}{m_c}(m_{B^*} - m_B),$$



$$\boldsymbol{r}_{c\bar{q}} = \boldsymbol{r}_{\bar{c}\bar{q}} + \boldsymbol{r}_{c\bar{c}} \text{ and } \boldsymbol{r}_{\bar{c}q} = \boldsymbol{r}_{cq} - \boldsymbol{r}_{c\bar{c}}$$
$$\Psi_T(\boldsymbol{r}_{cq}, \boldsymbol{r}_{\bar{c}\bar{q}}, \boldsymbol{r}_{c\bar{c}}) = \Psi_{c\bar{c}}(\boldsymbol{r}_{c\bar{c}})\Psi_{q\bar{q}}(\boldsymbol{r}_{cq}, \boldsymbol{r}_{\bar{c}\bar{q}}, \boldsymbol{r}_{c\bar{c}})$$

$$H_{q\bar{q}}\Psi_{q\bar{q}}(\boldsymbol{r}_{cq}, \boldsymbol{r}_{\bar{c}\bar{q}}, \boldsymbol{r}_{c\bar{c}}) = \Delta E(r_{c\bar{c}})\Psi_{q\bar{q}}(\boldsymbol{r}_{cq}, \boldsymbol{r}_{\bar{c}\bar{q}}, \boldsymbol{r}_{c\bar{c}})$$

$$\left(H_{c\bar{c}} + \Delta E(r_{c\bar{c}})\right)\Psi_{c\bar{c}}(\boldsymbol{r}_{c\bar{c}}) = E\Psi_{c\bar{c}}(\boldsymbol{r}_{c\bar{c}})$$

$$m_q = 308\text{MeV}, m_c = 1317\text{MeV}, \alpha_s(2M_c) = 0.331, k = 0.176\text{GeV}^2$$

$$V(r_{c\bar{c}}) = -\frac{4}{3}\alpha_s \frac{1}{r_{c\bar{c}}} + k r_{c\bar{c}}$$

$$T = |(c\bar{c})_{\mathbf{8}}(q\bar{q})_{\mathbf{8}}\rangle_{\mathbf{1}}$$

$$T_D = \sqrt{\frac{2}{3}}\left|(cq)_{\bar{\mathbf{3}}}(\bar{c}\bar{q})_{\mathbf{3}}\right\rangle - \sqrt{\frac{1}{3}}\left|(cq)_{\mathbf{6}}(\bar{c}\bar{q})_{\bar{\mathbf{6}}}\right\rangle$$

$$T_M = \sqrt{\frac{8}{9}}\left|(c\bar{q})_{\mathbf{1}}(\bar{c}q)_{\mathbf{1}}\right\rangle - \sqrt{\frac{1}{9}}\left|(c\bar{q})_{\mathbf{8}}(\bar{c}q)_{\mathbf{8}}\right\rangle$$

$$\left(T^a_{im}\delta_{jn} + \delta_{im}T^a_{jn}\right)\left(T^a_{mI}\delta_{nJ} + \delta_{mI}T^a_{nJ}\right) = (T^aT^a)_{iI}\delta_{jJ} + \delta_{iI}(T^aT^a)_{jJ} + 2T^a_{iI}T^a_{jJ}$$
$$= C(R_1)\delta_{iI}\delta_{jJ} + C(R_2)\delta_{iI}\delta_{jJ} + 2T^a_{iI}T^a_{jJ}$$

$$\bigoplus_k C(S_k)I_{D(S_k)}$$

$$R_1 \otimes R_2 = S_1 \oplus S_2 \oplus S_3 \dots$$

$$T^a_{iI}T^a_{jJ} = \lambda(S)\delta_{iI}\delta_{jJ}$$

$$\lambda(S) = \frac{1}{2}\left(C(S) - C(R_1) - C(R_2)\right)$$

$$\lambda_{cq} = \lambda_{\bar{c}\bar{q}} = \frac{2}{3}\left(\frac{1}{2}\left(\frac{4}{3} - \frac{8}{3}\right)\right) + \frac{1}{3}\left(\frac{1}{2}\left(\frac{10}{3} - \frac{8}{3}\right)\right) = -\frac{1}{3}$$

$$\lambda_{c\bar{c}} = \lambda_{q\bar{q}} = +\frac{1}{6}$$

$$\lambda_{c\bar{q}} = \lambda_{\bar{c}q} = -\frac{7}{6}$$

$$V_D(\boldsymbol{\zeta}) = -\frac{1}{3}\alpha_s\frac{1}{\zeta} + k\zeta$$

$$V_M(\boldsymbol{\zeta}) = -\frac{7}{6}\alpha_s\frac{1}{\zeta} + k\zeta$$

$$\psi_{\mathcal{C}}(\boldsymbol{\zeta}) = \sqrt{\frac{\mathcal{C}^3}{\pi}}e^{-\mathcal{C}\zeta} \text{ where } \mathcal{C} = D, M$$

$$E_{\mathcal{C}} = \langle\psi_{\mathcal{C}}(\boldsymbol{\zeta})| - \frac{\nabla^2}{2m_{cq}} + V_{\mathcal{C}}(\boldsymbol{\zeta})|\psi_{\mathcal{C}}(\boldsymbol{\zeta})\rangle = \frac{\mathcal{C}^2}{2m_{cq}} + \lambda_{\mathcal{C}}\alpha_s\mathcal{C} + \frac{3k}{2\mathcal{C}}\ \mathcal{C} = D, M$$

$$D = 0.413\text{GeV}\ \langle E_D\rangle_{\min} = 0.935\text{GeV}$$

$$M = 0.439\text{GeV}\ \langle E_M\rangle_{\min} = 0.818\text{GeV}.$$

$$\Psi_{q\bar{q}}\left(\boldsymbol{r}_{cq}, \boldsymbol{r}_{\bar{c}\bar{q}}, \boldsymbol{r}_{c\bar{c}}\right) = a_1(r_{c\bar{c}})\psi_D\left(\boldsymbol{r}_{cq}\right)\psi_D\left(\boldsymbol{r}_{\bar{c}\bar{q}}\right) + a_2(r_{c\bar{c}})\psi_M\left(\boldsymbol{r}_{c\bar{q}}\right)\psi_M\left(\boldsymbol{r}_{\bar{c}q}\right);$$

$$\Psi_{q\bar{q}}\left(\boldsymbol{r}_{cq}, \boldsymbol{r}_{\bar{c}\bar{q}}, \boldsymbol{r}_{c\bar{c}}\right) = \psi_D\left(\boldsymbol{r}_{cq}\right)\psi_D\left(\boldsymbol{r}_{\bar{c}\bar{q}}\right)\ \mathbf{3}, \bar{\mathbf{3}} + \mathbf{6}, \bar{\mathbf{6}}$$
$$\Psi_{q\bar{q}}\left(\boldsymbol{r}_{cq}, \boldsymbol{r}_{\bar{c}\bar{q}}, \boldsymbol{r}_{c\bar{c}}\right) = \psi_M\left(\boldsymbol{r}_{c\bar{q}}\right)\psi_M\left(\boldsymbol{r}_{\bar{c}q}\right)\ \mathbf{1}, \mathbf{1} + \mathbf{8}, \mathbf{8}$$
$$\boldsymbol{r}_{c\bar{q}} = \boldsymbol{r}_{\bar{c}\bar{q}} + \boldsymbol{r}_{c\bar{c}}, \boldsymbol{r}_{\bar{c}q} = \boldsymbol{r}_{cq} - \boldsymbol{r}_{c\bar{c}}$$

$$H_{q\bar{q}} = -\frac{\nabla^2_{r_{cq}}}{2m_{cq}} - \frac{\nabla^2_{r_{\bar{q}\bar{q}}}}{2m_{cq}} + V^{\mathrm{coul}} + V^{\mathrm{conf}} + V^{\mathrm{spin}}$$

$$\frac{d}{da_i}\langle \Psi_{q\bar{q}} | H_{q\bar{q}} | \Psi_{q\bar{q}} \rangle = 0$$

$$\begin{pmatrix} H_D - \Delta E(r_{c\bar{c}}) & H_{DM} - S^2_{DM}(r_{c\bar{c}})\Delta E(r_{c\bar{c}}) \\ H_{DM} - S^2_{DM}(r_{c\bar{c}})\Delta E(r_{c\bar{c}}) & H_M - \Delta E(r_{c\bar{c}}) \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = 0$$

$$S_{DM}(r_{c\bar{c}}) = \int_{\boldsymbol{r}_{cq}} \psi_D(\boldsymbol{r}_{cq})\psi_M(\boldsymbol{r}_{cq} - \boldsymbol{r}_{c\bar{c}}) = \int_{\boldsymbol{r}_{\bar{c}\bar{q}}} \psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}\bar{q}} - \boldsymbol{r}_{c\bar{c}})$$

$$\Psi_{q\bar{q}} = \sum_{i=1}^{N} a_i \Phi_i$$

$$\sum_i |a_i|^2 = 1$$

$$\sum_{j=1}^{N} \left(\langle \Phi_i | H_{q\bar{q}} | \Phi_j \rangle - \Delta E(r_{c\bar{c}})\langle \Phi_i \mid \Phi_j \rangle\right) a_j = 0$$

$$\langle \Phi_i \mid \Phi_j \rangle = \delta_{ij}$$

$$\begin{aligned} H_D &= \langle \psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) | H_{q\bar{q}} | \psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) \rangle \\ H_M &= \langle \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q}) | H_{q\bar{q}} | \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q}) \rangle \\ H_{DM} &= \langle \psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) | H_{q\bar{q}} | \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q}) \rangle \end{aligned}$$

$$\begin{aligned} \Delta E_{\pm}(r_{c\bar{c}}) = &\frac{1}{2(1 - S^4_{DM})}\Big(H_D + H_M - 2S^2_{DM}H_{DM} \\ &\pm \sqrt{(H_D + H_M - 2S^2_{DM}H_{DM})^2 - 4(1 - S^4_{DM})(H_D H_M - H^2_{DM})}\Big) \end{aligned}$$

$$I_0^{DM}(R) = \int_{\boldsymbol{r}_{cq}} \psi_D(\boldsymbol{r}_{cq})\left(-\nabla^2_{\boldsymbol{r}_{cq}}\right)\psi_M(\boldsymbol{r}_{cq} - \boldsymbol{r}_{c\bar{c}}) = \int_{\boldsymbol{r}_{\bar{c}\bar{q}}} \psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\left(-\nabla^2_{\boldsymbol{r}_{\bar{c}\bar{q}}}\right)\psi_M(\boldsymbol{r}_{\bar{c}\bar{q}} + \boldsymbol{r}_{c\bar{c}})$$

$$\begin{aligned} I_0^D &= \lim_{M \to D} \lim_{r_{c\bar{c}} \to 0} I_0^{DM}(r_{c\bar{c}}) = D^2 \\ I_0^M &= \lim_{D \to M} \lim_{r_{c\bar{c}} \to 0} I_0^{DM}(r_{c\bar{c}}) = M^2 \end{aligned}$$

$$V^{\mathrm{coul}} = -\frac{1}{3}\alpha_s \frac{1}{r_{cq}} - \frac{1}{3}\alpha_s \frac{1}{r_{\bar{c}\bar{q}}} - \frac{7}{6}\frac{1}{r_{c\bar{q}}} - \frac{7}{6}\alpha_s \frac{1}{r_{\bar{c}q}} + \frac{1}{6}\alpha_s \frac{1}{|\boldsymbol{r}_{cq} - \boldsymbol{r}_{\bar{c}\bar{q}} - \boldsymbol{r}_{c\bar{c}}|}$$

$$\begin{aligned} &\langle \psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) | K + V^{\mathrm{coul}} | \psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) \rangle \\ &= \frac{1}{m_{cq}} I_0^D + \alpha_s \left(-2\frac{1}{3} I_1^D(0) - 2\frac{7}{6} I_1^D(r_{c\bar{c}}) + \frac{1}{6} I_4^D(r_{c\bar{c}})\right) \end{aligned}$$

$$\langle\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})|K+V^{\text{coul}}|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$
$$=\frac{1}{m_{cq}}I_0^M+\alpha_s\left(-2\frac{7}{6}I_1^M(0)-2\frac{1}{3}I_2^M(r_{c\bar{c}})+\frac{1}{6}I_4^M(r_{c\bar{c}})\right)$$
$$\langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|K+V^{\text{coul}}|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle=$$
$$=S_{DM}(r_{c\bar{c}})\left(\frac{1}{m_{cq}}I_0^{DM}(r_{c\bar{c}})-2\frac{1}{3}\alpha_sI_2^{DM}(r_{c\bar{c}})-2\frac{7}{6}\alpha_sI_2^{MD}(r_{c\bar{c}})\right)+\frac{1}{6}\alpha_sI_6^{DM}(r_{c\bar{c}})$$

$$\langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|V^{\text{conf}}|\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\rangle$$

$$J_2^D=\int_{r_{cq}}\psi_D^2(\boldsymbol{r}_{cq})r_{cq}=\int_{r_{\bar{c}\bar{q}}}\psi_D^2(\boldsymbol{r}_{\bar{c}\bar{q}})r_{\bar{c}\bar{q}}$$

$$\langle\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})|V^{\text{conf}}|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$

$$J_2^M=\int_{r_{cq}}\psi_M^2(\boldsymbol{r}_{cq}-\boldsymbol{r}_{c\bar{c}})|\boldsymbol{r}_{cq}-\boldsymbol{r}_{c\bar{c}}|=\int_{r_{\bar{c}\bar{q}}}\psi_M^2(\boldsymbol{r}_{\bar{c}\bar{q}}+\boldsymbol{r}_{c\bar{c}})|\boldsymbol{r}_{\bar{c}\bar{q}}+\boldsymbol{r}_{c\bar{c}}|$$

$$J_2^{MD}(r_{c\bar{c}})=\int_{r_{cq}}\psi_D(\boldsymbol{r}_{cq})\psi_M(\boldsymbol{r}_{cq}-\boldsymbol{r}_{c\bar{c}})|\boldsymbol{r}_{cq}-\boldsymbol{r}_{c\bar{c}}|=\int_{r_{\bar{c}\bar{q}}}\psi_D(\boldsymbol{r}_{cq})\psi_M(\boldsymbol{r}_{\bar{c}\bar{q}}+\boldsymbol{r}_{c\bar{c}})|\boldsymbol{r}_{\bar{c}\bar{q}}+\boldsymbol{r}_{c\bar{c}}|$$

$$\langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|V^{\text{conf}}|\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\rangle=2kJ_2^D$$
$$\langle\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})|V^{\text{conf}}|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle=2kJ_2^M$$
$$\langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|V^{\text{conf}}|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle=2kS_{DM}(r_{c\bar{c}})J_2^{MD}(r_{c\bar{c}})$$

$$V^{\text{spin}}=\sum_{\text{pairs}}-\frac{\lambda_{ij}}{m_im_j}\frac{8\pi}{3}\alpha_s\delta^{(3)}(\boldsymbol{r}_i-\boldsymbol{r}_j)\boldsymbol{S}_i\cdot\boldsymbol{S}_j=\sum_{\text{pairs}}\mathcal{K}_{ij}(\mathbf{R}_{ij}^{\mathbf{c}})\boldsymbol{S}_i\cdot\boldsymbol{S}_j$$

$$|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\rangle_0|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\rangle_0$$

$$|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\rangle_1,|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\rangle_1$$

$$|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\rangle_1|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\rangle_2$$

$$V^{\text{spin},\pm}(0^{++})=\sum_{\text{pairs}}{}_0\langle(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}|\mathcal{K}_{ij}(\mathbf{R}_{ij}^{\mathbf{c}})\boldsymbol{S}_i\cdot\boldsymbol{S}_j|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\rangle_0$$
$$=\frac{1}{16}\left(\pm2\sqrt{49\mathcal{K}_{\bar{c}q}^2(\mathbf{1})-28\mathcal{K}_{\bar{c}q}(\mathbf{1})\left(\mathcal{K}_{cq}(\bar{\mathbf{3}})+\mathcal{K}_{q\bar{q}}(\mathbf{8})\right)+16\left(\mathcal{K}_{cq}^2(\bar{\mathbf{3}})-\mathcal{K}_{cq}(\bar{\mathbf{3}})\mathcal{K}_{q\bar{q}}(\mathbf{8})+\mathcal{K}_{q\bar{q}}^2(\mathbf{8})\right)}\right.$$
$$\left.-7\mathcal{K}_{\bar{c}q}(\mathbf{1})-4\left(\mathcal{K}_{cq}(\bar{\mathbf{3}})+\mathcal{K}_{q\bar{q}}(\mathbf{8})\right)\right)$$
$$V^{\text{spin}}(1^{++})=-\frac{7}{16}\mathcal{K}_{\bar{c}q}(\mathbf{1})-\frac{1}{4}\mathcal{K}_{cq}(\bar{\mathbf{3}})+\frac{1}{4}\mathcal{K}_{q\bar{q}}(\mathbf{8})$$
$$V^{\text{spin},\pm}(1^{+-})=\pm\frac{1}{9}\sqrt{\left(\frac{63}{16}\mathcal{K}_{\bar{c}q}(\mathbf{1})-\frac{9}{4}\mathcal{K}_{cq}(\bar{\mathbf{3}})\right)^2+\frac{81}{4}\mathcal{K}_{q\bar{q}}^2(\mathbf{8})}-\frac{1}{4}\mathcal{K}_{q\bar{q}}(\mathbf{8})$$
$$V^{\text{spin}}(2^{++})=\frac{7}{16}\mathcal{K}_{\bar{c}q}(\mathbf{1})+\frac{1}{4}\left(\mathcal{K}_{cq}(\bar{\mathbf{3}})+\mathcal{K}_{q\bar{q}}(\mathbf{8})\right)$$

$$K_{ij}(D;\mathbf{R}^{\mathbf{c}}_{ij})= \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|\mathcal{K}_{ij}(\mathbf{R}^{\mathbf{c}}_{ij})|\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\rangle$$
$$K_{ij}(M;\mathbf{R}^{\mathbf{c}}_{ij}) = \langle\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})|\mathcal{K}_{ij}(\mathbf{R}^{\mathbf{c}}_{ij})|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$
$$K_{ij}(D,M;\mathbf{R}^{\mathbf{c}}_{ij}) = \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|\mathcal{K}_{ij}(\mathbf{R}^{\mathbf{c}}_{ij})|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$

$$K_{c\bar{q}}(D,\mathbf{1}) = \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|\mathcal{K}_{c\bar{q}}(\mathbf{1})|\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\rangle$$
$$\propto \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|\delta(\boldsymbol{r}_{cq})|\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\rangle = \psi_D^2(0)$$

$$K_{ij}(D;\mathbf{R}^{\mathbf{c}}_{ij}), K_{ij}(M;\mathbf{R}^{\mathbf{c}}_{ij})$$

$$K_{ij}(D,M;\mathbf{R}^{\mathbf{c}}_{ij})$$

$$V^{\text{spin}}_{D,1^{++}}= \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|V^{\text{spin}}(1^{++})|\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\rangle$$
$$= -\frac{7}{16}K_{c\bar{q}}(D;\mathbf{1}) - \frac{1}{4}K_{cq}(D;\overline{\mathbf{3}}) + \frac{1}{4}K_{q\bar{q}}(D;\mathbf{8})$$
$$V^{\text{spin}}_{M,1^{++}} = \langle\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})|V^{\text{spin}}(1^{++})|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$
$$= -\frac{7}{16}K_{c\bar{q}}(M;\mathbf{1}) - \frac{1}{4}K_{cq}(M;\overline{\mathbf{3}}) + \frac{1}{4}K_{q\bar{q}}(M;\mathbf{8})$$
$$V^{\text{spin}}_{DM,1^{++}} = \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|V^{\text{spin}}(1^{++})|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$
$$= -\frac{7}{16}K_{c\bar{q}}(D,M;\mathbf{1}) - \frac{1}{4}K_{cq}(D,M;\overline{\mathbf{3}}) + \frac{1}{4}K_{q\bar{q}}(D,M;\mathbf{8})$$

$$H_{D,1^{++}} =2E_D - 2\frac{7}{6}\alpha_s I_2^D(r_{c\bar{c}}) + \frac{1}{6}\alpha_s I_4^D(r_{c\bar{c}}) + V^{\text{spin}}_{D,1^{++}}(r_{c\bar{c}})$$
$$H_{M,1^{++}} =2E_M - 2\frac{1}{3}\alpha_s I_2^M(r_{c\bar{c}}) + \frac{1}{6}\alpha_s I_4^D(r_{c\bar{c}}) + V^{\text{spin}}_{M,1^{++}}(r_{c\bar{c}})$$
$$H_{DM,1^{++}} =S_{DM}(r_{c\bar{c}})\left(\frac{1}{m_{cq}}I_0^{DM}(r_{c\bar{c}}) - 2\frac{1}{3}\alpha_s I_2^{DM}(r_{c\bar{c}}) - 2\frac{7}{6}\alpha_s I_2^{MD}(r_{c\bar{c}}) + 2kJ_2^{MD}(r_{c\bar{c}})\right)$$
$$+\frac{1}{6}\alpha_s I_6^{DM}(r_{c\bar{c}}) + V^{\text{spin}}_{DM,1^{++}}(r_{c\bar{c}})$$

$$\Psi_{q\bar{q},1} = \frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) + \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2(1+S_{DM}^2(r_{c\bar{c}}))}}$$
$$\Psi_{q\bar{q},2} = \frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) - \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2(1-S_{DM}^2(r_{c\bar{c}}))}}$$

$$\Psi_{q\bar{q}} = \frac{1}{\sqrt{c_1^2(r_{c\bar{c}}) + c_2^2(r_{c\bar{c}})}}\left(c_1(r_{c\bar{c}})\Psi_{q\bar{q},1} + c_2(r_{c\bar{c}})\Psi_{q\bar{q},2}\right)$$

$$\begin{pmatrix}\epsilon_{11}(r_{c\bar{c}}) - \Delta E^{\pm}(r_{c\bar{c}}) & -\epsilon_{12}(r_{c\bar{c}}) \\ -\epsilon_{12}(r_{c\bar{c}}) & \epsilon_{22}(r_{c\bar{c}}) - \Delta E^{\pm}(r_{c\bar{c}})\end{pmatrix}\begin{pmatrix}c_1^{\pm} \\ c_2^{\pm}\end{pmatrix} = 0$$

$$\epsilon_{11}(r_{c\bar{c}}) = \frac{H_M(r_{c\bar{c}}) + H_D(r_{c\bar{c}}) + 2H_{DM}(r_{c\bar{c}})}{2 + 2[S_{DM}^2(r_{c\bar{c}})]}$$

$$\epsilon_{22}(r_{c\bar{c}}) = \frac{H_M(r_{c\bar{c}}) + H_D(r_{c\bar{c}}) - 2H_{DM}(r_{c\bar{c}})}{2 - 2[S_{DM}^2(r_{c\bar{c}})]}$$

$$\epsilon_{12}(r_{c\bar{c}}) = \frac{H_D(r_{c\bar{c}}) - H_M(r_{c\bar{c}})}{2\sqrt{1 - S_{DM}^4(r_{c\bar{c}})}}$$

$$V_{-,1^{++}}^{\mathrm{BO}}(r_{c\bar{c}}) \to V_{-,1^{++}}^{\mathrm{BO}}(r_{c\bar{c}})$$

$$c_1^{\pm}(r_{c\bar{c}})/c_2^{\pm}(r_{c\bar{c}})\Delta E^{\pm}(r_{c\bar{c}})$$

$$c^{\pm}(r_{c\bar{c}}) = \frac{c_1^{\pm}(r_{c\bar{c}})}{c_2^{\pm}(r_{c\bar{c}})} = \frac{\epsilon_{22} - \epsilon_{11}}{2\epsilon_{12}} \pm \sqrt{1 + \left(\frac{\epsilon_{22} - \epsilon_{11}}{2\epsilon_{12}}\right)^2}$$

$$\Psi_{q\bar{q}}^{\pm} = \frac{1}{\sqrt{1 + (c^{\pm})^2}}\left(c^{\pm}(r_{c\bar{c}})\Psi_{q\bar{q},1} + \Psi_{q\bar{q},2}\right)$$

$$-\frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) + \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2(1 + S_{DM}(+\infty)^2)}} + \frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) - \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2(1 - S_{DM}(+\infty)^2)}}$$
$$\propto \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})$$

$$\frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) + \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2(1 + S_{DM}(+\infty)^2)}} + \frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}}) - \psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2(1 - S_{DM}(+\infty)^2)}}$$
$$\propto \psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})$$

$$V_{-,1^{++}}^{\mathrm{BO}}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E_{1^{++}}^{-}(r_{c\bar{c}})$$

$$V_{+,1^{++}}^{\mathrm{BO}}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E_{1^{++}}^{+}(r_{c\bar{c}}) + kr_{c\bar{c}}$$

$$V_{D,1^{+-}}^{\mathrm{spin},\pm} = \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|V^{\mathrm{spin},\pm}(1^{+-})|\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})\rangle$$
$$= \pm\frac{1}{9}\sqrt{\left(\frac{63}{16}K_{\bar{c}q}(D;\mathbf{1}) - \frac{9}{4}K_{cq}(D;\mathbf{3})\right)^2 + \frac{81}{4}K_{q\bar{q}}^2(D;\mathbf{8})} - \frac{1}{4}K_{q\bar{q}}(D;\mathbf{8})$$

$$V_{M,1^{+-}}^{\mathrm{spin},\pm} = \langle\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})|V^{\mathrm{spin},\pm}(1^{+-})|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$
$$= \pm\frac{1}{9}\sqrt{\left(\frac{63}{16}K_{\bar{c}q}(M;\mathbf{1}) - \frac{9}{4}K_{cq}(M;\mathbf{3})\right)^2 + \frac{81}{4}K_{q\bar{q}}^2(M;\mathbf{8})} - \frac{1}{4}K_{q\bar{q}}(M;\mathbf{8})$$

$$V_{DM,1^{+-}}^{\mathrm{spin},\pm} = \langle\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})|V^{\mathrm{spin},\pm}(1^{+-})|\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})\rangle$$
$$= \pm\frac{1}{9}\sqrt{\left(\frac{63}{16}K_{\bar{c}q}(D,M;\mathbf{1}) - \frac{9}{4}K_{cq}(D,M;\mathbf{3})\right)^2 + \frac{81}{4}K_{q\bar{q}}^2(D,M;\mathbf{8})} - \frac{1}{4}K_{q\bar{q}}(D,M;\mathbf{8})$$

$$V_{-,1^{+-}}^{\mathrm{BO},\pm}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E_{1^{+-}}^{-,\pm}(r_{c\bar{c}})$$

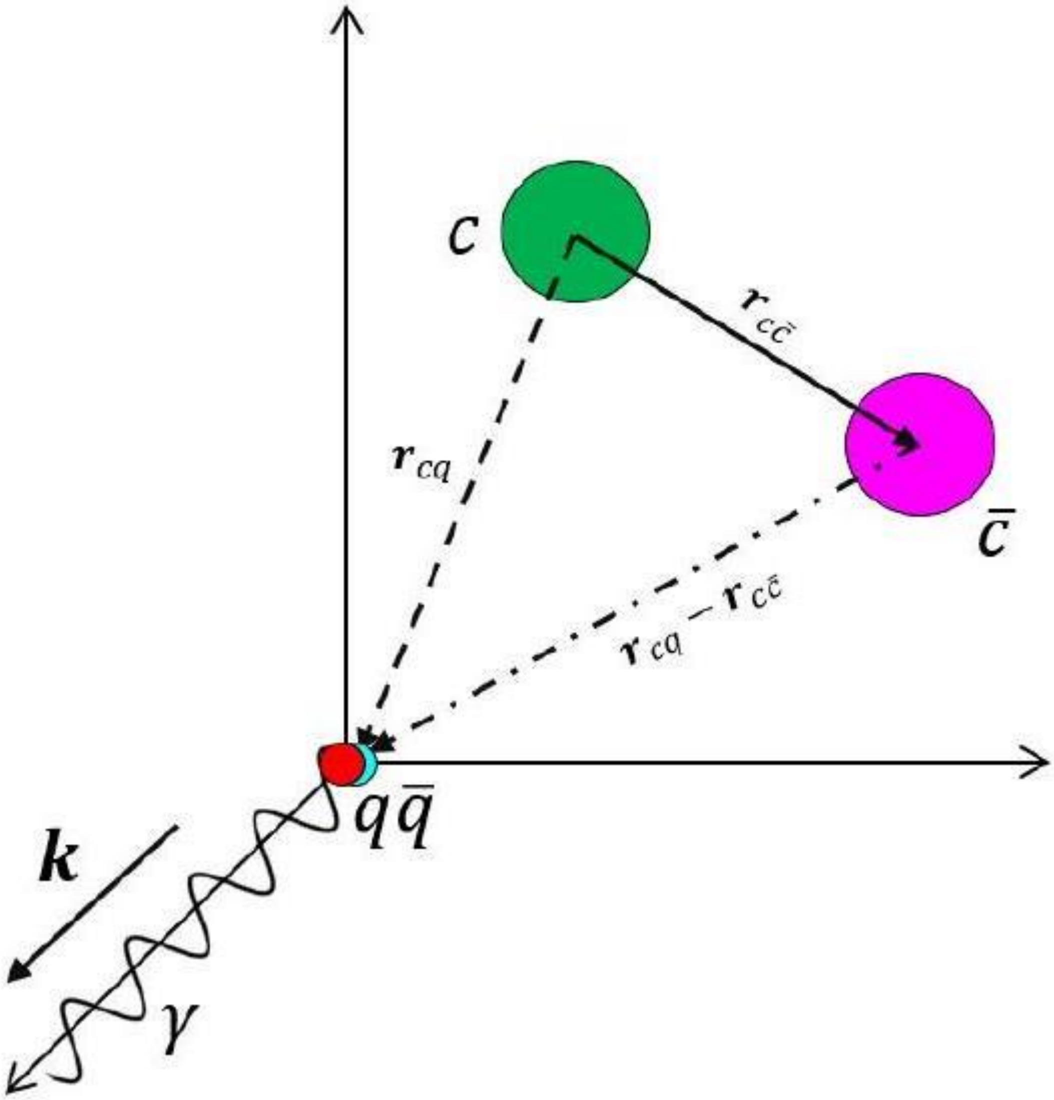
$$V_{+,1^{+-}}^{\mathrm{BO},\pm}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E_{1^{+-}}^{+,\pm}(r_{c\bar{c}}) + kr_{c\bar{c}}$$

$$V^{\mathrm{BO},\pm}_{-,0^{++}}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E^{-,\pm}_{0^{++}}(r_{c\bar{c}})$$

$$V^{\mathrm{BO},\pm}_{+,0^{++}}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E^{+,\pm}_{0^{++}}(r_{c\bar{c}}) + kr_{c\bar{c}}$$

$$V^{\mathrm{BO}}_{-,2^{++}}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E^{-}_{2^{++}}(r_{c\bar{c}})$$

$$V^{\mathrm{BO}}_{+,2^{++}}(r_{c\bar{c}}) = \frac{1}{6}\alpha_s\frac{1}{r_{c\bar{c}}} + \Delta E^{+}_{2^{++}}(r_{c\bar{c}}) + kr_{c\bar{c}}$$



$$\mathcal{R} = \frac{\mathrm{Br}(X \to \psi'\gamma)}{\mathrm{Br}(X \to \psi\gamma)}$$

$$A(X \to \psi^{(\prime)}\gamma) = \mathcal{F}\int_{\boldsymbol{r}_{c\bar{c}},\boldsymbol{r}_{cq}} e^{-i\boldsymbol{k}\cdot\left(\frac{\boldsymbol{r}_{c\bar{c}}}{2}-\boldsymbol{r}_{cq}\right)}\psi(|\boldsymbol{r}_{c\bar{c}}|)\Psi_{c\bar{c}q\bar{q}}(\boldsymbol{r}_{c\bar{c}},\boldsymbol{r}_{cq})$$

$$\Psi_{c\bar{c}q\bar{q}}(\boldsymbol{r}_{c\bar{c}},\boldsymbol{r}_{cq}) = \Psi_{c\bar{c}}(|\boldsymbol{r}_{c\bar{c}}|)\Psi_{q\bar{q}}(|\boldsymbol{r}_{cq}|,|\boldsymbol{r}_{cq} - \boldsymbol{r}_{c\bar{c}}|)$$

$$|\boldsymbol{k}| = \frac{M_X^2 - M_{\psi^{(\prime)}}^2}{2M_X}.$$

$$\mathcal{R} = \Phi\mathcal{P}\left|\frac{A(X\to\psi'\gamma)}{A(X\to\psi\gamma)}\right|^2 \approx 0.25\left|\frac{A(X\to\psi'\gamma)}{A(X\to\psi\gamma)}\right|^2$$

$$\Psi_{q\bar{q}}(\boldsymbol{r}_{cq},\boldsymbol{r}_{\bar{c}\bar{q}},\boldsymbol{r}_{c\bar{c}}) = \psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})$$

$$\Psi^-_{q\bar{q},1^{++}} = \frac{1}{\sqrt{1+\left(c^-_{1^{++}}\right)^2}}\left(c^-_{1^{++}}(r_{c\bar{c}})\frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})+\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2\left(1+S^2_{DM}(r_{c\bar{c}})\right)}}\right.$$
$$\left.+\frac{\psi_D(\boldsymbol{r}_{cq})\psi_D(\boldsymbol{r}_{\bar{c}\bar{q}})-\psi_M(\boldsymbol{r}_{c\bar{q}})\psi_M(\boldsymbol{r}_{\bar{c}q})}{\sqrt{2\left(1-S^2_{DM}(r_{c\bar{c}})\right)}}\right)$$

$$\psi_{\mathcal{C}}(\boldsymbol{\zeta}) = \sqrt{\frac{\mathcal{C}^3}{\pi}}e^{-\mathcal{C}r}$$

$$S_{AB}(R) = \int_{\xi}\psi_A(\boldsymbol{\xi})\psi_B(\boldsymbol{\xi}-\boldsymbol{R}) = \int_{\boldsymbol{\eta}}\psi_A(\boldsymbol{\eta})\psi_B(\boldsymbol{\eta}+\boldsymbol{R}) =$$
$$= \frac{8\sqrt{A^3B^3}}{R(A^2-B^2)^2}\left(R(Be^{-AR}+Ae^{-BR})+\frac{4AB}{A^2-B^2}(e^{-AR}-e^{-BR})\right)$$

$$I_0^{AB}(R) = \int_{\xi}\psi_A(\boldsymbol{\xi})(-\nabla^2_{\xi})\psi_B(\boldsymbol{\xi}-\boldsymbol{R}) = \int_{\boldsymbol{\eta}}\psi_A(\boldsymbol{\eta})(-\nabla^2_{\boldsymbol{\eta}})\psi_B(\boldsymbol{\eta}+\boldsymbol{R}) =$$
$$= \frac{8(AB)^{\frac{5}{2}}}{(A^2-B^2)^3}\left(e^{-BR}\left(\frac{2A^2+2B^2}{R}-A^2B+B^3\right)-e^{-AR}\left(\frac{2A^2+2B^2}{R}-AB^2+A^3\right)\right)$$

$$I_0^A = \int_{\xi}\psi_A(\boldsymbol{\xi})(-\nabla^2_{\xi})\psi_A(\boldsymbol{\xi}) = \int_{\boldsymbol{\eta}}\psi_A(\boldsymbol{\eta})(-\nabla^2_{\boldsymbol{\eta}})\psi_A(\boldsymbol{\eta}) = \lim_{B\to A}\lim_{R\to 0}I_0^{AB}(R) = A^2$$

$$I_0^B = \int_{\xi}\psi_B(\boldsymbol{\xi}-\boldsymbol{R})(-\nabla^2_{\xi})\psi_B(\boldsymbol{\xi}-\boldsymbol{R}) = \int_{\boldsymbol{\eta}}\psi_B(\boldsymbol{\eta}+\boldsymbol{R})(-\nabla^2_{\boldsymbol{\eta}})\psi_B(\boldsymbol{\eta}+\boldsymbol{R}) = B^2$$

$$I_1^A(R) = \int_{\xi}\psi_A^2(\boldsymbol{\xi})\frac{1}{|\boldsymbol{\xi}-\boldsymbol{R}|} = \int_{\boldsymbol{\eta}}\psi_A^2(\boldsymbol{\eta})\frac{1}{|\boldsymbol{\eta}+\boldsymbol{R}|} = \frac{1}{R}-Ae^{-2AR}\left(1+\frac{1}{AR}\right)$$
$$I_4^A(R) = \int_{\xi,\boldsymbol{\eta}}\psi_A^2(\boldsymbol{\xi})\psi_A^2(\boldsymbol{\eta})\frac{1}{|\boldsymbol{\xi}-\boldsymbol{R}-\boldsymbol{\eta}|} = A\left(\frac{1}{AR}-e^{-2AR}\left(\frac{1}{AR}+\frac{11}{8}+\frac{3}{4}AR+\frac{1}{6}A^2R^2\right)\right)$$

$$I_1^B(R) = \int_{\xi}\psi_B^2(\boldsymbol{\xi}-\boldsymbol{R})\frac{1}{\xi} = \int_{\xi'}\psi_B^2(\boldsymbol{\xi}')\frac{1}{|\boldsymbol{\xi}'+\boldsymbol{R}|} = \int_{\bar{\xi}}\psi_B^2(\bar{\boldsymbol{\xi}})\frac{1}{|\bar{\boldsymbol{\xi}}-\boldsymbol{R}|}$$
$$I_4^B(R) = \int_{\xi,\boldsymbol{\eta}}\psi_B^2(\boldsymbol{\xi}-\boldsymbol{R})\psi_B^2(\boldsymbol{\eta}+\boldsymbol{R})\frac{1}{|\boldsymbol{\xi}-\boldsymbol{R}-\boldsymbol{\eta}|} = \int_{\xi',\boldsymbol{\eta}'}\psi_B^2(\boldsymbol{\xi}')\psi_B^2(\boldsymbol{\eta}')\frac{1}{|\boldsymbol{\xi}'-\boldsymbol{R}-\boldsymbol{\eta}'|}$$

$$I_1^B(R) = \int_{\xi}\psi_B^2(\boldsymbol{\xi}-\boldsymbol{R})\frac{1}{\xi} = \int_{\bar{\xi}}\psi_B^2(\bar{\boldsymbol{\xi}})\frac{1}{|\bar{\boldsymbol{\xi}}+\boldsymbol{R}|} = \int_{\xi'}\psi_B^2(\boldsymbol{\xi}')\frac{1}{|\boldsymbol{\xi}'-\boldsymbol{R}|}$$
$$I_4^B(R) = \int_{\xi,\boldsymbol{\eta}}\psi_B^2(\boldsymbol{\xi}-\boldsymbol{R})\psi_B^2(\boldsymbol{\eta}+\boldsymbol{R})\frac{1}{|\boldsymbol{\xi}-\boldsymbol{R}-\boldsymbol{\eta}|} = \int_{\xi',\boldsymbol{\eta}'}\psi_B^2(\boldsymbol{\xi}')\psi_B^2(\boldsymbol{\eta}')\frac{1}{|\boldsymbol{\xi}'-\boldsymbol{R}-\boldsymbol{\eta}'|}$$

$$I_2^{AB}(R)=\int_{\xi}\psi_A(\boldsymbol{\xi})\psi_B(\boldsymbol{\xi}-\boldsymbol{R})\frac{1}{|\boldsymbol{\xi}|}=\int_{\boldsymbol{\eta}}\psi_A(\boldsymbol{\eta})\psi_B(\boldsymbol{\eta}+\boldsymbol{R})\frac{1}{|\boldsymbol{\eta}|}$$

$$=4\frac{\sqrt{A^3B^3}}{R}\left(\frac{R}{A^2-B^2}e^{-BR}+\frac{2B}{(A^2-B^2)^2}\left(e^{-AR}-e^{-BR}\right)\right)$$

$$I_6^{AB}(R)=\int_{\xi,\boldsymbol{\eta}}\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\frac{1}{|\boldsymbol{\xi}-\boldsymbol{\eta}-\boldsymbol{R}|}\psi_B(\boldsymbol{\xi}-\boldsymbol{R})\psi_B(\boldsymbol{\eta}+\boldsymbol{R})$$

$$J_2^{BA}(R)=\int_{\xi}\psi_A(\boldsymbol{\xi})\psi_B(\boldsymbol{\xi}-\boldsymbol{R})|\boldsymbol{\xi}-\boldsymbol{R}|=\int_{\boldsymbol{\eta}}\psi_A(\boldsymbol{\eta})\psi_B(\boldsymbol{\eta}+\boldsymbol{R})|\boldsymbol{\eta}+\boldsymbol{R}|$$

$$=\frac{8(AB)^{3/2}}{(A^2-B^2)^4R}\left(Ae^{-BR}\left(\frac{4A^2+20B^2}{R}-8A^2B+8B^3+R(A^2-B^2)^2\right)\right.$$
$$\left.-e^{-AR}\left(\frac{4A^3-20AB^2}{R}+A^4+2A^2B^2-3B^4\right)\right)$$

$$J_2^A=\int_{\xi}\psi_A^2(\boldsymbol{\xi})\xi=\int_{\boldsymbol{\eta}}\psi_A^2(\boldsymbol{\eta})\eta=\lim_{B\to A}\lim_{R\to 0}J_2^{BA}(R)=\frac{2}{3A}$$

$$J_2^B=\int_{\xi}\psi_B^2(\boldsymbol{\xi}-\boldsymbol{R})|\boldsymbol{\xi}-\boldsymbol{R}|=\int_{\boldsymbol{\eta}}\psi_B^2(\boldsymbol{\eta})|\boldsymbol{\eta}+\boldsymbol{R}|$$

$$J_2^B=\int_{\xi}\psi_B^2(\boldsymbol{\xi}-\boldsymbol{R})|\boldsymbol{\xi}-\boldsymbol{R}|=\int_{\xi'}\psi_B^2(\xi')\xi'=\lim_{A\to B}\lim_{R\to 0}J_2^{AB}(R)=\frac{2}{3B}$$

$$V^{\text{spin}}=2\kappa_{cq}^{\mathbf{R^c}}\mathbf{S}_c\cdot\mathbf{S}_q+2\kappa_{\bar{c}\bar{q}}^{\mathbf{R^c}}\mathbf{S}_{\bar{c}}\cdot\mathbf{S}_{\bar{q}}+2\kappa_{q\bar{q}}^{\mathbf{R^c}}\mathbf{S}_q\cdot\mathbf{S}_{\bar{q}}+2\kappa_{\bar{c}q}^{\mathbf{R^c}}\mathbf{S}_{\bar{c}}\cdot\mathbf{S}_q+2\kappa_{c\bar{q}}^{\mathbf{R^c}}\mathbf{S}_c\cdot\mathbf{S}_{\bar{q}}$$

$$\mathbf{S}_i\cdot\mathbf{S}_j\mathbf{S}_{ij}^{tot}$$

$$\kappa_{Qq}^{\mathbf{R^c}}=\kappa_{\bar{Q}\bar{q}}^{\overline{\mathbf{R}}^{\mathbf{c}}}$$

$$\kappa_{ij}^{\mathbf{R^c}}\mapsto\frac{1}{2}\mathcal{K}_{ij}(\mathbf{R^c})$$

$$\left|(c\bar{c})^{\mathbf{8}}(q\bar{q})^{\mathbf{8}}\right\rangle=\sqrt{\frac{2}{3}}\left|(cq)^{\bar{\mathbf{3}}}(\bar{c}\bar{q})^{\mathbf{3}}\right\rangle-\sqrt{\frac{1}{3}}\left|(cq)^{\mathbf{6}}(\bar{c}\bar{q})^{\bar{\mathbf{6}}}\right\rangle$$

$$\left|(c\bar{c})^{\mathbf{8}}(q\bar{q})^{\mathbf{8}}\right\rangle=\sqrt{\frac{8}{9}}\left|(c\bar{q})^{\mathbf{1}}(\bar{c}q)^{\mathbf{1}}\right\rangle-\sqrt{\frac{1}{9}}\left|(c\bar{q})^{\mathbf{8}}(\bar{c}q)^{\mathbf{8}}\right\rangle$$

$$|(c\bar{c})_0(q\bar{q})_1\rangle,|(c\bar{c})_1(q\bar{q})_0\rangle,|(c\bar{c})_1(q\bar{q})_1\rangle_1$$

$$C(q\bar{q})_0=+(q\bar{q})_0,C(q\bar{q})_1=-(q\bar{q})_1$$

$$|(c\bar{c})_0(q\bar{q})_1\rangle|(c\bar{c})_1(q\bar{q})_0\rangle|(c\bar{c})_1(q\bar{q})_1\rangle_1$$

$$|(c\bar{c})_0(q\bar{q})_1\rangle=A|(cq)_1(\bar{c}\bar{q})_0\rangle+B|(cq)_0(\bar{c}\bar{q})_1\rangle+C|(cq)_1(\bar{c}\bar{q})_1\rangle_1$$

$$\langle S_1S_2(S_{12})S_3S_4(S_{34})S \mid S_1S_3(S_{13})S_2S_4(S_{24})S\rangle =$$

$$\sqrt{(2S_{12}+1)(2S_{13}+1)(2S_{24}+1)(2S_{34}+1)}\begin{Bmatrix} S_1 & S_2 & S_{12} \\ S_3 & S_4 & S_{34} \\ S_{13} & S_{24} & S \end{Bmatrix}$$

$$\langle S_1S_2(S_{12})S_3S_4(S_{34})S \mid S_1S_4(S_{14})S_2S_3(S_{23})S\rangle =$$

$$(-1)^{S_3+S_4-S_{34}}\sqrt{(2S_{12}+1)(2S_{13}+1)}\sqrt{(2S_{14}+1)(2S_{23}+1)}\begin{Bmatrix} S_1 & S_2 & S_{12} \\ S_3 & S_4 & S_{34} \\ S_{14} & S_{23} & S \end{Bmatrix}$$

$$\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ 1 & 0 & 1 \end{Bmatrix} = -\frac{1}{6}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ 0 & 1 & 1 \end{Bmatrix} = \frac{1}{6}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 1 \\ 1 & 1 & 1 \end{Bmatrix} = \frac{1}{3\sqrt{6}}$$

$$|(c\bar{c})_0(q\bar{q})_1\rangle = -\frac{1}{2}|(cq)_1(\bar{c}\bar{q})_0\rangle + \frac{1}{2}|(cq)_0(\bar{c}\bar{q})_1\rangle + \frac{1}{\sqrt{2}}|(cq)_1(\bar{c}\bar{q})_1\rangle_1$$

$$|(c\bar{c})_1(q\bar{q})_0\rangle = \frac{1}{2}|(cq)_1(\bar{c}\bar{q})_0\rangle - \frac{1}{2}|(cq)_0(\bar{c}\bar{q})_1\rangle + \frac{1}{\sqrt{2}}|(cq)_1(\bar{c}\bar{q})_1\rangle_1$$

$$|(c\bar{c})_1(q\bar{q})_1\rangle_1 = \frac{1}{\sqrt{2}}|(cq)_0(\bar{c}\bar{q})_1\rangle + \frac{1}{\sqrt{2}}|(cq)_1(\bar{c}\bar{q})_0\rangle$$

$$B_S = \left\{\left|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_1, \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\right\rangle_1, \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_1\right\}$$

$$\left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_1 = \frac{1}{\sqrt{3}}\left|(cq)_0^{\bar{\mathbf{3}}}(\bar{c}\bar{q})_1^{\mathbf{3}}\right\rangle - \frac{1}{\sqrt{6}}\left|(cq)_0^{\mathbf{6}}(\bar{c}\bar{q})_1^{\bar{\mathbf{6}}}\right\rangle + \frac{1}{\sqrt{3}}\left|(cq)_1^{\bar{\mathbf{3}}}(\bar{c}\bar{q})_0^{\mathbf{3}}\right\rangle - \frac{1}{\sqrt{6}}\left|(cq)_1^{\mathbf{6}}(\bar{c}\bar{q})_0^{\bar{\mathbf{6}}}\right\rangle$$

$$B_S' = \left\{\frac{1}{\sqrt{2}}\left(\left|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle - \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\right\rangle\right), \frac{1}{\sqrt{2}}\left(\left|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle + \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\right\rangle\right), \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_1\right\}$$

$$V_{q\bar{q}}^{\text{spin}}(1^{++}) = {}_1\left\langle(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right|V_{q\bar{q}}^{\text{spin}}\left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_1 = -\frac{2}{3}\kappa_{cq}^{\bar{\mathbf{3}}} - \frac{1}{3}\kappa_{cq}^{\mathbf{6}} + \frac{1}{2}\kappa_{q\bar{q}}^{\mathbf{8}} - \frac{8}{9}\kappa_{\bar{c}q}^{\mathbf{1}} - \frac{1}{9}\kappa_{\bar{c}q}^{\mathbf{8}}$$

$$\left(\kappa_{ij}\right)^{\mathbf{R^c}} \mapsto \mathcal{K}_{ij}(\mathbf{R^c})/2$$

$$\begin{pmatrix} \langle -|V_{q\bar{q}}^{\text{spin}}|-\rangle & \langle -|V_{q\bar{q}}^{\text{spin}}|+\rangle \\ \langle -|V_{q\bar{q}}^{\text{spin}}|+\rangle & \langle +|V_{q\bar{q}}^{\text{spin}}|+\rangle \end{pmatrix}$$

$$|-\rangle = \frac{1}{\sqrt{2}}\left(\left|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle - \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\right\rangle\right)$$

$$|+\rangle = \frac{1}{\sqrt{2}}\left(\left|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle + \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\right\rangle\right)$$

$$V_{q\bar{q}}^{\text{spin},\pm}(1^{+-}) = \pm\frac{1}{9}\sqrt{\left[6\kappa_{cq}^{\bar{\mathbf{3}}} + 3\kappa_{cq}^{\mathbf{6}} - 8\kappa_{\bar{c}q}^{\mathbf{1}} - \kappa_{\bar{c}q}^{\mathbf{8}}\right]^2 + \left[9\kappa_{q\bar{q}}^{\mathbf{8}}\right]^2} - \frac{1}{2}\kappa_{q\bar{q}}^{\mathbf{8}}$$

$$|(c\bar{c})_0(q\bar{q})_0\rangle_0$$

$$|(c\bar{c})_1(q\bar{q})_1\rangle_0$$

$$|(c\bar{c})_0(q\bar{q})_0\rangle_0 = \frac{1}{2}|(cq)_0(\bar{c}\bar{q})_0\rangle_0 + \frac{\sqrt{3}}{2}|(cq)_1(\bar{c}\bar{q})_1\rangle_0 = -\frac{1}{2}|(\bar{c}q)_0(c\bar{q})_0\rangle_0 - \frac{\sqrt{3}}{2}|(\bar{c}q)_1(c\bar{q})_1\rangle_0$$
$$|(c\bar{c})_1(q\bar{q})_1\rangle_0 = \frac{\sqrt{3}}{2}|(cq)_0(\bar{c}\bar{q})_0\rangle_0 - \frac{1}{2}|(cq)_1(\bar{c}\bar{q})_1\rangle_0 = +\frac{\sqrt{3}}{2}|(\bar{c}q)_0(c\bar{q})_0\rangle_0 - \frac{1}{2}|(\bar{c}q)_1(c\bar{q})_1\rangle_0$$

$$|0\rangle = \left|(c\bar{c})_0^{\mathbf{8}}(q\bar{q})_0^{\mathbf{8}}\right\rangle$$
$$|1\rangle = \left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_0$$

$$\begin{pmatrix} \langle 0|V_{q\bar{q}}^{\text{spin}}|0\rangle & \langle 0|V_{q\bar{q}}^{\text{spin}}|1\rangle \\ \langle 1|V_{q\bar{q}}^{\text{spin}}|0\rangle & \langle 1|V_{q\bar{q}}^{\text{spin}}|1\rangle \end{pmatrix}$$

$$\langle 0|V_{q\bar{q}}^{\text{spin}}|0\rangle = -\frac{3}{2}\kappa_{q\bar{q}}^{\mathbf{8}}$$
$$\langle 1|V_{q\bar{q}}^{\text{spin}}|1\rangle = -\frac{4}{3}\kappa_{cq}^{\bar{\mathbf{3}}} - \frac{2}{3}\kappa_{cq}^{\mathbf{6}} + \frac{1}{2}\kappa_{q\bar{q}}^{\mathbf{8}} - \frac{2}{9}\kappa_{\bar{c}q}^{\mathbf{8}} - \frac{16}{9}\kappa_{\bar{c}q}^{\mathbf{1}}$$
$$\langle 0|V_{q\bar{q}}^{\text{spin}}|1\rangle = -\frac{2}{\sqrt{3}}\kappa_{cq}^{\bar{\mathbf{3}}} - \frac{1}{\sqrt{3}}\kappa_{cq}^{\mathbf{6}} + \frac{\sqrt{3}}{9}\kappa_{\bar{c}q}^{\mathbf{8}} + \frac{8\sqrt{3}}{9}\kappa_{\bar{c}q}^{\mathbf{1}}$$

$$\left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_2$$

$$2\kappa_{ij}^{\mathbf{R^c}}\boldsymbol{S}_i \cdot \boldsymbol{S}_j = \frac{1}{2}\kappa_{ij}^{\mathbf{R^c}}\ \forall i,j$$

$$V_{q\bar{q}}^{\text{spin}}(2^{++}) = {}_2\left\langle (c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right|V_{q\bar{q}}^{\text{spin}}\left|(c\bar{c})_1^{\mathbf{8}}(q\bar{q})_1^{\mathbf{8}}\right\rangle_2 = \frac{2}{3}\kappa_{cq}^{\bar{\mathbf{3}}} + \frac{1}{3}\kappa_{cq}^{\mathbf{6}} + \frac{1}{9}\kappa_{\bar{c}q}^{\mathbf{8}} + \frac{8}{9}\kappa_{\bar{c}q}^{\mathbf{1}} + \frac{1}{2}\kappa_{q\bar{q}}^{\mathbf{8}}$$

$$S_{AB}(R) = \int_{\xi}\psi_A(\boldsymbol{\xi})\psi_B(\boldsymbol{\xi}-\boldsymbol{R}) = \int_{\boldsymbol{\eta}}\psi_A(\boldsymbol{\eta})\psi_B(\boldsymbol{\eta}+\boldsymbol{R}) =$$
$$= \frac{8\sqrt{A^3B^3}}{R(A^2-B^2)^2}\left(R(Be^{-AR}+Ae^{-BR}) + \frac{4AB}{A^2-B^2}(e^{-AR}-e^{-BR})\right)$$

$$L^A(R) = \int_{\xi}\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\xi}-\boldsymbol{R}) = \int_{\boldsymbol{\eta}}\psi_A(\boldsymbol{\eta})\psi_A(\boldsymbol{\eta}+\boldsymbol{R}) = \lim_{B\to A}S_{AB}(R) =$$
$$= e^{-AR}\left(1 + AR + \frac{1}{3}A^2R^2\right)$$

$$\langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\delta(\boldsymbol{\xi}-\boldsymbol{R})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\delta(\boldsymbol{\eta}+\boldsymbol{R})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \psi_A^2(\boldsymbol{R})$$
$$\langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\delta(\boldsymbol{\xi})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\delta(\boldsymbol{\eta})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \psi_A^2(0)$$
$$\langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\delta(\boldsymbol{\xi}-\boldsymbol{\eta}-\boldsymbol{R})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \int_{\xi}\psi_A^2(\boldsymbol{\xi})\psi_A^2(\boldsymbol{\xi}-\boldsymbol{R}) = \frac{A^3}{8\pi}L^{2A}(R)$$
$$\langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\xi}-\boldsymbol{R})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\eta}+\boldsymbol{R})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = \psi_B^2(0)$$
$$\langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\xi})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\eta})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = \psi_B^2(\boldsymbol{R})$$
$$\langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\xi}-\boldsymbol{\eta}-\boldsymbol{R})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = \int_{\xi}\psi_B^2(\boldsymbol{\xi})\psi_B^2(\boldsymbol{\xi}-\boldsymbol{R}) = \frac{B^3}{8\pi}L^{2B}(R)$$

$$\langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\xi}-\boldsymbol{R})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\eta}+\boldsymbol{R})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = S_{AB}(R)\psi_B(0)\psi_A(\boldsymbol{R})$$

$$\langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\xi})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\eta})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = S_{AB}(R)\psi_B(\boldsymbol{R})\psi_A(0)$$

$$\langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\delta(\boldsymbol{\xi}-\boldsymbol{\eta}-\boldsymbol{R})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \int_{\xi}\psi_B(\boldsymbol{\xi}-\boldsymbol{R})\psi_B(\boldsymbol{\xi})\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\xi}-\boldsymbol{R}) = \frac{A^3B^3}{\pi(A+B)^3}L^{A+B}(R)$$

$$\mathcal{K}_{ij}(\mathbf{R}_{ij}^c) = -\frac{\lambda_{ij}}{m_i m_j}\frac{8\pi}{3}\alpha_s\delta^{(3)}(\boldsymbol{r}_i-\boldsymbol{r}_j)\,\lambda_{q\bar{q}}(\mathbf{8}) = +\frac{1}{6}\,\lambda_{cq}(\bar{\mathbf{3}}) = -\frac{2}{3}\,\lambda_{c\bar{q}}(\mathbf{1}) = -\frac{4}{3}$$

$$K_{c\bar{q}}(A;\mathbf{1}) = \langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\mathcal{K}_{c\bar{q}}(\mathbf{1})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \frac{4}{3M_c m_q}\alpha_s\frac{8\pi}{3}\psi_A^2(\boldsymbol{R})$$

$$K_{cq}(A;\bar{\mathbf{3}}) = \langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\mathcal{K}_{cq}(\bar{\mathbf{3}})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \frac{2}{3M_c m_q}\alpha_s\frac{8\pi}{3}\psi_A^2(0)$$

$$K_{q\bar{q}}(A;\mathbf{8}) = \langle\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})|\mathcal{K}_{q\bar{q}}(\mathbf{8})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = -\frac{1}{6m_q^2}\alpha_s\frac{8\pi}{3}\frac{A^3}{8\pi}L^{2A}(R)$$

$$K_{c\bar{q}}(B;\mathbf{1}) = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\mathcal{K}_{c\bar{q}}(\mathbf{1})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = \frac{4}{3M_c m_q}\alpha_s\frac{8\pi}{3}\psi_B^2(0)$$

$$K_{cq}(B;\bar{\mathbf{3}}) = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\mathcal{K}_{cq}(\bar{\mathbf{3}})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = \frac{2}{3M_c m_q}\alpha_s\frac{8\pi}{3}\psi_B^2(\boldsymbol{R})$$

$$K_{q\bar{q}}(B;\mathbf{8}) = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\mathcal{K}_{q\bar{q}}(\mathbf{8})|\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')\rangle = -\frac{1}{6m_q^2}\alpha_s\frac{8\pi}{3}\frac{B^3}{8\pi}L^{2B}(R)$$

$$K_{c\bar{q}}(A,B;\mathbf{1}) = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\mathcal{K}_{c\bar{q}}(\mathbf{1})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \frac{4}{3M_c m_q}\alpha_s\frac{8\pi}{3}S_{AB}(R)\psi_B(0)\psi_A(\boldsymbol{R})$$

$$K_{cq}(A,B;\bar{\mathbf{3}}) = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\mathcal{K}_{cq}(\bar{\mathbf{3}})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = \frac{2}{3M_c m_q}\alpha_s\frac{8\pi}{3}S_{AB}(R)\psi_B(\boldsymbol{R})\psi_A(0)$$

$$K_{q\bar{q}}(A,B;\mathbf{8}) = \langle\psi_B(\boldsymbol{\xi}')\psi_B(\boldsymbol{\eta}')|\mathcal{K}_{q\bar{q}}(\mathbf{8})|\psi_A(\boldsymbol{\xi})\psi_A(\boldsymbol{\eta})\rangle = -\frac{1}{6m_q^2}\alpha_s\frac{8\pi}{3}\frac{A^3B^3}{\pi(A+B)^3}L^{A+B}(R)$$

$$A\big(X\to\psi^{(\prime)}\gamma\big) = \mathcal{F}\int_{\boldsymbol{r}_{c\bar{c}},\boldsymbol{r}_{cq}}\cos\left[k\left(\cos\,\eta\left(\frac{R}{2}-\xi\cos\,\theta\right)-\xi\sin\,\theta\sin\,\eta\cos\,\phi\right)\right]\psi_c(r_{c\bar{c}})\Psi_{c\bar{c}q\bar{q}}(\boldsymbol{r}_{c\bar{c}},\boldsymbol{r}_{cq})$$

$$\boldsymbol{r}_{cq} = (\xi\sin\,\theta\cos\,\phi,\xi\sin\,\theta\sin\,\phi,\xi\cos\,\theta),\boldsymbol{r}_{c\bar{c}} = (0,0,R)\boldsymbol{k} = (k\sin\,\eta,0,k\cos\,\eta)$$

$$\partial_t u + \sum_{k=1}^{d}A_k(x)\partial_{x_k}u = \frac{iE(t,x)}{\varepsilon}Du + Cu$$
$$u(0,x) = u_0(x), x\in\Omega\subset\mathbb{R}^d$$

$$\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u}+\boldsymbol{b},\boldsymbol{u}(0) = \boldsymbol{u}_0$$

$$\frac{d\tilde{\mathbf{u}}}{dt} = \tilde{A}\tilde{\boldsymbol{u}},\tilde{\boldsymbol{u}} = \begin{bmatrix}\boldsymbol{u}\\ \boldsymbol{r}\end{bmatrix},\tilde{A} = \begin{bmatrix}A & \frac{I}{T}\\ \mathbf{0} & \mathbf{0}\end{bmatrix},\tilde{\boldsymbol{u}}(0) = \begin{bmatrix}\boldsymbol{u}_0\\ T\boldsymbol{b}\end{bmatrix}$$

$$\tilde{A} = H_1 + iH_2, H_1 = \frac{\tilde{A} + \tilde{A}^\dagger}{2}, H_2 = \frac{\tilde{A} - \tilde{A}^\dagger}{2i}$$

$$\frac{d\boldsymbol{v}}{dt} = -H_1 \partial_p \boldsymbol{v} + iH_2 \boldsymbol{v}, \boldsymbol{v}(0) = \xi(p)\tilde{\boldsymbol{u}}(0)$$

$$\xi(p) = e^{-|p|}$$

$$\xi(p) = \begin{cases} (-3 + 3e^{-1})p^3 + (-5 + 4e^{-1})p^2 - p + 1, & p \in (-1,0) \\ e^{-|p|}, & \text{otherwise} \end{cases}$$

$$p_j = L + j\Delta p, j = 0,1, \cdots, M$$

$$\phi_l(x) = e^{i\mu_l(x-L)}, \mu_l = \frac{2\pi(l-N)}{R-L}, l \in [M].$$

$$\Phi_p = (\phi_{jl})_{M\times M} = \left(\phi_l(p_j)\right)_{M\times M}, D_p = \text{diag}\{\mu_0, \cdots, \mu_{M-1}\}$$

$$i\frac{d\boldsymbol{w}}{dt} = \left(H_1 \otimes P_p - H_2 \otimes I_{M_p}\right)\boldsymbol{w}$$

$$\boldsymbol{w} = \sum_{j,k} v_j(t, p_k)|j\rangle|k\rangle$$

$$P_p = \Phi_p D_p (\Phi_p)^{-1} = P_p^\dagger$$

$$\tilde{\boldsymbol{w}} = \left(I_{M_x} \otimes (\Phi_p)^{-1}\right)\boldsymbol{w}$$

$$i\frac{d\tilde{\boldsymbol{w}}}{dt} = \left(H_1 \otimes D_p - H_2 \otimes I_{M_p}\right)\tilde{\boldsymbol{w}} =: H\tilde{\boldsymbol{w}}$$

$$s(H) = \mathcal{O}(s(\tilde{A})), \|H\|_{\max} \le \|H_1\|_{\max}/\Delta p + \|H_2\|_{\max},$$

$$\mathcal{O}\left(sT\|H\|_{\max} + \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right)$$

$$\mathcal{O}(m_H + n\text{polylog}(n))$$

$$e^{L+2\lambda_{\max}^+(H_1)T+R_p} \le \epsilon, e^{L+\lambda_{\max}^-(H_1)T+\lambda_{\max}^+(H_1)T+R_p} \le \epsilon$$

$$\lambda_{\max}^+(H_1) := \max\left\{\sup_{0<t<T}\{|\lambda| : \lambda \in \lambda(H_1(t)), \lambda > 0\}, 0\right\},$$
$$\lambda_{\max}^-(H_1) := \max\left\{\sup_{0<t<T}\{|\lambda| : \lambda \in \lambda(H_1(t)), \lambda < 0\}, 0\right\}.$$

$$\tilde{\boldsymbol{u}} = e^{p_k}\boldsymbol{v}(p_k), \text{or } \tilde{\boldsymbol{u}} = e^{p_k}\int_{p_k}^{\infty} \boldsymbol{v}\,dp$$

$$p_k \ge p_\star = \lambda_{\max}^+(H_1)T$$

$$\boldsymbol{v}(0) = \xi(p)\tilde{\boldsymbol{u}}(0), \text{ where } \xi(p) \in H^r(\mathbb{R}) \text{ satisfies } \xi(p) = e^{-p} \text{ for } p \ge 0$$

$$\|\tilde{\boldsymbol{u}}_h(T) - \tilde{\boldsymbol{u}}(T)\|_{L^2(\Omega_p)} \lesssim \Delta p^r e^{p_k}\|\tilde{\boldsymbol{u}}(T)\| + \epsilon\|\tilde{\boldsymbol{u}}_0\|,$$

$$\Omega_p = (p_k, p_k + R_p), R_p \geq 1$$

$$e_p^R = \mathcal{O}(1)$$

$$\lambda_1(H_1) \leq \lambda_2(H_1) \leq \cdots \leq \lambda_n(H_1),$$

$$p_k \geq \lambda_n(H_1)T$$

$$\frac{d\tilde{\boldsymbol{u}}^\lambda}{dt} = (H_1 - \lambda_0 I_{2n} + iH_2)\tilde{\boldsymbol{u}}^\lambda, \tilde{\boldsymbol{u}}^\lambda(0) = \tilde{\boldsymbol{u}}(0)$$

$$\boldsymbol{v}^\lambda = \xi(p)\tilde{\boldsymbol{u}}^\lambda$$

$$\tilde{\boldsymbol{u}}^\lambda = e^{p_k}\boldsymbol{v}^\lambda(p_k), \text{or } \tilde{\boldsymbol{u}}^\lambda = e^{p_k}\int_{p_k}^{\infty} \boldsymbol{v}^\lambda dp$$

$$p_k \geq p_\star = \max\{(\lambda_n(H_1) - \lambda_0)T, 0\}\tilde{\boldsymbol{u}}(T)e^{\lambda_0 T}\tilde{\boldsymbol{u}}^\lambda(T)$$

$$p_\star H_1 - \lambda_0 I_{2n}\frac{\lambda_1(H_1) + \lambda_n(H_1)}{2}$$

$$\|\tilde{\boldsymbol{u}}(0)/\tilde{\boldsymbol{u}}(T)\|$$

$$\Delta p^r e^{\lambda_n(H_1)T} > \epsilon\delta_T$$

$$\Delta p^r e^{\lambda_n(H_1)T} \leq \epsilon\delta_T$$

$$\Delta p^r < \epsilon\delta_T$$

$$\lambda_b := \max\left\{\lambda_n(H_1), \log\left(\frac{\Delta p^r}{\epsilon\delta_T}\right)/T\right\}$$

$$e^{-iHT}|\tilde{\psi}(0)\rangle = \frac{\tilde{\boldsymbol{w}}(0)}{\|\tilde{\boldsymbol{w}}(0)\|}|\tilde{\psi}(T)\rangle$$

$$I_{M_x} \otimes |p_k\rangle\langle p_k||\psi(T)\rangle$$

$$|\psi_k(T)\rangle \approx \frac{1}{\mathcal{N}}\left(\sum_j v_j(T, p_k)|j\rangle\right) \otimes |k\rangle, \mathcal{N} = \left(\sum_j \left|v_j(T, p_k)\right|^2\right)^{1/2}$$

$$P_r(T, p_k) = \frac{\|\boldsymbol{v}(T, p_k)\|^2}{\sum_l \|\boldsymbol{v}(T, p_l)\|^2}$$

$$P_r(T, p \geq p_\star) = \frac{1}{2}\frac{\|e^{-p_\star}\tilde{\boldsymbol{u}}(T)\|^2}{\|\tilde{\boldsymbol{u}}(0)\|^2} + \mathcal{O}(\Delta p)$$

$$\frac{\partial \boldsymbol{z}}{\partial t} = -\frac{\partial \boldsymbol{z}}{\partial s} - iH(s)\boldsymbol{z}, \boldsymbol{z}(0, s) = \delta(s)\tilde{\boldsymbol{w}}(0)$$

$$i\frac{d\tilde{\boldsymbol{z}}}{dt} = (D_s \otimes I + I_{M_s} \otimes H)\tilde{\boldsymbol{z}}, \tilde{\boldsymbol{z}}(0) = (\Phi_s^{-1} \otimes I)(\boldsymbol{\delta}_s \otimes \tilde{\boldsymbol{w}}(0))$$

$$I = I_{2n} \otimes I_{M_p}, \boldsymbol{\delta}_s = \sum_j \zeta_\omega(s_j)|j\rangle$$

$$\zeta_\omega(x) = \frac{1}{\omega}\zeta\left(\frac{x}{\omega}\right)\zeta(x) = 1 - |x|\zeta(x) = 1/2(1 + \cos(\pi x))$$

$$e^{L+\lambda_{\max}^{-}(H_1)T} \approx e^{L+\lambda_{\max}^{+}(H_1)T} \approx 0,$$

$$\Delta p = \mathcal{O}(\mu_{\max})$$

$$\|\boldsymbol{u}_h(T) - \boldsymbol{u}(T)\| \leq \frac{\epsilon}{2}\|\boldsymbol{u}(T)\|,$$

$$\Delta p = \mathcal{O}(\mu_{\max})$$

$$\tilde{\mathcal{O}}\left(\frac{\|\boldsymbol{u}(0)\| + T\|\boldsymbol{b}\|_{\mathrm{smax}}}{\|\boldsymbol{u}(T)\|}\left(\alpha_H T\mu_{\max} + \log\frac{\mu_{\max}(\|\boldsymbol{u}(0)\| + T\|\boldsymbol{b}\|_{\mathrm{smax}})}{\epsilon\|\boldsymbol{u}(T)\|}\right)\right)$$

$$\mathcal{O}\left(\frac{\|\boldsymbol{u}(0)\| + T\|\boldsymbol{b}\|_{\mathrm{smax}}}{\|\boldsymbol{u}(T)\|}\right)$$

$$\|\boldsymbol{b}\|_{\mathrm{smax}}^2 = \sum_i\left(\sup_{t\in[0,T]}|b_i(t)|\right)^2$$

$$\tilde{\mathcal{O}}\left(\frac{\|\boldsymbol{u}(0)\| + T\|\boldsymbol{b}\|_{\mathrm{smax}}}{\|\boldsymbol{u}(T)\|}\alpha_H T\log(1/\epsilon)\right)$$

$$\mathcal{O}\left(\frac{\|\boldsymbol{u}(0)\| + T\|\boldsymbol{b}\|_{\mathrm{smax}}}{\|\boldsymbol{u}(T)\|}\right)$$

$$\left[\xi(p_0), \cdots, \xi\left(p_{M_p-1}\right)\right]^{\top} \otimes \boldsymbol{u}_0$$

$$\partial_t u + c(x)\partial_x u + \lambda u = \frac{ia(x)}{\varepsilon}u, u(0,x) = u_0(x),$$

$$u(t,x) \in \mathbb{C}, x \in \Omega_x, t \geq 0$$

$$a(x) \geq a_0 > 0, \forall x \in \Omega_x$$

$$u_0(x) = f_0(x, \beta(x)/\varepsilon) \equiv f_0(x,\tau) \text{ with } \tau = \frac{\beta(x)}{\varepsilon}$$

$$u_0(x) = \sum_{k\in\mathbb{Z}} f_k(x)e^{ik\beta(x)/\varepsilon} \equiv \sum_{k\in\mathbb{Z}} u_k(0,x)$$

$$\partial_t u_k + c(x)\partial_x u_k + \lambda u_k = \frac{ia(x)}{\varepsilon}u_k, u_k(0,x) = f_k(x)e^{ik\beta(x)/\varepsilon}$$

$$u(t,x) = \sum_k u_k(t,x)$$

$$u_k(t,x) = \alpha_k(t,x)e^{iS_k(t,x)/\varepsilon}$$

$$\partial_t\alpha_k + c(x)\partial_x\alpha_k + \lambda\alpha_k + \frac{i}{\varepsilon}[\partial_t S_k + c(x)\partial_x S_k]\alpha_k = \frac{ia(x)}{\varepsilon}\alpha_k$$

$$\partial_t \alpha_k + c(x)\partial_x \alpha_k + \lambda \alpha_k = 0, \alpha_k(0,x) = f_k(x)$$
$$\partial_t S_k + c(x)\partial_x S_k = a(x), S_k(0,x) = k\beta(x)$$

$$\frac{d}{dt}\boldsymbol{\alpha}_k + icP_x\boldsymbol{\alpha}_k + \lambda\boldsymbol{\alpha}_k = \mathbf{0}$$

$$\boldsymbol{\alpha}_k(t) = \sum_j \alpha_k(t, x_j)|j\rangle$$

$$\frac{d}{dt}\boldsymbol{c}_k + icD_x\boldsymbol{c}_k + \lambda\boldsymbol{c}_k = \mathbf{0}$$

$$\frac{d}{dt}\boldsymbol{c}_k = -i\left(cD_x + \mathrm{Im}(\lambda)I_{M_x}\right)\Big)\boldsymbol{c}_k - \mathrm{Re}(\lambda)I_{M_x}\boldsymbol{c}_k$$

$$\tilde{\boldsymbol{c}}_k(t) = e^{\mathrm{Re}(\lambda)t}\boldsymbol{c}_k(t)$$

$$i\frac{d}{dt}\tilde{\boldsymbol{c}}_k = \left(cD_x + \mathrm{Im}(\lambda)I_{M_x}\right)\Big)\tilde{\boldsymbol{c}}_k, \tilde{\boldsymbol{c}}_k(0) = (\Phi_x)^{-1}\boldsymbol{\alpha}_k(0)$$

$$\frac{d}{dt}\boldsymbol{S}_k + icP_x\boldsymbol{S}_k = \boldsymbol{a}$$

$$\boldsymbol{S}_k(t) = \sum_j S_k(t, x_j)|j\rangle$$

$$\boldsymbol{a} = \sum_j a(x_j)|j\rangle$$

$$\boldsymbol{d}_k = (\Phi_x)^{-1}\boldsymbol{S}_k(t) \text{ and } \tilde{\boldsymbol{a}} = (\Phi_x)^{-1}\boldsymbol{a}$$

$$\frac{d}{dt}\boldsymbol{d}_k + icD_x\boldsymbol{d}_k = \tilde{\boldsymbol{a}}$$

$$\tilde{\boldsymbol{d}}_k = cD_x\boldsymbol{d}_k + i\tilde{\boldsymbol{a}}$$

$$i\frac{d}{dt}\tilde{\boldsymbol{d}}_k = cD_x\tilde{\boldsymbol{d}}_k, \tilde{\boldsymbol{d}}_k(0) = cD_x(\Phi_x)^{-1}\boldsymbol{S}_k(0) + i(\Phi_x)^{-1}\boldsymbol{a}.$$

$$\langle j|\frac{d}{dt}\boldsymbol{d}_k = \langle j|\tilde{\boldsymbol{a}}\langle j|\boldsymbol{d}_k$$

$$\frac{d}{dt}x = iHx + \lambda I_n x, \frac{d}{dt}y = iHy + F.$$

$$\tilde{x} = e^{-\mathrm{Re}(\lambda)t}x$$

$$N_{\mathrm{Gates}} = \mathcal{O}\left(m_x \log(m_x)\right)$$

$$\frac{d}{dt}\boldsymbol{\alpha}_k + iC(x)P_x\boldsymbol{\alpha}_k + \lambda\boldsymbol{\alpha}_k = \mathbf{0}$$
$$\frac{d}{dt}\boldsymbol{S}_k + iC(x)P_x\boldsymbol{S}_k = \boldsymbol{a}$$

$$C(x) = \mathrm{diag}\left[c(x_0), c(x_1), \cdots, c\left(x_{M_x-1}\right)\right]$$

$$i\frac{d}{dt}\boldsymbol{c}_k = \left(H_1 \otimes D_p - H_2 \otimes I_{M_p}\right)\boldsymbol{c}_k := H_\alpha \boldsymbol{c}_k$$

$$\boldsymbol{c}_k(0) = \left(I_{M_x} \otimes \left(\Phi_p\right)^{-1}\right)\sum_{j,k} \xi(p_k)\alpha_k\left(0, x_j\right)|j\rangle|k\rangle$$

$$H_1 = -\mathrm{Re}(\lambda)I_{M_x} - i\frac{C(x)P_x - P_xC(x)}{2}$$
$$H_2 = -\mathrm{Im}(\lambda)I_{M_x} - \frac{C(x)P_x + P_xC(x)}{2}$$

$$i\frac{d}{dt}\boldsymbol{d}_k = \left(H_1 \otimes D_p - H_2 \otimes I_{M_p}\right)\boldsymbol{d}_k := H_S \boldsymbol{d}_k$$

$$\boldsymbol{d}_k(0) = \left(I_{M_x} \otimes \left(\Phi_p\right)^{-1}\right)\sum_{j,k} \xi(p_k)S_k\left(0, x_j\right)|j\rangle|k\rangle$$

$$H_1 = \frac{1}{2}\begin{bmatrix} i(P_xC(x) - C(x)P_x) & A \\ A & \boldsymbol{0} \end{bmatrix}$$
$$H_2 = \frac{1}{2i}\begin{bmatrix} -i(C(x)P_x + P_xC(x)) & A \\ -A & \boldsymbol{0} \end{bmatrix}, A = \mathrm{diag}\{\boldsymbol{a}\}$$

$$\left|\tilde{\psi}_c(0)\right\rangle = \frac{\boldsymbol{c}_k(0)}{\|\boldsymbol{c}_k(0)\|}, \left|\tilde{\psi}_d(0)\right\rangle = \frac{\boldsymbol{d}_k(0)}{\|\boldsymbol{d}_k(0)\|}$$

$$\tilde{O}\left(\frac{T(|\lambda| + M_x\|c(x)\|_{\ell\infty})\|\boldsymbol{\alpha}_k(0)\|}{\|\boldsymbol{\alpha}_k(T)\|}\log(1/\epsilon)\right)$$

$$\tilde{O}\left(\frac{\|\boldsymbol{S}_k(0)\| + T\|\boldsymbol{a}\|_{\mathrm{smax}}}{\|\boldsymbol{S}_k(T)\|}(\|a(x)\|_{\ell^\infty} + M_x\|c(x)\|_{\ell^\infty})T\log(1/\epsilon)\right)$$

$$\frac{d\alpha_k^j(t)}{dt} + c(x_j)\frac{\alpha_k^j - \alpha_k^{j-1}}{\Delta x} + \lambda\alpha_k^j = 0, \alpha_k^j(0) = f_k(x_j),$$
$$\frac{dS_k^j(t)}{dt} + c(x_j)\frac{S_k^j - S_k^{j-1}}{\Delta x} = a(x_j), S_k^j(0) = k\beta(x_j),$$

$$S^+ := \sum_{j=1}^{M_x-1} |j\rangle\langle j-1| = \sum_{j=1}^{m_x} I_{2^{m_x-j}} \otimes \sigma_{10} \otimes \sigma_{01}^{\otimes(j-1)}, S^- = (S^+)^\dagger$$

$$\boldsymbol{\alpha}_k(t) = \sum_j \alpha_k^j(t)|j\rangle, \boldsymbol{S}_k = \sum_j S_k^j|j\rangle$$

$$D_x^- = \frac{1}{\Delta x}\left(I_{M_x} - S^+ - \sigma_{01}^{\otimes m_x}\right), D_x^+ = -(D_x^-)^\dagger$$

$$\frac{d\boldsymbol{\alpha}_k}{dt} = M_1\boldsymbol{\alpha}_k$$
$$\frac{d\boldsymbol{S}_k}{dt} = M_2\boldsymbol{S}_k + F_k$$

$$M_1 = -C(x)D_x^- - \lambda I_{M_x}, M_2 = -C(x)D_x^-$$

$$F_k = \sum_j a(x_j)|j\rangle$$

$$H_1 = -\mathrm{Re}(\lambda)I_{M_x} + \frac{D_x^+C(x) - C(x)D_x^-}{2}$$
$$H_2 = -\mathrm{Im}(\lambda)I_{M_x} - \frac{D_x^+C(x) + C(x)D_x^-}{2i}$$

$$H_1 = \frac{1}{2}\begin{bmatrix} D_x^+C(x) - C(x)D_x^- & A \\ A & \mathbf{0} \end{bmatrix}$$
$$H_2 = \frac{1}{2i}\begin{bmatrix} -D_x^+C(x) - C(x)D_x^- & A \\ -A & \mathbf{0} \end{bmatrix}, A = \mathrm{diag}\{F_k\}$$

$$u_0(x) = 1 + \frac{1}{2}\cos(2x) + i\left(1 + \frac{1}{2}\sin(2x)\right), x \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right].$$

$$u(t,x) = \exp(-(1 - i/\varepsilon)t)u_0(x - t)$$

$$u_0(x) = e^{i\frac{x}{\varepsilon}}\left(1 + \frac{1}{2}\cos(2x) + i\left(1 + \frac{1}{2}\sin(2x)\right)\right), x \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right].$$

$$\left\|\alpha_k^d(T,x) - \alpha_k(T,x)\right\|_\infty$$

$$\mathfrak{C}\left(\left\{p_j : \left\|\alpha_k^d(T,x,p_j) - \alpha_k(T,x)\right\|_\infty \le \Delta p\right\}\right)$$

$$\left[\frac{\lambda_1(H_1) + \lambda_n(H_1)}{2}, \lambda_n(H_1)\right]$$

$$\partial_t u + A(x)\partial_x u = \frac{iE(t,x)}{\varepsilon}Du + Cu, u(0,x) = u_0(x).$$

$$A(x) = \begin{bmatrix} a_1(x) & 0 \\ 0 & a_2(x) \end{bmatrix}, D = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}, C = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}.$$

$$U(t,x,S(t,x)/\varepsilon) = u(t,x)$$

$$\partial_t U_1 + a_1\partial_x U_1 + \frac{1}{\varepsilon}[\partial_t S + a_1\partial_x S]\partial_\tau U_1 = C_{11}U_1 + C_{12}U_2$$
$$\partial_t U_2 + a_2\partial_x U_2 + \frac{1}{\varepsilon}[\partial_t S + a_2\partial_x S]\partial_\tau U_2 = -\frac{iE}{\varepsilon}U_2 + C_{21}U_1 + C_{22}U_2$$

$$\partial_t S + a_2\partial_x S = E, S(0,x) = 0$$

$$\partial_t U_1 + a_1 \partial_x U_1 + \frac{1}{\varepsilon}[(a_1 - a_2)\partial_x S + E]\partial_\tau U_1 = C_{11}U_1 + C_{12}U_2$$
$$\partial_t U_2 + a_2 \partial_x U_2 = -\frac{E}{\varepsilon}[\partial_\tau U_2 + iU_2] + C_{21}U_1 + C_{22}U_2$$

$$\left\|\alpha_k^d(T,x,p_k) - \alpha_k(T,x)\right\|_\infty$$

$$p_k \in \left\{p_j: \left\|\alpha_k^d(T,x,p_j) - \alpha_k(T,x)\right\|_\infty \leq \Delta p\right\}$$

$$p_k \in \left\{p_j: \left\|\alpha_k^d(T,x,p_j) - \alpha_k(T,x)\right\|_\infty \leq \Delta p^2\right\}$$

$$p_k \in \{p_j: \|\alpha_k^d(T,x,p_j) - \alpha_k(T,x)\|_\infty \leq \Delta p \|\alpha_k(T,x)\|_\infty\}$$

$$\partial_t U_1 + a_1 \partial_x U_1 - C_{11}U_1 - C_{12}e^{-i\tau}V_2 = -\frac{1}{\varepsilon}[(a_1 - a_2)\partial_x S + E]\partial_\tau U_1,$$
$$\partial_t V_2 + a_2 \partial_x V_2 - C_{21}e^{i\tau}U_1 - C_{22}V_2 = -\frac{E}{\varepsilon}\partial_\tau V_2.$$

$$U_1(0,x,\tau) = f_1^{in} + \frac{i\varepsilon E C_{12}}{E^2 - \varepsilon^2 C_{12}C_{21}}\left(e^{-i\tau} - 1\right)f_2^{in}$$
$$U_2(0,x,\tau) = \frac{i\varepsilon E C_{21}}{E^2 - \varepsilon^2 C_{12}C_{21}}\left(e^{-i\tau} - 1\right)f_1^{in} + e^{-i\tau}f_2^{in}$$

$$u_0(x) = U(0,x,0) = \left(f_1^{in}(x), f_2^{in}(x)\right)^\top$$

$$\left(\left\{p_j: \left\|\alpha_k^d(T,x,p_j) - \alpha_k(T,x)\right\|_\infty \leq tol\right\}\right)$$

$$\Delta p \|\alpha_k(T,x)\|_\infty$$

$$\partial_t \boldsymbol{u} + i(A_1 P_x) \otimes I_{M_\tau}\boldsymbol{u} - C_{11}\boldsymbol{u} - C_{12}T_1\boldsymbol{v} = \frac{1}{\varepsilon}\mathrm{diag}\{(A_1 - A_2)P_x\boldsymbol{S} - i\boldsymbol{E}\} \otimes P_\tau \boldsymbol{u},$$
$$\partial_t \boldsymbol{v} + i(A_2 P_x) \otimes I_{M_\tau}\boldsymbol{v} - C_{21}T_2\boldsymbol{u} - C_{22}\boldsymbol{v} = -\frac{i}{\varepsilon}\mathrm{diag}\{\boldsymbol{E}\} \otimes P_\tau \boldsymbol{v},$$
$$\partial_t \boldsymbol{S} + iA_2 P_x \boldsymbol{S} = \boldsymbol{E},$$

$$\boldsymbol{u} = \sum_{j,k} U_1(t,x_j,\tau_k)|j\rangle|k\rangle, \boldsymbol{v} = \sum_{j,k} V_2(t,x_j,\tau_k)|j\rangle|k\rangle$$

$$\boldsymbol{S} = \sum_j S(t,x_j)|j\rangle$$

$$A_1 = \mathrm{diag}\left\{\sum_j a_1(x_j)|j\rangle\right\}, A_2 = \mathrm{diag}\left\{\sum_j a_2(x_j)|j\rangle\right\}, \boldsymbol{E} = \sum_j E(x_j)|j\rangle$$
$$T_1 = I_{M_x} \otimes \mathrm{diag}\left\{\sum_k e^{-i\tau_k}|k\rangle\right\}, T_2 = I_{M_x} \otimes \mathrm{diag}\left\{\sum_k e^{i\tau_k}|k\rangle\right\} = T_1^\dagger$$

$$M = \sigma_{00} \otimes \left(-i(A_1 P_x) \otimes I_{M_\tau} + C_{11}I_{M_x} \otimes I_{M_\tau} + \frac{1}{\varepsilon}\mathrm{diag}\{(A_1 - A_2)P_x\boldsymbol{S} - i\boldsymbol{E}\} \otimes P_\tau\right)$$
$$+\sigma_{11} \otimes \left(-i(A_2 P_x) \otimes I_{M_\tau} + C_{22}I_{M_x} \otimes I_{M_\tau} - \frac{i}{\varepsilon}\mathrm{diag}\{\boldsymbol{E}\} \otimes P_\tau\right)$$
$$+C_{12}\sigma_{01} \otimes T_1 + C_{21}\sigma_{10} \otimes T_2$$

$$H_1 = \sigma_{00} \otimes \left(\mathrm{Re}(C_{11}) I_{M_x} \otimes I_{M_\tau} - \frac{iA_1P_x - iP_xA_1}{2} \otimes I_{M_\tau} \right)$$
$$+\sigma_{11} \otimes \left(\mathrm{Re}(C_{22}) I_{M_x} \otimes I_{M_\tau} - \frac{iA_2P_x - iP_xA_2}{2} \otimes I_{M_\tau} \right)$$
$$+\frac{C_{12} + \overline{C_{21}}}{2} \sigma_{01} \otimes T_1 + \frac{\overline{C_{12}} + C_{21}}{2} \sigma_{10} \otimes T_2$$

$$H_2 = \sigma_{00} \otimes \left(\mathrm{Im}(C_{11}) I_{M_x} \otimes I_{M_\tau} - \frac{A_1P_x + P_xA_1}{2} \otimes I_{M_\tau} - \frac{1}{\varepsilon} \mathrm{diag}\{ i(A_1 - A_2)P_x\boldsymbol{S} + \boldsymbol{E} \} \otimes P_\tau \right)$$
$$+\sigma_{11} \otimes \left(\mathrm{Im}(C_{22}) I_{M_x} \otimes I_{M_\tau} - \frac{A_2P_x + P_xA_2}{2} \otimes I_{M_\tau} - \frac{1}{\varepsilon} \mathrm{diag}\{ \boldsymbol{E} \} \otimes P_\tau \right)$$
$$+i\frac{\overline{C_{21}} - C_{12}}{2} \sigma_{01} \otimes T_1 + i\frac{\overline{C_{12}} - C_{21}}{2} \sigma_{10} \otimes T_2$$

$$\lambda(H_1) = \frac{\mathrm{Re}(C_{11} + C_{22}) + \sqrt{\left(\mathrm{Re}(C_{11} - C_{22})\right)^2 + \left|C_{12} + \overline{C_{21}}\right|^2}}{2}$$

$$M = iH_2 \mathrm{Re}(C_{11}) = \mathrm{Re}(C_{22}) = C_{12} + \overline{C_{21}}$$

$$U_{j,k}(t) \approx U_1(t, x_j, \tau_k) V_{j,k} \approx V_2(t, x_j, \tau_k)$$

$$\frac{dU_{j,k}}{dt} + a_1(x_j) \frac{U_{j,k} - U_{j-1,k}}{\Delta x} - C_{11} U_{j,k} - C_{12} e^{-i\tau_k} V_{j,k}$$
$$= -\frac{1}{\varepsilon} \left(E_j + \left(a_1(x_j) - a_2(x_j) \right) \partial_x S(x_j) \right) \frac{U_{j,k} - U_{j,k-1}}{\Delta \tau}$$
$$\frac{dV_{j,k}}{dt} + a_2(x_j) \frac{V_{j,k} - V_{j-1,k}}{\Delta x} - C_{21} e^{i\tau_k} U_{j,k} - C_{22} V_{j,k}$$
$$= -\frac{1}{\varepsilon} E_j \frac{V_{j,k} - V_{j,k-1}}{\Delta \tau}$$

$$E_j = E(t, x_j)$$

$$\boldsymbol{u}(t) = \sum_{j,k} U_{j,k}(t) |j\rangle |k\rangle, \boldsymbol{v}(t) = \sum_{j,k} V_{j,k}(t) |j\rangle |k\rangle$$

$$M = \sigma_{00} \otimes \left(-(A_1 D_x^-) \otimes I_{M_\tau} + C_{11} I_{M_x} \otimes I_{M_\tau} - \frac{1}{\varepsilon} \mathrm{diag}\{ \boldsymbol{E} + (A_1 - A_2) \partial_x \boldsymbol{S} \} \otimes D_\tau^- \right)$$
$$+\sigma_{11} \otimes \left(-(A_2 D_x^-) \otimes I_{M_\tau} + C_{22} I_{M_x} \otimes I_{M_\tau} - \frac{1}{\varepsilon} \mathrm{diag}\{ \boldsymbol{E} \} \otimes D_\tau^- \right)$$
$$+C_{12} \sigma_{01} \otimes T_1 + C_{21} \sigma_{10} \otimes T_2$$

$$H_1 = \sigma_{00} \otimes \left(\left(\frac{D_x^+ A_1 - A_1 D_x^-}{2} \right) \otimes I_{M_\tau} + C_{11} I_{M_x} \otimes I_{M_\tau} + \frac{1}{\varepsilon} \mathrm{diag}\{ \boldsymbol{E} + (A_1 - A_2) \partial_x \boldsymbol{S} \} \otimes \frac{D_\tau^+ - D_\tau^-}{2} \right)$$
$$+\sigma_{11} \otimes \left(\left(\frac{D_x^+ A_2 - A_2 D_x^-}{2} \right) \otimes I_{M_\tau} + C_{22} I_{M_x} \otimes I_{M_\tau} + \frac{1}{\varepsilon} \mathrm{diag}\{ \boldsymbol{E} \} \otimes \frac{D_\tau^+ - D_\tau^-}{2} \right)$$
$$+\frac{C_{12} + C_{21}}{2} \sigma_{01} \otimes T_1 + \frac{C_{12} + C_{21}}{2} \sigma_{10} \otimes T_2$$

$$H_2 = i\sigma_{00} \otimes \left(\left(\frac{D_x^+ A_1 + A_1 D_x^-}{2} \right) \otimes I_{M_\tau} + \frac{1}{\varepsilon} \mathrm{diag}\{\boldsymbol{E} + (A_1 - A_2)\partial_x \boldsymbol{S}\} \otimes \frac{D_\tau^+ + D_\tau^-}{2} \right)$$
$$+ i\sigma_{11} \otimes \left(\left(\frac{D_x^+ A_2 + A_2 D_x^-}{2} \right) \otimes I_{M_\tau} + \frac{1}{\varepsilon} \mathrm{diag}\{\boldsymbol{E}\} \otimes \frac{D_\tau^+ + D_\tau^-}{2} \right)$$
$$+ i \frac{C_{21} - C_{12}}{2} \sigma_{01} \otimes T_1 + i \frac{C_{12} - C_{21}}{2} \sigma_{10} \otimes T_2$$

$$a_1(x) = 1, a_2(x) = 4, E(t,x) = 1.5 + \cos(x)$$

$$C = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$u(0,x) = \left(1 + \frac{1}{2}\cos(x) + i\sin(x), 1 + \frac{1}{2}\cos(x) + i\sin(x)\right), x \in [0,2\pi]$$

$$C = \frac{1}{2} \begin{bmatrix} 1+i & 1+i \\ -1+i & 1-i \end{bmatrix}$$

$$\Delta x = \frac{2\pi}{2^4}$$

$$\partial_t f^+ + v \cdot \nabla_x f^+ - \nabla_x (U + E) \cdot \nabla_v f^+ = \overline{b^i} f^i + b^i \overline{f^i}$$
$$\partial_t f^- + v \cdot \nabla_x f^- - \nabla_x (U - E) \cdot \nabla_v f^- = -\overline{b^i} f^i - b^i \overline{f^i}$$
$$\partial_t f^i + v \cdot \nabla_x f^i - \nabla_x U \cdot \nabla_v f^i = -i \frac{2E}{\varepsilon} f^i + b^i (f^- - f^+) + (b^+ - b^-) f^i$$

$$\left(f^+(t,x,v), f^-(t,x,v), f^i(t,x,v)\right) \in \mathbb{R} \times \mathbb{R} \times \mathbb{C}, (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d$$

$$\left(f^+(0,x,v), f^-(0,x,v), f^i(0,x,v)\right) = \left(f_{in}^+(x,v), f_{in}^-(x,v), f_{in}^i(x,v)\right).$$

$$\partial_t \boldsymbol{f} + \boldsymbol{v} \cdot \nabla_x \boldsymbol{f} - \nabla_x A \cdot \nabla_v \boldsymbol{f} = C\boldsymbol{f},$$

$$\boldsymbol{f} = \left(f^+, f^-, \mathrm{Re}(f^i), \mathrm{Im}(f^i)\right)^\top, \boldsymbol{v} = (v,v,v,v)^\top, A = \mathrm{diag}(U+E, U-E, U, U)$$
$$C = \begin{bmatrix} 0 & 0 & b^i + \overline{b^i} & -ib^i + i\overline{b^i} \\ 0 & 0 & -b^i - \overline{b^i} & ib^i - ib^i \\ -b^i & b^i & b^+ - b^- & 2E/\varepsilon \\ 0 & 0 & -2E/\varepsilon & b^+ - b^- \end{bmatrix}$$

$$\partial_t \boldsymbol{f} + \boldsymbol{v} \cdot \nabla_x \boldsymbol{f} = 0$$
$$\partial_t \boldsymbol{f} - \nabla_x A \cdot \nabla_v \boldsymbol{f} = 0$$
$$\partial_t \boldsymbol{f} = C\boldsymbol{f}$$
$$\partial_t S + v \cdot \nabla_x S - \nabla_x U \cdot \nabla_v S = 2E, S(0,x,v) = 0,$$

$$f^\pm(t,x,v) = F^\pm(t,x,v,\tau), f^i(t,x,v) = e^{-i\tau}(G + iH)(t,x,v,\tau)$$

$$G = \mathrm{Re}\left(e^{i\tau} f^i\right), H = \mathrm{Im}\left(e^{i\tau} f^i\right)$$

$$\partial_t F^+ + v\cdot\nabla_x F^+ - \nabla_x(U+E)\cdot\nabla_v F^+ = -\frac{\mathcal{E}^+}{\varepsilon}\partial_\tau F^+ + 2b^i G\cos\tau + 2b^i H\sin\tau$$
$$\partial_t F^- + v\cdot\nabla_x F^- - \nabla_x(U-E)\cdot\nabla_v F^- = -\frac{\mathcal{E}^-}{\varepsilon}\partial_\tau F^- - 2b^i G\cos\tau - 2b^i H\sin\tau$$
$$\partial_t G + v\cdot\nabla_x G - \nabla_x U\cdot\nabla_v G = -\frac{2E}{\varepsilon}\partial_\tau G + b^i(F^- - F^+)\cos\tau$$
$$\partial_t H + v\cdot\nabla_x H - \nabla_x U\cdot\nabla_v H = -\frac{2E}{\varepsilon}\partial_\tau H + b^i(F^- - F^+)\sin\tau$$

$$\mathcal{E}^\pm = 2E \mp \nabla_x E\cdot\nabla_v S$$

$$F^+(0,x,v,\tau) = f_{in}^+ - i\frac{\varepsilon}{2E}\left(b^i f_{in}^i(1-e^{-i\tau}) - b^i\overline{f_{in}^i}(1-e^{i\tau})\right)$$
$$F^-(0,x,v,\tau) = f_{in}^- + i\frac{\varepsilon}{2E}\left(b^i f_{in}^i(1-e^{-i\tau}) - b^i\overline{f_{in}^i}(1-e^{i\tau})\right)$$
$$G(0,x,v,\tau) = \mathrm{Re}(f_{in}^i) - \frac{\varepsilon}{2E}b^i(f_{in}^+ - f_{in}^-)\sin\tau$$
$$H(0,x,v,\tau) = \mathrm{Im}(f_{in}^i) + \frac{\varepsilon}{2E}b^i(f_{in}^+ - f_{in}^-)(\cos\tau - 1)$$

$$\partial_t \boldsymbol{g} + v\partial_x \boldsymbol{g} + A\partial_v \boldsymbol{g} + B\partial_\tau \boldsymbol{g} = C\boldsymbol{g}$$

$$A = \partial_x \mathrm{diag}(-U-E, -U+E, -U, -U), B = \mathrm{diag}\left(\frac{\mathcal{E}^+}{\varepsilon}, \frac{\mathcal{E}^-}{\varepsilon}, \frac{2E}{\varepsilon}, \frac{2E}{\varepsilon}\right),$$
$$C = \begin{bmatrix} 0 & 0 & 2b^i\cos\tau & 2b^i\sin\tau \\ 0 & 0 & -2b^i\cos\tau & -2b^i\sin\tau \\ -b^i\cos\tau & b^i\cos\tau & 0 & 0 \\ -b^i\sin\tau & b^i\sin\tau & 0 & 0 \end{bmatrix}.$$

$$\frac{d}{dt}\tilde{\boldsymbol{g}} = \Bigg(-i\Bigg(P_x \otimes I_4 \otimes \mathrm{diag}\Big\{\sum_j v_j|j\rangle\Big\} \otimes I_{M_\tau} + \sum_i |i\rangle\langle i| \otimes A(x_i) \otimes P_v \otimes I_{M_\tau}$$
$$+ \sum_{i,j} |i\rangle\langle i| \otimes B(t, x_i, v_j) \otimes I_{M_v} \otimes P_\tau\Bigg) + \sum_{i,j,k} |i\rangle\langle i| \otimes |j\rangle\langle j| \otimes |k\rangle\langle k| \otimes C(x_i, v_j, \tau_k)\Bigg)\tilde{\boldsymbol{g}}$$

$$\tilde{\boldsymbol{g}} = \sum_{i,j,k} \boldsymbol{g}(t, x_i, v_j, \tau_k)|i\rangle|j\rangle|k\rangle$$

$$H_1 = \sum_{i,j,k} |i\rangle\langle i| \otimes |j\rangle\langle j| \otimes |k\rangle\langle k| \otimes \frac{C(x_i, v_j, \tau_k) + C^T(x_i, v_j, \tau_k)}{2}$$

$$H_2 = -\Bigg(P_x \otimes I_4 \otimes \mathrm{diag}\Big\{\sum_j v_j|j\rangle\Big\} \otimes I_{M_\tau} + \sum_i |i\rangle\langle i| \otimes A(x_i) \otimes P_\tau \otimes I_{M_\tau}$$
$$+ \sum_i |i\rangle\langle i| \otimes B(x_i) \otimes I_{M_v} \otimes P_\tau\Bigg)$$
$$-i\sum_{i,j,k} |i\rangle\langle i| \otimes |j\rangle\langle j| \otimes |k\rangle\langle k| \otimes \frac{C(x_i, v_j, \tau_k) - C^T(x_i, v_j, \tau_k)}{2}$$

$$\lambda_n(H_1) = \frac{\|b^i\|_\infty}{\sqrt{2}}$$

$$f^+(0,x,v) = f^-(0,x,v) = \left(1+\frac{1}{2}\cos(x)\right)\frac{e^{-v^2/2}}{\sqrt{2\pi}}$$

$$f^i(0,x,v) = f^-(0,x,v) = \left(\left(1+\frac{1}{2}\sin(x)\right) + i\left(1+\frac{1}{2}\cos(x)\right)\right)\frac{e^{-v^2/2}}{\sqrt{2\pi}}$$

$$U(x) = 0, E(x) = 1-\cos(x/2)+\varepsilon, b^i(x,v) = -\frac{1}{2}\sin(v+1), b^\pm = 0$$

$$M_\tau = 2^k, M_v = 2^l, M_x = 2^m, M_p = 2^n$$

$$\rho^{\pm,i}(T,x,v) = \int_{-2\pi}^{2\pi} f^{\pm,i}(T,x,v)dp$$

$$\lambda_0 = \frac{\sqrt{2}}{4}$$

$$\partial_t u + \sum_{k=1}^{d} A_k(x)\partial_{x_k} u = \frac{iE(t,x)}{\varepsilon}Du + Cu$$

$$|\Psi_P\rangle_E = \mathcal{P}\exp\left\{i\int_{E_0}^{E} dp^- \mathcal{G}(p^-)\right\}|\Psi_P\rangle_{E_0}$$

$$\mathcal{G}(p^-) \equiv \int_p \delta\left(p^- - \frac{\boldsymbol{p}^2}{2p^+}\right) G(p^+,\boldsymbol{p}^2);$$

$$\begin{aligned} G(p^+,\boldsymbol{p}) = g\int_{k^-<p^-;(k-p)^-<p^-} & A_i^a(k^+,\boldsymbol{k})\frac{2p^+(k^+-p^+)}{k^+} \\ \times\Bigg\{ & \left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{p^+}-1\right)+\epsilon_{ki}\epsilon_{jl}\right]\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}A_l^\dagger(p^+,\boldsymbol{p})T^a A_k^\dagger(k^+-p^+,\boldsymbol{k}-\boldsymbol{p}) \\ - & \left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+-p^+}-1\right)+\epsilon_{ki}\epsilon_{jl}\right]\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}A_l^\dagger(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^a A_k^\dagger(p^+,\boldsymbol{p})\Bigg\} + \text{h.c.} \end{aligned}$$

$$\langle 0|A(p)A^\dagger(p)|0\rangle = \frac{(2\pi)^3}{2p^+}$$

$$G(p^+,\boldsymbol{p}) = A_i^\dagger(p^+,\boldsymbol{p})C_i(p^+,\boldsymbol{p}) + A_i(p^+,\boldsymbol{p})C_i^\dagger(p^+,\boldsymbol{p})$$

$$\begin{aligned} C_i^a(p^+,\boldsymbol{p}) = g\int_{p^->k^-,p^->(k-p)^-} & \frac{2p^+(k^+-p^+)}{k^+} \\ & \times\left\{\left[\delta_{kl}\delta_{ji}\left(\frac{2k^+}{p^+}-1\right)+\epsilon_{lk}\epsilon_{ji}\right]+\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+-p^+}-1\right)+\epsilon_{ik}\epsilon_{jl}\right]\right\} \\ & \times\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}A_l^\dagger(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^a A_k(k^+,\boldsymbol{k}) \end{aligned}$$

$$F^i_{lk}(k,p)=\frac{2p^+(k^+-p^+)}{k^+}\left\{\left[\delta_{kl}\delta_{ji}\left(\frac{2k^+}{p^+}-1\right)+\epsilon_{lk}\epsilon_{ji}\right]+\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+-p^+}-1\right)+\epsilon_{ik}\epsilon_{jl}\right]\right\}\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}$$
$$=\frac{4p^+(k^+-p^+)}{k^+}\left\{\delta_{kl}\delta_{ji}\frac{k^+}{p^+}+\delta_{ki}\delta_{jl}\frac{k^+}{k^+-p^+}-\delta_{kj}\delta_{il}\right\}\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}$$

$$C^a_i(p^+,\boldsymbol{p}) \;= g\int_{k^-<p^-;\,(k-p)^-<p^-} F^i_{lk}(k,p)A^\dagger_l(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^aA_k(k^+,\boldsymbol{k})$$
$$C^{a\dagger}_i(p^+,\boldsymbol{p}) \;= g\int_{k^-<p^-;\,(k+p)^-<p^-} F^i_{kl}(k+p,p)A^\dagger_l(k^++p^+,\boldsymbol{k}+\boldsymbol{p})T^aA_k(k^+,\boldsymbol{k})$$

$$S=1-\frac{1}{2(N_c^2-1)}\int_q \langle\Psi_T|\gamma_j^{\dagger b}(q)\gamma_j^b(q)|\Psi_T\rangle O(q)$$

$$\langle\Psi_T|\gamma_j^{\dagger b}(q)\gamma_j^b(q)|\Psi_T\rangle$$

$$O(q)=\langle\Psi_P|\mathcal{C}^a_i(q^-,\boldsymbol{q})\mathcal{C}^{a\dagger}_i(q^-,\boldsymbol{q})|\Psi_P\rangle_E$$
$$\mathcal{C}^{a\dagger}_i(q^-,\boldsymbol{q})=g\int_{k:k^-<q^-} f^i_{lk}(k,q)A^\dagger_l(k^+,\boldsymbol{k}+\boldsymbol{q})T^aA_k(k^+,\boldsymbol{k})$$

$$f^i_{jk}(k,q)=2k^+\frac{\boldsymbol{q}^i}{\boldsymbol{q}^2}\delta^{jk}+4k^+\epsilon^{il}\frac{\boldsymbol{q}^l}{\boldsymbol{q}^2}\epsilon^{jk}\frac{1}{\frac{2q^-k^+}{\boldsymbol{q}^2}-1}$$

$$O(q)=O_1(q)+O_2(q)$$

$$O_1(q) \;= g^2N_c\int_{k:k^-<q^-}\frac{1}{2k^+}f^i_{lk}(k,q)f^i_{lm}(k,q)\langle\Psi_P|A^{a\dagger}_k(k^+,\boldsymbol{k})A^a_m(k^+,\boldsymbol{k})|\Psi_P\rangle_E$$
$$O_2(q) \;= g^2\int_{\{k,l:(k-q)^-<q^-;k^-<q^-;(l-q)^-<q^-;l^-<q^-\}} f^i_{lk}(k,q)f^i_{nm}(l,q)$$
$$\times\langle\Psi_P|:A^\dagger_l(k^+,\boldsymbol{k}-\boldsymbol{q})T^aA_k(k^+,\boldsymbol{k})A^\dagger_m(l^+,\boldsymbol{l}+\boldsymbol{q})T^aA_n(l^+,\boldsymbol{l}):|\Psi_P\rangle_E$$

$$O_1(q)=\frac{g^2N_c}{2}\int_{k^-<q^-}\frac{dk^+}{2\pi}\frac{d^2\boldsymbol{k}}{(2\pi)^2}\frac{1}{(2k^+)^2}f^i_{lk}(k,q)f^i_{lk}(k,q)\mathcal{T}(k)$$

$$\left[f^{Ti}(k,q)f^i(k,q)\right]_{st}=\frac{(2k^+)^2}{\boldsymbol{q}^2}\left[1+\frac{4}{\left(\frac{2q^-k^+}{\boldsymbol{q}^2}-1\right)^2}\right]\delta_{st}$$

$$\hat{T}(k)\equiv a^{\dagger a}_i(k)a^a_i(k);\;\mathcal{T}(k)\equiv\langle\Psi_P|\hat{T}(k)|\Psi_P\rangle_E$$

$$\left[f^{Ti}(k,q)f^i(k,q)\right]_{st}\approx\frac{(2k^+)^2}{\boldsymbol{q}^2}\frac{1}{\epsilon}\delta(k^+-\bar{q}^+)\delta_{st}$$

$$\epsilon=\Delta q^-/\boldsymbol{q}^2$$

$$\bar{O}_1(q)=\frac{g^2N_c}{4\pi}\frac{1}{\boldsymbol{q}^2}\int_{\boldsymbol{k}^2<\boldsymbol{q}^2=2k^+E}\frac{d^2\boldsymbol{k}}{(2\pi)^2}\mathcal{T}\left(\boldsymbol{k},k^+=\frac{\boldsymbol{q}^2}{2q^-}\right)$$

$$k^-=\frac{\boldsymbol{k}^2}{2k^+}<E$$

$$\langle\hat{O}\rangle_E = \langle\Psi_P|\hat{O}|\Psi_P\rangle_E$$

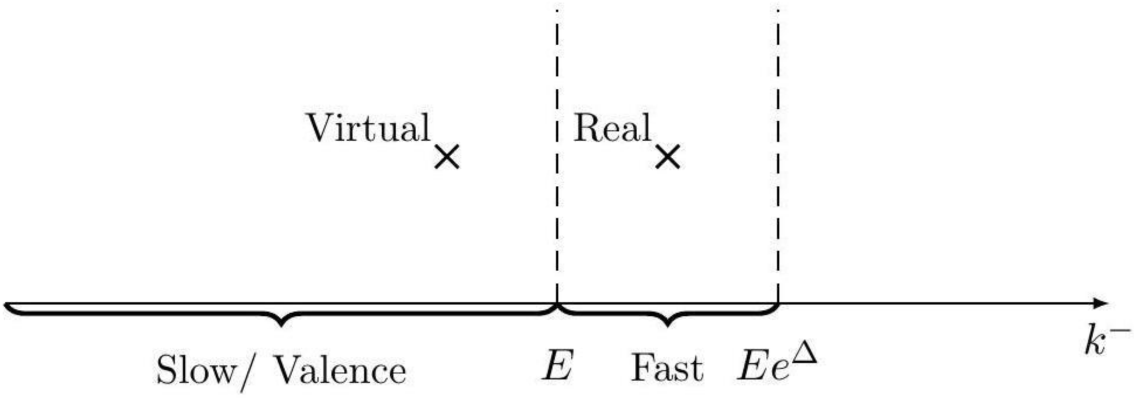
$$E < p^- < Ee^{\Delta}$$

$$\delta\langle\hat{O}\rangle \equiv \langle\hat{O}\rangle_{Ee^{\Delta}} - \langle\hat{O}\rangle_E$$

$$|\Psi_P\rangle_E = |0\rangle_F \otimes |\Psi_P\rangle_E$$

$$\frac{\partial\langle\hat{O}\rangle}{\partial\eta} = \lim_{\Delta\to 0}\frac{\delta\langle\hat{O}\rangle}{\Delta};\ \eta \equiv \ln\, E/E_0$$

$$\delta\langle\hat{O}\rangle = \langle\hat{O}\rangle_{Ee^{\Delta}}$$



$$\delta\langle\hat{O}\rangle = \int_{E<p^-<Ee^{\Delta}} \frac{d^3p}{(2\pi)^3}\frac{1}{2p^+}\left\langle C^\dagger(p)\hat{O}C(p) - \frac{1}{2}C^\dagger(p)C(p)\hat{O} - \frac{1}{2}\hat{O}C^\dagger(p)C(p)\right\rangle_E$$
$$= \frac{1}{2}\int_{E<p^-<Ee^{\Delta}} \frac{d^3p}{(2\pi)^3}\frac{1}{2p^+}\langle\{C^\dagger(p)[\hat{O},C(p)] + \text{h.c.}\}\rangle_E$$

$$\int \frac{dp^+d^2\boldsymbol{p}}{(2\pi)^3}f(p) = \int \frac{dp^+}{2\pi}\frac{1}{4\pi}\int dp^2 f(p) = \Delta\frac{1}{4\pi}\int \frac{dp^+}{2\pi}2p^+Ef(\boldsymbol{p}^2 = 2p^+E, p^+)$$
$$= \Delta\frac{1}{2\pi}\int \frac{d^2\boldsymbol{p}}{(2\pi)^2}\frac{\boldsymbol{p}^2}{2E}f\left(\boldsymbol{p}^2, p^+ = \frac{\boldsymbol{p}^2}{2E}\right)$$

$$\delta\mathcal{T}(k) \equiv \langle\hat{T}\rangle_{Ee^{\Delta}} - \langle\hat{T}\rangle_E;\ \delta\mathcal{T}(k) = \delta\mathcal{T}^L(k) + \delta\mathcal{T}^{NL}(k)$$

$$\delta\mathcal{T}^L(k) = \frac{g^2N_c}{2}\int_{k^-,(k\pm p)^-<E;E<p^-<Ee^{\Delta}}\int \frac{d^3p}{(2\pi)^3}\frac{1}{2p^+}\Big[\frac{1}{4k^+(k^++p^+)}F^l_{st}(k+p,p)F^l_{st}(k+p,p)\mathcal{T}(k+p)$$
$$-\frac{1}{4k^+(k^+-p^+)}F^l_{st}(k,p)F^l_{st}(k,p)\mathcal{T}(k)\Big]$$

$$\delta\mathcal{T}^{NL}(k) = \frac{g^2}{2}\int \frac{d^3p}{(2\pi)^3}\int \frac{d^3l}{(2\pi)^3}\frac{1}{2p^+}$$
$$\times\big[F^i_{lk}(l,p)F^i_{nm}(k+p,p)\langle\Psi_P|{:}A^\dagger_l(l^+-p^+,\boldsymbol{l}-\boldsymbol{p})T^aA_k(l^+,\boldsymbol{l})A^\dagger_m(k^++p^+,\boldsymbol{k}+\boldsymbol{p})T^aA_n(k^+,\boldsymbol{k}){:}|\Psi_P\rangle_E$$
$$-F^i_{lk}(l,p)F^i_{nm}(k,p)\langle\Psi_P|{:}A^\dagger_l(l^+-p^+,\boldsymbol{l}-\boldsymbol{p})T^aA_k(l^+,\boldsymbol{l})A^\dagger_m(k^+,\boldsymbol{k})T^aA_n(k^+-p^+,\boldsymbol{k}-\boldsymbol{p}){:}|\Psi_P\rangle_E\big] + h.c.$$

$$F^i_{ln}(k,p)F^i_{ln}(k,p) = 32(k^+)^2\zeta(1-\zeta)\left[\frac{\zeta}{1-\zeta} + \frac{1-\zeta}{\zeta} + \zeta(1-\zeta)\right]\frac{1}{\boldsymbol{p}^2};\ \zeta \equiv \frac{p^+}{k^+}$$

$$\int \frac{d^3p}{(2\pi)^3}\frac{1}{2p^+}\frac{1}{4k^+(k^+-p^+)}F_{st}^l(k,p)F_{st}^l(k,p)\mathcal{T}(\boldsymbol{k},x) = \frac{\Delta}{2\pi^2}\int_0^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\mathcal{T}(\boldsymbol{k},x)$$

$$\int \frac{d^3p}{(2\pi)^3}\frac{1}{2p^+}\frac{1}{4k^+(k^++p^+)}F_{st}^l(k+p,p)F_{st}^l(k+p,p)\mathcal{T}(\boldsymbol{k}+\boldsymbol{p},k^++p^+)$$
$$= \frac{\Delta}{2\pi^2}\int d\boldsymbol{n}\int_0^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\frac{1}{1-\zeta}\mathcal{T}\left(\boldsymbol{k}_\zeta,\frac{x}{1-\zeta}\right)$$

$$\zeta \equiv \frac{p^+}{k^++p^+}$$

$$\boldsymbol{k}_\zeta \equiv \boldsymbol{k}+\boldsymbol{n}\left[2Ek^+\frac{\zeta}{1-\zeta}\right]^{1/2}$$

$$\frac{\partial}{\partial\eta}\mathcal{T}(\boldsymbol{k},x) = -\frac{g^2N_c}{4\pi^2}\int_0^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\left[\mathcal{T}(\boldsymbol{k},x)-\frac{1}{1-\zeta}\int d\boldsymbol{n}\mathcal{T}\left(\boldsymbol{k}_\zeta,\frac{x}{1-\zeta}\right)\right]$$

$$\boldsymbol{k}^2 \gg 2k^+E\frac{\zeta}{1-\zeta}$$

$$\zeta < \frac{k^-/E}{1+k^-/E} \approx \frac{k^-}{E}$$

$$\frac{\partial}{\partial\eta}\mathcal{T}(\boldsymbol{k},x) = -\frac{g^2N_c}{4\pi^2}\int_{\frac{k^-}{E}}^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\mathcal{T}(\boldsymbol{k},x)+\cdots$$

$$\ln\left(\frac{\boldsymbol{k}^2}{\boldsymbol{p}^2}\right)-\ln\left(\frac{p^+}{k^+}\right)$$

$$\frac{\partial T(k^+,\boldsymbol{k}^2;\mu^2;\xi)}{\partial \ln\,\mu^2} = -\frac{\alpha_s}{2\pi}N_c\int_{\xi/k^+}^{1-\xi/k^+} d\zeta\left[\frac{1-\zeta}{\zeta}+\frac{\zeta}{1-\zeta}+\zeta(1-\zeta)\right]T(k^+,\boldsymbol{k}^2;\mu^2;\xi)$$
$$\frac{\partial T(k^+,\boldsymbol{k}^2;\mu^2;\xi)}{\partial \ln\,\frac{1}{\xi}} = -\frac{\alpha_s}{2\pi}2N_c\int_{\boldsymbol{k}^2}^{\mu^2}\frac{dp^2}{p^2}T(k^+,\boldsymbol{k}^2;\mu^2;\xi)$$

$$\mathcal{T}(\boldsymbol{k},k^+;E) = T(k^+,\boldsymbol{k};\mu^2(E);\xi(E))$$

$$\ln\frac{\mu^2(E)}{\boldsymbol{k}^2} = \frac{1}{\sqrt{2}}a\ln\frac{E}{k^-};\ \ln\frac{k^+}{\xi(E)} = \frac{1}{\sqrt{2}}\frac{1}{a}\ln\frac{E}{k^-}$$

$$\frac{\partial}{\partial \ln\,E}\mathcal{T}(\boldsymbol{k},k^+;E) = \left[\frac{\partial \ln\,\mu^2}{\partial \ln\,E}\frac{\partial}{\partial \ln\,\mu^2}+\frac{\partial \ln\,1/\xi}{\partial \ln\,E}\frac{\partial}{\partial \ln\,1/\xi}\right]T(\boldsymbol{k},k^+;\mu^2(E),\xi(E))$$

$$\ln\frac{\mu^2}{\boldsymbol{k}^2} = 2\ln\frac{k^+}{\xi}$$

$$\ln\frac{\mu^2(E)}{\boldsymbol{k}^2} = \frac{1}{\sqrt{2}}a\ln\frac{E}{k^-};\ \ln\frac{k^+}{\xi(E)}-\frac{11}{12} = \frac{1}{\sqrt{2}}\frac{1}{a}\left[\ln\frac{E}{k^-}-\frac{11}{12}\right]$$

$$\langle\Psi_P|:A_l^{\dagger b}(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^a_{bc}A^c_k(k^+,\boldsymbol{k})A_m^{\dagger d}(l^++p^+,\boldsymbol{l}+\boldsymbol{p})T^a_{de}A^e_n(l^+,\boldsymbol{l}):|\Psi_P\rangle_E$$
$$=\frac{1}{4V(N_c^2-1)^2}\delta^3(k-l-p)\delta^{km}\delta^{ln}\delta^{cd}\delta^{be}T^a_{bc}T^a_{de}$$
$$\times\langle\Psi_P|:\left[A^\dagger(l^+,\boldsymbol{l})A(l^+,\boldsymbol{l})\right]\left[A^\dagger(l^++p^+,\boldsymbol{l}+\boldsymbol{p})A(l^++p^+,\boldsymbol{l}+\boldsymbol{p})\right]:|\Psi_P\rangle_E$$
$$=\frac{N_c}{4V(N_c^2-1)}\delta^3(k-l-p)\delta^{km}\delta^{ln}\langle\Psi_P|:\left[A^\dagger(l^+,\boldsymbol{l})A(l^+,\boldsymbol{l})\right]\left[A^\dagger(l^++p^+,\boldsymbol{l}+\boldsymbol{p})A(l^++p^+,\boldsymbol{l}+\boldsymbol{p})\right]:|\Psi_P\rangle_E$$

$$(|\Psi_P\rangle=|k_1,k_2,\dots k_n\rangle)$$

$$|\Phi\rangle=\int_{\boldsymbol{q},\boldsymbol{s}}\Phi(\boldsymbol{q},\boldsymbol{s})|\boldsymbol{q},\boldsymbol{s}\rangle$$

$$\langle\Phi|A^\dagger(\boldsymbol{k}-\boldsymbol{p})A^\dagger(\boldsymbol{l}+\boldsymbol{p})A(\boldsymbol{l})A(\boldsymbol{k})|\Phi\rangle=\Phi^*(\boldsymbol{k}-\boldsymbol{p},\boldsymbol{l}+\boldsymbol{p})\Phi(\boldsymbol{k},\boldsymbol{l})$$

$$\Phi(\boldsymbol{k},\boldsymbol{l})\;=\int_{\boldsymbol{x}^2<R^2,\boldsymbol{y}^2<R^2}e^{i\boldsymbol{k}\cdot\boldsymbol{x}+i\boldsymbol{l}\cdot\boldsymbol{y}}\chi_1(\boldsymbol{x}+\boldsymbol{y})\chi_2(\boldsymbol{x}-\boldsymbol{y})$$
$$\approx\int_{|\boldsymbol{x}+\boldsymbol{y}|<R}e^{\frac{i}{2}(\boldsymbol{k}+\boldsymbol{l})\cdot(\boldsymbol{x}+\boldsymbol{y})}\chi_1(\boldsymbol{x}+\boldsymbol{y})\int_{|\boldsymbol{x}-\boldsymbol{y}|<R}e^{\frac{i}{2}(\boldsymbol{k}-\boldsymbol{l})\cdot(\boldsymbol{x}-\boldsymbol{y})}\chi_2(\boldsymbol{x}-\boldsymbol{y})$$
$$\approx\bar{\chi}_1(\boldsymbol{k}+\boldsymbol{l})e^{i|\boldsymbol{k}-\boldsymbol{l}|R}\psi(\boldsymbol{k}-\boldsymbol{l})$$

$$\Phi^*(\boldsymbol{k}-\boldsymbol{p},\boldsymbol{l}+\boldsymbol{p})\Phi(\boldsymbol{k},\boldsymbol{l})\propto e^{iR(|\boldsymbol{k}-\boldsymbol{l}|-|\boldsymbol{k}-\boldsymbol{l}+2\boldsymbol{p}|)}$$

$$|\boldsymbol{k}|\sim|\boldsymbol{l}|\sim|\boldsymbol{p}|\gg\frac{1}{R}$$

$$\langle\Psi_P|:A_l^{\dagger b}(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^a_{bc}A^c_k(k^+,\boldsymbol{k})A_m^{\dagger d}(l^++p^+,\boldsymbol{l}+\boldsymbol{p})T^a_{de}A^e_n(l^+,\boldsymbol{l}):|\Psi_P\rangle_E$$
$$=\frac{N_c}{4S_\perp(N_c^2-1)}\sqrt{l^+(l^++p^+)}\delta^3(k-l-p)\delta^{km}\delta^{ln}$$
$$\times\langle\Psi_P|:\left[A^\dagger(l^+,\boldsymbol{l})A(l^+,\boldsymbol{l})\right]\left[A^\dagger(l^++p^+,\boldsymbol{l}+\boldsymbol{p})A(l^++p^+,\boldsymbol{l}+\boldsymbol{p})\right]:|\Psi_P\rangle_E$$

$$\delta\mathcal{T}^{NL}(k)=\frac{g^2N_c}{(2\pi)^3}\frac{1}{4S_\perp(N_c^2-1)}\int\frac{d^3p}{(2\pi)^3}\frac{1}{2p^+}\frac{1}{2k^+}$$
$$\times\left[\frac{\sqrt{k^+(k^++p^+)}}{2(k+p)^+}F^i_{lk}(k+p,p)F^i_{lk}(k+p,p)\mathcal{T}_2(k,k+p)-\frac{\sqrt{k^+(k^+-p^+)}}{2(k-p)^+}F^i_{lk}(k,p)F^i_{lk}(k,p)\mathcal{T}_2(k,k-p)\right]$$

$$\mathcal{T}_2(k,q)\equiv\langle\Psi_P|:\left[a^\dagger(k^+,\boldsymbol{k})a(k^+,\boldsymbol{k})\right]\left[a^\dagger(q^+,\boldsymbol{q})a(q^+,\boldsymbol{q})\right]:|\Psi_P\rangle_E$$

$$\mathcal{T}_2(k,q)\approx\mathcal{T}(k)\mathcal{T}(q)$$

$$\frac{\partial}{\partial\eta}\mathcal{T}(\boldsymbol{k},x)=-\frac{g^2N_c}{4\pi^2}\int_0^{1/2}d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]$$
$$\times\left[\mathcal{T}(\boldsymbol{k},x)\left\{1+\frac{x\sqrt{1-\zeta}}{16\pi^2S_\perp(N_c^2-1)}\int d\boldsymbol{n}\mathcal{T}\left(\boldsymbol{k}_{\zeta'},(1-\zeta)x\right)\right\}\right.$$
$$\left.-\frac{1}{1-\zeta}\int d\boldsymbol{n}\mathcal{T}\left(\boldsymbol{k}_\zeta,\frac{x}{1-\zeta}\right)\left\{1+\frac{x}{16\pi^2S_\perp(N_c^2-1)\sqrt{1-\zeta}}\mathcal{T}(\boldsymbol{k},x)\right\}\right]$$

$$\boldsymbol{k}_\zeta = \boldsymbol{k} + \boldsymbol{n}\left[2k^+E\frac{\zeta}{1-\zeta}\right]^{1/2} = \boldsymbol{k} + \boldsymbol{n}\left[\boldsymbol{k}^2\frac{E}{k^-}\frac{\zeta}{1-\zeta}\right]^{1/2}$$

$$\boldsymbol{k}_{\zeta'} = \boldsymbol{k} + \boldsymbol{n}[2k^+E\zeta]^{1/2} = \boldsymbol{k} + \boldsymbol{n}\left[\boldsymbol{k}^2\frac{E}{k^-}\zeta\right]^{1/2}$$

$$\mathcal{T}(\boldsymbol{q}, q^+) \propto \frac{1}{\boldsymbol{q}^2}\frac{1}{q^+}\zeta > \frac{k^-}{E}$$

$$(1-\zeta)^{1/2}\mathcal{T}\big(\boldsymbol{k}_{\zeta'}, (1-\zeta)x\big) - \frac{1}{(1-\zeta)^{3/2}}\mathcal{T}\left(\boldsymbol{k}_\zeta, \frac{x}{1-\zeta}\right)$$

$$\approx \frac{1}{(1-\zeta)^{1/2}}\mathcal{T}\left(\boldsymbol{n}\left[\boldsymbol{k}^2\frac{E}{k^-}\zeta\right]^{1/2}, x\right) - (1-\zeta)^{1/2}\mathcal{T}\left(\boldsymbol{n}\left[\boldsymbol{k}^2\frac{E}{k^-}\zeta\right]^{1/2}, x\right) \approx \zeta\mathcal{T}\left(\boldsymbol{n}\left[\boldsymbol{k}^2\frac{E}{k^-}\zeta\right]^{1/2}, x\right)$$

$$\begin{aligned}
&-\frac{g^2N_c}{4\pi^2}\int_0^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta} + \frac{1-\zeta}{\zeta} + \zeta(1-\zeta)\right]\mathcal{T}(\boldsymbol{k}, x) \\
&\quad\times\frac{x}{16\pi^2S_\perp(N_c^2-1)}\int d\boldsymbol{n}\left\{(1-\zeta)^{1/2}\mathcal{T}\big(\boldsymbol{k}_{\zeta'}, (1-\zeta)x\big) - \frac{1}{(1-\zeta)^{3/2}}\int \mathcal{T}\left(\boldsymbol{k}_\zeta, \frac{x}{1-\zeta}\right)\right\} \\
&\quad= -\frac{g^2N_c}{4\pi^2}\frac{x}{16\pi^2S_\perp(N_c^2-1)}\mathcal{T}(\boldsymbol{k}, x)\int_{\boldsymbol{k}^-/E}^{1/2} d\zeta\int d\boldsymbol{n}\mathcal{T}\left(\boldsymbol{n}\left[\boldsymbol{k}^2\frac{E}{k^-}\zeta\right]^{1/2}, x\right) \\
&\quad= -\frac{g^2N_c}{4\pi^2}\frac{x}{4\pi S_\perp(N_c^2-1)}\frac{1}{\boldsymbol{k}^2}\frac{k^-}{E}\mathcal{T}(\boldsymbol{k}, x)\int_{\boldsymbol{p}^2=\boldsymbol{k}^2}^{\boldsymbol{p}^2=k^+E}\frac{d^2\boldsymbol{p}}{(2\pi)^2}\mathcal{T}(\boldsymbol{p}, x)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial}{\partial\eta}\mathcal{T}(\boldsymbol{k}, x) = &-\frac{g^2N_c}{4\pi^2}\left[\int_{k^-/E}^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta} + \frac{1-\zeta}{\zeta} + \zeta(1-\zeta)\right]\right. \\
&\left. + \frac{x}{4\pi S_\perp(N_c^2-1)}\frac{1}{\boldsymbol{k}^2}\frac{k^-}{E}\int_{\boldsymbol{p}^2=\boldsymbol{k}^2}^{\boldsymbol{p}^2=k^+E}\frac{d^2\boldsymbol{p}}{(2\pi)^2}\mathcal{T}(\boldsymbol{p}, x)\right]\mathcal{T}(\boldsymbol{k}, x)
\end{aligned}$$

$$\begin{aligned}
\frac{\partial}{\partial\eta}[x\mathcal{T}(\boldsymbol{k}, x)] = &-\frac{g^2N_c}{4\pi^2}\left[\int_{\boldsymbol{k}^2/Q^2}^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta} + \frac{1-\zeta}{\zeta} + \zeta(1-\zeta)\right]\right. \\
&\left. + \frac{1}{4\pi(N_c^2-1)}\frac{1}{Q^2S_\perp}\int_{\boldsymbol{p}^2=\boldsymbol{k}^2}^{\boldsymbol{p}^2=Q^2}\frac{d^2\boldsymbol{p}}{(2\pi)^2}[x\mathcal{T}(\boldsymbol{p}, x)]\right][x\mathcal{T}(\boldsymbol{k}, x)]
\end{aligned}$$

$$\delta\langle\hat{O}\rangle = \int_{p,\bar{p}:p^-=\bar{p}^-=E}\langle\Psi_P|C_i^{\dagger a}(p)\langle 0|A_i^a(p)\hat{O}A_j^{\dagger b}(\bar{p})|0\rangle_F C_j^b(\bar{p})|\Psi_P\rangle_E$$

$$\delta\mathcal{T}(\boldsymbol{k}, k^+; k^- = E) = \frac{1}{2k^+}\langle\Psi_P|C_i^{\dagger a}(k)C_i^a(k)|\Psi_P\rangle_E$$

$$\begin{aligned}
\delta\mathcal{T}(\boldsymbol{k}, k^+; k^- = E) = &\frac{g^2N_c}{4\pi^3}\frac{1}{\boldsymbol{k}^2}\int d^2\boldsymbol{q}\int_x^{\min\left(\frac{\boldsymbol{k}^2}{\boldsymbol{q}^2}, \frac{\boldsymbol{k}^2}{\boldsymbol{k}^2+(\boldsymbol{q}-\boldsymbol{k})^2}\right)} d\zeta\frac{1}{\zeta}\left[\frac{\zeta}{1-\zeta} + \frac{1-\zeta}{\zeta} + \zeta(1-\zeta)\right] \\
&\times\mathcal{T}\left(\boldsymbol{q}, \frac{k^+}{\zeta}\right)\left[1 + \frac{1}{16\pi^2S_\perp(N_c^2-1)}\frac{k^+(1-\zeta)^{1/2}}{\zeta}\mathcal{T}\left(\boldsymbol{q}-\boldsymbol{k}, k^+\frac{1-\zeta}{\zeta}\right)\right]
\end{aligned}$$

$$\delta[x\mathcal{T}(\boldsymbol{k},x;k^-=E)]=\frac{g^2N_c}{4\pi^3}\frac{1}{\boldsymbol{k}^2}\int d^2\boldsymbol{q}\int_x^{\min\left(\frac{\boldsymbol{k}^2}{\boldsymbol{q}^2},\frac{\boldsymbol{k}^2}{\boldsymbol{k}^2+(\boldsymbol{q}-\boldsymbol{k})^2}\right)} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]$$
$$\times\left[\frac{x}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)\right]\left[1+\frac{1}{16\pi^2S_\perp(N_c^2-1)}\frac{1}{(1-\zeta)^{1/2}}\left[x\frac{1-\zeta}{\zeta}\mathcal{T}\left(\boldsymbol{q}-\boldsymbol{k},x\frac{1-\zeta}{\zeta}\right)\right]\right]$$

$$\boldsymbol{q}^2=(\boldsymbol{q}-\boldsymbol{k})^2\gg\boldsymbol{k}^2$$

$$\zeta<\boldsymbol{k}^2/\boldsymbol{q}^2$$

$$\delta[x\mathcal{T}(\boldsymbol{k},x;k^-=E)]=\delta[x\mathcal{T}(\boldsymbol{k},x;k^-=E)]^{DGLAP}+\delta[x\mathcal{T}(\boldsymbol{k},x;k^-=E)]^{BFKL}$$

$$\delta[x\mathcal{T}(\boldsymbol{k},x;k^-=E)]^{DGLAP}=\frac{g^2N_c}{4\pi^3}\frac{1}{\boldsymbol{k}^2}\int_x^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]$$
$$\times\int^{\boldsymbol{q}^2<\boldsymbol{k}^2} d^2\,d^2\boldsymbol{q}\left[\frac{x}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)\right]\left[1+\frac{1}{16\pi^2S_\perp(N_c^2-1)}\frac{1}{(1-\zeta)^{1/2}}\left[x\frac{1-\zeta}{\zeta}\mathcal{T}\left(\boldsymbol{k},x\frac{1-\zeta}{\zeta}\right)\right]\right]$$

$$\delta[x\mathcal{T}(\boldsymbol{k},x;k^-=E)]^{BFKL}=\frac{g^2N_c}{4\pi^3}\frac{1}{\boldsymbol{k}^2}\int_x^1 d\zeta\frac{1}{\zeta}\int_{\boldsymbol{q}^2=\boldsymbol{k}^2}^{\boldsymbol{q}^2=\frac{\boldsymbol{k}^2}{\zeta}} d^2\boldsymbol{q}\left[\frac{x}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)\right]$$

$$\ln\ 1/x\ln\ \frac{\boldsymbol{k}^2}{\Lambda_{QCD}^2}$$

$$\ln\ k^-/E_0-\Delta/2\ln\ k^-/E_0+\Delta/2$$

$$\frac{\partial}{\partial\eta}\left[x\mathcal{T}_{\text{real}}^{\text{DGLAP}}(\boldsymbol{k},x)\right]=\frac{g^2N_c}{4\pi^3}\frac{1}{\boldsymbol{k}^2}\int_x^{1/2} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]$$
$$\times\int^{\boldsymbol{q}^2<\boldsymbol{k}^2} d^2\,d^2\boldsymbol{q}\left[\frac{x}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)\right]\left[1+\frac{1}{16\pi^2S_\perp(N_c^2-1)}\frac{1}{(1-\zeta)^{1/2}}\left[x\frac{1-\zeta}{\zeta}\mathcal{T}\left(\boldsymbol{k},x\frac{1-\zeta}{\zeta}\right)\right]\right]\delta\left(\eta-\ln\ \frac{k^-}{E_0}\right)$$

$$\frac{\partial}{\partial\eta}\left[x\mathcal{T}_{\text{real}}^{\text{BFKL}}(\boldsymbol{k},x)\right]=\frac{g^2N_c}{4\pi^3}\frac{1}{\boldsymbol{k}^2}\int_x^1 d\zeta\frac{1}{\zeta}\int_{\boldsymbol{q}^2=\boldsymbol{k}^2}^{\boldsymbol{q}^2=\frac{\boldsymbol{k}^2}{\zeta}} d^2\boldsymbol{q}\left[\frac{x}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)\right]\delta\left(\eta-\ln\ \frac{k^-}{E_0}\right)$$

$$G(x,E)\equiv\int d^2\boldsymbol{k}\mathcal{T}(\boldsymbol{k},k^+;E)=\int_0^{2k^+E} d^2\boldsymbol{k}\mathcal{T}(\boldsymbol{k},k^+;E)$$

$$Q^2=2k^+E=2xs,x=k^+/P^+$$

$$\frac{\partial}{\partial\ln\ E}G(x,E)=(2k^+E)\pi\mathcal{T}(\boldsymbol{k}^2=2k^+E,k^+;E)+\int_0^{2k^+E} d^2\boldsymbol{k}\frac{\partial}{\partial\ln\ E}\mathcal{T}(\boldsymbol{k},k^+;E)$$

$$\frac{g^2N_c}{2}\int\frac{d^3p}{(2\pi)^3}\frac{1}{2p^+}\frac{1}{4k^+(k^++p^+)}F_{st}^l(k+p,p)F_{st}^l(k+p,p)\mathcal{T}(\boldsymbol{k}+\boldsymbol{p},k^++p^+)$$
$$=\frac{g^2N_c}{2}\frac{\Delta}{\pi}\frac{1}{Ek^+}\int\frac{d^2\boldsymbol{p}}{(2\pi)^2}\bar{\zeta}\left[\frac{\bar{\zeta}}{1-\bar{\zeta}}+\frac{1-\bar{\zeta}}{\bar{\zeta}}+\bar{\zeta}(1-\bar{\zeta})\right]\mathcal{T}\left(\boldsymbol{k}+\boldsymbol{p},\frac{x}{\bar{\zeta}}\right)$$

$$\bar{\zeta}\equiv\frac{k^+}{k^++p^+}=\frac{1}{1+\frac{p^2}{2Ek^+}}$$

$$\frac{g^2N_c}{2}\int d^2\boldsymbol{k}\frac{\Delta}{\pi}\frac{1}{Ek^+}\int \frac{d^2\boldsymbol{p}}{(2\pi)^2}\bar{\zeta}\left[\frac{\bar{\zeta}}{1-\bar{\zeta}}+\frac{1-\bar{\zeta}}{\bar{\zeta}}+\bar{\zeta}(1-\bar{\zeta})\right]\mathcal{T}\left(\boldsymbol{k}+\boldsymbol{p},\frac{x}{\bar{\zeta}}\right)$$

$$=\frac{g^2N_c}{2}\frac{\Delta}{2\pi^2}\int d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\int_\Omega d^2\boldsymbol{q}\frac{1}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)$$

$$q^- < E;\ (q-p)^- < E$$

$$\boldsymbol{q}^2 < \frac{2Ek^+}{\zeta};\ \text{or } \zeta < \frac{2\mathrm{E}k^+}{\mathrm{q}^2}$$

$$\boldsymbol{q}^2+\boldsymbol{p}^2-2|\boldsymbol{p}||\boldsymbol{q}|\cos\phi < 2Ek^+;\ \frac{\boldsymbol{q}^2}{2Ek^+}-2\sqrt{\frac{\boldsymbol{q}^2}{2Ek^+}}\sqrt{\frac{1-\zeta}{\zeta}}\cos\phi < \frac{2\zeta-1}{\zeta}$$

$$q^2 \ll 2Ek^+\frac{1-\zeta}{\zeta}$$

$$\frac{1}{2}<\zeta<1$$

$$\log Q^2/\Lambda_{QCD}^2$$

$$\frac{1}{2}+\beta_-\left(\cos\phi,\frac{\boldsymbol{q}^2}{2Ek^+}\right)<\zeta<1+\beta_+\left(\cos\phi,\frac{\boldsymbol{q}^2}{2Ek^+}\right)$$

$$\ln\left(2Ek^+/\Lambda_{QCD}^2\right)$$

$$\frac{\boldsymbol{q}^2}{2Ek^+}<\frac{1}{\zeta}-2\sqrt{\frac{1-\zeta}{\zeta}}$$

$$\frac{\boldsymbol{q}^2}{2Ek^+}>\frac{1}{\zeta}+2\sqrt{\frac{1-\zeta}{\zeta}}$$

$$\ln\frac{Q^2}{\Lambda_{QCD}^2}$$

$$\cos\phi>\frac{1}{2}\sqrt{\frac{\boldsymbol{q}^2}{2Ek^+}}$$

$$\boldsymbol{q}^2=4Ek^+\ -\frac{\pi}{4}<\phi<\frac{\pi}{4}$$

$$\frac{g^2N_c}{2}\int d^2\boldsymbol{k}\frac{\Delta}{\pi}\frac{1}{Ek^+}\int \frac{d^2\boldsymbol{p}}{(2\pi)^2}\bar{\zeta}^2\frac{1}{\bar{\zeta}}\left[\frac{\bar{\zeta}}{1-\bar{\zeta}}+\frac{1-\bar{\zeta}}{\bar{\zeta}}+\bar{\zeta}(1-\bar{\zeta})\right]\mathcal{T}\left(\boldsymbol{k}+\boldsymbol{p},\frac{x}{\bar{\zeta}}\right)$$

$$\approx\frac{g^2N_c}{2}\frac{\Delta}{2\pi^2}\int_{1/2}^{1} d\zeta\frac{1}{\zeta}\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\int_0^{2Ek^+/\zeta} d^2\boldsymbol{q}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)$$

$$\frac{\partial}{\partial\ln Q^2}[xG(x,E)]^{\text{gain}}=\frac{g^2N_c}{4\pi^2}\int_{1/2}^{1} d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\int_0^{Q^2/\zeta} d^2\boldsymbol{q}\left[\frac{x}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{x}{\zeta}\right)\right]$$

$$-\frac{g^2N_c}{2}\int\frac{d^3p}{(2\pi)^3}\frac{1}{8p^+k^+(k^+-p^+)}F_{st}^l(k,p)F_{st}^l(k,p)\mathcal{T}(k)$$
$$=-\Delta\frac{g^2N_c}{8\pi^2}\int_0^1 d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\mathcal{T}(\boldsymbol{k},x)$$

$$\frac{\partial}{\partial\ln\,Q^2}[xG(x,E)]^{loss}=-\frac{g^2N_c}{8\pi^2}\int_0^1 d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\int_0^{Q^2}d^2\boldsymbol{k}[x\mathcal{T}(\boldsymbol{k},x)]$$

$$q^-<E;\;(q-k)^-<E$$

$$\boldsymbol{q}^2<2Ek^+/\zeta$$

$$\frac{\boldsymbol{q}^2}{2Ek^+}-2\sqrt{\frac{\boldsymbol{q}^2}{2Ek^+}}\cos\,\phi<\frac{1-2\zeta}{\zeta}$$

$$\zeta<\frac{1}{2}$$

$$\frac{\boldsymbol{q}^2}{2Ek^+}<\frac{1}{\zeta}-2\sqrt{\frac{1-\zeta}{\zeta}}$$

$$\frac{\boldsymbol{q}^2}{2Ek^+}>\frac{1}{\zeta}+2\sqrt{\frac{1-\zeta}{\zeta}}$$

$$Q^2\pi\mathcal{T}(\boldsymbol{k}^2=Q^2,k^+,E)=\frac{g^2N_c}{4\pi^2}\int_x^{1/2}d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\int^{Q^2/\zeta}\frac{d^2\boldsymbol{q}}{(2\pi)^2}\frac{d^2\boldsymbol{q}}{(2\pi)^2}\frac{1}{\zeta}\mathcal{T}\left(\boldsymbol{q},\frac{k^+}{\zeta}\right)$$

$$P_{gg}(\zeta)=\left[\frac{\zeta}{1-\zeta}\right]_++\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)$$

$$\frac{\partial}{\partial\ln\,Q^2}[xG(x,Q^2)]=\frac{\alpha_s}{2\pi}\int_x^1 d\zeta P_{gg}(\zeta)\left[\frac{x}{\zeta}G\left(\frac{x}{\zeta},\frac{Q^2}{\zeta}\right)\right]$$

$$\frac{\partial}{\partial\ln\,Q^2}G(x,Q^2)=Q^2\pi T(\boldsymbol{k}^2=Q^2,x;Q^2,\xi)+\int_k\frac{\partial}{\partial Q^2}T(\boldsymbol{k}^2,x;Q^2,\xi)$$

$$\left(\frac{k^+}{\zeta},\boldsymbol{q}^2\right)\to(k^+,Q^2)+\left(\frac{k^+}{\zeta},\boldsymbol{q}^2\right)\text{with }Q^2\ll\boldsymbol{q}^2\ll\frac{Q^2}{\zeta}$$

$$\int_{\boldsymbol{k}^2}^{Q^2}d^2\boldsymbol{p}\mathcal{T}(\boldsymbol{p},x)\mathcal{T}(\boldsymbol{k},x)=\frac{1}{\pi}\frac{\partial}{\partial\boldsymbol{k}^2}\left[\int_0^{Q^2}d^2\boldsymbol{p}\mathcal{T}(\boldsymbol{p},x)\int_0^{\boldsymbol{k}^2}d^2\boldsymbol{q}\mathcal{T}(\boldsymbol{q},x)-\frac{1}{2}\left[\int_0^{\boldsymbol{k}^2}d^2\boldsymbol{q}\mathcal{T}(\boldsymbol{q},x)\right]^2\right]$$

$$\int^{Q^2}d^2\,d^2\boldsymbol{k}\int_{\boldsymbol{k}^2}^{Q^2}d^2\boldsymbol{p}\mathcal{T}(\boldsymbol{p},x)\mathcal{T}(\boldsymbol{k},x)=\frac{1}{2}\left[\int_0^{Q^2}d^2\boldsymbol{p}\mathcal{T}(\boldsymbol{p},x)\right]^2=\frac{1}{2}G^2(Q^2,x)$$

$$\frac{\partial}{\partial\ln\,Q^2}[xG(Q^2,x)]_{virt}^{NL}=-\frac{\alpha_sN_c}{4\pi}\frac{1}{(2\pi)^3}\frac{1}{N_c^2-1}\frac{1}{Q^2S_\perp}[xG(Q^2,x)]^2$$

$$\frac{1}{(1-\zeta)^{1/2}}x\frac{1-\zeta}{\zeta}\mathcal{T}\left(\boldsymbol{k},x\frac{1-\zeta}{\zeta}\right)\approx\sqrt{2}x\mathcal{T}(\boldsymbol{k},x)$$

$$\frac{\alpha_s N_c}{\pi^2}\frac{\sqrt{2}}{16\pi^2}\frac{1}{Q^2 S_\perp(N_c^2-1)}\int_x^{1/2}d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\left[\frac{x}{\zeta}G\left(Q^2,\frac{x}{\zeta}\right)\right][x\mathcal{T}(\boldsymbol{k},x)]$$

$$\frac{\partial}{\partial E}[xG(Q^2,x)]_{real}^{NL}=\frac{\alpha_s^2 N_c}{\pi^3}\frac{\sqrt{2}}{16\pi^2}\frac{1}{Q^2 S_\perp(N_c^2-1)}\int_x^{1/2}d\zeta\left[\frac{\zeta}{1-\zeta}+\frac{1-\zeta}{\zeta}+\zeta(1-\zeta)\right]\left[\frac{x}{\zeta}G\left(Q^2,\frac{x}{\zeta}\right)\right]$$
$$\times\int_x^{1/2}d\xi\left[\frac{\xi}{1-\xi}+\frac{1-\xi}{\xi}+\xi(1-\xi)\right]\left[\frac{x}{\xi}G\left(\frac{Q^2}{\xi},\frac{x}{\xi}\right)\right]$$

$$\ln\frac{Q^2}{\boldsymbol{k}^2}=\frac{1}{2}\ln\frac{k^+}{\xi}$$

$$\frac{1}{N_c^2-1}\frac{1}{Q^2 S_\perp}S_\perp\sim\frac{1}{\Lambda_{QCD}^2}$$

$$\boldsymbol{k}^2>\frac{\Lambda_{QCD}^2}{\alpha_s}$$

$$\Lambda_{QCD}<|\boldsymbol{k}|<\frac{\Lambda_{QCD}}{g}$$

$$\int_k\equiv\int\frac{d^2\boldsymbol{k}dk^+}{(2\pi)^3}$$

$$\mathcal{T}(\boldsymbol{k},k^+)\equiv P^+\mathcal{T}(\boldsymbol{k},x)$$

$$|\Psi_{in}\rangle=|\Psi_P\rangle\otimes|\Psi_T\rangle$$

$$\hat{S}=\lim_{\tau\to\infty}\mathcal{T}\exp\left\{i\int_0^\tau dx^+H_{PT}^I(x^+)\right\}$$

$$U(0,\tau)=\mathcal{T}\exp\left\{i\int_0^\tau dx^+H_{SF}^I(x^+)\right\}$$

$$\Omega=\lim_{\tau\to\infty}U(0,\tau)$$

$$|\Psi_P\rangle=\Omega|0\rangle_F\otimes|\psi_0\rangle_S$$

$$\mathcal{L}_{YM}=-\frac{1}{4}F_a^{\mu\nu}F_{\mu\nu}^a=\frac{1}{2}(F^{+-})^2+F^{+i}F^{-i}-\frac{1}{4}F^{ij}F_{ij}$$

$$F^{+-}=\partial^+A^- - D^-A^+;\quad F^{+i}=\partial^+A^i-D^iA^+$$
$$F^{-i}=\partial^-A^i-D^iA^-;\quad F^{ij}=\partial^iA^j-D^jA^i$$

$$D^{ab}A^b=\partial A^a-gf^{abc}A^bA^c$$

$$D^-F^{+-}+D^iF^{-i}=D^-\partial^+A^-+D^i\left[\partial^-A^i-D^iA^-\right]=\partial^-\partial^+A^- -\partial^2A^-+\partial^i\partial^-A^i+O(g)=0$$

$$\Pi_i^a(x)=\partial^+A_i^a(x)$$

$$H = \frac{1}{2}\int_{x^-,\boldsymbol{x}} [\Pi^a(x^-,\boldsymbol{x})\Pi^a(x^-,\boldsymbol{x}) + B(x^-,\boldsymbol{x})B(x^-,\boldsymbol{x})]$$

$$\Pi^a(x^-,\boldsymbol{x}) \equiv F_a^{+-}(x^-,\boldsymbol{x}) = \frac{1}{\partial^+} D_i^{ab}\partial^+ A_i^b = \partial_i A_i^a - g\frac{1}{\partial^+} f^{abc} A_i^b \partial^+ A_i^c$$

$$B^a(x^-,\boldsymbol{x}) = \epsilon_{ij}\left[\partial_i A_j^a - \frac{g}{2} f^{abc} A_i^b A_j^c\right]$$

$$A_a^i(x^-,\boldsymbol{x}) = \int \frac{d^3k}{(2\pi)^3}\left[A_a^i(k^+,\boldsymbol{k})e^{-ik\cdot x} + A_a^{\dagger i}(k^+,\boldsymbol{k})e^{ik\cdot x}\right]$$

$$k\cdot x \equiv k^+x^- - \boldsymbol{k}\cdot\boldsymbol{x}\Pi^a$$

$$\Pi^a(p^+,\boldsymbol{p}) = -i\boldsymbol{p}_i A_i^a(p^+,\boldsymbol{p}) + gf^{abc}\int_{k^+>0} A_i^b(p^+ + k^+,\boldsymbol{p}+\boldsymbol{k})\frac{2k^+ + p^+}{p^+} A_i^{c\dagger}(k^+,\boldsymbol{k})$$

$$+gf^{abc}\int_{p^+>k^+>0} A_i^b(k^+,\boldsymbol{k})\frac{k^+}{p^+} A_i^c(p^+ - k^+,\boldsymbol{p}-\boldsymbol{k})$$

$$\int_k \equiv \int \frac{d^3k}{(2\pi)^3}$$

$$A_i^a(k) \equiv \frac{1}{\sqrt{2k^+}}\hat{a}_i^a(k);\; A_i^{a\dagger}(k) \equiv \frac{1}{\sqrt{2k^+}}\hat{a}_i^{a\dagger}(k)$$

$$\left[A_i^a(p), A_j^{b\dagger}(q)\right] = (2\pi)^3\delta_{ij}^{ab}\frac{1}{2p^+}\delta^3(p-q)$$

$$\Pi^a(-p^+,-\boldsymbol{p}) = \Pi^{a\dagger}(p^+,\boldsymbol{p})$$

$$B^a(p^+,\boldsymbol{p}) = \epsilon_{ij}\Bigg[-i\boldsymbol{p}_i A_j^a(p^+,\boldsymbol{p}) - gf^{abc}\int_{k^+} A_i^b(k^+ + p^+,\boldsymbol{k}+\boldsymbol{p}) A_j^{c\dagger}(k^+,\boldsymbol{k})$$

$$-\frac{g}{2}f^{abc}\int_{p^+>k^+>0} A_i^b(p^+ - k^+,\boldsymbol{p}-\boldsymbol{k}) A_j^c(k^+,\boldsymbol{k})\Bigg]$$

$$B^a(-p^+,-\boldsymbol{p}) = \epsilon_{ij}\Bigg[i\boldsymbol{p}_i A_j^{a\dagger}(p^+,\boldsymbol{p}) - gf^{abc}\int_{k^+} A_i^{b\dagger}(k^+ + p^+,\boldsymbol{k}+\boldsymbol{p}) A_j^c(k^+,\boldsymbol{k})$$

$$-\frac{g}{2}f^{abc}\int_{p^+>k^+>0} A_i^{b\dagger}(p^+ - k^+,\boldsymbol{p}-\boldsymbol{k}) A_j^{c\dagger}(k^+,\boldsymbol{k})\Bigg]$$

$$H = \frac{1}{2}\int_p \left[\Pi^a(p^+,\boldsymbol{p})\Pi^{\dagger a}(p^+,\boldsymbol{p}) + B^a(p^+,\boldsymbol{p})B^{\dagger a}(p^+,\boldsymbol{p})\right]$$

$$A_i^a(k) = A_{Si}^a(k)\theta\left(E - \frac{\boldsymbol{k}^2}{2k^+}\right) + A_{Fi}^a(k)\theta\left(\frac{\boldsymbol{k}^2}{2k^+} - E\right)$$

$$\Omega_{BFKL}: p^- > k^-; p^+ \ll k^+; \boldsymbol{p}^2 \sim \boldsymbol{k}^2;\; \Omega_{DGLAP}: p^- > k^-; p^+ \sim k^+; \boldsymbol{p}^2 \gg \boldsymbol{k}^2$$

$$\mathcal{H}(p) = \frac{1}{2}\left[\Pi_F^a(p^+,\boldsymbol{p})\Pi_F^{\dagger a}(p^+,\boldsymbol{p}) + B_F^a(p^+,\boldsymbol{p})B_F^{\dagger a}(p^+,\boldsymbol{p})\right]$$

$$\rho^a(p^+,\boldsymbol{p}) = -if^{abc}\int_{k\in\Omega_{BFKL}} (2k^+ + p^+)A_{Sj}^{b\dagger}(k^+ + p^+, \boldsymbol{k}+\boldsymbol{p})A_{Sj}^c(k^+,\boldsymbol{k})$$
$$-if^{abc}\int_{k\in\Omega_{DGLAP}} (2k^+ + p^+)A_{Sj}^{b\dagger}(k^+ + p^+, \boldsymbol{k}+\boldsymbol{p})A_{Sj}^c(k^+,\boldsymbol{k})$$
$$\approx -2if^{abc}\int_{k\in\Omega_{BFKL}} k^+A_{Sj}^{b\dagger}(k^+, \boldsymbol{k}+\boldsymbol{p})A_{Sj}^c(k^+,\boldsymbol{k})$$

$$b^a(p^+,\boldsymbol{p}) = -g\epsilon_{ij}f^{abc}\int_{k\in\Omega_{BFKL}} A_{Si}^{b\dagger}(k^+ + p^+, \boldsymbol{k}+\boldsymbol{p})A_{Sj}^c(k^+,\boldsymbol{k})$$
$$-g\epsilon_{ij}f^{abc}\int_{k\in\Omega_{DGLAP}} A_{Si}^{b\dagger}(k^+ + p^+, \boldsymbol{k}+\boldsymbol{p})A_{Sj}^c(k^+,\boldsymbol{k})$$

$$gf^{abc}\int_{k^+>0} A_i^b(p^+ + k^+, \boldsymbol{p}+\boldsymbol{k})\frac{2k^+ + p^+}{p^+}A_i^{c\dagger}(k^+,\boldsymbol{k}) \rightarrow$$
$$gf^{abc}\left[\int_{k\in\Omega_{DGLAP}} A_{Si}^b(k^+,\boldsymbol{k})\frac{2k^+ - p^+}{p^+}A_{Fi}^{c\dagger}(k^+ - p^+, \boldsymbol{k}-\boldsymbol{p}) + A_{Fi}^b(p^+ + k^+, \boldsymbol{p}+\boldsymbol{k})\frac{2k^+ + p^+}{p^+}A_{Si}^{c\dagger}(k^+,\boldsymbol{k})\right]$$
$$+gf^{abc}\int_{p^+\gg k^+} A_{Fi}^b(p^+ + k^+, \boldsymbol{p}+\boldsymbol{k})\frac{2k^+ + p^+}{p^+}A_{Si}^{c\dagger}(k^+,\boldsymbol{k})$$

$$f^{abc}\int_{p^+>k^+>0} A_i^b(k^+,\boldsymbol{k})\frac{k^+}{p^+}A_i^c(p^+ - k^+, \boldsymbol{p}-\boldsymbol{k}) \rightarrow f^{abc}\int_{k\in\Omega_{DGLAP}} A_{Si}^b(k^+,\boldsymbol{k})\frac{2k^+ - p^+}{p^+}A_{Fi}^c(p^+ - k^+, \boldsymbol{p}-\boldsymbol{k})$$
$$+f^{abc}\int_{p^+\gg k^+} A_{Si}^b(k^+,\boldsymbol{k})\frac{2k^+ - p^+}{p^+}A_{Fi}^c(p^+ - k^+, \boldsymbol{p}-\boldsymbol{k})$$

$$\Pi_F^a(p) = -i\boldsymbol{p}_i A_{Fi}^a(p^+,\boldsymbol{p}) - 2gf^{abc}\int_{k\in\Omega_{BFKL}} \frac{k^+}{p^+}A_{Sj}^{b\dagger}(p^+, \boldsymbol{k}-\boldsymbol{p})A_{Sj}^c(k^+,\boldsymbol{k})$$
$$+gf^{abc}\left\{\int_{p^+\gg k^+;\boldsymbol{k}^2\sim\boldsymbol{p}^2} \left[A_{Fi}^b(p^+, \boldsymbol{p}+\boldsymbol{k})\alpha_i^{c\dagger}(k^+,\boldsymbol{k}) + A_{Fi}^b(p^+, \boldsymbol{p}+\boldsymbol{k})\alpha_i^c(k^+,-\boldsymbol{k})\right]\right.$$
$$+\left[\int_{k\in\Omega_{DGLAP}} A_{Si}^b(k^+,\boldsymbol{k})\frac{2k^+ - p^+}{p^+}A_{Fi}^{c\dagger}(k^+ - p^+, \boldsymbol{k}-\boldsymbol{p}) + A_{Fi}^b(p^+ + k^+, \boldsymbol{p}+\boldsymbol{k})\frac{2k^+ + p^+}{p^+}A_{Si}^{c\dagger}(k^+,\boldsymbol{k})\right]$$
$$\left.+\int_{k\in\Omega_{DGLAP}} A_{Si}^b(k^+,\boldsymbol{k})\frac{2k^+ - p^+}{p^+}A_{Fi}^c(p^+ - k^+, \boldsymbol{p}-\boldsymbol{k})\right\}$$

$$\epsilon_{ij}gf^{abc}\int_{k^+} A_i^b(k^+ + p^+, \boldsymbol{k}+\boldsymbol{p})A_j^{c\dagger}(k^+,\boldsymbol{k}) \rightarrow$$
$$\epsilon_{ij}gf^{abc}\int_{k\in\Omega_{DGLAP}} \left[A_{Fi}^b(k^+ + p^+, \boldsymbol{k}+\boldsymbol{p})A_{Sj}^{c\dagger}(k^+,\boldsymbol{k}) + A_{Fi}^{b\dagger}(k^+ - p^+, -\boldsymbol{k}-\boldsymbol{p})A_{Sj}^c(k^+,-\boldsymbol{k})\right]$$
$$+\epsilon_{ij}gf^{abc}\int_{p^+\gg k^+} A_{Fi}^b(k^+ + p^+, \boldsymbol{k}+\boldsymbol{p})\alpha_j^{c\dagger}(k^+,\boldsymbol{k})$$
$$\frac{g}{2}\epsilon_{ij}f^{abc}\int_i^b (p^+ - k^+, \boldsymbol{p}-\boldsymbol{k})A_j^c(k^+,\boldsymbol{k}) \rightarrow$$
$$g\epsilon_{ij}f^{abc}\int_{k\in\Omega_{DGLAP}} A_{Fi}^b(p^+ - k^+, \boldsymbol{p}-\boldsymbol{k})A_{Sj}^c(k^+,\boldsymbol{k}) + g\epsilon_{ij}f^{abc}\int_{p^+\gg k^+} A_{Fi}^b(p^+ - k^+, \boldsymbol{p}-\boldsymbol{k})\alpha_j^c(k^+,\boldsymbol{k})$$

$$B_F^a(p) = -\epsilon_{ij}\Big\{i\boldsymbol{p}_i A_{Fj}^a(p^+,\boldsymbol{p}) + gf^{abc}\int_{p^+\gg k^+;\boldsymbol{k}^2\sim\boldsymbol{p}^2}\left[A_{Fi}^b(p^+,\boldsymbol{k}+\boldsymbol{p})\alpha_j^{c\dagger}(k^+,\boldsymbol{k})\right.$$
$$\left.+A_{Fi}^b(p^+,\boldsymbol{p}-\boldsymbol{k})\alpha_j^c(k^+,\boldsymbol{k})\right] + gf^{abc}\int_{k\in\Omega_{DGLAP}}\left[A_{Fi}^b(k^+ + p^+,\boldsymbol{k}+\boldsymbol{p})A_{Sj}^{c\dagger}(k^+,\boldsymbol{k})\right.$$
$$\left.+A_{Fi}^{b\dagger}(k^+ - p^+,-\boldsymbol{k}-\boldsymbol{p})A_{Sj}^c(k^+,-\boldsymbol{k}) + A_{Fi}^b(p^+ - k^+,\boldsymbol{p}-\boldsymbol{k})A_{Sj}^c(k^+,\boldsymbol{k})\right]\Big\}$$

$$P_i^{ab} \equiv \boldsymbol{p}_i\delta^{ab} + igf^{abc}\int_{k^+\ll p^+;k^-\ll p^-}\left[\alpha_i^{\dagger c}(k^+,\boldsymbol{k}) + \alpha_i^c(k^+,-\boldsymbol{k})\right] \approx \boldsymbol{p}_i\delta^{ab} + igf^{abc}\alpha_i^c$$

$$\Pi_F^a(p) = -iP_i^{ab}A_{Fi}^b(p^+,\boldsymbol{p}) + 2gf^{abc}\int_{k\in\Omega_{BFKL}}\frac{k^+}{p^+}A_{Sj}^{b\dagger}(k^+ + p^+,\boldsymbol{k}-\boldsymbol{p})A_{Sj}^c(k^+,\boldsymbol{k})$$
$$+gf^{abc}\int_{k\in\Omega_{DGLAP}}\Bigg[A_{Si}^b(k^+,\boldsymbol{k})\frac{2k^+ - p^+}{p^+}\left[A_{Fi}^{c\dagger}(k^+ - p^+,\boldsymbol{k}-\boldsymbol{p}) + A_{Fi}^c(p^+ - k^+,\boldsymbol{p}-\boldsymbol{k})\right]$$
$$-A_{Si}^{b\dagger}(k^+,\boldsymbol{k})\frac{2k^+ + p^+}{p^+}A_{Fi}^c(p^+ + k^+,\boldsymbol{p}+\boldsymbol{k})\Bigg];$$

$$B_F^a(p) = -i\epsilon_{ij}P_i^{ab}A_{Fj}^b(p) - \epsilon_{ij}gf^{abc}\int_{k\in\Omega_{DGLAP}}\left\{A_{Fi}^b(k^+ + p^+,\boldsymbol{k}+\boldsymbol{p})A_{Sj}^{c\dagger}(k^+,\boldsymbol{k})\right.$$
$$\left.+\left[A_{Fi}^{b\dagger}(k^+ - p^+,-\boldsymbol{k}-\boldsymbol{p}) + A_{Fi}^b(p^+ - k^+,\boldsymbol{p}-\boldsymbol{k})\right]A_{Sj}^c(k^+,-\boldsymbol{k})\right\}$$

$$\mathcal{H}_0(p) = \frac{1}{2}A_{Fi}^a(p^+,\boldsymbol{p})\left[\boldsymbol{P}^2\delta_{ij} + [\boldsymbol{P}_i,\boldsymbol{P}_j]\right]^{ab}A_{Fj}^b(p^+,\boldsymbol{p})$$

$$\mathcal{H}_I^{BFKL}(p) = g\frac{1}{p^+}\left[A_{Fi}^{\dagger a}(p)\boldsymbol{P}_i^{ab}\rho^b(p^+,-\boldsymbol{p}) + A_{Fi}^a(p)\boldsymbol{P}_i^{ab}\rho^b(p^+,\boldsymbol{p})\right]$$

$$\mathcal{H}_I^{DGLAP} = -ig\int_{k\in\Omega_{DGLAP}}A_{Si}^a(k^+,\boldsymbol{k})f^{abc}\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{p^+} - 1\right) + \epsilon_{ki}\epsilon_{jl}\right]\boldsymbol{P}_j^{bd}A_{Fl}^{\dagger d}(p^+,\boldsymbol{p})A_{Fk}^{\dagger c}(k^+ - p^+,\boldsymbol{k}-\boldsymbol{p})$$
$$+ \text{h.c.}$$

$$\mathcal{H}_I^1 = -ig\int_{k\in\Omega_{DGLAP}}A_{Si}^a(k^+,\boldsymbol{k})f^{abc}\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{p^+} - 1\right) + \epsilon_{ki}\epsilon_{jl}\right]\boldsymbol{P}_j^{bd}A_{Fl}^{\dagger d}(p^+,\boldsymbol{p})A_{Fk}^c(p^+ - k^+,\boldsymbol{p}-\boldsymbol{k}) + h.c.$$
$$\mathcal{H}_I^2 = -ig\int_{k\in\Omega_{DGLAP}}A_{Si}^{\dagger a}(k^+,\boldsymbol{k})f^{abc}\left[\delta_{ki}\delta_{jl}\left(-\frac{2k^+}{p^+} - 1\right) + \epsilon_{ki}\epsilon_{jl}\right]\boldsymbol{P}_j^{bd}A_{Fl}^{\dagger d}(p^+,\boldsymbol{p})A_{Fk}^c(p^+ + k^+,\boldsymbol{p}+\boldsymbol{k}) + h.c$$

$$\Delta\mathcal{H}(p) = -igf^{abc}A_{Fj}^{\dagger b}(p)A_{Fj}^c(p)\int_{k^+\ll p^+;k^-\ll p^-}\frac{\boldsymbol{k}_i}{k^+}\left[\alpha_i^a(k^+,\boldsymbol{k}) - \alpha_i^{\dagger a}(k^+,-\boldsymbol{k})\right]$$

$$H_0 = \int_p\mathcal{H}_0(p);\ \ \mathcal{H}_0(p) = \frac{1}{2}A_i^a(p^+,\boldsymbol{p})\left[\boldsymbol{P}^2\delta_{ij} + [\boldsymbol{P}_i,\boldsymbol{P}_j]\right]^{ab}A_j^b(p^+,\boldsymbol{p})$$

$$H_I = \int_p\mathcal{H}_I(p);\mathcal{H}_I(p) = -ig\int_{\max(k^-,(k-p)^-)<p^-}A_i^a(k^+,\boldsymbol{k})f^{abc}$$
$$\times\left\{\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{p^+} - 1\right) + \epsilon_{ki}\epsilon_{jl}\right]\boldsymbol{P}_j^{bd}A_l^{\dagger d}(p^+,\boldsymbol{p})A_k^{\dagger c}(k^+ - p^+,\boldsymbol{k}-\boldsymbol{p})\right.$$
$$\left.+\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+ - p^+} - 1\right) + \epsilon_{ki}\epsilon_{jl}\right](\boldsymbol{K}-\boldsymbol{P})_j^{bd}A_l^{\dagger d}(k^+ - p^+,\boldsymbol{k}-\boldsymbol{p})A_k^{\dagger c}(p^+,\boldsymbol{p})\right\} + h.c.$$

$$\mathcal{H}_I(p) \approx -ig\int_{\max(k^-,(k-p)^-)<p^-} A_i^a(k^+,\boldsymbol{k})f^{abc}$$
$$\times\left\{\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{p^+}-1\right)+\epsilon_{ki}\epsilon_{jl}\right]\boldsymbol{p}_j A_l^{\dagger b}(p^+,\boldsymbol{p})A_k^{\dagger c}(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})\right.$$
$$\left.-\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+-p^+}-1\right)+\epsilon_{ki}\epsilon_{jl}\right]\boldsymbol{p}_j A_l^{\dagger b}(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})A_k^{\dagger c}(p^+,\boldsymbol{p})\right\}+\text{ h.c.}$$

$$\Omega_p = 1 + iG(p^+,\boldsymbol{p}) \approx e^{iG(p^+,\boldsymbol{p})};\ G(p^+,\boldsymbol{p}) = \mathcal{H}_I(p)D$$

$$D^{-1} \equiv k^- - p^- - (k-p)^- = \frac{\boldsymbol{k}^2}{2k^+} - \frac{\boldsymbol{p}^2}{2p^+} - \frac{(\boldsymbol{k}-\boldsymbol{p})^2}{2(k^+-p^+)} \approx -\frac{\boldsymbol{p}^2 k^+}{2p^+(k^+-p^+)}$$

$$G(p^+,\boldsymbol{p}) = g\int_{k^-<p^-;(k-p)^-<p^-} A_i^a(k^+,\boldsymbol{k})\frac{2p^+(k^+-p^+)}{k^+}$$
$$\times\left\{\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{p^+}-1\right)+\epsilon_{ki}\epsilon_{jl}\right]\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}A_l^\dagger(p^+,\boldsymbol{p})T^a A_k^\dagger(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})\right.$$
$$\left.-\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+-p^+}-1\right)+\epsilon_{ki}\epsilon_{jl}\right]\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}A_l^\dagger(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^a A_k^\dagger(p^+,\boldsymbol{p})\right\}+\text{ h.c.}$$

$$G(p^+,\boldsymbol{p}) = A_i^\dagger(p^+,\boldsymbol{p})C_i(p^+,\boldsymbol{p}) + A_i(p^+,\boldsymbol{p})C_i^\dagger(p^+,\boldsymbol{p})$$

$$C_i^a(p^+,\boldsymbol{p}) = g\int_{p^->k^-,p^->(k-p)^-}\frac{2p^+(k^+-p^+)}{k^+}$$
$$\times\left\{\left[\delta_{kl}\delta_{ji}\left(\frac{2k^+}{p^+}-1\right)+\epsilon_{lk}\epsilon_{ji}\right]+\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+-p^+}-1\right)+\epsilon_{ik}\epsilon_{jl}\right]\right\}$$
$$\times\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}A_l^\dagger(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^a A_k(k^+,\boldsymbol{k})$$

$$F_{lk}^i(k,p) = \frac{2p^+(k^+-p^+)}{k^+}\left\{\left[\delta_{kl}\delta_{ji}\left(\frac{2k^+}{p^+}-1\right)+\epsilon_{lk}\epsilon_{ji}\right]+\left[\delta_{ki}\delta_{jl}\left(\frac{2k^+}{k^+-p^+}-1\right)+\epsilon_{ik}\epsilon_{jl}\right]\right\}\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}$$
$$= \frac{4p^+(k^+-p^+)}{k^+}\left\{\delta_{kl}\delta_{ji}\frac{k^+}{p^+}+\delta_{ki}\delta_{jl}\frac{k^+}{k^+-p^+}-\delta_{kj}\delta_{il}\right\}\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}$$

$$\epsilon_{ij}\epsilon_{kl} = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}$$

$$C_i^a(p^+,\boldsymbol{p}) = g\int_{k^-<p^-;\,(k-p)^-<p^-} F_{lk}^i(k,p)A_l^\dagger(k^+-p^+,\boldsymbol{k}-\boldsymbol{p})T^a A_k(k^+,\boldsymbol{k})$$
$$C_i^{a\dagger}(p^+,\boldsymbol{p}) = g\int_{k^-<p^-;\,(k+p)^-<p^-} F_{kl}^i(k+p,p)A_l^\dagger(k^++p^+,\boldsymbol{k}+\boldsymbol{p})T^a A_k(k^+,\boldsymbol{k})$$

$$|\Psi_P\rangle_E = \mathcal{P}\exp\left\{i\int_{E_0}^{E} dp^-\mathcal{G}(p^-)\right\}|\Psi_P\rangle_{E_0}$$

$$\mathcal{G}(p^-) \equiv \int_p \delta\left(p^- - \frac{\boldsymbol{p}^2}{2p^+}\right)G(p^+,\boldsymbol{p}^2)$$

$$\lambda = \delta = \sqrt{\frac{k^-}{p^-}}$$

$$\frac{k^+}{p^+} = \frac{p^2}{\boldsymbol{k}^2}$$

$$k^+ > p^+ \sqrt{\frac{p^-}{k^-}} \left[\boldsymbol{p}^2 < \boldsymbol{k}^2 \sqrt{\frac{p^-}{k^-}} \right]$$

$$\boldsymbol{p}^2 > \boldsymbol{k}^2 \sqrt{\frac{p^-}{k^-}} \left[\text{or} \quad k^+ < p^+ \sqrt{\frac{p^-}{k^-}} \right]$$

$$H_I = H_I^{BFKL} + H_I^{DGLAP}$$

$$H_I^{BFKL} = g \int_p \frac{1}{p^+} [A_i^{\dagger a}(p) \boldsymbol{p}_i \rho^a(p^+, -\boldsymbol{p}) + A_i^a(p) \boldsymbol{p}_i \rho^{*a}(p^+, -\boldsymbol{p})]$$

$$\rho^a(p^+, \boldsymbol{p}) = -2if^{abc} \int_{k^+ > \sqrt{\frac{p^-}{k^-}} p^+, \max(k^-, (k+p)^-) < p^-} k^+ A_j^{b\dagger}(k^+, \boldsymbol{k} + \boldsymbol{p}) A_j^c(k^+, \boldsymbol{k}),$$

$$H_I^{DGLAP} = -ig \int_{\boldsymbol{p}^2 > \sqrt{\frac{p^-}{k^-}} \boldsymbol{k}^2; p^+ < k^+/2; k^- < p^-} A_i^a(k^+, \boldsymbol{k}) f^{abc}$$
$$\times \left\{ \left[\delta_{ki} \delta_{jl} \left(\frac{2k^+}{p^+} - 1 \right) + \epsilon_{ki} \epsilon_{jl} \right] \boldsymbol{p}_j A_l^{\dagger b}(p^+, \boldsymbol{p}) A_k^{\dagger c}(k^+ - p^+, -\boldsymbol{p}) \right.$$
$$\left. - \left[\delta_{ki} \delta_{jl} \left(\frac{2k^+}{k^+ - p^+} - 1 \right) + \epsilon_{ki} \epsilon_{jl} \right] \boldsymbol{p}_j A_l^{\dagger b}(k^+ - p^+, -\boldsymbol{p}) A_k^{\dagger c}(p^+, \boldsymbol{p}) \right\} + \text{ h.c.}$$

$$|\Psi_P\rangle_E = \mathcal{P}\exp \left\{ i \int_{E_0}^{E} dp^- [\mathcal{G}^{BFKL}(p^-) + \mathcal{G}^{DGLAP}(p^-)] \right\} |\Psi_P\rangle_{E_0}$$

$$\mathcal{G}^{BFKL}(p^-) \equiv \int_p \delta \left(p^- - \frac{\boldsymbol{p}^2}{2p^+} \right) G^{BFKL}(p^+, \boldsymbol{p})$$
$$\mathcal{G}^{DGLAP}(p^-) \equiv \int_p \delta \left(p^- - \frac{\boldsymbol{p}^2}{2p^+} \right) G^{DGLAP}(p^+, \boldsymbol{p})$$

$$G^{BFKL}(p^+, \boldsymbol{p}) = 2g \left[A_i^{\dagger a}(p) \frac{\boldsymbol{p}_i}{\boldsymbol{p}^2} \rho^a(p^+, -\boldsymbol{p}) + A_i^a(p) \frac{\boldsymbol{p}_i}{\boldsymbol{p}^2} \rho^{\dagger a}(p^+, -\boldsymbol{p}) \right]$$

$$G^{DGLAP}(p^+, \boldsymbol{p}) = -ig \int_{p^2 > \sqrt{\frac{p^-}{k^-}} k^2; p^+ < k^+/2; k^- < p^-} f^{abc} A_i^a(k^+, \boldsymbol{k}) \frac{2p^+(k^+ - p^+)}{k^+}$$
$$\times \left\{ \left[\delta_{ki} \delta_{jl} \left(\frac{2k^+}{p^+} - 1 \right) + \epsilon_{ki} \epsilon_{jl} \right] \frac{\boldsymbol{p}_j}{\boldsymbol{p}^2} A_l^{\dagger b}(p^+, \boldsymbol{p}) A_k^{\dagger c}(k^+ - p^+, -\boldsymbol{p}) \right.$$
$$\left. + \left[\delta_{li} \delta_{jk} \left(\frac{2k^+}{k^+ - p^+} - 1 \right) + \epsilon_{li} \epsilon_{jk} \right] \frac{\boldsymbol{p}_j}{\boldsymbol{p}^2} A_l^{\dagger b}(p^+, \boldsymbol{p}) A_k^{\dagger c}(k^+ - p^+, -\boldsymbol{p}) \right\} + \text{ h.c.}$$

$$S = \langle \Psi_{in} | \hat{S} | \Psi_{in} \rangle = \langle \Psi_P | \langle \Psi_T | \hat{S} | \Psi_T \rangle | \Psi_P \rangle$$

$$\hat{S}_P = \langle \Psi_T | \hat{S} | \Psi_T \rangle$$

$$\tilde{F}_a^{+i} = \partial^+ \tilde{A}_a^i$$
$$\tilde{F}_a^{-i} = \left(\partial^- \tilde{A}_a^i - \partial^i \tilde{A}_a^- - g f^{abc} \tilde{A}_b^- \tilde{A}_c^i \right) - g f^{abc} \tilde{A}_b^- \gamma_c^i - g f^{abc} \gamma_b^- \tilde{A}_c^i$$
$$\tilde{F}_a^{ij} = \partial^i \tilde{A}_a^j - \partial^j \tilde{A}_a^i - g f^{abc} \tilde{A}_b^i \gamma_c^j - g f^{abc} \gamma_b^i \tilde{A}_c^j - g f^{abc} \tilde{A}_b^i \tilde{A}_c^j$$

$$\mathcal{L}_{YM} = \frac{1}{2}\left(\partial^+ \tilde{A}_a^-\right)^2 + \partial^+ \tilde{A}_a^i\left(\partial^- \tilde{A}_a^i - \partial^i \tilde{A}_a^- - gf^{abc}\tilde{A}_b^- \tilde{A}_c^i\right) - \frac{1}{4}\left(\partial^i \tilde{A}_a^j - \partial^j \tilde{A}_a^i - gf^{abc}\tilde{A}_b^i \tilde{A}_c^j\right)^2$$

$$-\partial^+ \tilde{A}_a^i\left(gf^{abc}\tilde{A}_b^- \gamma_c^i + gf^{abc}\gamma_b^- \tilde{A}_c^i\right) + gf^{abc}\gamma_b^i \tilde{A}_c^j\left(\partial^i \tilde{A}_a^j - \partial^j \tilde{A}_a^i - gf^{ade}\tilde{A}_d^i \tilde{A}_e^j\right) + \frac{1}{2}gf^{abc}\tilde{A}_b^i \tilde{A}_c^j\left(\partial^i \gamma_a^j - \partial^j \gamma_a^i\right)$$

$$-(\partial^+)^2 \tilde{A}_a^- + \partial^i \partial^+ \tilde{A}_a^i - gf^{abc}\left(\tilde{A}_b^i + \gamma_b^i\right)\partial^+ \tilde{A}_c^i = 0$$

$$\gamma_a^- = \frac{\partial_i}{\partial^2}\partial^- \gamma_a^i + O(g)$$

$$H_{PT} = gf^{abc}\int d^3x\left\{\partial^+ \tilde{A}_a^i\left(\tilde{A}_b^- \gamma_c^i + \gamma_b^- \tilde{A}_c^i\right) - \gamma_b^i \tilde{A}_c^j\left(\partial^i \tilde{A}_a^j - \partial^j \tilde{A}_a^i\right) - \frac{1}{2}\tilde{A}_b^i \tilde{A}_c^j\left(\partial^i \gamma_a^j - \partial^j \gamma_a^i\right)\right\}$$

$$= gf^{abc}\int d^3x\left\{-\gamma_a^i \tilde{A}_b^i \partial^j \tilde{A}_c^j - \partial^i \gamma_a^j \tilde{A}_b^i \tilde{A}_c^j - \gamma_b^i \tilde{A}_c^j\left(\partial^i \tilde{A}_a^j - \partial^j \tilde{A}_a^i\right) + \left[\partial^- \frac{\partial^i}{\partial^2}\gamma_a^i\right]\tilde{A}_b^j \partial^+ \tilde{A}_c^j\right\}$$

$$= gf^{abc}\int d^3x\left\{\left[\partial^- \frac{\partial^i}{\partial^2}\gamma_a^i\right]\tilde{A}_b^j \partial^+ \tilde{A}_c^j - \gamma_a^i \tilde{A}_b^j \partial^i \tilde{A}_c^j + 2\left[\partial^j \gamma_a^i\right]\tilde{A}_b^i \tilde{A}_c^j\right\}$$

$$\frac{1}{2}\left(\partial^+ \tilde{A}_a^-\right)^2 - \partial^i \tilde{A}_a^i \partial^+ \tilde{A}_a^- = -\frac{1}{2}\left(\partial^i \tilde{A}_a^i\right)^2$$

$$\gamma_a^i(x^+, \boldsymbol{x}) = \int \frac{dq^- d^2q}{(2\pi)^3}\left[\gamma_a^i(q^-, \boldsymbol{q})e^{-iq\cdot x} + \gamma_a^{*i}(q^-, \boldsymbol{q})e^{iq\cdot x}\right]$$

$$H_{PT}(x^+) = igf^{abc}\int \frac{d^3k}{(2\pi)^3}\frac{dq^-}{2\pi}\frac{d^2\boldsymbol{q}}{(2\pi)^2}e^{-iD^{-1}x^+}\gamma_a^i(q)\tilde{A}_b^{\dagger j}(k+q)\tilde{A}_c^k(k)$$

$$\times\left[\delta^{jk}\left(\frac{2k^+ q^-}{\boldsymbol{q}^2}\boldsymbol{q}^i - \left(2\boldsymbol{k}^i + \boldsymbol{q}^i\right)\right) + 2\epsilon^{il}\boldsymbol{q}^l \epsilon^{jk}\right] + h.c$$

$$D = \frac{1}{q^- + \frac{\boldsymbol{k}^2}{2k^+} - \frac{(\boldsymbol{k}+\boldsymbol{q})^2}{2k^+}}$$

$$D \approx \frac{2k^+}{2q^- k^+ - \boldsymbol{q}^2}$$

$$\hat{S}_P = \langle \Psi_T | \exp\left\{i\int_q \tilde{G}(q)\right\} | \Psi_T \rangle$$

$$\tilde{G}(q) = gf^{abc}\int_{k:k^- < q^-}\gamma_i^a(q) f_{jk}^i(k,q)\tilde{A}_b^{\dagger j}(k^+, \boldsymbol{k}+\boldsymbol{q})\tilde{A}_c^k(k^+, \boldsymbol{k}) + h.c.$$

$$f_{jk}^i(k,q) = 2k^+ \frac{\boldsymbol{q}^i}{\boldsymbol{q}^2}\delta^{jk} + 4k^+ \epsilon^{il}\frac{\boldsymbol{q}^l}{\boldsymbol{q}^2}\epsilon^{jk}\frac{1}{\frac{2q^- k^+}{\boldsymbol{q}^2} - 1}$$

$$S = 1 - \frac{1}{2(N_c^2 - 1)}\int_q \langle \Psi_T | \gamma_j^{\dagger b}(q)\gamma_j^b(q) | \Psi_T \rangle O(q)$$

$$\langle \Psi_T | \gamma_j^{\dagger b}(q)\gamma_j^b(q) | \Psi_T \rangle$$

$$O(q) = \langle \Psi_P | \mathcal{C}_i^a(q^-, \boldsymbol{q}) \mathcal{C}_i^{a\dagger}(q^-, \boldsymbol{q}) | \Psi_P \rangle_E$$
$$\mathcal{C}_i^{a\dagger}(q^-, \boldsymbol{q}) = g \int_{k:k^-<q^-} f_{lk}^i(k,q) A_l^\dagger(k^+, \boldsymbol{k}+\boldsymbol{q}) T^a A_k(k^+, \boldsymbol{k})$$

$$\langle \Psi_T | \gamma_j^{\dagger b}(q) \gamma_j^b(q) | \Psi_T \rangle$$

$$q^- \gg \frac{q^2}{2k^+}$$

$$f_{lk}^i(k,q) \to 2k^+ \frac{\boldsymbol{q}_i}{\boldsymbol{q}^2} \delta_{kl}; \; \mathcal{C}_i^{a\dagger}(q^-, q) \to \frac{\boldsymbol{q}_i}{\boldsymbol{q}^2} \rho^a(\bar{q}^+, \boldsymbol{q}); \; \bar{q}^+ \equiv \frac{\boldsymbol{q}^2}{2q^-}$$

$$f_{jk}^i(k,q) \to 4k^+ \epsilon^{il} \frac{\boldsymbol{q}^l}{\boldsymbol{q}^2} \epsilon^{jk} \frac{1}{\frac{k^+}{\bar{q}^+} - 1} = 4k^+ \frac{\boldsymbol{q}^k \delta^{ij} - \boldsymbol{q}^j \delta^{ik}}{2q^- k^+ - \boldsymbol{q}^2}.$$

$$O(q) = O_1(q) + O_2(q)$$

$$O_1(q) \; = g^2 N_c \int_{k:k^-<q^-} \frac{1}{2k^+} f_{lk}^i(k,q) f_{lm}^i(k,q) \langle \Psi_P | A_k^{a\dagger}(k^+, \boldsymbol{k}) A_m^a(k^+, \boldsymbol{k}) | \Psi_P \rangle_E$$
$$O_2(q) \; = g^2 \int_{\{k,l:(k-q)^-<q^-;k^-<q^-;(l-q)^-<q^-;l^-<q^-\}} f_{lk}^i(k,q) f_{nm}^i(l,q)$$
$$\times \langle \Psi_P | : A_l^\dagger(k^+, \boldsymbol{k}-\boldsymbol{q}) T^a A_k(k^+, \boldsymbol{k}) A_m^\dagger(l^+, \boldsymbol{l}+\boldsymbol{q}) T^a A_n(l^+, \boldsymbol{l}) : | \Psi_P \rangle_E$$

$$O_1(q) = \frac{g^2 N_c}{2} \int_{k:k^-<q^-} \frac{1}{2k^+} f_{lk}^i(k,q) f_{lk}^i(k,q) \langle \Psi_P | A_m^{a\dagger}(k^+, \boldsymbol{k}) A_m^a(k^+, \boldsymbol{k}) | \Psi_P \rangle_E$$
$$= \frac{g^2 N_c}{2} \int_{k:k^-<q^-} \frac{1}{(2k^+)^2} f_{lk}^i(k,q) f_{lk}^i(k,q) T(k)$$

$$\left[f^{Ti}(k,q) f^i(k,q) \right]_{st} = \frac{(2k^+)^2}{\boldsymbol{q}^2} \left[1 + \frac{4}{\left(\frac{k^+}{\bar{q}^+} - 1 \right)^2} \right] \delta_{st}$$

$$\hat{T}(k) \equiv a_i^{\dagger a}(k) a_i^a(k); \; T(k) \equiv \langle \Psi_P | \hat{T}(k) | \Psi_P \rangle_E$$

$$\left[f^{Ti}(k,q) f^i(k,q) \right]_{st} \to \frac{(2k^+)^2}{\boldsymbol{q}^2}$$

$$\left[f^{Ti}(k,q) f^i(k,q) \right]_{st} \approx \frac{(2k^+)^2}{\boldsymbol{q}^2} \frac{1}{\epsilon} \delta(k^+ - \bar{q}^+) \delta_{st}.$$

$$\bar{O}_1(q) = \frac{g^2 N_c}{4\pi} \frac{1}{q^2} \int_{\boldsymbol{k}:\boldsymbol{k}^2<\boldsymbol{q}^2=2k^+q^-} T(k^+ = \bar{q}, \boldsymbol{k})$$

$$G(x, Q^2) = \int_{\boldsymbol{k}:\boldsymbol{k}^2<Q^2} T(k^+, \boldsymbol{k})$$

$$\Lambda_+ e^{-\Delta} < k^+ < \Lambda_+$$

$$E e^{\Delta} > k^- > E$$

$$\frac{1}{\sqrt{2k^+}}\langle \boldsymbol{k},b,i \mid \Psi_{NLO}\rangle = F_i^1\rho^b(-k) + \int_p \left[iF_i^2 f^{abc}\{\rho^c(p-k),\rho^a(-p)\}_+ + F_i^3\rho^b(-k)\rho^a(p)\rho^a(-p)\right]$$

$$F_i^2(k,p) = \frac{1}{2(2\pi)^{3/2}}\frac{g^3}{(2\pi)^3}\sum_{n=3}^{7}\psi_i^n(k,p)$$

$$\psi_i^3 = \frac{k^+ + p^+}{(k^+ - p^+)^2}\frac{1}{p^+}\frac{\boldsymbol{p}_i}{\boldsymbol{k}^2\boldsymbol{p}^2}$$

$$\psi_i^4 = -\frac{k^+ - p^+}{(k^+ + p^+)^2}\frac{k^+}{p^+}\frac{\boldsymbol{p}_i}{\boldsymbol{k}^2[k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2]}$$

$$\psi_i^5 = \theta(p^+ - k^+)\frac{1}{\boldsymbol{k}^2\boldsymbol{p}^2}\frac{k^+}{p^+}\frac{1}{[k^+(\boldsymbol{k}-\boldsymbol{p})^2 + (p^+ - k^+)\boldsymbol{k}^2]}\times$$
$$\left\{\left[-\frac{k^+ + p^+}{(k^+ - p^+)^2}(\boldsymbol{k}-\boldsymbol{p})^2 + \frac{1}{k^+ - p^+}(\boldsymbol{k}^2 - \boldsymbol{p}^2) - 2\frac{1}{p^+}\boldsymbol{p}^2\right]\boldsymbol{p}_i + 2\left[\frac{\boldsymbol{p}^2}{p^+} - \frac{\boldsymbol{p}(\boldsymbol{k}-\boldsymbol{p})}{k^+}\right]\boldsymbol{k}_i\right\}$$

$$\psi_i^6 = \theta(k^+ - p^+)\frac{1}{\boldsymbol{k}^2\boldsymbol{p}^2}\frac{1}{[p^+(\boldsymbol{k}-\boldsymbol{p})^2 + (k^+ - p^+)\boldsymbol{p}^2]}\times$$
$$\left\{\left[-\frac{k^+ + p^+}{(k^+ - p^+)^2}(\boldsymbol{k}-\boldsymbol{p})^2 + \frac{1}{k^+ - p^+}(\boldsymbol{k}^2 - \boldsymbol{p}^2) - 2\frac{1}{p^+}\boldsymbol{p}^2\right]\boldsymbol{p}_i + 2\left[\frac{\boldsymbol{p}^2}{p^+} - \frac{\boldsymbol{p}(\boldsymbol{k}-\boldsymbol{p})}{k^+}\right]\boldsymbol{k}_i\right\}$$

$$\psi_i^7 = 2\frac{1}{\boldsymbol{k}^2}\frac{1}{p^+}\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\boldsymbol{k}_i$$

$$\bar{\psi}_i^n \equiv \int_{k^+,p^+}\psi_i^n;\ n = 3\ldots 7$$

$$\bar{\psi}_i^5 + \bar{\psi}_i^3 + \bar{\psi}_i^4 + \bar{\psi}_i^6 = -(2B^+ - A^+)\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2} + [B^+ - A^+ - C^+]\frac{\boldsymbol{p}\cdot\boldsymbol{k}\boldsymbol{k}_i - \boldsymbol{k}^2\boldsymbol{p}_i}{\boldsymbol{k}^2(\boldsymbol{k}-\boldsymbol{p})^2}$$
$$+[B^+ + A^+ - C^+]\frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2};\ \bar{\psi}_i^7 = 2B^+\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}$$

$$A^+ = \int_{p^+,k^+}\frac{1}{k^+ + p^+}\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}$$
$$= \frac{1}{\boldsymbol{p}^2}\left(\Delta - \frac{1}{2}\ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right)\ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\theta\left[\Delta - \ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right] + \frac{1}{2}\frac{1}{\boldsymbol{p}^2}\Delta^2\theta\left[\ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \Delta\right]$$

$$B^+ = \int_{p^+,k^+}\frac{1}{p^+}\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}$$
$$= \frac{1}{\boldsymbol{p}^2}\left\{\left[\frac{1}{2}\Delta^2 + \Delta\ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \frac{1}{2}\ln^2\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\theta\left[\Delta - \ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right] + \Delta^2\theta\left[\ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \Delta\right]\right\}$$

$$C^+ = \int_{p^+,k^+}\theta(k^+ - p^+)\frac{1}{p^+}\frac{1}{[p^+(\boldsymbol{k}-\boldsymbol{p})^2 + (k^+ - p^+)\boldsymbol{p}^2]}$$
$$= \frac{1}{2\boldsymbol{p}^2}\Delta^2$$

$$B^+ - A^+ - C^+ = 0$$
$$B^+ + A^+ - C^+ = 2\left[\Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \frac{1}{2}\ln^2 \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\theta\left[\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right] + \Delta^2\theta\left[\ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \Delta\right]$$
$$2B^+ - A^+ = \frac{1}{\boldsymbol{p}^2}\left[\Delta^2 + \Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \frac{1}{2}\ln^2 \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\theta\left[\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right] + \frac{3}{2}\frac{1}{\boldsymbol{p}^2}\Delta^2\theta\left[\ln \frac{p^2}{k^2} - \Delta\right]$$

$$\Delta \gg \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\ln^2 \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}$$

$$[\bar{\psi}_i^5 + \bar{\psi}_i^3 + \bar{\psi}_i^4 + \bar{\psi}_i^6] = \left[\frac{1}{\boldsymbol{p}^2}\Delta^2 + \frac{1}{\boldsymbol{p}^2}\Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2} + \frac{2}{\boldsymbol{p}^2}\Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}$$

$$[\bar{\psi}_i^5 + \bar{\psi}_i^3 + \bar{\psi}_i^4 + \bar{\psi}_i^6] \simeq \frac{1}{\boldsymbol{p}^2}\left[\Delta^2 + \Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}$$

$$A^- \equiv \int_{p^+,k^+} \frac{1}{k^- + p^-}\frac{1}{k^-\boldsymbol{p}^2 + p^-\boldsymbol{k}^2}$$
$$B^- \equiv \int_{p^+,k^+} \frac{1}{\boldsymbol{p}^2}\frac{1}{k^-}\frac{1}{k^- + p^-}$$
$$C^- \equiv \int_{p^+,k^+} \theta\left(p^- - k^-\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right)\frac{1}{\boldsymbol{p}^2}\frac{1}{p^-}\frac{1}{k^-}$$

$$A^- = \frac{1}{\boldsymbol{p}^2 - \boldsymbol{k}^2}\left[\Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \frac{1}{2}\ln^2 \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\theta\left(\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right) + \frac{1}{2\boldsymbol{p}^2}\Delta^2\theta\left(\ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \Delta\right)$$
$$B^- = \frac{1}{2\boldsymbol{p}^2}\Delta^2$$
$$C^- = \frac{1}{2\boldsymbol{p}^2}\left[\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]^2\theta\left(\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right)$$

$$B^- - A^- - C^- = 0$$
$$2B^- - A^- = \frac{1}{2\boldsymbol{p}^2}\Delta^2 + \frac{1}{2\boldsymbol{p}^2}\left[\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]^2\theta\left(\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right)$$
$$B^- + A^- - C^- = \frac{2}{\boldsymbol{p}^2}\left[\Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \frac{1}{2}\ln^2 \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\theta\left(\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right) + \frac{1}{\boldsymbol{p}^2}\Delta^2\theta\left(\ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \Delta\right)$$

$$\begin{aligned}
[\bar{\psi}_i^5 + \bar{\psi}_i^3 + \bar{\psi}_i^4 + \bar{\psi}_i^6] &= \left[\frac{1}{2\boldsymbol{p}^2}\Delta^2 + \frac{1}{2\boldsymbol{p}^2}\left[\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]^2\theta\left(\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right)\right]\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2} \\
&+ \left\{\frac{2}{\boldsymbol{p}^2}\left[\Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \frac{1}{2}\ln^2 \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\theta\left(\Delta - \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right) + \frac{1}{\boldsymbol{p}^2}\Delta^2\theta\left(\ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2} - \Delta\right)\right\}\frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2} \\
&\approx \frac{1}{\boldsymbol{p}^2}\Delta^2\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2} - \frac{1}{\boldsymbol{p}^2}\Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\left[\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2} - \frac{2\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}\right] \\
&\simeq \frac{1}{\boldsymbol{p}^2}\left[\Delta^2 - \Delta \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}
\end{aligned}$$

$$\ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\Delta < \ln \frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\frac{\boldsymbol{p}(\boldsymbol{k}-\boldsymbol{p})}{\boldsymbol{p}^2(\boldsymbol{k}-\boldsymbol{p})^2}$$

$$\langle \rho(p)\rho(-p)\rangle \sim \mu^2\boldsymbol{p}^2/(\boldsymbol{p}^2 + Q_s^2)$$

$$\Delta = \ln \frac{E}{E_0}$$

$$\rho^a(p^+,\boldsymbol{p}) = \rho^a(p) + \delta\rho^a(p);$$
$$\rho^a(p) = -2if^{abc}\int_{q^-<E_0} q^+ A_j^{b\dagger}(q^+,\boldsymbol{q}+\boldsymbol{p})A_j^c(q^+,\boldsymbol{q})$$
$$\delta\rho^a(p) = -2if^{abc}\int_{E_0<q^-<p^-} q^+ A_j^{b\dagger}(q^+,\boldsymbol{q}+\boldsymbol{p})A_j^c(q^+,\boldsymbol{q})$$

$$|\Psi_3\rangle \equiv |\Psi_P\rangle_E|_{\rho\rho\rho} = 8g^3\int_{p^-<q^-<m^-}\Big[\rho^c(-m)\frac{\boldsymbol{m}_k}{\boldsymbol{m}^2}A_k^{\dagger c}(m^+,\boldsymbol{m})\rho^{*b}(-q)\frac{\boldsymbol{q}_j}{\boldsymbol{q}^2}A_j^b(q^+,\boldsymbol{q})\rho^a(-p)\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}A_i^{\dagger a}(p^+,\boldsymbol{p})$$
$$+\rho^{*c}(-m)\frac{\boldsymbol{m}_k}{\boldsymbol{m}^2}A_k^c(m^+,\boldsymbol{m})\rho^b(-q)\frac{\boldsymbol{q}_j}{\boldsymbol{q}^2}A_j^{\dagger b}(q^+,\boldsymbol{q})\rho^a(-p)\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}A_i^{\dagger a}(p^+,\boldsymbol{p})\Big]|0\rangle_F$$
$$= 8g^3\int_{p^-<q^-}\left[\frac{1}{2p^+}\frac{\boldsymbol{q}_i}{\boldsymbol{q}^2\boldsymbol{p}^2}\rho^a(-q)\rho^{*b}(-p)\rho^b(-p)A_i^{\dagger a}(q^+,\boldsymbol{q}) + \frac{1}{2q^+}\frac{\boldsymbol{p}_i}{\boldsymbol{q}^2\boldsymbol{p}^2}\rho^a(-p)\rho^{*b}(-q)\rho^b(-q)A_i^{\dagger a}(p^+,p)\right]|0\rangle_F$$
$$= 8g^3\int_{p,q}\frac{1}{2p^+}\frac{\boldsymbol{q}_i}{\boldsymbol{q}^2\boldsymbol{p}^2}\rho^a(-q)\rho^{*b}(-p)\rho^b(-p)A_i^{\dagger a}(q^+,\boldsymbol{q})|0\rangle_F$$

$$\frac{1}{\sqrt{2k^+}}\langle\boldsymbol{k}\mid\Psi_3\rangle = \frac{4g^3}{(2\pi)^{3/2}[2k^+]}\int_{E_0}^{E}\frac{dp^-}{2\pi}\int\frac{d^2\boldsymbol{p}}{(2\pi)^2}\frac{1}{p^+}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2\boldsymbol{p}^2}\rho^a(-k)\rho^{*b}(-p)\rho^b(-p)$$

$$G^{BFKL}(p^+,\boldsymbol{p}^2) = 2g\left[A_i^{\dagger a}(p)P_j[Q^{-1}]_{ij}^{ab}\rho^b(p^+,-\boldsymbol{p}) + A_i^a(p)P_j[Q^{-1}]_{ij}^{ab}\rho^{\dagger b}(p^+,-\boldsymbol{p})\right]$$

$$Q_{ij}^{ab} \equiv \left(\boldsymbol{P}^2\delta_{ij} + [\boldsymbol{P}_i,\boldsymbol{P}_j]\right)^{ab}\|$$

$$[Q^{-1}]_{ij}^{ab} = \frac{1}{\boldsymbol{p}^2}\left(\delta^{ab}\delta_{ij} - 2igf^{abc}\frac{\boldsymbol{p}_k\alpha_k^c}{\boldsymbol{p}^2}\delta_{ij} + igf^{abc}\frac{\boldsymbol{p}_i\alpha_j^c}{\boldsymbol{p}^2} + igf^{abc}\frac{\boldsymbol{p}_j\alpha_i^c}{\boldsymbol{p}^2}\right)$$
$$\boldsymbol{P}_j[Q^{-1}]_{ij}^{ab} = \frac{1}{\boldsymbol{p}^2}\left(\delta^{ab}\boldsymbol{p}_i - igf^{abc}\frac{\boldsymbol{p}_i\boldsymbol{p}_k\alpha_k^c}{\boldsymbol{p}^2} + 2igf^{abc}\alpha_i^c\right) = \frac{1}{\boldsymbol{p}^2}\left(\delta^{ab}\boldsymbol{p}_i + igf^{abc}\left[\frac{\boldsymbol{p}_i\boldsymbol{p}_k}{\boldsymbol{p}^2} - 2\left(\frac{\boldsymbol{p}_i\boldsymbol{p}_k}{\boldsymbol{p}^2} - \delta_{ik}\right)\right]\alpha_k^c\right)$$

$$|\Psi_P\rangle = \mathcal{P}\exp\left\{2\int_{p:E_0<p^-<E}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}\left[A_i^{\dagger a}(p)\rho^b(p^+,-\boldsymbol{p}) + A_i^a(p)\rho^{\dagger b}(p^+,-\boldsymbol{p})\right]\right.$$
$$\left.\times\left[g\delta^{ab} + ig^2f^{abc}\frac{\boldsymbol{p}_j}{\boldsymbol{p}^2}\int_{k:k^+\ll p^+;k^-\ll p^-}\left[\alpha_j^{\dagger c}(-k) + \alpha_j^c(k)\right]\right]\right\}|0\rangle_F$$

$$|\Psi_{eik}\rangle = 8g^3\int_{E_0<p^-<q^-<m^-<E}\left\{\frac{\boldsymbol{m}_k}{\boldsymbol{m}^2}\frac{\boldsymbol{q}_j}{\boldsymbol{q}^2}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}[\delta\rho^c(-m)\rho^{*b}(-q)\rho^a(-p) + \rho^c(-m)\delta\rho^{*b}(-q)\rho^a(-p)]\right.$$
$$\times A_k^{\dagger c}(m^+,\boldsymbol{m})A_j^b(q^+,\boldsymbol{q})A_i^{\dagger a}(p^+,\boldsymbol{p})$$
$$\left.+\frac{\boldsymbol{m}_k}{\boldsymbol{m}^2}\frac{\boldsymbol{q}_j}{\boldsymbol{q}^2}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}[\delta\rho^{*c}(-m)\rho^b(-q)\rho^a(-p) + \rho^{*c}(-m)\delta\rho^b(-q)\rho^a(-p)]A_k^c(m^+,\boldsymbol{m})A_j^{\dagger b}(q^+,\boldsymbol{q})A_i^{\dagger a}(p^+,\boldsymbol{p})\right\}|0\rangle_F$$

$$|\Psi_{eik}\rangle = 8g^3\int_{p^-<q^-}\frac{1}{2q^+}\frac{1}{\boldsymbol{q}^2}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}[\delta\rho^{*b}(-q)\rho^b(-q)\rho^a(-p) + \rho^{*b}(-q)\delta\rho^b(-q)\rho^a(-p)]A_i^{\dagger a}(p^+,\boldsymbol{p})|0\rangle_F$$

$$|\Psi_{eik}\rangle = -i4g^3\int_{p^-<q^-;p^+<q^+}\frac{1}{q^+}\frac{1}{\boldsymbol{q}^2}\frac{(\boldsymbol{p}-\boldsymbol{q})_i}{(\boldsymbol{p}-\boldsymbol{q})^2}f^{abc}\rho^a(-p+q)\rho^b(-q)A_i^{\dagger c}(p^+,\boldsymbol{p})|0\rangle_F$$

$$\psi_{eik}^{a}(k) \equiv \frac{1}{\sqrt{2k^+}}\langle \boldsymbol{k} \mid \Psi_{eik}\rangle \;= i\frac{4g^3}{(2\pi)^{3/2}[2k^+]}\int_{k^-<p^-;k^+>p^+}\frac{1}{p^+}\frac{1}{\boldsymbol{p}^2}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(-k+p)\rho^c(-p)$$

$$= i\frac{4g^3}{(2\pi)^{3/2}[2k^+]}\left[\int_{k^-<p^-} - \int_{k^-<p^-;p^+>k^+}\right]\frac{1}{p^+}\frac{1}{\boldsymbol{p}^2}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(-k+p)\rho^c(-p)$$

$$\left|\Psi_{soft}\right\rangle = i8g^3\int_{p^->q^->k^-;q^+>k^+}\frac{\boldsymbol{p}_i\boldsymbol{q}_j(\boldsymbol{q}+\boldsymbol{k})_l}{\boldsymbol{p}^2\boldsymbol{q}^2(\boldsymbol{q}+\boldsymbol{k})^2}f^{abc}\rho^{*d}(-p)\rho^b(-q-k)A_i^d(p)\alpha_l^{\dagger c}(k)A_j^{\dagger a}(q)|0\rangle_F$$

$$-i8g^3\int_{p^->q^-;p^->k^-;p^+>k^+}\frac{(\boldsymbol{p}+\boldsymbol{k})_j\boldsymbol{p}_i\boldsymbol{q}_l}{(\boldsymbol{p}+\boldsymbol{k})^2\boldsymbol{p}^2\boldsymbol{q}^2}f^{abc}\rho^{*b}(-p-k)\rho^d(-q)\alpha_j^{\dagger c}(k^+,-\boldsymbol{k})A_i^a(p^+,\boldsymbol{p})A_l^{\dagger d}(q^+,\boldsymbol{q})|0\rangle_F$$

$$= i4g^3\int_{p^->k^-;p^+>k^+}\frac{1}{p^+}\frac{(\boldsymbol{p}+\boldsymbol{k})_i}{\boldsymbol{p}^2(\boldsymbol{p}+\boldsymbol{k})^2}f^{abc}\rho^a(p)\rho^b(-p-k)\alpha_i^{\dagger c}(k)|0\rangle_F$$

$$\psi_{\text{soft}}^{a}(k) \equiv \frac{1}{\sqrt{2k^+}}\langle \boldsymbol{k} \mid \Psi_{\text{soft}}\rangle$$

$$= \frac{i4g^3}{(2\pi)^{3/2}[2k^+]}\int_{p^->k^-;p^+>k^+}\frac{1}{p^+}\frac{(\boldsymbol{p}+\boldsymbol{k})_i}{\boldsymbol{p}^2(\boldsymbol{p}+\boldsymbol{k})^2}f^{abc}\rho^b(p)\rho^c(-p-k)$$

$$= \frac{i4g^3}{(2\pi)^{3/2}[2k^+]}\int_{p^->k^-;p^+>k^+}\frac{1}{p^+}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{\boldsymbol{p}^2(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(p-k)\rho^c(-p)$$

$$\psi_{eik}^{a}(k) + \psi_{soft}^{a}(k) = i\frac{4g^3}{(2\pi)^{3/2}[2k^+]}\left[2\int_{k^-<p^-;p+} - \int_{k^-<p^-;p^+>k^+}\right]\frac{1}{p^+}\frac{1}{\boldsymbol{p}^2}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(p-k)\rho^c(-p)$$

$$\psi_{eik}^{a}(k) + \psi_{soft}^{a}(k) = i\frac{4g^3}{(2\pi)^{3/2}[2k^+]}\int\frac{d^2\boldsymbol{p}}{(2\pi)^2}\left[2\ln\frac{E}{k^-} - \ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\frac{1}{\boldsymbol{p}^2}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(p-k)\rho^c(-p)$$

$$\int\frac{dk^+}{2\pi}\left[\psi_{eik}^{a}(k) + \psi_{soft}^{a}(k)\right] = \frac{i2g^3}{(2\pi)^{5/2}}\int\frac{dk^+}{k^+}\int\frac{d^2\boldsymbol{p}}{(2\pi)^2}\left[2\ln\frac{E}{k^-} - \ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\frac{1}{\boldsymbol{p}^2}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(p-k)\rho^c(-p)$$

$$= \frac{i2g^3}{(2\pi)^{5/2}}\int_E^{Ee^\Delta}\frac{dk^-}{k^-}\int\frac{d^2\boldsymbol{p}}{(2\pi)^2}\left[2\ln\frac{E}{k^-} - \ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\frac{1}{\boldsymbol{p}^2}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(p-k)\rho^c(-p)$$

$$= \frac{i2g^3}{(2\pi)^{5/2}}\int\frac{d^2\boldsymbol{p}}{(2\pi)^2}\left[\Delta^2 - \Delta\ln\frac{\boldsymbol{p}^2}{\boldsymbol{k}^2}\right]\frac{1}{\boldsymbol{p}^2}\frac{(\boldsymbol{p}-\boldsymbol{k})_i}{(\boldsymbol{p}-\boldsymbol{k})^2}f^{abc}\rho^b(p-k)\rho^c(-p)$$

$$\psi_i^{3u} = \theta(p^+ - k^+)\psi_i^3;\; \psi_i^{3d} = \theta(k^+ - p^+)\psi_i^3$$

$$\psi_i^4 = -\frac{k^+ - p^+}{(k^+ + p^+)^2}\frac{k^+}{p^+}\frac{\boldsymbol{p}_i}{\boldsymbol{k}^2[k^+p^2 + p^+\boldsymbol{k}^2]}$$

$$\psi_i^5 + \psi_i^{3u} = \theta(p^+ - k^+)\frac{1}{\boldsymbol{k}^2\boldsymbol{p}^2}\frac{k^+}{p^+}\frac{1}{[k^+(\boldsymbol{k}-\boldsymbol{p})^2 + (p^+ - k^+)\boldsymbol{k}^2]}\times$$
$$\left\{\left[-\frac{p^+\boldsymbol{k}^2 + k^+\boldsymbol{p}^2}{k^+(k^+ - p^+)} - 2\frac{1}{p^+}\boldsymbol{p}^2\right]\boldsymbol{p}_i + 2\left[\frac{\boldsymbol{p}^2}{p^+} - \frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{k^+}\right]\boldsymbol{k}_i\right\}$$

$$\psi_i^6 + \psi_i^{3d} = \theta(k^+ - p^+)\frac{1}{\boldsymbol{k}^2\boldsymbol{p}^2}\frac{1}{[p^+(\boldsymbol{k}-\boldsymbol{p})^2 + (k^+ - p^+)\boldsymbol{p}^2]}\times$$
$$\left\{\left[\frac{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}{p^+(k^+ - p^+)} - 2\frac{1}{p^+}\boldsymbol{p}^2\right]\boldsymbol{p}_i + 2\left[\frac{\boldsymbol{p}^2}{p^+} - \frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{k^+}\right]\boldsymbol{k}_i\right\}$$

$$\psi_i^5 = \frac{1}{\boldsymbol{k}^2(\boldsymbol{p}-\boldsymbol{k})^2}\frac{1}{p^+ + k^+}\frac{1}{p^+}\frac{k^+\boldsymbol{p}^2}{[k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2]}\times$$

$$\left\{2\left[-\frac{k^+}{p^+} - \frac{\boldsymbol{p}\cdot\boldsymbol{k}}{\boldsymbol{p}^2} - \frac{(\boldsymbol{k}-\boldsymbol{p})^2}{\boldsymbol{p}^2}\frac{p^+}{k^+ + p^+}\right]\boldsymbol{p}_i + 2\left[\frac{k^+}{p^+} + \frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{\boldsymbol{p}^2}\frac{p^+}{k^+} + \frac{\boldsymbol{p}\cdot\boldsymbol{k}}{p^2}\right]\boldsymbol{k}_i\right\}$$

$$\psi_i^{3u} = -\frac{2k^+ + p^+}{(p^+)^2}\frac{1}{p^+ + k^+}\frac{1}{\boldsymbol{k}^2(\boldsymbol{p}-\boldsymbol{k})^2}(\boldsymbol{k}_i - \boldsymbol{p}_i)$$

$$\psi_i^5 = \frac{2k^+ + p^+}{(p^+)^2(p^+ + k^+)}\frac{1}{\boldsymbol{k}^2}\frac{k^+p^2}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2} + \frac{k^+ - p^+}{(k^+ + p^+)^2p^+}\frac{1}{\boldsymbol{k}^2}\frac{k^+\boldsymbol{p}^2}{(k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2)}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}$$

$$+\frac{1}{(p^+ + k^+)p^+}\frac{k^+}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\left[\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2} - \frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}\right] + 2\frac{1}{(p^+ + k^+)(k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2)}\frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}$$

$$\psi_i^{3u} = -\frac{2k^+ + p^+}{(p^+)^2(p^+ + k^+)}\frac{1}{\boldsymbol{k}^2}\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2}$$

$$\psi_i^4 = -\frac{k^+ - p^+}{(k^+ + p^+)^2p^+}\frac{1}{\boldsymbol{k}^2}\frac{k^+\boldsymbol{p}^2}{(k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2)}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}$$

$$\psi_i^5 = -\psi_i^{3u} - \psi_i^4 - \left(\frac{2}{p^+} - \frac{1}{p^+ + k^+}\right)\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2}$$

$$+\left(\frac{1}{p^+} - \frac{1}{p^+ + k^+}\right)\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\left[\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2} - \frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}\right] + \frac{2}{p^+ + k^+}\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}$$

$$= -\psi_i^{3u} - \psi_i^4$$

$$-\frac{1}{p^+}\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2} - \left(\frac{1}{p^+} - \frac{1}{p^+ + k^+}\right)\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2} + \frac{2}{p^+ + k^+}\frac{1}{k^+\boldsymbol{p}^2 + p^+\boldsymbol{k}^2}\frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p}^2)}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}$$

$$\psi_i^6 + \psi_i^{3d} = \theta(k^+ - p^+)\frac{1}{\boldsymbol{k}^2\boldsymbol{p}^2}\frac{1}{[p^+(\boldsymbol{k}-\boldsymbol{p})^2 + (k^+ - p^+)\boldsymbol{p}^2]}\left\{\left[\frac{\boldsymbol{p}^2 + \boldsymbol{k}^2}{k^+ - p^+} - \frac{1}{p^+}\boldsymbol{p}^2\right]\boldsymbol{p}_i + 2\left[\frac{\boldsymbol{p}^2}{p^+} - \frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{k^+}\right]\boldsymbol{k}_i\right\}$$

$$\psi_i^6 + \psi_i^{3d} = \theta(k^+ - p^+)\frac{1}{\boldsymbol{k}^2(\boldsymbol{p}-\boldsymbol{k})^2}\frac{1}{[p^+(\boldsymbol{k}-\boldsymbol{p})^2 + (k^+ - p^+)\boldsymbol{p}^2]}\left[(\boldsymbol{k}^2\boldsymbol{p}_i - \boldsymbol{p}\cdot\boldsymbol{k}\boldsymbol{k}_i)\frac{1}{p^+} + \boldsymbol{p}\cdot(\boldsymbol{p}-\boldsymbol{k})\boldsymbol{k}_i\left[\frac{1}{p^+} - \frac{2}{k^+}\right]\right]$$

$$\frac{(\boldsymbol{k}-\boldsymbol{p})_i}{(\boldsymbol{k}-\boldsymbol{p})^2} - \frac{\boldsymbol{k}_i}{\boldsymbol{k}^2} = -\frac{\boldsymbol{k}^2\boldsymbol{p}_i - \boldsymbol{p}\cdot\boldsymbol{k}\boldsymbol{k}_i}{\boldsymbol{k}^2(\boldsymbol{k}-\boldsymbol{p})^2} + \frac{\boldsymbol{p}\cdot(\boldsymbol{k}-\boldsymbol{p})}{(\boldsymbol{k}-\boldsymbol{p})^2}\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}$$

$$\frac{g}{2p^+}\boldsymbol{P}_i^{ab}\rho^b(-p) + \frac{1}{2}\left[\boldsymbol{P}^2\delta_{ij} + [\boldsymbol{P}_i, \boldsymbol{P}_j]\right]^{ab}A_j^b(p)$$

$$+igp^+f^{abc}\int_{k^+\ll p^+;k^-\ll p^-}\frac{\boldsymbol{k}_j}{k^+}\left[\alpha_j^b(k^+,\boldsymbol{k}) - \alpha_j^{\dagger b}(k^+,-\boldsymbol{k})\right]A_i^c(p) = 0$$

$$A_i^a(p^+,\boldsymbol{p}) = -g\frac{1}{p^+}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}\rho^a(-p) - ig^2\frac{1}{p^+}\frac{1}{\boldsymbol{p}^2}f^{abc}\int_{k^+\ll p^+;k^-\ll p^-}\left[\alpha_i^{\dagger c}(k^+,\boldsymbol{k}) + \alpha_i^c(k^+,-\boldsymbol{k})\right]\rho^b(-p)$$

$$-2ig^2\frac{\boldsymbol{p}_i}{\boldsymbol{p}^4}\frac{1}{p^+}f^{abc}\int_{k^+\ll p^+;k^-\ll p^-}\left[\boldsymbol{p}_j - \frac{p^+}{k^+}\boldsymbol{k}_j\right]\left[\alpha_j^{\dagger b}(k^+,\boldsymbol{k}) + \alpha_j^b(k^+,\boldsymbol{k})\right]\rho^c(-p) = -g\frac{1}{p^+}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}\rho^a(-p)$$

$$+ig^2\frac{1}{\boldsymbol{p}^2}\frac{1}{p^+}f^{abc}\int_{k^+\ll p^+;k^-\ll p^-}\left\{\left[\delta_{ij} - \frac{2\boldsymbol{p}_i\boldsymbol{p}_j}{\boldsymbol{p}^2}\right] + \frac{2p^+}{k^+}\frac{\boldsymbol{p}_i\boldsymbol{k}_j}{\boldsymbol{p}^2}\right\}\left[\alpha_j^{\dagger b}(k^+,\boldsymbol{k}) + \alpha_j^b(k^+,\boldsymbol{k})\right]\rho^c(-p)$$

$$A_i^a(p^+,\boldsymbol{p}) = -g\frac{1}{p^+}\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}\rho^a(-\boldsymbol{p}) + ig^2\frac{1}{\boldsymbol{p}^2}\left[\delta_{ij} - \frac{2\boldsymbol{p}_i\boldsymbol{p}_j}{\boldsymbol{p}^2}\right]\frac{1}{p^+}f^{abc}\int_{k^+\ll p^+;k^-\ll p^-}\left[\alpha_j^{\dagger b}(k^+,\boldsymbol{k}) + \alpha_j^b(k^+,\boldsymbol{k})\right]\rho^c(-\boldsymbol{p})$$

$$h = p^-A_i^{a\dagger}A_i^a + \rho^a(p)A^{a-}(p) + k^-\alpha_i^{a\dagger}\alpha_i^a + \rho^a(k)\alpha^{a-}(k)$$

$$U=\mathcal{P}e^{i\int_0^\infty dt[\rho^a(p)A^{a-}(t,p)+\rho^a(k)\alpha^{a-}(t,k)]^I}$$

$$U=1+i\int_0^\infty dt\left[\rho^a(p)A^{a-}(p)e^{-ip^-t}+\rho^a(k)\alpha^{a-}(k)e^{-ik^-t}\right]=1+\left[\frac{1}{p^-}\rho^a(p)A^{a-}(p)+\frac{1}{k^-}\rho^a(k)\alpha^{a-}(k)\right]$$
$$=1+i\left[\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}\rho^a(p)A_i^a(p)+\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}\rho^a(k)\alpha_i^a(k)\right]\approx e^{i\left[\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}\rho^a(p)A_i^a(p)+\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}\rho^a(k)\alpha_i^a(k)\right]}$$

$$U_2=-\int_0^\infty dt_1[\rho^a(p)A^{a-}(p)e^{-ip^-t_1}+\rho^a(k)\alpha^{a-}(k)e^{-ik^-t_1}]\int_0^{t_1}dt_2[\rho^a(p)A^{a-}(p)e^{-ip^-t_2}+\rho^a(k)\alpha^{a-}(k)e^{-ik^-t_2}]$$
$$\approx-\int_0^\infty dt_1\int_0^{t_1}dt_2[\rho^a(p)A^{a-}(p)e^{-ip^-t_1}\rho^b(k)\alpha^{b-}(k)e^{-ik^-t_2}+\rho^a(k)\alpha^{a-}(k)e^{-ik^-t_1}\rho^b(p)A^{b-}(p)e^{-ip^-t_2}]$$
$$=-\frac{1}{2}\int_0^\infty dt_1\int_0^\infty dt_2[\rho^a(p)A^{a-}(p)\rho^b(k)\alpha^{b-}(k)e^{-ip^-t_1-ik^-t_2}+\rho^a(k)\alpha^{a-}(k)\rho^b(p)A^{b-}(p)e^{-ik^-t_1-ip^-t_2}]$$
$$+\frac{1}{2}\int_0^\infty dt_1\int_{t_1}^\infty dt_2([\rho^a(p)A^{a-}(p),\rho^b(k)\alpha^{b-}(k)]e^{-ip^-t_1-ik^-t_2}+[\rho^a(k)\alpha^{a-}(k),\rho^b(p)A^{b-}(p)]e^{-ik^-t_1-ip^-t_2})$$

$$\delta U_2=\frac{1}{2}if^{abc}\rho^c(p)A^{b-}(p)\alpha^{c-}(k)\int_0^\infty dt_1\int_{t_1}^\infty dt_2\{e^{-ip^-t_1}e^{-ik^-t_2}-e^{-ik^-t_1}e^{-ip^-t_2}\}$$
$$=\frac{1}{2}if^{abc}\rho^c(p)A^{b-}(p)\alpha^{c-}(k)\left[\frac{1}{p^-k^-}-\frac{1}{p^-p^-}\right]=\frac{1}{2}if^{abc}\rho^c(p)\frac{\boldsymbol{p}_i\boldsymbol{k}_j}{\boldsymbol{p}^2\boldsymbol{k}^2}\left[1-\frac{\boldsymbol{k}^2}{\boldsymbol{p}^2}\frac{p^+}{k^+}\right]A_i^b(p)\alpha_j^c(k)$$

$$U=\exp\left\{i\left[\frac{\boldsymbol{p}_i}{\boldsymbol{p}^2}\rho^a(p)A_i^a(p)+\frac{\boldsymbol{k}_i}{\boldsymbol{k}^2}\rho^a(k)\alpha_i^a(k)\right]+\frac{1}{2}if^{abc}\rho^c(p)\frac{\boldsymbol{p}_i\boldsymbol{k}_j}{\boldsymbol{p}^2\boldsymbol{k}^2}\left[1-\frac{\boldsymbol{k}^2}{\boldsymbol{p}^2}\frac{p^+}{k^+}\right]A_i^b(p)\alpha_j^c(k)\right\}$$

$$\frac{d}{dt}\rho^a(p)=-if^{abc}\alpha^{-b}(k)\rho^c(p)$$

$$\rho^a(p,t)=\left[\mathcal{P}\exp\left\{-i\int_0^t d\tau T\alpha^-(\tau)\right\}\right]^{ab}\rho^b(p)$$

$$\rho^a(p,t)\approx[\exp\{-iT\alpha^-t\}]^{ab}\rho^b(p)$$

$$U(A)=1-i\int_0^\infty dt\rho^a(p,t)A^{a-}(p,t)=1+i\rho^a(p)\int_0^\infty dt\left[e^{-i(-T\alpha^-+p^-)t}\right]_{ab}A^{-b}$$
$$=1+\rho^a(p)\left[\frac{1}{p^--T\alpha^-}\right]_{ab}A^{-b}\approx\exp\left\{i\frac{p_i}{p^+}\rho^a(p)\left[\frac{1}{p^--T\alpha^-}\right]_{ab}A_i^b(p)\right\}$$

$$P^-\equiv\frac{\boldsymbol{P}^2}{2p^+}$$

$$A_i^a(p,t)=\left[e^{-i(P^-+T\alpha^-)t}\right]_{ab}A_i^b(p)$$

$$U(A)=1-i\int_0^\infty dt\rho^a(p,t)A^{a-}(p,t)=1+i\rho^a(p)\int_0^\infty dt\left[e^{iT\alpha^-t}e^{-i(P^-+T\alpha^-)t}\right]_{ab}A^{-b}(p)$$
$$=1+i\rho^a(p)\left[\frac{\boldsymbol{P}_i}{\boldsymbol{P}^2}\right]_{ab}A_i^b(p)\approx e^{i\rho^a(p)\left[\frac{\boldsymbol{P}_i}{\boldsymbol{P}^2}\right]_{ab}A_i^b(p)}$$

$$|k,i\rangle=\frac{a^{i\dagger}(k^+,\boldsymbol{k})}{(2\pi)^{3/2}}|0\rangle$$

$$\hat{H}_{\mathrm{PF}} = \hat{T}_{\mathrm{N}} + \hat{H}_{\mathrm{e}} + \sum_{\lambda,k}^{2N_{\mathrm{c}}} \left[\frac{p_{\lambda k}^2}{2} + \frac{\omega_k^2}{2} \left(q_{\lambda k} + \sqrt{\frac{2}{\hbar\omega_k}} \eta_k \hat{\mathbf{e}}_\lambda \cdot \hat{\boldsymbol{\mu}} \right)^2 \right]$$

$$\hat{H}_{\mathrm{e}} = \hat{T}_{\mathrm{e}} + \hat{V}_{\mathrm{ee}} + \hat{V}_{\mathrm{eN}} + \hat{V}_{\mathrm{NN}}$$

$$\hat{\mu} = -\sum_{i=1}^{N_{\mathrm{e}}} \hat{r}_i + \sum_{j=1}^{N_{\mathrm{N}}} Z_j \hat{R}_j$$

$$\eta_k = \sqrt{\hbar/2\omega_k \varepsilon_0 \mathcal{V}} = \eta/\sqrt{k}$$

$$\hat{H}_{\mathrm{PF}} = \hat{T}_{\mathrm{N}} + \hat{T}_{\mathrm{c}} + \hat{H}_{\mathrm{CBO}}$$

$$\hat{H}_{\mathrm{CBO}} = \hat{H}_{\mathrm{e}} + \sum_{\lambda,k}^{2N_{\mathrm{c}}} \frac{\omega_k^2}{2} \left(q_{\lambda k} + \sqrt{\frac{2}{\hbar\omega_k}} \eta_k \hat{\mathbf{e}}_\lambda \cdot \hat{\boldsymbol{\mu}} \right)^2,$$

$$\hat{H}_{\mathrm{CBO}} |\nu\rangle = V_{\mathrm{CBO},\nu}(\mathbf{R}, \mathbf{q}) |\nu\rangle.$$

$$\hat{H}_{\mathrm{e}} |n\rangle = V_{\mathrm{BO},n}(\mathbf{R}) |n\rangle.$$

$$q_{\lambda k} = -\sqrt{2/\hbar\omega_k} \eta_k \hat{\mathbf{e}}_\lambda \cdot \hat{\boldsymbol{\mu}} = 0$$

$$\begin{aligned} H_{nn} =& V_{\mathrm{BO},n}(\mathbf{R}) + \sum_{\lambda,k}^{2N_{\mathrm{c}}} \left[\frac{\omega_k^2}{2} q_{\lambda k}^2 \right. \\ & \left. + \sqrt{2/\hbar} \omega_k^{3/2} \eta_k q_{\lambda k} \langle n|\hat{\mu}_\lambda|n\rangle + \frac{\omega_k}{\hbar} \eta_k^2 \langle n|\hat{\mu}_\lambda^2|n\rangle \right] \end{aligned}$$

$$\begin{aligned} H_{mn} =& \sum_{\lambda,k}^{2N_{\mathrm{c}}} \left[\sqrt{2/\hbar} \omega_k^{3/2} \eta_k q_{\lambda k} \langle m|\hat{\mu}_\lambda|n\rangle \right. \\ & \left. + \frac{\omega_k}{\hbar} \eta_k^2 \langle m|\hat{\mu}_\lambda^2|n\rangle \right] \text{ for } m \neq n \end{aligned}$$

$$\hat{H}^{(0)} = \sum_n H_{nn} |n\rangle\langle n|$$

$$\Delta\hat{V} = \hat{H}_{\mathrm{CBO}} - \hat{H}^{(0)}$$

$$\Delta\hat{V} = \sum_{m \neq n} H_{mn} |m\rangle\langle n|$$

$$E_0^{(2)} = \sum_{n \neq 0} \frac{|\langle 0|\Delta\hat{V}|n\rangle|^2}{E_0 - E_n}$$

$$
\begin{aligned}
E_0^{(2)} =& \eta^2 q^2 \frac{2\omega_c^3}{\hbar} \sum_{n\neq 0} \frac{\langle 0|\hat{\mu}|n\rangle^2}{V_{\mathrm{BO},0} - V_{\mathrm{BO},n}} \\
&+\eta^3 q \sqrt{\frac{8\omega_c^5}{\hbar^3}} \sum_{n\neq 0} \frac{\langle 0|\hat{\mu}^2|n\rangle\langle 0|\hat{\mu}|n\rangle}{V_{\mathrm{BO},0} - V_{\mathrm{BO},n}} \\
&+\eta^4 \frac{\omega_c^2}{\hbar^2} \sum_{n\neq 0} \frac{\langle 0|\hat{\mu}^2|n\rangle^2}{V_{\mathrm{BO},0} - V_{\mathrm{BO},n}} \\
&-\eta^3 q^3 \sqrt{\frac{8\omega_c^9}{\hbar^3}} \sum_{n\neq 0} \frac{(\langle 0|\hat{\mu}|0\rangle - \langle n|\hat{\mu}|n\rangle)\langle 0|\hat{\mu}|n\rangle^2}{\left(V_{\mathrm{BO},0} - V_{\mathrm{BO},n}\right)^2} \\
&+O(\eta^4)
\end{aligned}
$$

$$
\begin{aligned}
\langle 0|\hat{\mu}^2|0\rangle =& \sum_n \langle 0|\hat{\mu}|n\rangle\langle n|\hat{\mu}|0\rangle \\
=& \langle 0|\hat{\mu}|0\rangle^2 + \sum_{n\neq 0} \langle 0|\hat{\mu}|n\rangle\langle n|\hat{\mu}|0\rangle
\end{aligned}
$$

$$
q_{\min} = -\sqrt{2/\hbar}\eta\omega_c^{-1/2}\langle 0|\hat{\mu}|0\rangle
$$

$$
\hat{\mu} = \sum_i \hat{\mu}_i
$$

$$
V_{\mathrm{cCBO}}(\mathbf{R}, q_{\min}) = \sum_{i=1}^{N} \left[V_{\mathrm{BO},0}(\mathbf{R}_i) + \frac{\eta^2\omega}{\hbar}\left(\langle 0|\hat{\mu}_i^2|0\rangle - \langle 0|\hat{\mu}_i|0\rangle^2\right) \right],
$$

$$
\eta_N = \eta_1/\sqrt{N},
$$

$$
C^{\mathrm{PT}} = -\frac{2\omega_c^3\eta^2}{\hbar} N\alpha_1
$$

$$
\alpha_1 = -2\sum_{n\neq 0} \langle 0|\hat{\mu}|n\rangle^2 / \left(V_0(\mathbf{R}_{\mathrm{eq}}) - V_{\mathrm{BO},n}(\mathbf{R}_{\mathrm{eq}})\right)
$$

$$
\begin{aligned}
\omega_c'^2 =& C + C^{\mathrm{PT}} \\
=& \omega_c^2 \left(1 - \frac{2\omega_c\eta^2}{\hbar} N\alpha_1\right) \\
=& \omega_c^2 \left(1 - \frac{N\alpha_1}{\varepsilon_0 \mathcal{V}}\right) \\
=& \omega_c^2/n^2 \left(\frac{N\alpha_1}{\varepsilon_0 \mathcal{V}} \ll 1\right)
\end{aligned}
$$

$$
\begin{aligned}
\hat{\mu}^2 =& \left(\sum_{i=1}^{N_e} \hat{r}_i\right)^2 - 2\sum_{i=1}^{N_e} \hat{r}_i \sum_{j=1}^{N_N} Z_j \hat{R}_j + \left(\sum_{j=1}^{N_N} Z_j \hat{R}_j\right)^2 \\
=& \left(\sum_{i=1}^{N_e} \hat{r}_i\right)^2 + 2\hat{\mu}_e\mu_N + \mu_N^2
\end{aligned}
$$

$$\left(\sum_{i=1}^{N_e} \hat{r}_i\right)^2 = \sum_i \hat{r}_i^2 + \sum_{i\neq j} \hat{r}_i\hat{r}_j$$

$$\langle 0|\sum_{i\neq j} \hat{r}_i\hat{r}_j|0\rangle = \sum_{n\neq m}^{\text{occupied}} [4\langle\phi_n|\hat{r}|\phi_n\rangle\langle\phi_m|\hat{r}|\phi_m\rangle \\ -2\langle\phi_n|\hat{r}|\phi_m\rangle\langle\phi_m|\hat{r}|\phi_n\rangle]$$

$$\langle 0|\hat{\mu}|\Psi_m^n\rangle = \langle\phi_m|\hat{r}|\phi_n\rangle$$

$$\langle 0|\sum_i \hat{r}_i^2|\Psi_m^n\rangle = \langle\phi_m|\hat{r}^2|\phi_n\rangle$$

$$\langle 0|\sum_{i\neq j} \hat{r}_i\hat{r}_j|\Psi_m^n\rangle = 2\sum_p [4\langle\phi_m|\hat{r}|\phi_n\rangle\langle\phi_p|\hat{r}|\phi_p\rangle \\ -2\langle\phi_m|\hat{r}|\phi_p\rangle\langle\phi_p|\hat{r}|\phi_n\rangle].$$

$$(\hat{\boldsymbol{\mu}} \otimes \hat{\boldsymbol{\mu}}) = \begin{pmatrix} \hat{\mu}_x\hat{\mu}_x & \hat{\mu}_x\hat{\mu}_y & \hat{\mu}_x\hat{\mu}_z \\ \hat{\mu}_y\hat{\mu}_x & \hat{\mu}_y\hat{\mu}_y & \hat{\mu}_y\hat{\mu}_z \\ \hat{\mu}_z\hat{\mu}_x & \hat{\mu}_z\hat{\mu}_y & \hat{\mu}_z\hat{\mu}_z \end{pmatrix}.$$

$$A_{ij} \equiv \frac{\partial^2 V_{\text{BO},0}}{\partial R_i \partial R_j} + \sqrt{2/\hbar}\,\omega_c^{3/2} q\eta \frac{\partial^2}{\partial R_i \partial R_j}\langle 0|\hat{\mu}_1|0\rangle \\ + \frac{\omega_c}{\hbar}\eta^2 \left[\frac{\partial^2}{\partial R_i \partial R_j}\langle 0|\hat{\mu}_1^2|0\rangle + \sum_{m\neq 1} \langle 0|\hat{\mu}_m|0\rangle \frac{\partial^2}{\partial R_i \partial R_j}\langle 0|\hat{\mu}_1|0\rangle\right] \\ = \frac{\partial^2 V_{\text{BO},0}}{\partial R_i \partial R_j} + \frac{\omega_c}{\hbar}\eta^2 \left[\frac{\partial^2}{\partial R_i \partial R_j}\langle 0|\hat{\mu}_1^2|0\rangle - (N+1)\langle 0|\hat{\mu}_1|0\rangle \frac{\partial^2}{\partial R_i \partial R_j}\langle 0|\hat{\mu}_1|0\rangle\right]$$

$$G_{ij} \equiv \frac{\omega_c}{\hbar}\eta^2 \frac{\partial}{\partial R_i}\langle 0|\hat{\mu}_1|0\rangle \frac{\partial}{\partial R_j}\langle 0|\hat{\mu}_1|0\rangle$$

$$B_i \equiv \frac{\partial^2 V_{\text{cCBO}}}{\partial q \partial R_i} = \sqrt{2/\hbar}\,\omega_c^{3/2}\eta \frac{\partial}{\partial R_i}\langle 0|\hat{\mu}_1|0\rangle$$

$$C \equiv \frac{\partial^2 V_{\text{cCBO}}}{\partial q^2} = \omega_c^2.$$

$$\mathbf{H} = \begin{pmatrix} \mathbf{A} & \mathbf{G} & \mathbf{G} & \cdots & \mathbf{B} \\ \mathbf{G} & \mathbf{A} & \mathbf{G} & \cdots & \mathbf{B} \\ \mathbf{G} & \mathbf{G} & \mathbf{A} & \cdots & \mathbf{B} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{B}^{\text{T}} & \mathbf{B}^{\text{T}} & \mathbf{B}^{\text{T}} & \cdots & C \end{pmatrix}$$

$$\omega_m'^2 = \omega_m^2 + \frac{\omega_c}{\hbar M_{\text{HF}}}\eta^2 \left[\frac{\partial^2}{\partial R^2}\langle 0|\hat{\mu}^2|0\rangle - 2\langle 0|\hat{\mu}_1|0\rangle \frac{\partial^2}{\partial R^2}\langle 0|\hat{\mu}_1|0\rangle\right],$$

$$\left(\left(\frac{\partial\langle\hat{\mu}\rangle}{\partial \mathbf{R}}, \frac{\partial\langle\hat{\mu}\rangle}{\partial \mathbf{R}}, \frac{\partial\langle\hat{\mu}\rangle}{\partial \mathbf{R}}, \ldots, 0\right)^{\text{T}} \cdot \mathbf{v}\right)^2$$

$$E_0^{(2),\eta^2} = \frac{2\omega_c^2\eta^2}{\hbar} q^2 \sum_{n\neq 0} \frac{\langle 0|\hat{\mu}|n\rangle^2}{V_0(\mathbf{R}) - V_n(\mathbf{R})}$$
$$\equiv -\frac{\omega_c^2\eta^2}{\hbar} q^2 \alpha_1(\mathbf{R})$$

$$A_{ij}^{\mathrm{PT}} = -\frac{\eta^2\omega_c^3}{\hbar} q^2 \frac{\partial^2}{\partial R_i \partial R_j}\alpha_1(\mathbf{R})$$
$$= -\eta^4 \frac{\omega_c^2}{\hbar^2} N^2 \langle 0|\hat{\mu}_1|0\rangle^2 \frac{\partial^2}{\partial R_i \partial R_j}\alpha_1(\mathbf{R})$$
$$B_i^{\mathrm{PT}} = -\frac{2\eta^2\omega_c^3}{\hbar} q \frac{\partial}{\partial R_i}\alpha_1(\mathbf{R})$$
$$= \eta^3 \sqrt{\frac{8\omega_c^5}{\hbar^3}} N \langle 0|\hat{\mu}_1|0\rangle \frac{\partial}{\partial R_i}\alpha_1(\mathbf{R})$$
$$C^{\mathrm{PT}} = -\frac{2\eta^2\omega_c^3}{\hbar}\alpha_N(\mathbf{R})$$
$$= -\eta^2 \frac{2\omega_c^3}{\hbar} N\alpha_1(\mathbf{R}).$$

$$A_{ij}^{\langle\hat{\mu}\rangle^2} \equiv \frac{\partial^2 V_{\mathrm{BO},0}}{\partial R_i \partial R_j} + \sqrt{2/\hbar}\,\omega_c^{3/2} q\eta \frac{\partial^2}{\partial R_i \partial R_j}\langle 0|\hat{\mu}_1|0\rangle$$
$$+2\frac{\omega_c}{\hbar}\eta^2\left[\frac{\partial\langle 0|\hat{\mu}_1|0\rangle}{\partial R_i}\frac{\partial\langle 0|\hat{\mu}_1|0\rangle}{\partial R_j} + N\langle 0|\hat{\mu}_1|0\rangle \frac{\partial^2}{\partial R_i \partial R_j}\langle 0|\hat{\mu}_1|0\rangle\right]$$

$$= \frac{\partial^2 V_{\mathrm{BO},0}}{\partial R_i \partial R_j} + 2\frac{\omega_c}{\hbar}\eta^2 \frac{\partial\langle 0|\hat{\mu}_1|0\rangle}{\partial R_i}\frac{\partial\langle 0|\hat{\mu}_1|0\rangle}{\partial R_j}$$

$$\mathbf{H} = \begin{pmatrix} \mathbf{A} + (N-1)\mathbf{G} & \sqrt{N}\mathbf{B} \\ \sqrt{N}\mathbf{B}^{\mathrm{T}} & C \end{pmatrix},$$

$$E_0^{(2)} = \sum_{n\neq 0} \frac{\left(\sum_{\lambda,k}\left[\sqrt{2/\hbar}\,\omega_c^{3/2}\eta k q_{\lambda,k}\hat{\mathbf{e}}_\lambda \cdot \langle 0|\hat{\boldsymbol{\mu}}|n\rangle + \frac{\omega_c}{\hbar}\eta^2\langle 0|(\hat{\mathbf{e}}_\lambda\cdot\hat{\boldsymbol{\mu}})^2|n\rangle\right]\right)^2}{V_0(\mathbf{R}) - V_n(\mathbf{R}) + \eta\sum_{\lambda,k}\left[\sqrt{2/\hbar}\,\omega_c^{3/2} k q_{\lambda,k}\hat{\mathbf{e}}_\lambda \cdot (\langle 0|\hat{\boldsymbol{\mu}}|0\rangle - \langle n|\hat{\boldsymbol{\mu}}|n\rangle)\right] + O(\eta^2)}$$
$$= \sum_{n\neq 0} \eta^2 \frac{2\omega_c^3}{\hbar} \frac{\left(\sum_{\lambda,k} k q_{\lambda,k}\hat{\mathbf{e}}_\lambda \cdot \langle 0|\hat{\boldsymbol{\mu}}|n\rangle\right)^2}{V_0(\mathbf{R}) - V_n(\mathbf{R})}$$
$$+\eta^3 2\sqrt{\frac{2\omega_c^5}{\hbar^3}} \frac{\left[\sum_{\lambda,k}\langle 0|(\hat{\mathbf{e}}_\lambda\cdot\hat{\boldsymbol{\mu}})^2|n\rangle\right]\left[\sum_{\lambda',k'} k' q_{\lambda',k'}\hat{\mathbf{e}}_{\lambda'} \cdot \langle 0|\hat{\boldsymbol{\mu}}|n\rangle\right]}{V_0(\mathbf{R}) - V_n(\mathbf{R})}$$
$$+\eta^4 \frac{\omega_c^2}{\hbar^2} \frac{\left(\sum_{\lambda,k}\langle 0|(\hat{\mathbf{e}}_\lambda\cdot\hat{\boldsymbol{\mu}})^2|n\rangle\right)^2}{V_0(\mathbf{R}) - V_n(\mathbf{R})}$$
$$-\eta^3\sqrt{\frac{8\omega_c^9}{\hbar^3}}\left[\sum_{\lambda,k} k q_{\lambda,k}\hat{\mathbf{e}}_\lambda \cdot (\langle 0|\hat{\boldsymbol{\mu}}|0\rangle - \langle n|\hat{\boldsymbol{\mu}}|n\rangle)\right]\left(\sum_{\lambda',k'} k' q_{\lambda',k'}\hat{\mathbf{e}}_{\lambda'} \cdot \langle 0|\hat{\boldsymbol{\mu}}|n\rangle\right)^2$$
$$+O(\eta^4)$$

$$\hat{V}_{\mathrm{dipole}} = \frac{1}{2}\sum_\alpha (\omega_\alpha \hat{q}_\alpha - \lambda_\alpha \cdot \hat{\mu})^2.$$

$$\hat{H}_e(R,q)|\psi(R,q)\rangle = U(R,q)|\psi(R,q)\rangle$$
$$\left(\hat{T}_{\text{nuc}} + \hat{T}_{\text{pht}} + \bar{U}(R,q)\right)\left|\Phi^{\text{nuc,pht}}\right\rangle = E\left|\Phi^{\text{nuc,pht}}\right\rangle$$

$$(\lambda_\alpha \cdot \hat{\mu})^2 \overset{\text{MF}}{\approx} 2(\lambda_\alpha \cdot \langle\hat{\mu}\rangle)(\lambda_\alpha \cdot \hat{\mu}) - (\lambda_\alpha \cdot \langle\hat{\mu}\rangle)^2.$$

$$\hat{H}_e^{\text{MF}}(\psi; R, q) = \hat{T}_e + \hat{V}_{\text{Coulomb}}(R)$$
$$+\sum_\alpha \frac{1}{2}(\omega_\alpha q_\alpha)^2 - (\omega_\alpha q_\alpha - \lambda_\alpha \cdot \mu(\psi, R))(\lambda_\alpha \cdot \hat{\mu})$$
$$-\frac{1}{2}(\lambda_\alpha \cdot \mu(\psi, R))^2$$

$$\epsilon(\psi; R) \approx \left\langle \hat{T}_e + \hat{V}_{\text{Coulomb}}(R) \right\rangle_\psi$$

$$\bar{\epsilon}(R) = \epsilon(\bar{\psi}; R) = \min_\psi \epsilon(\psi; R).$$

$$U(\psi; R, q) = \epsilon(\psi; R) + \frac{1}{2}\sum_\alpha (\omega_\alpha q_\alpha - \lambda_\alpha \cdot \mu(\psi, R))^2$$

$$\bar{U}(R, q) = U(\bar{\psi}_U; R, q) = \min_\psi U(\psi; R, q).$$

$$\mathcal{E}_\alpha = \omega_\alpha q_\alpha - \lambda_\alpha \cdot \bar{\mu}_U(R, q)$$

$$\mathcal{F}(\psi; R, \mathcal{E}) = \epsilon(\psi; R) - \mathbb{E}(\mathcal{E}) \cdot \mu(\psi, R_I)$$

$$\overline{\mathcal{F}}(R, \mathcal{E}) = \mathcal{F}(\bar{\psi}_\mathcal{F}; R, q) = \min_\psi \mathcal{F}(\psi; R, \mathcal{E})$$

$$\mathfrak{F} := U - \sum_\alpha \mathcal{D}_\alpha \mathcal{E}_\alpha$$

$$\mathcal{E}_\alpha := \frac{\partial U}{\partial \mathcal{D}_\alpha} \quad (14) \quad \mathcal{D}_\alpha := -\frac{\partial \mathfrak{F}}{\partial \mathcal{E}_\alpha}$$

$$\mathfrak{F}(\psi, R, \mathcal{E}) = \bar{\epsilon}(\psi, R) - \sum_\alpha \mathcal{E}_\alpha \lambda_\alpha \cdot \bar{\mu}_\mathcal{F}(\psi, R) - \frac{1}{2}\sum_\alpha \mathcal{E}_\alpha^2.$$

$$dU = \frac{\partial U}{\partial \psi} d\psi + \frac{\partial U}{\partial R} dR + \mathcal{E} d\mathcal{D}$$

$$d\mathfrak{F} = \frac{\partial \mathfrak{F}}{\partial \psi} d\psi + \frac{\partial \mathfrak{F}}{\partial R} dR - \mathcal{D} d\mathcal{E}$$

$$\mathfrak{F} := U - \sum_\alpha \mathcal{D}_\alpha \mathcal{E}_\alpha$$

$$d\mathfrak{F} = dU - \mathcal{E} d\mathcal{D} - \mathcal{D} d\mathcal{E}$$

$$d\mathfrak{F} = \frac{\partial U}{\partial \psi} d\psi + \frac{\partial U}{\partial R} dR - \mathcal{D} d\mathcal{E}$$

$$\left.\frac{d\mathfrak{F}}{d\psi}\right|_{R\mathcal{E}} = \left.\frac{dU}{d\psi}\right|_{R\mathcal{D}} \frac{\partial U}{\partial \psi}$$

$$F_I = -\left.\frac{d\bar{U}}{dR_I}\right|_{\mathcal{D}} = -\left.\frac{d\bar{\mathcal{F}}}{dR_I}\right|_{\mathcal{E}}$$

$$F_\alpha = -\left.\frac{d\bar{U}}{dq_\alpha}\right|_R = -\omega_\alpha \left.\frac{d\bar{U}}{d\mathcal{D}_\alpha}\right|_R = -\omega_\alpha \mathcal{E}_\alpha$$

$$\mathcal{E}_\alpha(R,q) = \omega_\alpha q_\alpha - \lambda_\alpha \cdot \bar{\mu}_{\mathcal{F}}\left(R, \sum_\beta \lambda_\beta \mathcal{E}_\beta(R,q)\right)$$

$$\bar{\mu} = \bar{\mu}_0 + \sum_I Z_I^* \Delta R_I + \chi \mathbb{E}$$

$$Z_{Ii} = \frac{d\bar{\mu}_i}{dR_I} \chi_{ij} = \frac{d\bar{\mu}_i}{d\mathbb{E}_j}$$

$$\mathcal{E}_\alpha = \omega_\alpha \Delta q_\alpha - \lambda_\alpha \cdot \sum_I Z_I^* \Delta R_I - \lambda_\alpha^T \chi \sum_\beta \lambda_\beta \mathcal{E}_\beta$$

$$\Delta q_\alpha = q_\alpha - \frac{\lambda_\alpha \cdot \bar{\mu}_0}{\omega_\alpha}$$

$$\mathcal{E}_\alpha = \sum_\beta [(\mathbb{I} + \mathbb{X})^{-1}]_{\alpha\beta} \left(\omega_\beta \Delta q_\beta - \lambda_\beta \cdot \sum_I Z_I^* \Delta R_I\right)$$

$$\mathbb{X}_{\alpha\beta} = \lambda_\alpha^T \chi \lambda_\beta$$

$$\mathbb{E} = \sum_\alpha \lambda_\alpha \mathcal{E}_\alpha$$

$$\bar{U}(R,\mathcal{E}) = \epsilon(\bar{\psi}_{\mathcal{F}}; R) + \frac{1}{2}\sum_\alpha \mathcal{E}_\alpha^2$$

$$d\bar{\mathcal{F}}/d\mathcal{E}_\alpha = \partial\bar{\mathcal{F}}/\partial\mathcal{E}_\alpha$$

$$\frac{d\epsilon(\bar{\psi}_{\mathcal{F}}; R)}{d\mathcal{E}_\alpha} = \sum_\beta \mathcal{E}_\beta \lambda_\beta \left(\chi \lambda_\alpha + \frac{d\chi}{d\mathcal{E}_\alpha} \sum_\gamma \mathcal{E}_\gamma \lambda_\gamma\right)$$

$$C_{IJ} = \frac{\partial^2 \bar{U}}{\partial R_I \partial R_J}$$

$$\begin{aligned}\bar{U} &= \bar{U}(R_0, q_0) + \frac{1}{2} C_{IJ} \Delta R_I \Delta R_J \\ &+ \frac{1}{2}\left(\delta_{\alpha\beta} + \lambda_\beta \chi \lambda_\alpha\right) \mathcal{E}_\alpha \mathcal{E}_\beta\end{aligned}$$

$$\bar{U} = \bar{U}(R_0, q_0) + \frac{1}{2}\Delta R_I C_{IJ} \Delta R_J + \frac{1}{2}[\omega_\alpha \Delta q_\alpha - \lambda_\alpha Z_I \Delta R_I][(\mathbb{I} + \mathbb{X})^{-1}]_{\alpha\gamma}[\omega_\gamma \Delta q_\gamma - \lambda_\gamma Z_J \Delta R_J]$$

$$\bar{\mu} = \bar{\mu}_0 + \chi \left[\sum_{\alpha} \lambda_\alpha (\omega_\alpha q_\alpha - \lambda_\alpha \cdot \mu) \right] + \sum_i \mathbf{Z}_i^* \Delta R_i$$

$$\bar{\mu} = \bar{\mu}_0 + \Delta\bar{\mu}$$

$$\Delta\bar{\mu} + \sum_{\alpha} (\chi\lambda_\alpha)\lambda_\alpha \cdot \Delta\bar{\mu} = \chi \sum_{\alpha} \lambda_\alpha \omega_\alpha \Delta q_\alpha + \sum_i \mathbf{Z}_i^* \Delta R_i$$

$$\Lambda = 1 + \sum_{\alpha} \chi \lambda_\alpha \lambda_\alpha^T$$

$$\Delta\bar{\mu} = \Lambda^{-1} \left(\chi \sum_{\alpha} \lambda_\alpha \omega_\alpha \Delta q_\alpha + \sum_i \mathbf{Z}_i^* \Delta R_i \right)$$

$$\left[-\frac{\hbar^2}{2M} \sum_i \nabla_i^2 - \frac{\hbar^2}{2m} \nabla^2 - \lambda\delta(x - x_1) - \lambda\delta(x - x_2) \right] \Psi(x; x_1, x_2) = E\Psi(x; x_1, x_2)$$

$$\Psi(x; x_1, x_2) = \phi(x \mid x_1, x_2)\psi(x_1, x_2)$$

$$\left[-\frac{\hbar^2}{2M} \sum_i \nabla_i^2 \psi(x_1, x_2) \right] \phi(x \mid x_1, x_2) + \left[-\frac{\hbar^2}{2M} \sum_i \nabla_i^2 \phi(x \mid x_1, x_2) \right] \psi(x_1, x_2)$$
$$- \frac{\hbar^2}{2M} \sum_i \frac{\partial\phi}{\partial x_i} \frac{\partial\psi}{\partial x_i} + \left[\left(-\frac{\hbar^2}{2m} \nabla_x^2 - \lambda\delta(x - x_1) - \lambda\delta(x - x_2) \right) \phi(x \mid x_1, x_2) \right] \psi(x_1, x_2)$$
$$= E\phi(x \mid x_1, x_2)\psi(x_1, x_2)$$

$$-\frac{\hbar^2}{2m} \nabla_x^2 \phi(x \mid x_1, x_2) - \lambda[\delta(x - x_1) + \delta(x - x_2)]\phi(x \mid x_1, x_2) = E(x_1, x_2)\phi(x \mid x_1, x_2).$$

$$\left[-\frac{\hbar^2}{2M} \sum_i \nabla_i^2 + E(x_1, x_2) \right] \psi(x_1, x_2)\phi(x \mid x_1, x_2) + \left[-\frac{\hbar^2}{2M} \sum_i \nabla_i^2 \phi(x \mid x_1, x_2) \right] \psi(x_1, x_2)$$
$$- \frac{\hbar^2}{2M} \sum_i \frac{\partial\phi}{\partial x_i} \frac{\partial\psi}{\partial x_i} = E\phi(x \mid x_1, x_2)\psi(x_1, x_2)$$

$$\left[-\frac{\hbar^2}{2M} \sum_i \nabla_i^2 + E(x_1, x_2) \right] \psi(x_1, x_2) = E\psi(x_1, x_2)$$

$$\phi(x \mid x_1, x_2) = \sum_{i=1}^{2} \int_0^\infty \frac{dt}{\hbar} K_t(x, x_i) e^{-\frac{\nu^2}{\hbar} t}$$

$$-\frac{\hbar^2}{2m} \nabla^2 K_t(x, y) + \hbar \frac{\partial K_t(x, y)}{\partial t} = 0$$

$$K_t(x, y) = K_t(y, x), \text{ and } \lim_{t \to 0^+} K_t(x, y) = \delta(x - y)$$

$$K_t(x, y) = \sqrt{\frac{2m}{4\pi\hbar t}} e^{-\frac{2m}{4\hbar t}|x - y|^2}$$

$$\frac{1}{\lambda} - \frac{1}{\hbar}\int_0^\infty dtK_t(x_2,x_2)e^{-\frac{\nu^2}{\hbar}t} = \frac{1}{\hbar}\int_0^\infty dtK_t(x_1,x_2)e^{-\frac{\nu^2 t}{\hbar}}$$

$$\begin{aligned}\int_0^\infty \frac{dt}{\hbar}\left(-\frac{\hbar^2}{2m}\right)\frac{\partial^2}{\partial x^2}K_t(x,x_i)e^{-\frac{\nu^2}{\hbar}t} &= -\int_0^\infty \frac{dt}{\hbar}\hbar\frac{\partial}{\partial t}K_t(x,x_i)e^{-\frac{\nu^2}{\hbar}t} \\ &= -\int_0^\infty dt\left(\frac{\partial}{\partial t}\left(K_t(x,x_i)e^{-\frac{\nu^2}{\hbar}t}\right) - K_t(x,x_i)e^{-\frac{\nu^2}{\hbar}t}\right) \\ &= \delta(x-x_i) - (-\nu^2)\int_0^\infty \frac{dt}{\hbar}K_t(x,x_i)e^{-\frac{\nu^2}{\hbar}t}\end{aligned}$$

$$\frac{1}{2\lambda} = \frac{1}{\hbar}\int_0^\infty dtK_t(x_1,x_1)e^{-\frac{\nu_0^2}{\hbar}t} = \sqrt{\frac{m}{2\hbar^2\nu_0^2}}$$

$$\nu_0^2 = \frac{2m\lambda^2}{\hbar^2}$$

$$\begin{aligned}\frac{1}{\lambda} - \sqrt{\frac{m}{2\pi\hbar}}\int_0^\infty \frac{dt}{\hbar}\frac{e^{-\frac{\nu^2-\Delta E}{\hbar}t}}{\sqrt{t}} &= \sqrt{\frac{m}{2\pi\hbar}}\int_0^\infty \frac{dt}{\hbar}\frac{e^{-\frac{(\nu^2-\Delta E_1)}{\hbar}t-\frac{mz^2}{2\hbar t}}}{\sqrt{t}} \\ &= \sqrt{\frac{m}{2\hbar^2(\nu_0^2-\Delta E)}}e^{\frac{|z|}{\hbar}\sqrt{2m(\nu_0^2-\Delta E)}}\end{aligned}$$

$$\frac{1}{\lambda} - \sqrt{\frac{m}{2\hbar^2(\nu_0^2-\Delta E)}} = \sqrt{\frac{m}{2\hbar^2(\nu_0^2-\Delta E)}}e^{-\frac{\nu_0|z|\sqrt{2m}}{\hbar}}$$

$$\Delta E = \lambda^3|z|\left(\frac{2m}{\hbar^2}\right)^2$$

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}\psi + |z|\lambda^3\left(\frac{2m}{\hbar^2}\right)^2\psi = \delta E\psi$$

$$\beta^3 = (2\mu)\left(\frac{2m}{\hbar^3}\right)^2\lambda^3, \quad \beta = \left(\frac{\mu}{m}\right)^{1/3}\frac{\nu_0^2}{\lambda}$$

$$u = |z| - \left(\frac{\hbar^2}{2m}\right)^2\frac{\delta E}{\lambda^3} \quad \sigma = \beta u$$

$$\psi_\pm(z) = C\binom{\mathrm{sgn}(z)}{1}Ai\left((2\mu)^{\frac{1}{3}}\frac{(2m)^{\frac{2}{3}}}{\hbar^2}\lambda\left(|z| - \left(\frac{\hbar^2}{2m}\right)^2\frac{\delta E}{\lambda^3}\right)\right)$$

$$\delta E_n = (-\sigma_n)\frac{2m\lambda^2}{\hbar^2}\left(\frac{m}{\mu}\right)^{1/3} = (-\sigma_n)\nu_0^2\left(\frac{m}{\mu}\right)^{1/3}$$

$$2C_n^2\int_{\sigma_n}^\infty d\sigma|Ai(\sigma)|^2 = 1$$

$$\frac{1}{2C_n^2} = \left(\frac{\partial Ai(\sigma)}{\partial\sigma}\right)^2\Bigg|_{\sigma=\sigma_n} - \sigma_n Ai(\sigma_n)^2.$$

$$\frac{1}{2C_n^2} = -\sigma_n Ai(\sigma_n)^2$$

$$\frac{1}{2C_n^2} = \left(\frac{\partial Ai(\sigma)}{\partial \sigma}\right)^2\bigg|_{\sigma=\sigma_n}$$

$$\psi_n(z) = C_n\left(\frac{\mu}{m}\right)^{1/6}\frac{\nu_0}{\lambda^{1/2}}\binom{\mathrm{sgn}(z)}{1}Ai\left((2\mu)^{\frac{1}{3}}\frac{(2m)^{\frac{2}{3}}}{\hbar^2}\lambda\left(|z| - \left(\frac{\hbar^2}{2m}\right)^2\frac{\delta E_n}{\lambda^3}\right)\right)$$

$$\left(\frac{\mu}{m}\right)^{1/6}\frac{\nu_0}{\lambda^{1/2}} = (2\mu)^{1/6}\frac{(2m)^{1/3}\lambda^{1/2}}{\hbar}$$

$$(2C_n^2)\int_{\sigma_n}^{\infty} d\sigma\left(\frac{\sigma\hbar^2}{(2\mu)^{\frac{1}{3}}(2m)^{\frac{2}{3}}\lambda} + \left(\frac{\hbar^2}{2m}\right)^2\frac{\delta E}{\lambda^3}\right)|Ai(\sigma)|^2 = -\frac{2}{3}\frac{\sigma_n}{\lambda}\frac{\hbar^2}{(2\mu)^{\frac{1}{3}}(2m)^{\frac{2}{3}}}$$
$$= \left[-\frac{2}{3}\sigma_n\right]\frac{\lambda}{\nu_0^2}\left(\frac{m}{\mu}\right)^{1/3}$$

$$< z^2 >= 2C_n^2\int_{\sigma_n}^{\infty} d\sigma|Ai(\sigma)|^2\left(\frac{\sigma\hbar^2}{(2\mu)^{\frac{1}{3}}(2m)^{\frac{2}{3}}\lambda} + \left(\frac{\hbar^2}{2m}\right)^2\frac{\delta E}{\lambda^3}\right)^2$$

$$\frac{\hbar^4}{(2\mu)^{\frac{2}{3}}(2m)^{\frac{4}{3}}\lambda^2}(2C_n^2)\int_{\sigma_n}^{\infty} d\sigma\sigma^2|Ai(\sigma)|^2 = \frac{1}{5}\frac{\sigma_n^2}{\lambda^2}\frac{\hbar^4}{(2\mu)^{\frac{2}{3}}(2m)^{\frac{4}{3}}}\left(1 - \frac{1}{\sigma_n{}^3}\right)$$

$$< z^2 >= \frac{8}{15}\frac{\sigma_n^2}{\lambda^2}\frac{\hbar^4}{(2\mu)^{\frac{2}{3}}(2m)^{\frac{4}{3}}} - \frac{1}{5}\frac{\hbar^4}{(2\mu)^{\frac{2}{3}}(2m)^{\frac{4}{3}}\lambda^2\sigma_n} = A_n\left(\frac{m}{\mu}\right)^{2/3}\left(\frac{\lambda}{\nu_0^2}\right)^2$$

$$H = \int dx\phi^\dagger(x)\left[-\frac{\nabla^2}{2m}\right]\phi(x) + \int dx\psi^\dagger(x)\left[-\frac{\nabla^2}{2M}\right]\psi(x) - \lambda\int dx\phi^\dagger(x)\psi^\dagger(x)\phi(x)\psi(x)$$

$$\chi(x)\chi^\dagger(y) = \delta(x-y)\Pi_0,$$
$$\chi(x)\chi(y) = 0 = \chi^\dagger(x)\chi^\dagger(y),$$

$$\Pi_1 = \int dx\chi^\dagger(x)\chi(x), \Pi_0 = 1 - \Pi_1$$

$$\mathcal{F}_M \otimes \mathcal{F}_m$$

$$\mathcal{F}_M \otimes \mathcal{F}_m \oplus \mathcal{F}_M \otimes \mathcal{F}_m \otimes L^2(\mathbf{R})$$

$$\hat{H} - E\Pi_0 = \begin{pmatrix} (H_0 - E)\Pi_0 & \int dx\psi^\dagger(x)\phi^\dagger(x)\chi(x) \\ \int dy\psi(y)\phi(y)\chi^\dagger(y) & \frac{1}{\lambda}\Pi_1 \end{pmatrix} \equiv \begin{pmatrix} a & b^\dagger \\ b & d \end{pmatrix}$$

$$\left(\hat{H} - E\Pi_0\right)^{-1} \equiv \begin{pmatrix} \alpha & \beta^\dagger \\ \beta & \delta \end{pmatrix}$$

$$\alpha = \left(a - b^{\dagger} d^{-1} b\right)^{-1} = (H - E)^{-1} = a^{-1} + a^{-1} b^{\dagger} \Phi^{-1} b a^{-1}$$

$$\Phi \equiv d - b a^{-1} b^{\dagger}$$

$$\Phi = \frac{1}{\lambda}\Pi_1 - \int dx \phi(x)\psi(x)\chi^{\dagger}(x)\frac{1}{H_0 - E}\int dy \psi^{\dagger}(y)\phi^{\dagger}(y)\chi(y)$$

$$[dp] = \frac{dp}{2\pi}$$

$$\Phi = \frac{1}{\lambda}\Pi_1 - \int [dpdq]\chi^{\dagger}(p+q)\frac{1}{H_0 + v_0^2 - \delta' E + p^2/2M + q^2/2m}\chi(p+q)$$
$$-\int [dpdqdr]\chi^{\dagger}(p+q)\psi^{\dagger}(r)\frac{1}{H_0 + v_0^2 - \delta' E + p^2/2M + r^2/2M + q^2/2m}\psi(p)\chi(r+q)$$

$$\int [dPd\eta]\chi^{\dagger}(P)\frac{1}{H_0 + v_0^2 - \delta' E + P^2/2(M+m) + \eta^2/2\mu}\chi(P)$$

$$\frac{1}{2\hbar}\sqrt{\frac{2mM}{m+M}}\int [dP]\chi^{\dagger}(P)\frac{1}{\sqrt{H_0 + v_0^2 - \delta' E + P^2/2(M+m)}}\chi(P)$$

$$\Phi(E) \mid \omega >= 0$$

$$\Phi = \frac{1}{\lambda}\Pi_1 - \frac{\sqrt{2m}}{2\hbar v_0}\int [dP]\chi^{\dagger}(P)\left[1 - \frac{1}{2}\frac{\left(H_0 - \delta' E + \frac{P^2}{2M}\right)}{v_0^2} + \frac{3}{8}\frac{\left(H_0 - \delta' E + \frac{P^2}{2M}\right)^2}{v_0^4} + \cdots\right]\chi(P)$$
$$-\int [dpdqdr]\chi^{\dagger}(p+q)\psi^{\dagger}(r)\left[\frac{1}{\left(v_0^2 + \frac{q^2}{2m}\right)} - \frac{\left(\frac{p^2}{2M} + \frac{r^2}{2M} - \delta' E\right)}{\left(v_0^2 + \frac{q^2}{2m}\right)^2} + \frac{\left(\frac{p^2}{2M} + \frac{r^2}{2M} - \delta' E\right)^2}{\left(v_0^2 + \frac{q^2}{2m}\right)^3} + \cdots\right]$$
$$\times \psi(p)\chi(q+r)$$

$$\left|\omega >= \int [d\xi dQ] f(\xi) e^{-iQX/\hbar}\chi^{\dagger}\left(\frac{Q}{2} + \xi\right)\psi^{\dagger}\left(\frac{Q}{2} - \xi\right)\right| \Omega >,$$

$$\left(\frac{1}{\lambda} - \frac{1}{2}\frac{\sqrt{2m}}{\hbar v_0}\right)\Pi_1 \left|\omega > + \frac{1}{4}\frac{\sqrt{2m}}{\hbar v^3}\int [dP]\chi^{\dagger}(P)\left(H_0 - \delta' E + \frac{P^2}{2M}\right)\chi(P)\right|\omega >$$
$$= \left(\frac{1}{\lambda} - \frac{1}{2}\frac{\sqrt{2m}}{\hbar v_0}\right)\Pi_1 \left|\ \omega > + \frac{1}{4}\frac{\sqrt{2m}}{\hbar v^3}\int [dQd\xi] f(\xi) e^{-i\frac{QX}{\hbar}}\left(\frac{1}{2}\frac{Q^2}{2M} + 2\frac{\xi^2}{2M} - \delta' E\right)\right.$$
$$\left.\times \chi^{\dagger}\left(\frac{Q}{2} + \xi\right)\psi^{\dagger}\left(\frac{Q}{2} - \xi\right)\right| \Omega >$$

$$\left(\frac{1}{\lambda} - \frac{1}{2}\frac{\sqrt{2m}}{\hbar v_0}\right) f(z) + \frac{1}{4}\frac{\sqrt{2m}}{\hbar v^3}\left[\frac{1}{2}\frac{Q^2}{2M} - \frac{\hbar^2}{2\mu}\nabla_z^2 - \delta' E\right] f(z).$$

$$\int [dpdqdr]\chi^{\dagger}(p+q)\psi^{\dagger}(r)\frac{1}{\nu_0^2+\frac{q^2}{2m}}\psi(p)\chi(q+r)\bigg|\,\omega>$$

$$=\int [dqdQd\xi]f(\xi)e^{-iQX/\hbar}\frac{1}{\nu_0^2+\frac{q^2}{2m}}\chi^{\dagger}\left(\frac{Q}{2}-\xi+q\right)\psi^{\dagger}\left(\frac{Q}{2}+\xi-q\right)\bigg|\,\Omega>$$

$$\int [dqdQd\xi]f(q-\xi)e^{-iQX/\hbar}\frac{1}{\nu_0^2+\frac{q^2}{2m}}\chi^{\dagger}\left(\frac{Q}{2}+\xi\right)\psi^{\dagger}\left(\frac{Q}{2}-\xi\right)\bigg|\,\Omega>$$

$$\int [dqdQd\xi]f(q-\xi)e^{-iQX/\hbar}\frac{1}{\nu_0^2+\frac{q^2}{2m}}\chi^{\dagger}\left(\frac{Q}{2}+\xi\right)\psi^{\dagger}\left(\frac{Q}{2}-\xi\right)\bigg|\Omega>\mapsto\frac{1}{2}\frac{\sqrt{2m}}{\hbar\nu_0}e^{-\frac{\sqrt{2m}}{\hbar}\nu_0\left|z\right|}f(z).$$

$$\left(\frac{1}{\lambda}-\frac{1}{2}\frac{\sqrt{2m}}{\hbar\nu_0}\right)f(z)+\frac{1}{4}\frac{\sqrt{2m}}{\hbar\nu_0^3}\left[\frac{1}{2}\frac{Q^2}{2M}-\frac{\hbar^2}{2\mu}\nabla_z^2-\delta' E\right]f(z)-\frac{1}{2}\frac{\sqrt{2m}}{\hbar\nu_0}e^{-\frac{\sqrt{2m}}{\hbar}\nu_0|z|}f(z).$$

$$\int [dpdqdr]\chi^{\dagger}(p+q)\psi^{\dagger}(r)\frac{\left(\frac{p^2}{2M}+\frac{r^2}{2M}-\delta' E\right)}{\left(\nu_0^2+\frac{q^2}{2m}\right)^2}\psi(p)\chi(q+r)\bigg|\,\omega>$$

$$=\int [dqdQd\xi]f(\xi)e^{-iQX/\hbar}\left(\frac{\frac{\left(\frac{Q}{2}-\xi\right)^2}{2M}+\frac{\left(\frac{Q}{2}+\xi-q\right)^2}{2M}-\delta' E}{\left(\nu_0^2+\frac{q^2}{2m}\right)^2}\right)\chi^{\dagger}\left(\frac{Q}{2}-\xi+q\right)\psi^{\dagger}\left(\frac{Q}{2}+\xi-q\right)\bigg|\,\Omega>$$

$$=\int [dqdQd\xi]f(\xi-q)e^{-iQX/\hbar}\left(\frac{\frac{\left(\frac{Q}{2}+\xi-q\right)^2}{2M}+\frac{\left(\frac{Q}{2}-\xi\right)^2}{2M}-\delta' E}{\left(\nu_0^2+\frac{q^2}{2m}\right)^2}\right)\chi^{\dagger}\left(\frac{Q}{2}+\xi\right)\psi^{\dagger}\left(\frac{Q}{2}-\xi\right)\bigg|\,\Omega>$$

$$\frac{\left(\frac{Q}{2}+\xi-q\right)^2}{2M}=\frac{\left(\frac{Q}{2}+\xi\right)^2}{2M}\underbrace{-\frac{2m}{2M}\frac{2q\left(\frac{Q}{2}+\xi\right)}{2m}+\left(\frac{2m}{2M}\right)\frac{q^2}{2m}}_{(*)},$$

$$\mapsto-\frac{2m}{M}\left(\frac{1}{4}\frac{\left(\frac{Q}{2}-i\hbar\frac{\partial}{\partial z}\right)}{2m}\frac{\hbar}{i}\frac{\partial}{\partial z}+\frac{1}{8}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\right)\frac{\sqrt{2m}}{\hbar\nu_0^3}e^{-\frac{\sqrt{2m}}{\hbar}\nu_0|z|}\left[1+\frac{\sqrt{2m}}{\hbar}\nu_0|z|\right]f(z)\qquad(*)$$

$$\frac{\nu_0^2}{8}\left(\frac{\sqrt{2m}}{\hbar\nu_0^3}\right)\left[\frac{iQ}{\sqrt{2m}\nu_0}\left(O\left(\frac{m}{\mu}\right)^{\frac{4}{3}}+O\left(\frac{m}{\mu}\right)^{\frac{5}{3}}+\cdots\right)+\left(O\left(\frac{m}{\mu}\right)+O\left(\frac{m}{\mu}\right)^{\frac{4}{3}}+O\left(\frac{m}{\mu}\right)^{\frac{5}{3}}+\cdots\right)\right].$$

$$\int [dqdQd\xi]f(\xi-q)\,e^{-iQX/\hbar}\left(\frac{\frac{\left(\frac{Q}{2}+\xi\right)^2}{2M}+\frac{\left(\frac{Q}{2}-\xi\right)^2}{2M}-\delta' E}{\left(\nu_0^2+\frac{q^2}{2m}\right)^2}\right)\chi^{\dagger}\left(\frac{Q}{2}+\xi\right)\psi^{\dagger}\left(\frac{Q}{2}-\xi\right)\bigg|\,\Omega>\mapsto$$

$$\mapsto\frac{1}{4}\frac{\sqrt{2m}}{\hbar\nu_0^3}\left[\frac{1}{2}\frac{Q^2}{2M}-\frac{\hbar^2}{2\mu}\nabla_z^2-\delta' E\right]e^{-\frac{\sqrt{2m}}{\hbar}\nu_0|z|}\left[1+\frac{\sqrt{2m}}{\hbar}\nu_0|z|\right]f(z)$$

$$\int [dqdQd\xi]f(\xi)e^{-iQX/\hbar}\left(\frac{\frac{\left(\frac{Q}{2}-\xi\right)^2}{2M}+\frac{\left(\frac{Q}{2}+\xi-q\right)^2}{2M}-\delta' E}{\left(v_0^2+\frac{q^2}{2m}\right)^2}\right)\chi^\dagger\left(\frac{Q}{2}-\xi+q\right)\psi^\dagger\left(\frac{Q}{2}+\xi-q\right)\Bigg|\Omega>$$

$$=\int [dqdQd\xi]f(\xi-q)e^{-iQX/\hbar}\left(\frac{\frac{\left(\frac{Q}{2}+\xi-q\right)^2}{2M}+\frac{\left(\frac{Q}{2}-\xi+q\right)^2}{2M}-\delta' E}{\left(v_0^2+\frac{q^2}{2m}\right)^2}\right)\chi^\dagger\left(\frac{Q}{2}+\xi\right)\psi^\dagger\left(\frac{Q}{2}-\xi\right)\Bigg|\Omega>.$$

$$\left(-\frac{\hbar^2}{2\mu}\nabla_z^2\right)V(z)+V(z)\left(-\frac{\hbar^2}{2\mu}\nabla_z^2\right)$$

$$\left(\frac{1}{\lambda}-\frac{1}{2}\frac{\sqrt{2m}}{\hbar v_0}\right)f(z)+\frac{1}{4}\frac{\sqrt{2m}}{\hbar v_0^3}\left[\frac{1}{2}\frac{Q^2}{2M}-\frac{\hbar^2}{2\mu}\nabla_z^2-\delta' E\right]f(z)-\frac{1}{2}\frac{\sqrt{2m}}{\hbar v_0}e^{-\frac{\sqrt{2m}}{\hbar}v_0|z|}f(z)$$
$$+\frac{1}{8}\frac{\sqrt{2m}}{\hbar v_0^3}\left[\left[\frac{1}{2}\frac{Q^2}{2M}-\frac{\hbar^2}{2\mu}\nabla_z^2-\delta' E\right],e^{-\frac{\sqrt{2m}}{\hbar}v_0|z|}\left[1+\frac{\sqrt{2m}}{\hbar}v_0|z|\right]\right]_+ f(z)=0$$

$$\left(\frac{1}{\lambda}-\frac{\sqrt{2m}}{\hbar v_0}\right)f(z)+\frac{1}{2}\frac{\sqrt{2m}}{\hbar v_0^3}\left[\frac{1}{2}\frac{Q^2}{2M}-\frac{\hbar^2}{2\mu}\nabla_z^2-\delta' E\right]f(z)+\frac{1}{2}\frac{2m}{\hbar^2}|z|f(z)=0$$

$$v_0^2=\frac{2m\lambda^2}{\hbar^2}$$

$$\left(-\frac{\hbar^2}{2\mu}\nabla_z^2-\left[\delta' E-\frac{1}{2}\frac{Q^2}{2M}\right]\right)f(z)+\frac{\sqrt{2m}}{\hbar}v_0^3|z|f(z)=0$$

$$\delta E=\delta' E-\frac{1}{2}\frac{Q^2}{2M}$$

$$\left(-\frac{\hbar^2}{2\mu}\nabla_z^2-\delta E\right)f(z)+\left(\frac{2m}{\hbar^2}\right)^2\lambda^3|z|f(z)=0$$

$$\frac{1}{8}\frac{\sqrt{2m}}{\hbar v_0^3}(2C_n^2)\int_{\sigma_n}^{\infty}d\sigma Ai(\sigma)\left(-\frac{\hbar^2}{2\mu}\nabla_z^2 e^{-\frac{\sqrt{2m}}{\hbar}v_0|z|}\left[\frac{\sqrt{2m}}{\hbar}v_0|z|+1\right]\right)Ai(\sigma)$$
$$=-\frac{\sqrt{2m}}{8\hbar v_0^3}\frac{\hbar^2}{2\mu}(2C_n^2)\int_{\sigma_n}^{\infty}d\sigma Ai(\sigma)\left(\nabla_z^2\left[-\frac{1}{2}\frac{2m}{\hbar^2}v_0^2z^2+\frac{1}{3}\frac{(2m)^{\frac{3}{2}}}{\hbar^3}v_0^3|z|^3-\frac{1}{8}\frac{(2m)^2}{\hbar^4}v_0^4z^4+\cdots\right]\right)Ai(\sigma)$$
$$=-\frac{\sqrt{2m}}{8\hbar v_0^3}\frac{\hbar^2}{2\mu}(2C_n^2)\int_{\sigma_n}^{\infty}d\sigma Ai(\sigma)\left(-\frac{2m}{\hbar^2}v_0^2+2\frac{(2m)^{\frac{3}{2}}}{\hbar^3}v_0^3|z|-\frac{3}{2}\frac{(2m)^2}{\hbar^4}v_0^4z^2\right)Ai(\sigma)$$
$$=\frac{\sqrt{2m}}{\hbar v_0^3}\left[O\left(v_0^2\left(\frac{m}{\mu}\right)\right)+O\left(v_0^2\left(\frac{m}{\mu}\right)^{\frac{4}{3}}\right)+O\left(v_0^2\left(\frac{m}{\mu}\right)^{\frac{5}{3}}\right)+\cdots\right]$$

$$\Phi = \frac{1}{\lambda}\Pi_1 - \frac{\sqrt{2m}}{\hbar\nu_0}\int [dP]\chi^\dagger(P)\left[1 - \frac{1}{2}\frac{\left(H_0 - \delta_1 E - \delta_2 E + \frac{P^2}{2M}\right)}{\nu_0^2} + \frac{3}{8}\frac{\left(H_0 - \delta_1 E + \frac{P^2}{2M}\right)^2}{\nu_0^4} + \cdots\right]\chi(P)$$

$$-\int [dpdqdr]\chi^\dagger(p+q)\psi^\dagger(r)\left[\frac{1}{\nu_0^2 + \frac{q^2}{2m}} - \frac{\left(\frac{p^2}{2M} + \frac{r^2}{2M} - \delta_1 E - \delta_2 E\right)}{\left(\nu_0^2 + \frac{q^2}{2m}\right)^2} + \frac{\left(\frac{p^2}{2M} + \frac{r^2}{2M} - \delta_1 E\right)^2}{\left(\nu_0^2 + \frac{q^2}{2m}\right)^3} + ..\right] \times \psi(p)\chi(q+r)$$

$$\Phi(E)|\omega >= \omega(E)|\omega >$$

$$\omega(\nu_0 + \delta_1 E + \delta_2 E) + \delta_2\omega(\nu_0 + \delta_1 E) = 0$$

$$\langle\omega_1|\delta_2\Phi|\omega_1\rangle + <\omega_1\left|\frac{\partial\Phi}{\partial E}\right|\omega_1 > \delta_2 E = -\frac{1}{4}\frac{\sqrt{2m}}{\hbar\nu_0^3}\delta_2 E - \frac{1}{4}\frac{(2m)^{\frac{3}{2}}}{\hbar^3}\nu_0 < z^2 >$$

$$-\frac{3}{16}\frac{\sqrt{2m}}{\hbar\nu_0^5}\int [dP] < \omega_1\left|\chi^\dagger(P)\left(H_0 - \delta_1 E + \frac{P^2}{2M}\right)^2\chi(P)\right|\omega_1 >$$

$$-\int [dpdqdr] < \omega_1\left|\chi^\dagger(p+q)\psi^\dagger(r)\frac{(\delta_2 E)}{\left(\nu_0^2 + \frac{q^2}{2m}\right)^2}\psi(p)\chi(q+r)\right|\omega_1 >$$

$$-\int [dpdqdr] < \omega_1\left|\chi^\dagger(p+q)\psi^\dagger(r)\frac{\left(\frac{p^2}{2M} + \frac{r^2}{2M} - \delta_1 E\right)^2}{\left(\nu_0^2 + \frac{q^2}{2m}\right)^3}\psi(p)\chi(q+r)\right|\omega_1 >$$

$$(*) = -\frac{3}{16}\frac{\sqrt{2m}}{\hbar\nu_0^5}\int [dP] < \omega_1\left|\chi^\dagger(P)\left(H_0 - \delta_1 E + \frac{P^2}{2M}\right)^2\chi(P)\right|\omega_1 >$$

$$= -\frac{3}{16}\frac{\sqrt{2m}}{\hbar\nu_0^5}(2C_n^2)\int_{\sigma_n}^{\infty} d\sigma Ai(\sigma)\left(\frac{\hbar^4}{(2\mu)^2}\nabla_z^4 + 2\delta_1 E\frac{\hbar^2}{2\mu}\nabla_z^2 + \delta_1 E^2\right)Ai(\sigma)$$

$$\frac{\sigma\hbar^2}{(2m)^{\frac{2}{3}}(2\mu)^{\frac{1}{3}}\lambda} + \frac{\delta_1 E}{\lambda^3}\left(\frac{\hbar^2}{2m}\right)^2 = z$$

$$-\sigma_n = (2\mu)^{\frac{1}{3}}\frac{\hbar^2}{(2m)^{\frac{4}{3}}\lambda^2}\delta_1 E^{(n)}$$

$$(*) = -a_n\left(\frac{m}{\mu}\right)^{\frac{2}{3}}\frac{1}{\lambda} = -a_n\frac{\sqrt{2m}}{\hbar\nu_0}\left(\frac{m}{\mu}\right)^{\frac{2}{3}}$$

$$-\frac{1}{4}\frac{(2m)^{\frac{3}{2}}}{\hbar^3}\nu_0 < z^2 >= -b_n\left(\frac{m}{\mu}\right)^{\frac{2}{3}}\frac{1}{\lambda} = -b_n\frac{\sqrt{2m}}{\hbar\nu_0}\left(\frac{m}{\mu}\right)^{\frac{2}{3}}$$

$$(**) = -\int [dpdqdr] < \omega_1\left|\chi^\dagger(p+q)\psi^\dagger(r)\frac{\delta_2 E}{\left(\nu_0^2 + \frac{q^2}{2m}\right)^2}\psi(p)\chi(q+r)\right|\omega_1 >$$

$$(**) = -\frac{1}{4}\frac{\sqrt{2m}}{\hbar v_0^3}\delta_2 E$$

$$(***) = -\int [dpdqdr] < \omega_1 \left| \chi^\dagger(p+q)\psi^\dagger(r)\frac{\left(\frac{p^2}{2M}+\frac{r^2}{2M}-\delta_1 E\right)^2}{\left(v_0^2+\frac{q^2}{2m}\right)^3}\psi(p)\chi(q+r)\right| \omega_1 >$$

$$\left(\frac{-\hbar^2}{2\mu}\nabla_z^2\right)^2 V(z) + \frac{-\hbar^2}{2\mu}\nabla_z^2 V(z)\frac{-\hbar^2}{2\mu}\nabla_z^2 + V(z)\left(\frac{-\hbar^2}{2\mu}\nabla_z^2\right)^2$$

$$(***) = -d_n\frac{\sqrt{2m}}{\hbar v_0}\left(\frac{m}{\mu}\right)^{\frac{2}{3}}$$

$$\delta_2 E^{(n)} = -\alpha_n v_0^2\left(\frac{m}{\mu}\right)^{\frac{2}{3}}$$

$$H = \frac{1}{2}\int dx{:}\pi^2 + \phi(-\nabla^2+m^2)\phi{:} + \int dx\Psi^\dagger(x)\left(-\frac{\nabla^2}{2M}\right)\Psi(x) - \lambda\int \phi^{(-)}(x)\Psi^\dagger(x)\Psi(x)\phi^{(+)}(x)dx$$

$$\phi(x,t) = \int \frac{[dk]}{\sqrt{2\omega(k)}}\left(a^\dagger(k)e^{-ikx+i\omega(k)t} + a(k)e^{ikx-i\omega(k)t}\right)$$

$$\left[a(k), a^\dagger(p)\right] = \delta[k-p] \text{ and } \omega(k) = \sqrt{k^2+m^2}.$$

$$\phi^{(+)}(x,t) = \int \frac{[dk]}{\sqrt{2\omega(k)}}a(k)e^{ikx-i\omega(k)t}$$

$$H^{(0)} = \int [dk]\sqrt{k^2+m^2}a^\dagger(k)a(k) - \lambda\sum_{i=1,2}\phi^{(-)}(x_i)\phi^{(+)}(x_i)$$

$$\Phi(\mu(|z|)) = \begin{cases} \frac{1}{\lambda}-\frac{1}{2}\int_{-\infty}^{\infty}[dp]\frac{1}{\left(\sqrt{p^2+m^2}\right)\left(\sqrt{p^2+m^2}-\mu(|z|)\right)} & \text{if } i=j \\ -\frac{1}{2}\int_{-\infty}^{\infty}[dp]\frac{e^{ipz}}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu(|z|)\right)} & \text{if } i\neq j \end{cases}$$

$$\frac{1}{\lambda}-\int_{-\infty}^{\infty}\frac{[dp]}{2}\frac{1}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu(|z|)\right)} = \int_{-\infty}^{\infty}\frac{[dp]}{2}\frac{e^{ipz}}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu(|z|)\right)}$$

$$\frac{1}{\lambda}-\int_{-\infty}^{\infty}\frac{[dp]}{2}\frac{1}{\left(\sqrt{p^2+m^2}\right)\left(\sqrt{p^2+m^2}-\mu_0\right)} = \int_{-\infty}^{\infty}\frac{[dp]}{2}\frac{1}{\left(\sqrt{p^2+m^2}\right)\left(\sqrt{p^2+m^2}-\mu_0\right)}$$

$$\int_{-\infty}^{\infty}[dp]\frac{1}{\left(\sqrt{p^2+m^2}\right)\left(\sqrt{p^2+m^2}-\mu_0\right)} = \int_0^1 du\int_{-\infty}^{\infty}[dp]\frac{1}{\left(\sqrt{p^2+m^2}-\mu_0 u\right)^2}$$

$$\frac{1}{\left(\sqrt{p^2+m^2}-\mu_0 u\right)^2}=\int_0^\infty dtte^{-t\left(\sqrt{p^2+m^2}-\mu_0 u\right)}$$

$$e^{-t\sqrt{p^2+m^2}}=\frac{1}{2\sqrt{\pi}}\int_0^\infty ds\frac{t}{s^{\frac{3}{2}}}e^{-s(p^2+m^2)-\frac{t^2}{4s}}$$

$$\int_{-\infty}^{\infty}[dp]\frac{1}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu_0\right)}=\frac{1}{2\sqrt{\pi}}\int_0^1 du\int_0^\infty dtt^2e^{ut\mu_0}\int_0^\infty ds\frac{1}{s^{\frac{3}{2}}}e^{-m^2s-\frac{t^2}{4s}}\int_{-\infty}^{\infty}[dp]e^{-sp^2}$$

$$\int_{-\infty}^{\infty}[dp]\frac{1}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu_0\right)}=\frac{1}{4\pi}\int_0^1 du\int_0^\infty dtt^2e^{ut\mu_0}\int_0^\infty ds\frac{1}{s^2}e^{-sm^2-\frac{t^2}{4s}}$$

$$K_\nu(w)=\frac{1}{2}\left(\frac{w}{2}\right)^\nu\int_0^\infty ds\frac{e^{-s-\frac{w^2}{4s}}}{s^{\nu+1}}$$

$$\int_{-\infty}^{\infty}[dp]\frac{1}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu_0\right)}=\frac{m}{\pi}\int_0^1 du\int_0^\infty dtte^{ut\mu_0}K_1(mt)=\frac{m}{\pi\mu_0}\int_0^\infty dt(e^{\mu_0 t}-1)K_1(mt)$$

$$K_1(mt)=-\frac{1}{m}\frac{\partial K_0(mt)}{\partial t}$$

$$\int_0^\infty dtK_1(mt)(e^{\mu_0 t}-1)=\frac{1}{m}(1-e^{\mu_0 t})K_0(mt)\Big|_0^\infty+\frac{\mu_0}{m}\int_0^\infty dte^{\mu_0 t}K_0(mt)$$

$$(e^{\mu_0 t}-1)K_0(mt)|_0^\infty=0$$

$$\int_0^\infty dte^{\mu_0 t}K_0(mt)=\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}$$

$$\int_{-\infty}^{\infty}[dp]\frac{1}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu_0\right)}=\frac{1}{\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}$$

$$\frac{1}{\lambda}=\frac{1}{\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}$$

$$\left[-\frac{1}{2M}\sum_i\nabla_i^2+\mu(|x_1-x_2|)\right]\psi(x_1,x_2)=E\psi(x_1,x_2)$$

$$\frac{1}{\lambda}-\int_{-\infty}^{\infty}\frac{[dp]}{2}\frac{1}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-(\mu_0+\delta\mu)\right)}=\int_{-\infty}^{\infty}\frac{[dp]}{2}\frac{e^{ipz}}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-(\mu_0+\delta\mu(|z|))\right)}$$

$$\frac{1}{\lambda}-\frac{1}{2\pi}\frac{\arccos\left(-\frac{(\mu_0+\delta\mu)}{m}\right)}{\sqrt{m^2-(\mu_0+\delta\mu)^2}}=\int_{-\infty}^{\infty}\frac{[dp]}{2}\frac{e^{ipz}}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-(\mu_0+\delta\mu)\right)}$$

$$\int_{-\infty}^{\infty}[dp]\frac{e^{ipz}}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-(\mu_0+\delta\mu)\right)}=\frac{1}{4\pi}\int_0^1 du\int_0^{\infty}dtt^2e^{ut(\mu_0+\delta\mu)}\int_0^{\infty}ds\frac{e^{-m^2s-\frac{(t^2+z^2)}{4s}}}{s^2}$$

$$=\frac{m}{(\mu_0+\delta\mu)\pi}\int_0^{\infty}dtt\frac{\left(e^{t(\mu_0+\delta\mu)}-1\right)K_1\left(m\sqrt{t^2+z^2}\right)}{\sqrt{t^2+z^2}}$$

$$\frac{tK_1\left(m\sqrt{t^2+z^2}\right)}{\sqrt{t^2+z^2}}=-\frac{1}{m}\frac{\partial K_0\left(m\sqrt{t^2+z^2}\right)}{\partial t}$$

$$\int_{-\infty}^{\infty}[dp]\frac{e^{ipz}}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-(\mu_0+\delta\mu)\right)}=\frac{1}{\pi}\int_0^{\infty}dte^{t(\mu_0+\delta\mu)}K_0\left(m\sqrt{t^2+z^2}\right)$$

$$\frac{1}{\lambda}-\frac{1}{2\pi}\frac{\arccos\left(-\frac{(\mu_0+\delta\mu)}{m}\right)}{\sqrt{m^2-(\mu_0+\delta\mu)^2}}=\frac{1}{2\pi}\int_0^{\infty}dte^{t(\mu_0+\delta\mu)}K_0\left(m\sqrt{t^2+z^2}\right)$$

$$\frac{1}{\lambda}-\frac{1}{2\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}-\frac{\delta\mu}{2\pi}\left(\mu_0\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{(m^2-\mu_0^2)^{\frac{3}{2}}}+\frac{1}{m^2-\mu_0^2}\right)=\frac{1}{2\pi}\int_0^{\infty}dte^{t(\mu_0+\delta\mu)}K_0\left(m\sqrt{t^2+z^2}\right)$$

$$\frac{1}{\lambda}-\frac{1}{\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}-\frac{\delta\mu}{m^2-\mu_0^2}\left(\frac{\mu_0}{2\lambda}+\frac{1}{2\pi}\right)=\frac{1}{2\pi}\int_0^{\infty}dt\left[e^{t(\mu_0+\delta\mu)}K_0\left(m\sqrt{t^2+z^2}\right)-e^{t\mu_0}K_0(mt)\right]$$

$$\delta\mu\int_0^{\infty}dtte^{t\mu_0}K_0\left(m\sqrt{t^2+z^2}\right)\to\delta\mu\int_0^{\infty}dtte^{t\mu_0}K_0(mt)=\delta\mu\frac{\partial}{\partial\mu_0}\int_0^{\infty}dte^{t\mu_0}K_0(mt)$$

$$\delta\mu\frac{\partial}{\partial\mu_0}\int_0^{\infty}dte^{t\mu_0}K_0(mt)=\delta\mu\left[\mu_0\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{(m^2-\mu_0^2)^{\frac{3}{2}}}+\frac{1}{m^2-\mu_0^2}\right]$$

$$\frac{1}{\lambda}-\frac{1}{\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}-\frac{\delta\mu}{m^2-\mu_0^2}\left(\frac{\mu_0}{\lambda}+\frac{1}{\pi}\right)=\frac{1}{2\pi}\int_0^{\infty}dte^{t\mu_0}\left[K_0\left(m\sqrt{t^2+z^2}\right)-K_0(mt)\right]$$

$$-\frac{\delta\mu}{m^2-\mu_0^2}\left(\frac{\mu_0}{\lambda}+\frac{1}{\pi}\right)=-\frac{1}{4}|z|$$

$$\delta\mu(z)=\frac{|z|}{4}\frac{(m^2-\mu_0^2)\lambda}{\left(\mu_0+\frac{1}{\pi}\lambda\right)}$$

$$\left[-\frac{1}{M}\frac{\partial^2}{\partial z^2}+\frac{|z|}{4}\frac{(m^2-\mu_0^2)\lambda}{\left(\mu_0+\frac{1}{\pi}\lambda\right)}\right]\psi(z)=\left(E-\frac{Q^2}{4M}\right)\psi(z)=\delta E\psi(z)$$

$$\Phi=\frac{1}{\lambda}\Pi_1-\int[dpdq]\chi^{\dagger}(p+q)\frac{1}{2\sqrt{q^2+m^2}\left[\sqrt{q^2+m^2}+H_0+\frac{p^2}{2M}-(\mu_0+\delta'E)\right]}\chi(p+q)$$

$$-\int[dpdqdr]\chi^{\dagger}(p)\Psi^{\dagger}(r-q)\frac{1}{2\sqrt{q^2+m^2}\left[\frac{r^2}{2M}+\frac{p^2}{2M}+\sqrt{q^2+m^2}-(\mu_0+\delta'E)\right]}\Psi(p-q)\chi(r),$$

$$\int [dpdq]\chi^{\dagger}(p+q)\frac{1}{\sqrt{q^2+m^2}\left[\sqrt{q^2+m^2}+H_0+\frac{p^2}{2M}-(\mu_0+\delta' E)\right]}\chi(p+q)=$$

$$\frac{1}{2\sqrt{\pi}}\int [dpdq]\chi^{\dagger}(p+q)\int_0^1 du\int_0^{\infty} dtt^2 e^{-ut\left(H_0+\frac{p^2}{2M}-(\mu_0+\delta' E)\right)}\int_0^{\infty} ds\frac{e^{-s(m^2+q^2)-\frac{t^2}{4s}}}{s^{\frac{3}{2}}}\chi(p+q)$$

$$\frac{tup^2}{2M}+sq^2=A(p+q)^2+B(p-\alpha q)^2.$$

$$\alpha=\frac{2Ms}{tu}, A=\frac{stu}{2M}\left(\frac{1}{\frac{tu}{2M}+s}\right) \text{ and } B=\left(\frac{tu}{2M}\right)^2\left(\frac{1}{\frac{tu}{2M}+s}\right).$$

$$[dpdq]=\left(\frac{tu}{2M}\right)\left(\frac{1}{\frac{tu}{2M}+s}\right)[dRdQ].$$

$$\int [dpdq]\chi^{\dagger}(p+q)\frac{1}{\sqrt{q^2+m^2}\left[\sqrt{q^2+m^2}+H_0+\frac{p^2}{2M}-(\mu_0+\delta' E)\right]}\chi(p+q)$$
$$=\frac{1}{2\sqrt{\pi}}\int [dR]\chi^{\dagger}(R)e^{-AR^2}\int_0^1 du\int_0^{\infty} dtt^2 e^{-ut[H_0-(\mu_0+\delta' E)]}$$
$$\times\int_0^{\infty} ds\frac{e^{-sm^2-\frac{t^2}{4s}}}{s^{\frac{3}{2}}}\int [dQ]\left(\frac{tu}{2M}\right)\frac{e^{-BQ^2}}{\left(\frac{tu}{2M}+s\right)}\chi(R)$$

$$\frac{1}{4\pi}\int [dR]\chi^{\dagger}(R)e^{-AR^2}\int_0^1 du\int_0^{\infty} dtt^2 e^{-ut\left(H_0-(\mu_0+\delta' E)\right)}\int_0^{\infty} ds\frac{e^{-sm^2-\frac{t^2}{4s}}}{s^{\frac{3}{2}}\sqrt{\frac{tu}{2M}+s}}\chi(R)$$

$$\frac{1}{4\pi}\int [dR]\chi^{\dagger}(R)\int_0^1 du\int_0^{\infty} dtt^2 e^{-ut\left(H_0+\frac{R^2}{2M}-(\mu_0+\delta' E)\right)}\int_0^{\infty} ds\frac{e^{-sm^2-\frac{t^2}{4s}}}{s^2}\chi(R)$$
$$=-\frac{m}{\pi}\int [dR]\chi^{\dagger}(R)\int_0^{\infty} dt\frac{\left(e^{-t\left(H_0+\frac{R^2}{2M}-(\mu_0+\delta' E)\right)}-1\right)}{\left(H_0+\frac{R^2}{2M}-(\mu_0+\delta' E)\right)}K_1(mt)\chi(R)$$
$$=\frac{1}{\pi}\int [dR]\chi^{\dagger}(R)\frac{\arccos\left(\frac{H_0+\frac{R^2}{2M}-\delta' E-\mu_0}{m}\right)}{\sqrt{m^2-\left(H_0+\frac{R^2}{2M}-\delta' E-\mu_0\right)}}\chi(R)$$

$$A=\left(\frac{stu}{2M}\right)\left(\frac{1}{\frac{tu}{2M}+s}\right)\to\frac{tu}{2M}$$

$$\Phi=\frac{1}{\lambda}\Pi_1-\frac{1}{2\pi}\int\;[dR]\chi^{\dagger}(R)\frac{\arccos\left(\frac{\frac{R^2}{2M}+H_0-\mu_0-\delta' E}{m}\right)}{\sqrt{m^2-\left(\frac{R^2}{2M}+H_0-\mu_0-\delta' E\right)^2}}\chi(R)$$
$$-\int\;[dpdqdr]\chi^{\dagger}(p)\Psi^{\dagger}(r-q)\frac{1}{2\sqrt{q^2+m^2}\left(\sqrt{q^2+m^2}-\mu_0+\frac{r^2}{2M}+\frac{p^2}{2M}-\delta' E\right)}\Psi(p-q)\chi(r)$$

$$\frac{\arccos\left(\frac{\frac{R^2}{2M}+H_0-\mu_0-\delta\mu}{m}\right)}{\sqrt{m^2-\left(\frac{R^2}{2M}+H_0-\mu_0-\delta' E\right)^2}}=\left(\arccos\left(-\frac{\mu_0}{m}\right)-\frac{H_0+\frac{R^2}{2M}-\delta' E}{\sqrt{m^2-\mu_0^2}}\right)$$
$$\times\frac{1}{\sqrt{m^2-\mu_0^2}}\left(1-\mu_0\frac{\left(H_0+\frac{R^2}{2M}-\delta' E\right)}{m^2-\mu_0^2}\right)+\cdots$$

$$\int\;[dpdqdr]\chi^{\dagger}(p)\Psi^{\dagger}(r-q)\frac{1}{2\sqrt{q^2+m^2}\left(\sqrt{q^2+m^2}-\mu_0+\frac{r^2}{2M}+\frac{p^2}{2M}-\delta' E\right)}\Psi(p-q)\chi(r)$$
$$=\int\;[dpdqdr]\chi^{\dagger}(p)\Psi^{\dagger}(r-q)\frac{1}{2\sqrt{q^2+m^2}\left(\sqrt{q^2+m^2}-\mu_0\right)}\Psi(p-q)\chi(r)$$
$$-\int\;[dpdqdr]\chi^{\dagger}(p)\Psi^{\dagger}(r-q)\frac{\left(\frac{r^2}{2M}+\frac{p^2}{2M}-\delta' E\right)}{2\sqrt{q^2+m^2}\left(\sqrt{q^2+m^2}-\mu_0\right)^2}\Psi(p-q)\chi(r)+\cdots$$

$$\Phi=\left[\frac{1}{\lambda}-\frac{1}{2\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}\right]\Pi_1$$
$$+\frac{1}{2\pi}\left(\mu_0\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{(m^2-\mu_0^2)^{\frac{3}{2}}}+\frac{1}{m^2-\mu_0^2}\right)\int\;[dR]\chi^{\dagger}(R)\left(H_0+\frac{R^2}{2M}-\delta' E\right)\chi(R)$$
$$-\frac{1}{2}\int\;[dpdqdr]\chi^{\dagger}(p)\Psi^{\dagger}(r-q)\frac{1}{\sqrt{q^2+m^2}\left(\sqrt{q^2+m^2}-\mu_0\right)}\Psi(p-q)\chi(r)$$
$$+\frac{1}{2}\int\;[dpdqdr]\chi^{\dagger}(p)\Psi^{\dagger}(r-q)\frac{\left(\frac{r^2}{2M}+\frac{p^2}{2M}-\delta' E\right)}{\sqrt{q^2+m^2}\left(\sqrt{q^2+m^2}-\mu_0\right)^2}\Psi(p-q)\chi(r)+\cdots$$

$$\left|\omega>=\int\;[dQd\xi]e^{-iQX}f(\xi)\chi^{\dagger}(Q/2+\xi)\Psi^{\dagger}(Q/2-\xi)\right|\Omega>$$

$$\Phi(\mu_0+\delta' E)\mid\omega>=0$$

$$\frac{1}{\sqrt{q^2+m^2}\left(\sqrt{q^2+m^2}-\mu_0\right)^2}$$

$$\begin{aligned}\int_{-\infty}^{\infty}[dp]\frac{e^{ipz}}{\sqrt{p^2+m^2}\left(\sqrt{p^2+m^2}-\mu_0\right)^2} &= \frac{1}{4\pi}\int_0^1 udu\int_0^{\infty} dtt^3 e^{ut\mu_0}\int_0^{\infty} ds\frac{e^{-m^2 s-\frac{(t^2+z^2)}{4s}}}{s^2}\\ &= \frac{m}{\pi\mu_0}\int_0^1 udu\int_0^{\infty} dtt^3\frac{e^{ut\mu_0}K_1\left(m\sqrt{t^2+z^2}\right)}{\sqrt{t^2+z^2}}\\ &= \frac{m}{\pi\mu_0}\frac{\partial}{\partial\mu_0}\int_0^1 du\int_0^{\infty} dtt^2\frac{e^{ut\mu_0}K_1\left(m\sqrt{t^2+z^2}\right)}{\sqrt{t^2+z^2}}\\ &= \frac{1}{\pi}\frac{\partial}{\partial\mu_0}\int_0^{\infty} dte^{\mu_0 t}K_0\left(m\sqrt{t^2+z^2}\right)\end{aligned}$$

$$\begin{aligned}&\left(\frac{1}{\lambda}-\frac{1}{2\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}\right)f(z)+\frac{1}{2\pi}\left(\mu_0\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{(m^2-\mu_0^2)^{\frac{3}{2}}}+\frac{1}{m^2-\mu_0^2}\right)\left(-\frac{\nabla_z^2}{M}+\frac{1}{2}\frac{Q^2}{2M}-\delta' E\right)f(z)\\ &-\frac{1}{2\pi}\left(\int_0^{\infty} dte^{\mu_0 t}K_0\left(m\sqrt{t^2+z^2}\right)\right)f(z)\\ &+\frac{1}{2}\left[-\frac{\nabla_z^2}{M}+\frac{1}{2}\frac{Q^2}{2M}-\delta' E,\frac{1}{2\pi}\frac{\partial}{\partial\mu_0}\int_0^{\infty} dte^{\mu_0 t}K_0\left(m\sqrt{t^2+z^2}\right)\right]_+ f(z)=0\end{aligned}$$

$$\begin{aligned}&\left(\frac{1}{\lambda}-\frac{1}{\pi}\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}}\right)f(z)\\ &+\frac{1}{\pi}\left(\mu_0\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{(m^2-\mu_0^2)^{\frac{3}{2}}}+\frac{1}{m^2-\mu_0^2}\right)\left(-\frac{\nabla_z^2}{M}-\delta E\right)f(z)+\frac{1}{4}|z|f(z)=0\end{aligned}$$

$$\left(-\frac{\nabla_z^2}{M}+\frac{1}{2}\frac{Q^2}{2M}-\delta E\right)f(z)+\frac{1}{4}\frac{(m^2-\mu_0^2)}{\left(\mu_0+\frac{1}{\pi}\lambda\right)}\lambda|z|f(z)=0$$

$$\phi(x\mid x_1,x_2)=\frac{N}{\hbar}\left[\int_0^{\infty} dtK_t(x,x_1)e^{-\frac{\nu^2}{\hbar}t}+\int_0^{\infty} dtK_t(x,x_2)e^{-\frac{\nu^2}{\hbar}t}\right]$$

$$\int_{-\infty}^{\infty} dx|\phi(x\mid x_1,x_2)|^2=1$$

$$\int dxK_{t_1}(x,x_1)K_{t_2}(x,x_2)=K_{t_1+t_2}(x_1,x_2)$$

$$1=2\frac{N^2}{\hbar^2}\left[\iint dt_1dt_2K_{t_1+t_2}(x_1,x_1)e^{-\frac{\nu^2}{\hbar}(t_1+t_2)}+\int dt_1dt_2K_{t_1+t_2}(x_1,x_2)e^{-\frac{\nu^2}{\hbar}(t_1+t_2)}\right]$$

$$t=t_1+t_2,\ \text{and}\ s=t_1-t_2$$

$$1=\frac{N^2}{\hbar^2}\left[\int_0^{\infty} dtt[K_t(x_1,x_1)+K_t(x_2,x_2)]e^{-\frac{\nu^2}{\hbar}t}+2\int_0^{\infty} dttK_t(x_1,x_2)e^{-\frac{\nu^2}{\hbar}t}\right]$$

$$1=\frac{N^2}{2}\frac{\sqrt{2m}}{\hbar\nu^3}\left[1+\left[1+\frac{\sqrt{2m}}{\hbar}\nu|x_1-x_2|\right]e^{-\frac{\sqrt{2m}}{\hbar}\nu|x_1-x_2|}\right]$$

$$\phi(x\mid x_1,x_2)=\frac{\sqrt{\nu}}{\sqrt{2}}\frac{(2m)^{\frac{1}{4}}}{\sqrt{\hbar}}\frac{1}{\sqrt{\left[1+\left[1+\frac{\sqrt{2m}}{\hbar}\nu|x_1-x_2|\right]e^{-\frac{\sqrt{2m}}{\hbar}\nu|x_1-x_2|}\right]}}\left[e^{-\frac{\sqrt{2m}}{\hbar}\nu|x-x_1|}+e^{-\frac{\sqrt{2m}}{\hbar}\nu|x-x_2|}\right]$$

$$X=\frac{x_1+x_2}{2}\ \text{and}\ z=x_1-x_2$$

$$\phi(x,z)=\frac{1}{\sqrt{2}}\frac{(2m)^{\frac{1}{4}}}{\sqrt{\hbar}}\sqrt{\nu}\frac{1}{\sqrt{\left[1+\left[1+\frac{\sqrt{2m}}{\hbar}\nu|z|\right]e^{-\frac{\sqrt{2m}}{\hbar}\nu|z|}\right]}}\left[e^{-\frac{\sqrt{2m}}{\hbar}\nu\left|x-\frac{z}{2}\right|}+e^{-\frac{\sqrt{2m}}{\hbar}\nu\left|x+\frac{z}{2}\right|}\right].$$

$$\frac{1}{\lambda}=\sqrt{\frac{m}{2\hbar^2\nu^2(z)}}\left(e^{-\sqrt{2m}\nu(z)/\hbar}+1\right).$$

$$\phi(z;x)=A(z)(\epsilon_+(x,z)+\epsilon_-(x,z))$$

$$\epsilon_+=e^{-\frac{\sqrt{2m}}{\hbar}\nu\left|x+\frac{z}{2}\right|}\ \text{and}\ \epsilon_-=e^{-\frac{\sqrt{2m}}{\hbar}\nu\left|x-\frac{z}{2}\right|}$$

$$\nu^2(z)=\nu_0^2+\delta E_1(z)$$

$$\nu_0=\frac{\sqrt{2m}}{\hbar}\lambda\ \text{and}\ \delta E_1=-|z|\lambda^3\left(\frac{2m}{\hbar^2}\right)^2.$$

$$\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)\phi(x,z)\psi(z)=\psi(z)\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)\phi(x,z)+\phi(x,z)\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)\psi(z)$$
$$+2\frac{\partial\psi}{\partial x_1}\frac{\partial\phi}{\partial x_1}+2\frac{\partial\psi}{\partial x_2}\frac{\partial\phi}{\partial x_2}$$

$$\psi(z)\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)\phi(x,z)+2\frac{\partial\psi}{\partial x_1}\frac{\partial\phi}{\partial x_1}+2\frac{\partial\psi}{\partial x_2}\frac{\partial\phi}{\partial x_2}$$

$$\frac{\partial}{\partial x_1}=\frac{1}{2}\frac{\partial}{\partial X}+\frac{\partial}{\partial z}\ \text{and}\ \frac{\partial}{\partial x_2}=\frac{1}{2}\frac{\partial}{\partial X}-\frac{\partial}{\partial z},$$

$$2\psi(z)\frac{\partial^2}{\partial z^2}\phi(x,z)\ \text{and}\ 4\frac{\partial\psi}{\partial z}\frac{\partial\phi}{\partial z}.$$

$$\frac{\partial\epsilon_+}{\partial z}=\frac{1}{2}\frac{\partial\epsilon_+}{\partial x}-\frac{\sqrt{2m}}{\hbar}\frac{\partial\nu}{\partial z}\left|x+\frac{z}{2}\right|\epsilon_+$$
$$\frac{\partial\epsilon_-}{\partial z}=-\frac{1}{2}\frac{\partial\epsilon_-}{\partial x}-\frac{\sqrt{2m}}{\hbar}\frac{\partial\nu}{\partial z}\left|x-\frac{z}{2}\right|\epsilon_-$$

$$4\frac{\partial\phi}{\partial z}\frac{\partial\psi}{\partial z}=4\frac{\partial\psi}{\partial z}\left[\frac{\partial A}{\partial z}(\epsilon_++\epsilon_-)+A\left(\frac{1}{2}\left[\frac{\partial\epsilon_+}{\partial x}-\frac{\partial\epsilon_-}{\partial x}\right]-\frac{\sqrt{2m}}{\hbar}\frac{\partial\nu}{\partial z}\left(\left|x-\frac{z}{2}\right|\epsilon_-+\left|x+\frac{z}{2}\right|\epsilon_+\right)\right)\right].$$

$$-\frac{4\hbar^2}{2\mu}\int dxdz\phi\psi\frac{\partial\phi}{\partial z}\frac{\partial\psi}{\partial z}=-\frac{\hbar^2}{\mu}\left[\int dz\psi\frac{\partial\psi}{\partial z}\int dx\left[2\frac{\partial A}{\partial z}(\epsilon_+ +\epsilon_-)+A\left(\frac{\partial\epsilon_+}{\partial x}-\frac{\partial\epsilon_-}{\partial x}\right)\right]A(\epsilon_+ +\epsilon_-)\right.$$

$$\left.-\frac{\sqrt{2m}}{\hbar}\frac{\partial v}{\partial z}\left(\left|x-\frac{z}{2}\right|\epsilon_- +\left|x+\frac{z}{2}\right|\epsilon_+\right)A^2(\epsilon_- +\epsilon_+)\right]$$

$$=-\frac{\hbar^2}{2\mu}\int dz\psi\frac{\partial\psi}{\partial z}\int dx\left[4A\frac{\partial A}{\partial z}(\epsilon_+ +\epsilon_-)^2+2A^2\left(\epsilon_+\frac{\partial\epsilon_+}{\partial x}-\epsilon_-\frac{\partial\epsilon_-}{\partial x}\right)\right.$$

$$+2A^2\epsilon_+\epsilon_-\left(\frac{1}{\epsilon_+}\frac{\partial\epsilon_+}{\partial x}-\frac{1}{\epsilon_-}\frac{\partial\epsilon_-}{\partial x}\right)$$

$$\left.-2A^2\frac{\sqrt{2m}}{\hbar}\frac{\partial v}{\partial z}\left(\left|x-\frac{z}{2}\right|\epsilon_- +\left|x+\frac{z}{2}\right|\epsilon_+\right)(\epsilon_- +\epsilon_+)\right].$$

$$\frac{\partial v}{\partial z}\approx-\frac{1}{2}\mathrm{sgn}(z)\left(\frac{2m}{\hbar^2}\right)^{3/2}\lambda^2$$

$$(1)=-\frac{\hbar^2}{2\mu}4\int dz\psi\frac{\partial\psi}{\partial z}\frac{\partial}{\partial z}\ln A$$

$$(3)=-2\frac{\hbar^2}{2\mu}\int dxdz\psi\frac{\partial\psi}{\partial z}A^2\epsilon_+\epsilon_-\frac{\partial}{\partial x}\ln\left(\frac{\epsilon_+}{\epsilon_-}\right)$$

$$\frac{\partial}{\partial z}\ln A\approx\frac{\partial}{\partial z}\ln\sqrt{v}\approx-\frac{1}{4}\lambda\frac{2m}{\hbar^2}\mathrm{sgn}(z)$$

$$\left|\frac{\hbar^2}{2\mu}v_0\frac{\sqrt{2m}}{\hbar}\int dz\mathrm{sgn}(z)\psi\frac{\partial\psi}{\partial z}\right|\le v_0\sqrt{\frac{m}{\mu}}\left|\int dz\left|\frac{\hbar}{\sqrt{2\mu}}\frac{\partial\psi}{\partial z}\right|^2\right|^{\frac{1}{2}}\left|\int dz\left|\mathrm{sgn}(z)\psi\right|^2\right|^{\frac{1}{2}}\le v_0^2\left(\frac{m}{\mu}\right)^{\frac{2}{3}},$$

$$2\left|\frac{\hbar^2}{2\mu}\frac{\sqrt{2m}}{\hbar}v_0\int dz\psi\frac{\partial\psi}{\partial z}A^2\int_{-\frac{|z|}{2}}^{\frac{|z|}{2}}dxe^{-\frac{\sqrt{2m}}{\hbar}v\left(\left|x+\frac{z}{2}\right|+\left|x-\frac{z}{2}\right|\right)}\frac{\partial}{\partial x}\left(\left|x+\frac{z}{2}\right|-\left|x-\frac{z}{2}\right|\right)\right|$$

$$\le 16\frac{2m}{\hbar\sqrt{2\mu}}v_0^2\left|\int dz\left|\frac{\hbar}{\sqrt{2\mu}}\frac{\partial\psi}{\partial z}\right|^2\right|^{\frac{1}{2}}\left|\int dzz^2\left|\psi\right|^2\right|^{\frac{1}{2}}\approx\frac{2m}{\hbar\sqrt{2\mu}}v_0^3\left(\frac{m}{\mu}\right)^{\frac{1}{6}}\sqrt{<z^2>}\approx C\frac{m}{\mu}v_0^2$$

$$\int dx\epsilon_-\epsilon_+\left|x-\frac{z}{2}\right|.$$

$$2\int dxe^{-\frac{\sqrt{2m}}{\hbar}v|x|}(|x|+|z|)$$

$$(4)\le 8\frac{\hbar^2}{\mu}\frac{\sqrt{2m}}{\hbar}\int dzA^2\left|\frac{\partial v}{\partial z}\frac{\partial\psi}{\partial z}\right|\psi\int dxe^{-\frac{\sqrt{2m}}{\hbar}v|x|}(|x|+|z|)$$

$$(4')\le 8\frac{\hbar}{\sqrt{\mu}}\left(\frac{\sqrt{2m}}{\hbar}\right)^5v_0\left(\frac{\sqrt{2m}}{\hbar}v_0\right)^{-2}\lambda^2\left[\int dz(\mathrm{sgn}(z)\psi)^2\right]^{1/2}\left[\frac{\hbar^2}{2\mu}\int dz\left|\frac{\partial\psi}{\partial z}\right|^2\right]^{1/2}$$

$$(4') \leq C_4 \left(\frac{m}{\mu}\right)^{2/3} v_0^2$$

$$\Lambda = \frac{\hbar^2}{\mu}\int dxdz\psi^2 A(\epsilon_+ + \epsilon_-)\left[\frac{\partial^2 A}{\partial z^2}(\epsilon_+ + \epsilon_-) + 4\frac{\partial A}{\partial z}\left(\frac{\partial \epsilon_+}{\partial x} - \frac{\partial \epsilon_-}{\partial x}\right) + 4A\left(\frac{\partial^2 \epsilon_+}{\partial x^2} + \frac{\partial^2 \epsilon_-}{\partial x^2}\right)\right]$$

$$\phi = \frac{\hbar^2}{\mu}\int dxdz\psi^2 A(\epsilon_+ + \epsilon_-)\frac{\sqrt{2m}}{\hbar}\frac{\partial A}{\partial z}\frac{\partial v}{\partial z}\left[\epsilon_+\left|x + \frac{z}{2}\right| + \epsilon_-\left|x - \frac{z}{2}\right|\right]$$

$$\varphi = \frac{\hbar^2}{\mu}\int dxdz\psi^2 A^2\left[\left(\frac{\partial \epsilon_+}{\partial x} - \frac{\partial \epsilon_-}{\partial x}\right) - \frac{\sqrt{2m}}{\hbar}\frac{\partial v}{\partial z}\left(\epsilon_+\left|x + \frac{z}{2}\right| + \epsilon_-\left|x - \frac{z}{2}\right|\right)\right] \times \frac{\sqrt{2m}}{\hbar}\frac{\partial v}{\partial z}\left[\epsilon_+\left|x + \frac{z}{2}\right| + \epsilon_-\left|x - \frac{z}{2}\right|\right].$$

$$\int dxdzA^2(\epsilon_+ + \epsilon_-)\psi\frac{\partial \psi}{\partial z}\frac{\sqrt{2m}}{\hbar}\frac{\partial v}{\partial z}\left[\epsilon_+\left|x + \frac{z}{2}\right| + \epsilon_-\left|x - \frac{z}{2}\right|\right]$$

$$(1^a) = -2\frac{\hbar^2}{2\mu}\int dz|\psi|^2\frac{1}{A}\frac{\partial^2}{\partial z^2}A$$

$$(1^b) = -4\frac{\hbar^2}{2\mu}\int dxdz|\psi|^2\left(\frac{\partial}{\partial z}A^2\right)\left(\epsilon_+\epsilon_-\frac{\partial}{\partial x}\ln\left(\frac{\epsilon_+}{\epsilon_-}\right) + \frac{1}{2}\frac{\partial}{\partial x}(\epsilon_+^2 + \epsilon_-^2)\right)$$

$$(1^c) = -8\frac{\hbar^2}{2\mu}\int dxdz|\psi|^2 A^2\left(\frac{\partial^2 \epsilon_+}{\partial x^2} + \frac{\partial^2 \epsilon_-}{\partial x^2}\right)(\epsilon_+ + \epsilon_-)$$

$$\frac{1}{A}\frac{\partial^2}{\partial z^2}A = \frac{\partial^2}{\partial z^2}\ln A + \left(\frac{\partial}{\partial z}\ln A\right)^2$$

$$-2\frac{\hbar^2}{2\mu}\int dz|\psi|^2\frac{\partial^2}{\partial z^2}\ln A = 4\frac{\hbar^2}{2\mu}\int dz\psi\frac{\partial \psi}{\partial z}\frac{\partial \ln A}{\partial z}$$

$$\leq \sqrt{\frac{m}{\mu}}v_0\left|\int dz\left|\frac{\hbar}{\sqrt{2\mu}}\frac{\partial \psi}{\partial z}\right|^2\right|^{\frac{1}{2}}\left|\int dz\left|\psi\right|^2\right|^{\frac{1}{2}} \approx \left(\frac{m}{\mu}\right)^{\frac{2}{3}} v_0^2$$

$$-2\frac{\hbar^2}{2\mu}\int dz|\psi|^2\left(\frac{\partial}{\partial z}\ln A\right)^2 \approx \frac{m}{\mu}v_0^2$$

$$4\frac{\hbar^2}{2\mu}\left|\int dz\left|\psi\right|^2\left(\frac{\partial}{\partial z}A^2\right)\int_{-|z|/2}^{|z|/2} dx\epsilon_+\epsilon_-\frac{\partial}{\partial x}\ln\left(\frac{\epsilon_+}{\epsilon_-}\right)\right| \leq 8\frac{\hbar^2}{2\mu}\frac{(2m)^{\frac{3}{2}}}{\hbar^3}v_0^3\left[\int dz|z||\psi|^2\right]$$

$$\langle |z| \rangle = C\frac{\lambda}{v_0^2}\left(\frac{m}{\mu}\right)^{1/3}$$

$$\leq 8\frac{\hbar^2}{2\mu}\frac{(2m)^{\frac{3}{2}}}{\hbar^3}C\frac{\lambda}{v_0^2}\left(\frac{m}{\mu}\right)^{1/3} v_0^3 \approx \left(\frac{m}{\mu}\right)^{\frac{4}{3}} v_0^2$$

$$\int dx\left(\epsilon_+\frac{\partial\epsilon_+}{\partial x}+\epsilon_-\frac{\partial\epsilon_-}{\partial x}\right)=\frac{1}{2}\int dx\frac{\partial}{\partial x}(\epsilon_+^2+\epsilon_-^2)$$

$$(1^c)=-8\frac{\hbar^2}{2\mu}\int dxdz|\psi|^2A^2\left(\frac{\partial^2\epsilon_+}{\partial x^2}+\frac{\partial^2\epsilon_-}{\partial x^2}\right)(\epsilon_++\epsilon_-)\approx C_8\frac{m}{\mu}v_0^2$$

$$\int dx\epsilon_\pm\epsilon_\pm\left|x\pm\frac{z}{2}\right|$$

$$A\frac{\partial A}{\partial z}\frac{1}{2}\frac{\partial A^2}{\partial z}\frac{\sqrt{2m}}{\hbar}\frac{\partial v}{\partial z}$$

$$\frac{\partial v}{\partial z}\approx-\frac{1}{2}\mathrm{sgn}(z)\left(\frac{\sqrt{2m}}{\hbar}\right)^3\lambda^2$$

$$|(2)|\le C_9'\frac{\hbar^2}{\mu}\int dz\psi^2\left(\frac{\sqrt{2m}}{\hbar}\right)^2\left[\left(\frac{\sqrt{2m}}{\hbar}\right)^3\lambda^2\right]^2\left(\frac{\sqrt{2m}}{\hbar}v\right)^{-2}\le C_9\frac{m}{\mu}v_0^2$$

$$\int dxdz\psi^2A^2(\epsilon_+-\epsilon_-)\frac{\sqrt{2m}}{\hbar}\frac{\partial v}{\partial z}\frac{\partial}{\partial x}\left(\epsilon_+\left|x+\frac{z}{2}\right|+\epsilon_-\left|x-\frac{z}{2}\right|\right)$$

$$|(3^a)|\le C_{10}'\frac{\hbar^2}{\mu}\int dz\left(\frac{\sqrt{2m}}{\hbar}\right)^2v\left|\frac{\partial v}{\partial z}\right|\left(\frac{\sqrt{2m}}{\hbar}v\right)\int dxe^{-\frac{\sqrt{2m}}{\hbar}v|x|}|x|\le C_{10}\frac{m}{\mu}v_0^2.$$

$$\int dx\epsilon_\pm\epsilon_\pm\left|x\pm\frac{z}{2}\right|^2$$

$$\int dxe^{-\frac{\sqrt{2m}}{\hbar}}[|x|^2+2|x||z|+|z|^2]$$

$$\left|(3^b)\right|\le C_{11}'\frac{\hbar^2}{\mu}\int dz\psi^2\left(\frac{\sqrt{2m}}{\hbar}v\right)\left(\frac{\sqrt{2m}}{\hbar}\right)^2\left|\frac{\partial v}{\partial z}\right|^2\left(\frac{\sqrt{2m}}{\hbar}v\right)^{-3}\le C_{11}\frac{m}{\mu}v_0^2$$

$$\int_0^\infty dte^{t\mu_0}K_0\left(m\sqrt{t^2+z^2}\right)=\frac{1}{2}\sum_{k=0}^\infty\frac{\mu_0^k}{k!}\int_0^\infty dtt^k\int_0^\infty\frac{du}{u}e^{-u(t^2+z^2)-\frac{m^2}{4u}}$$

$$\begin{aligned}\int_0^\infty dte^{t\mu_0}K_0\left(m\sqrt{t^2+z^2}\right)&=\frac{1}{2}\sum_{k=0}^\infty\frac{\mu_0^k}{k!}\int_0^\infty dtt^ke^{-ut^2}\int_0^\infty\frac{du}{u}e^{-uz^2-\frac{m^2}{4u}}\\&=\frac{1}{2}\sum_{k=0}^\infty\frac{\mu_0^k}{k!}\int_0^\infty dtt^ke^{-t^2}\int_0^\infty\frac{du}{u^{\frac{k+1}{2}+1}}e^{-uz^2-\frac{m^2}{4u}}\\&=\frac{1}{4}\sum_{k=0}^\infty\Gamma\left(\frac{k+1}{2}\right)\frac{\mu_0^k}{k!}|z|^{k+1}\int_0^\infty\frac{du}{u^{\frac{k+1}{2}+1}}e^{-u-\frac{m^2z^2}{4u}}\end{aligned}$$

$$\int_0^\infty dte^{t\mu_0}K_0\left(m\sqrt{t^2+z^2}\right)=\frac{1}{2}\sum_{k=0}^\infty\Gamma\left(\frac{k+1}{2}\right)\frac{\mu_0^k}{k!}2^{\frac{k+1}{2}}\left(\frac{|z|}{m}\right)^{\frac{k+1}{2}}K_{\frac{k+1}{2}}(m|z|)$$

$$\Gamma(x)\Gamma\left(x+\frac{1}{2}\right)=2^{1-2x}\sqrt{\pi}\Gamma(2z),$$

$$(*) = \int_0^\infty dt e^{t\mu_0} K_0\left(m\sqrt{t^2+z^2}\right) = \sqrt{\pi}\sum_{k=0}^{\infty} \frac{\mu_0^k}{2^{\frac{k+1}{2}}\Gamma\left(\frac{k}{2}+1\right)}\left(\frac{|z|}{m}\right)^{\frac{k+1}{2}} K_{\frac{k+1}{2}}(m|z|)$$

$$(*) = \sqrt{\pi}\sum_{n=0}^{\infty} \frac{\mu_0^{2n}}{2^{n+\frac{1}{2}}\Gamma(n+1)}\left(\frac{|z|}{m}\right)^{n+\frac{1}{2}} K_{n+\frac{1}{2}}(m|z|) + \sqrt{\pi}\sum_{n=1}^{\infty} \frac{\mu_0^{2n-1}}{2^n\Gamma\left(n+\frac{1}{2}\right)}\left(\frac{|z|}{m}\right)^{n} K_n(m|z|).$$

$$K_{n+\frac{1}{2}}(x) = \sqrt{\frac{\pi}{2x}} e^{-x}\sum_{k=0}^{n} \frac{\Gamma(n+k+1)}{k!\,\Gamma(n-k+1)(2x)^k}$$

$$K_n(x) = \frac{1}{2}\sum_{k=0}^{n-1} (-1)^k \frac{(n-k-1)!}{k!\left(\frac{x}{2}\right)^{n-2k}}$$

$$+(-1)^{n+1}\sum_{k=0}^{\infty} \frac{\left(\frac{x}{2}\right)^{n+2k}}{k!\,(n+k)!}\left[\ln\left(\frac{x}{2}\right) - \frac{1}{2}\psi(k+1) - \frac{1}{2}\psi(k+n+1)\right].$$

$$\Sigma_1 = \sqrt{\pi}\sum_{n=0}^{\infty} \frac{\mu_0^{2n}}{2^{n+\frac{1}{2}}\Gamma(n+1)}\left(\frac{|z|}{m}\right)^{n+\frac{1}{2}} K_{n+\frac{1}{2}}(m|z|)$$

$$= \pi\sum_{n=0}^{\infty}\sum_{k=0}^{n} \frac{\mu_0^{2n}}{2^{n+k+1}k!}\frac{\Gamma(n+k+1)}{\Gamma(n+1)\Gamma(n-k+1)}\frac{|z|^{n-k}}{m^{n+k+1}} e^{-m|z|}$$

$$= \pi\sum_{n=0}^{\infty}\sum_{k=0}^{n} \frac{\mu_0^{2n}}{2^{n+k+1}k!}\frac{\Gamma(n+k+1)}{\Gamma(n+1)\Gamma(n-k+1)}\frac{|z|^{n-k}}{m^{n+k+1}}\left(1 - m|z| + \frac{1}{2}m^2z^2 + \cdots\right)$$

$$\pi\sum_{n=0}^{\infty} \frac{\mu_0^{2n}}{2^{2n+1}(\Gamma(n+1))^2}\frac{\Gamma(2n+1)}{m^{2n+1}}\left(1 - m|z| + \frac{1}{2}m^2z^2 + \cdots\right)$$

$$C_1 = \pi\sum_{n=0}^{\infty} \frac{\mu_0^{2n}}{2^{2n+1}(\Gamma(n+1))^2}\frac{\Gamma(2n+1)}{m^{2n+1}}$$

$$C_2|z| = -\pi\sum_{n=0}^{\infty} \left(\frac{\mu_0}{m}\right)^{2n} \frac{\Gamma(2n+1)}{2^{2n+1}(\Gamma(n+1))^2}|z|.$$

$$= \pi\sum_{n=1}^{\infty} \left(\frac{\mu_0}{m}\right)^{2n} \frac{\Gamma(2n)}{2^{2n}\Gamma(n)\Gamma(n+1)}|z|.$$

$$\pi\sum_{n=0}^{\infty} \frac{\mu_0^{2n}}{2^{2n+1}(\Gamma(n+1))^2}\frac{\Gamma(2n+1)}{m^{2n+1}} - \frac{\pi}{2}|z|.$$

$$\Sigma_2 = \sqrt{\pi}\sum_{n=1}^{\infty} \frac{\mu_0^{2n-1}}{2^n\Gamma\left(n+\frac{1}{2}\right)}\left(\frac{|z|}{m}\right)^{n} K_n(m|z|) = \sqrt{\pi}\frac{1}{2}\sum_{n=1}^{\infty}\sum_{k=0}^{n-1} (-1)^k \frac{\mu_0^{2n-1}}{2^{2k}\Gamma\left(n+\frac{1}{2}\right)}\frac{(n-k-1)!}{k!}\frac{|z|^{2k}}{m^{2n-2k}}$$

$$+\sqrt{\pi}\sum_{n=1}^{\infty}\sum_{k=0}^{\infty} (-1)^{n+1} \frac{\mu_0^{2n-1}}{2^{2k+2n}\Gamma\left(n+\frac{1}{2}\right)}\frac{m^{2k}|z|^{2n+2k}}{k!\,(k+n)!}\left[\ln\left(\frac{m|z|}{2}\right) - \frac{1}{2}\psi(k+1) - \frac{1}{2}\psi(k+n+1)\right].$$

$$\sqrt{\pi}\frac{1}{2}\sum_{n=1}^{\infty}\sum_{k=0}^{n-1}(-1)^k\frac{\mu_0^{2n-1}}{2^{2k}\Gamma\left(n+\frac{1}{2}\right)}\frac{(n-k-1)!}{k!}\frac{|z|^{2k}}{m^{2n-2k}}\rightarrow\sqrt{\pi}\frac{1}{2}\sum_{n=1}^{\infty}\frac{\mu_0^{2n-1}}{\Gamma\left(n+\frac{1}{2}\right)}\frac{\Gamma(n)}{m^{2n}}$$

$$\pi\sum_{n=0}^{\infty}\frac{\mu_0^{2n}}{2^{2n+1}(\Gamma(n+1))^2}\frac{\Gamma(2n+1)}{m^{2n+1}}+\frac{\sqrt{\pi}}{2}\sum_{n=1}^{\infty}\frac{\mu_0^{2n-1}}{\Gamma\left(n+\frac{1}{2}\right)}\frac{\Gamma(n)}{m^{2n}}$$
$$=\frac{\sqrt{\pi}}{2}\sum_{n=0}^{\infty}\frac{\mu_0^{2n}}{m^{2n+1}}\frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma(n+1)}+\frac{\sqrt{\pi}}{2}\sum_{n=0}^{\infty}\frac{\mu_0^{2n+1}}{m^{2n+2}}\frac{\Gamma(n+1)}{\Gamma\left(n+\frac{3}{2}\right)}$$
$$=\frac{1}{m}\frac{\sqrt{\pi}}{2}\sum_{n=0}^{\infty}\left(\frac{\mu_0}{m}\right)^{2n}\left(\frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma(n+1)}+\frac{\mu_0}{m}\frac{\Gamma(n+1)}{\Gamma\left(n+\frac{3}{2}\right)}\right)=\frac{\arccos\left(-\frac{\mu_0}{m}\right)}{\sqrt{m^2-\mu_0^2}},$$

$$\frac{1}{\pi}\int_0^{\infty}dte^{t\mu_0}\left[K_0\left(m\sqrt{t^2+z^2}\right)-K_0(mt)\right]=-\frac{1}{2}|z|+O(z^2)$$

$$\frac{1}{4\pi m}\int[dR]\chi^{\dagger}(R)\exp\left[-\frac{stu}{2}\left(\frac{m}{M}\right)\frac{1}{tu\frac{m}{2M}+s}\left(\frac{R^2}{m^2}\right)\right]$$
$$\times\int_0^1du\int_0^{\infty}dtt^2e^{-ut[H_0-(\mu_0+\delta'E)]/m}\int_0^{\infty}ds\frac{e^{-s-\frac{t^2}{4s}}}{s^{\frac{3}{2}}\sqrt{tu\frac{m}{2M}+s}}\chi(R)$$

$$\exp\left[-\frac{stu}{2}\left(\frac{m}{M}\right)\frac{1}{tu\frac{m}{2M}+s}\left(\frac{R^2}{m^2}\right)\right]=\exp\left[-s\frac{tu}{s}\left(\frac{m}{2M}\right)\frac{1}{\frac{tu}{s}\frac{m}{2M}+1}\left(\frac{R^2}{m^2}\right)\right]$$

$$\frac{1}{4\pi m}\int[dR]\chi^{\dagger}(R)\chi(R)\int_0^1du\int_0^{(m/M)^2}ds\int_0^{s^{1/2}}t^2dt\frac{e^{-s-\frac{t^2}{4s}}}{s^{\frac{3}{2}}\sqrt{tu\frac{m}{2M}+s}}$$

$$\int_0^1du\int_0^{m/M}t^2dt\left[\int_0^{(m/M)^2}ds\frac{e^{-\frac{t^2}{2s}}}{s^3}\right]^{1/2}\left[\int_0^{(m/M)^2}\frac{ds}{tu\frac{m}{2M}+s}\right]^{1/2}$$

$$\int_0^1 du \int_0^{m/M} t^2 dt \left[\int_0^{(m/M)^2} ds \frac{e^{-\frac{t^2}{2s}}}{s^3}\right]^{1/2} \left[\int_0^{(m/M)^2} \frac{ds}{tu\frac{m}{2M}+s}\right]^{1/2}$$
$$= \int_0^1 du \int_0^{m/M} t^2 dt \left[\frac{1}{t^4}\int_0^{(m/M)^2/t^2} ds \frac{e^{-\frac{1}{2s}}}{s^3}\right]^{1/2} \left[\ln\left(\frac{tu\frac{m}{2M}+(m/M)^2}{tu\frac{m}{2M}}\right)\right]^{1/2}$$
$$\leq \int_0^1 du \int_0^{m/M} dt \left[\int_0^{\infty} ds \frac{e^{-\frac{1}{2s}}}{s^3}\right]^{1/2} \left[\ln\left(\frac{tu\frac{M}{2m}+1}{tu\frac{M}{2m}}\right)\right]^{1/2}$$
$$= \frac{m}{M}\left[\int_0^{\infty} ds \frac{e^{-\frac{1}{2s}}}{s^3}\right]^{1/2} \int_0^1 du \int_0^1 dv \ln^{1/2}\left(\frac{uv/2+1}{uv/2}\right)$$
$$\leq C\frac{m}{M}$$

$$H = H_s(\vec{X}) + H_f(\vec{X},\vec{Y}),$$

$$\frac{\partial}{\partial t}\rho = -\frac{i}{\hbar}[H,\rho] + \mathcal{L}\rho,$$

$$\mathcal{L}\rho = \frac{1}{2}\sum_k \left(2L_k\rho L_k^\dagger - \rho L_k^\dagger L_k - L_k^\dagger L_k \rho\right),$$

$$\rho(t_0+dt) = \left(1 - \sum_k dp_k\right)|\phi_0\rangle\langle\phi_0| + \sum_k dp_k|\phi_k\rangle\langle\phi_k|,$$

$$dp_k = \langle\phi(t_0)|L_k^\dagger L_k|\phi(t_0)\rangle dt$$

$$|\phi_0\rangle = \frac{(1 - iH_{\text{eff}}dt/\hbar)|\phi(t_0)\rangle}{\sqrt{1-\sum_k dp_k}}$$
$$|\phi_k\rangle = \frac{L_k|\phi(t_0)\rangle}{\|L_k|\phi(t_0)\rangle\|}$$

$$H_{\text{eff}} = H - \frac{i}{2}\hbar\sum_k L_k^\dagger L_k$$

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = H_{\text{eff}}|\Psi(t)\rangle.$$

$$H_{\text{eff}} = H_s(\vec{X}) + H_f'(\vec{X},\vec{Y})$$

$$H_f'(\vec{X},\vec{Y}) = H_f(\vec{X},\vec{Y}) - \frac{i}{2}\sum_k L_k^\dagger L_k$$

$$|\psi_n^R(\vec{X})\rangle\langle\psi_n^L(\vec{X})|E_n(\vec{X})$$

$$\langle\psi_m^L \mid \psi_n^R\rangle = \delta_{mn}$$

$$\langle\psi_n^R \mid \psi_n^R\rangle = 1$$

$$|\Phi\rangle = \sum_{n=1}^{N} c_n|\varphi_n(\vec{X})\rangle|\psi_n^R(\vec{X},\vec{Y})\rangle,$$

$$\sum_m \langle\psi_n^L|H_s(\vec{X})|\psi_m^R\rangle|\varphi_m(\vec{X})\rangle + E_n(\vec{X})|\varphi_n(\vec{X})\rangle = E|\varphi_n(\vec{X})\rangle$$

$$H_{n,m}(\vec{X}) = \langle\psi_n^L|H_s(\vec{X})|\psi_m^R\rangle$$

$$(\mathcal{H}_0 + \mathcal{H}_\mathcal{P})\varphi = E\varphi,$$

$$\mathcal{H}_0 = \begin{bmatrix} H_1 + E_1(\vec{X}) & 0 & \cdots & 0 \\ 0 & H_2 + E_2(\vec{X}) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & H_N + E_N(\vec{X}) \end{bmatrix},$$

$$\mathcal{H}_\mathcal{P} = \begin{bmatrix} 0 & H_{1,2} & \cdots & H_{1,N} \\ H_{2,1} & 0 & \cdots & N_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ H_{N,1} & H_{N,2} & \cdots & 0 \end{bmatrix}, \varphi = \begin{bmatrix} |\varphi_1\rangle \\ |\varphi_2\rangle \\ \vdots \\ |\varphi_n\rangle \end{bmatrix}.$$

$$\tilde{\varphi}_{1,k}^{R[0]} = \begin{bmatrix} \left|\varphi_{1,k}^{R[0]}\right\rangle \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \tilde{\varphi}_{2,k}^{R[0]} = \begin{bmatrix} 0 \\ \left|\varphi_{2,k}^{R[0]}\right\rangle \\ \vdots \\ 0 \end{bmatrix},$$

$$\cdots, \qquad \tilde{\varphi}_{N,k}^{R[0]} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ \left|\varphi_{N,k}^{R[0]}\right\rangle \end{bmatrix},$$

$$\mathcal{H}_n \left|\varphi_{n,k}^{R[0]}\right\rangle = E_{n,k}^{[0]} \left|\varphi_{n,k}^{R[0]}\right\rangle,$$

$$\mathcal{H}_n = \left(H_n(\vec{X}) + E_n(\vec{X})\right)$$

$$\left|\frac{\left\langle\varphi_{n',k'}^{L[0]}\right| H_{n',n} \left|\varphi_{n,k}^{R[0]}\right\rangle}{E_{n',k'}^{[0]} - E_{n,k}^{[0]}}\right| \ll 1, \text{for all } k', n' \neq k, n,$$

$$H_{\text{eff}} = H_s'(\vec{X}) + H_f(\vec{X},\vec{Y})$$

$$H_s'(\vec{X}) = H_s(\vec{X}) - \frac{i}{2}\sum_k X_k^\dagger X_k$$

$$H_{n,m}(\vec{X}) = \langle\psi_n|\left(H_s(\vec{X}) - \frac{i}{2}\sum_k X_k^\dagger X_k\right)|\psi_m\rangle$$

$$\langle\psi_n| - \frac{i}{2}\sum_k X_k^\dagger X_k|\psi_n\rangle$$

$$|\Phi\rangle = \sum_{n,k} c_{n,k} \left|\varphi_{n,k}^{[0]}\right\rangle \left|\psi_n^{(R)}\right\rangle$$

$$H = \hbar\omega a^\dagger a - \hbar\chi a^\dagger a x + \frac{p^2}{2m} + \frac{1}{2} m\Omega^2 x^2,$$

$$H_{\text{eff}} = \hbar\left(\omega - \frac{i}{2}\gamma\right) a^\dagger a - \hbar g a^\dagger a\left(b + b^\dagger\right) + \hbar\Omega\left(b^\dagger b + \frac{1}{2}\right)$$

$$b = \sqrt{\frac{m\Omega}{2\hbar}}\left(x + \frac{ip}{m\Omega}\right) \text{ and } g = \chi\sqrt{\frac{\hbar}{2m\Omega}}$$

$$H_{\text{eff}} = H_s + H_f$$

$$H_s = \hbar\Omega\left(b^\dagger b + \frac{1}{2}\right)$$

$$H_f = \hbar\left(\omega - \frac{1}{2} i\gamma\right) a^\dagger a - \hbar g a^\dagger a\left(b + b^\dagger\right)$$

$$\left|\psi_{n_a}^R\right\rangle = |n_a\rangle$$

$$\left\langle\psi_{n_a}^L\right| = \langle n_a|$$

$$E_{n_a} = \hbar(\omega - i\gamma)n_a - \hbar g n_a\left(b + b^\dagger\right)$$

$$\mathcal{H}_{n_a} = \hbar\Omega\left(b^\dagger b + \frac{1}{2}\right) - \hbar g n_a\left(b + b^\dagger\right) + \hbar\left(\omega - \frac{1}{2} i\gamma\right) n_a.$$

$$\left|\varphi_{n_a,n_b}^R\right\rangle = D\left(\alpha(n_a)\right)|n_b\rangle$$

$$E_{n_a,n_b} = \hbar\Omega\left(n_b + \frac{1}{2}\right) + \hbar\left(\omega - \frac{1}{2} i\gamma\right) n_a - \frac{\hbar g^2}{\Omega} n_a^2$$

$$D(\alpha) = e^{A^\dagger\alpha - A\alpha^*}$$

$$\alpha(n_a) = \frac{n_a g}{\Omega}|n_b\rangle$$

$$|\Phi(0)\rangle = \frac{1}{2}(|0\rangle + |1\rangle)(|0\rangle + |1\rangle)$$

$$\rho(t) = \frac{1}{N}\sum_{i}^{N} |\psi_i(t)\rangle\langle\psi_i(t)|$$

$$F(\rho_1, \rho_2) = \text{Tr}\sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}}$$

$$H_{\text{eff}} = \hbar\omega a^\dagger a - \hbar g a^\dagger a\left(b + b^\dagger\right) + \hbar\Omega\left(b^\dagger b + \frac{1}{2}\right) - \frac{1}{2} i\hbar\kappa b^\dagger \notin$$

$$H_{\text{eff}} = H_s + H_f$$

$$H_s = \hbar\Omega\left(b^\dagger b + \frac{1}{2}\right) - \frac{1}{2} i\hbar\kappa b^\dagger b$$

$$H_f = \hbar\omega a^\dagger a - \hbar g a^\dagger a\left(b + b^\dagger\right)$$

$$|\psi\rangle = |n_a\rangle$$

$$E_{n_a} = \hbar\omega n_a - \hbar g n_a\left(b + b^\dagger\right)$$

$$\mathcal{H}_{n_a} = \hbar\Omega_0\left(b^\dagger b + \frac{1}{2}\right) - \hbar g n_a\left(b + b^\dagger\right) + \hbar\omega n_a + \frac{1}{2}i\hbar\kappa$$

$$\hbar\Omega_0 = \hbar\Omega - \frac{1}{2}i\hbar\kappa$$

$$\alpha_0 = \frac{n_a g}{\Omega_0}$$

$$\vec{B} = \vec{B}(z) = B\left(\sin\,\theta\cos\,\frac{2\pi z}{L}, \sin\,\theta\sin\,\frac{2\pi z}{L}, \cos\,\theta\right)$$

$$H = H(z) = \frac{\vec{p}^2}{2M} + \mu\vec{B}\cdot\vec{\sigma} = H_K + H_S,$$

$$\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)L_2 = \sqrt{\kappa}\sigma^-$$

$$\begin{aligned} H_{\mathrm{eff}} &= \mu\vec{B}\cdot\vec{\sigma} - \frac{1}{2}i\hbar\kappa\sigma^+\sigma^- \\ &= \mu B\begin{pmatrix} \cos\,\theta - \frac{1}{2}ig & \sin\,\theta e^{-2\pi zi/L} \\ \sin\,\theta e^{2\pi zi/L} & -\cos\,\theta \end{pmatrix} \end{aligned}$$

$$\begin{aligned} |\psi_+^R\rangle &= \frac{1}{N}\left(\cos\,\frac{\alpha}{2}|1\rangle + \sin\,\frac{\alpha}{2}e^{2\pi zi/L}|0\rangle\right) \\ |\psi_-^R\rangle &= \frac{1}{N}\left(\sin\,\frac{\alpha}{2}|1\rangle - \cos\,\frac{\alpha}{2}e^{2\pi zi/L}|0\rangle\right) \end{aligned}$$

$$\begin{aligned} \langle\psi_+^L| &= N\left(\cos\,\frac{\alpha}{2}\langle 1| + \sin\,\frac{\alpha}{2}e^{-2\pi zi/L}\langle 0|\right) \\ \langle\psi_-^L| &= N\left(\sin\,\frac{\alpha}{2}\langle 1| - \cos\,\frac{\alpha}{2}e^{-2\pi zi/L}\langle 0|\right), \end{aligned}$$

$$E_\pm = -\frac{1}{2}ig \pm \frac{1}{2}\sqrt{16 - g^2 - 8ig\cos\,\theta}$$

$$\tan\,\alpha = \frac{4\sin\,\theta}{4\cos\,\theta - ig}$$

$$N = \sqrt{\left|\cos\,\frac{\alpha}{2}\right|^2 + \left|\sin\,\frac{\alpha}{2}\right|^2}.$$

$$\left|\sin\,\frac{\alpha}{2}\right|^2 + \left|\cos\,\frac{\alpha}{2}\right|^2 = 1$$

$$\mathcal{H}_n = -\frac{\hbar^2}{2M}\left(\nabla - i\vec{A}_n\right)^2 + E_n$$

$$\vec{A}_n = i\langle\psi_n^L|\nabla|\psi_n^R\rangle, n = +, -$$

$$\Gamma(g) = \max\left\{\left|\frac{\left\langle\varphi_{n',k'}^{L[0]}\middle|O_{n',n}\middle|\varphi_{n,k}^{R[0]}\right\rangle}{E_{n',k'}^{[0]} - E_{n,k}^{[0]}}\right|\right\},$$

$$O_{n',n} = -\frac{\hbar}{2M}\left(2\langle\psi_{n'}^{L}|\nabla|\psi_n^R\rangle\nabla + \langle\psi_{n'}^{L}|\nabla^2|\psi_n^R\rangle\right)$$

$$H_{n,m} = \langle\psi_n|H_s|\psi_m\rangle - \frac{1}{2}i\sum_k \langle\psi_n|X_k^\dagger X_k|\psi_m\rangle$$

$$3(D-2)/(3-D)(D-1) = b_{ho}^2/r_{2D}^2,$$

$$\boldsymbol{R}_i = \mathbf{x}_j - \mathbf{x}_k \text{ and } \boldsymbol{r}_i = \mathbf{x}_i - \frac{m_j\mathbf{x}_j + m_k\mathbf{x}_k}{m_j + m_k}$$

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \equiv \Psi(\boldsymbol{R}, \boldsymbol{r}) = \sum_{i=1}^{3} \psi^{(i)}(\boldsymbol{R}_i, \boldsymbol{r}_i)$$

$$\left[\frac{1}{2\eta_i}\nabla_{\boldsymbol{R}_i}^2 + \frac{1}{2\mu_i}\nabla_{\boldsymbol{r}_i}^2 - E_3\right]\psi^{(i)}(\boldsymbol{R}_i, \boldsymbol{r}_i) = 0$$

$$\eta_i = m_j m_k/(m_j + m_k)$$

$$\mu_i = m_i(m_j + m_k)/(m_i + m_j + m_k)$$

$$\left[\frac{\partial}{\partial R_i} R_i^{\frac{D-1}{2}} \Psi(\boldsymbol{R}_i, \boldsymbol{r}_i)\right]_{R_i\to 0} = \frac{3-D}{2}\left[\frac{\Psi(\boldsymbol{R}_i, \boldsymbol{r}_i)}{R_i^{\frac{3-D}{2}}}\right]_{R_i\to 0}$$

$$\boldsymbol{R}_i' = \sqrt{\eta_i}\boldsymbol{R}_i$$

$$\boldsymbol{r}_i' = \sqrt{\mu_i}\boldsymbol{r}_i$$

$$\boldsymbol{R}_j' = -\boldsymbol{R}_k'\cos\,\theta_i + \boldsymbol{r}_k'\sin\,\theta_i,$$
$$\boldsymbol{r}_j' = -\boldsymbol{R}_k'\sin\,\theta_i - \boldsymbol{r}_k'\cos\,\theta_i,$$

$$\tan\,\theta_i = \left[m_i M/(m_j m_k)\right]^{1/2}$$

$$M = m_1 + m_2 + m_3$$

$$F^{(i)}(R_i', r_i') = (R_i' r_i')^{(D-1)/2}\psi^{(i)}(R_i', r_i')$$

$$F^{(i)}(\rho, \alpha_i) = C^{(i)}\chi(\rho)G^{(i)}(\alpha_i)$$

$$\rho^2 = R_i'^2 + r_i'^2, \alpha_i = \arctan\,(R_i'/r_i')$$

$$\left[-\frac{\partial^2}{\partial\rho^2}+\frac{s_n^2-1/4}{\rho^2}+2\kappa_0^2\right]\chi(\rho)=0$$

$$\left[-\frac{\partial^2}{\partial\alpha_i^2}-s_n^2+\frac{(D-1)(D-3)}{\sin^2\ 2\alpha_i}\right]G^{(i)}(\alpha_i)=0$$

$$G^{(i)}(z)=(1-z^2)^{1/4}g^{(i)}(z)$$

$$G^{(i)}(\alpha_i)=\sqrt{\sin\ 2\alpha_i}\left[P_{s_n/2-1/2}^{D/2-1}(\cos\ 2\alpha_i)\right.$$
$$\left.-\frac{2}{\pi}\tan\left[\pi(s_n-1)/2\right]Q_{s_n/2-1/2}^{D/2-1}(\cos\ 2\alpha_i)\right]$$

$$\psi^{(i)}(R_i',r_i')=\mathcal{C}^{(i)}\frac{K_{s_n}\left(\sqrt{2}\kappa_0\sqrt{R_i'^2+r_i'^2}\right)}{\left(R_i'^2+r_i'^2\right)^{D/2-1/2}}$$
$$\times\frac{\sqrt{\sin\left[2\arctan\left(R_i'/r_i'\right)\right]}}{\left\{\cos\left[\arctan\left(R_i'/r_i'\right)\right]\sin\left[\arctan\left(R_i'/r_i'\right)\right]\right\}^{D/2-1/2}}$$
$$\times\left[P_{s_n/2-1/2}^{D/2-1}\{\cos\left[2\arctan\left(R_i'/r_i'\right)\right]\}\right.$$
$$\left.-\frac{2}{\pi}\tan\left[\pi(s_n-1)/2\right]Q_{s_n/2-1/2}^{D/2-1}\{\cos\left[2\arctan\left(R_i'/r_i'\right)\right]\}\right]$$

$$\frac{\mathcal{C}^{(i)}}{2}\left[(\cot\ \alpha_i)^{\frac{D-1}{2}}\left(\sin\ 2\alpha_i\frac{\partial}{\partial\alpha_i}+D-3\right)G^{(i)}(\alpha_i)\right]_{\alpha_i\to 0}$$

$$+(D-2)\left[\frac{\mathcal{C}^{(j)}G^{(j)}(\theta_k)}{(\sin\ \theta_k\cos\ \theta_k)^{\frac{D-1}{2}}}+\frac{\mathcal{C}^{(k)}G^{(k)}(\theta_j)}{(\sin\ \theta_j\cos\ \theta_j)^{\frac{D-1}{2}}}\right]=0$$

$$H=-\frac{\hbar^2}{2\eta_B}\nabla_R^2+V_B(|\mathbf{R}|)+\left(-\frac{\hbar^2}{2\mu_B}\nabla_r^2+\sum_{j=1}^{2}V_A\left(\left|\mathbf{r}+(-1)^j\frac{\eta_B}{m_A}\mathbf{R}\right|\right)\right)$$

$$\Psi(\mathbf{r},\mathbf{R})=\phi(\mathbf{R})\psi_R(\mathbf{r})$$

$$\left[-\frac{\hbar^2}{2\mu_B}\nabla_r^2+\sum_{j=1}^{2}V_A\left(\left|\mathbf{r}+(-1)^j\frac{\mathbf{R}}{2}\right|\right)\right]\psi_R(\mathbf{r})=\epsilon(R)\psi_R(\mathbf{r})$$

$$\left[-\frac{\hbar^2}{2\eta_B}\nabla_R^2+\epsilon(R)\right]\phi(\mathbf{R})=E_3\phi(\mathbf{R})$$

$$\left[-\frac{d^2}{dR^2}+\frac{(D-3+2L)(D-1+2L)}{4R^2}-\frac{m_A}{\hbar^2}|\epsilon(R)|\right]\chi(R)=-\frac{m_A}{\hbar^2}E_3\chi(R)$$

$$-\lim_{R\to 0}|\epsilon(R)|=-\frac{\hbar^2}{2\mu_B}\frac{(N-2)g(D)}{R^2}$$

$$g(D)=\left[-\frac{\pi\csc(D\pi/2)}{2^{\frac{D}{2}}\Gamma(D/2)K_{\frac{D-2}{2}}(\sqrt{g(D)})}\right]^{\frac{4}{2-D}}$$

$$\left[-\frac{d^2}{dR^2}+\frac{s_n^2-1/4}{R^2}\right]\chi(R)=\frac{m_A}{\hbar^2}E_3\chi(R),$$

$$s_n^2=-\frac{m_A g(D)}{2\mu_B}+\frac{(D-2+2L)^2}{4}$$

$$(N-2)\frac{m_A}{2\mu_B}g(D)>\frac{(D-2+2L)^2}{4}.$$

$$\chi(R)=\sqrt{R}K_{is_0}(\kappa_0 R).$$

$$\psi_R(r)=-\frac{R^{2-D}}{(2\pi)^{\frac{D}{2}}}\frac{2\mu_B}{\hbar^2}g(D)^{\frac{D-2}{4}}\times\left\{\left(\frac{r^2}{R^2}+\frac{1}{4}+\frac{r}{R}\cos(\theta_{rR})\right)^{\frac{2-D}{4}}K_{\frac{D-2}{2}}\left(\sqrt{g(D)\left[\frac{r^2}{R^2}+\frac{1}{4}+\frac{r}{R}\cos(\theta_{rR})\right]}\right)+\left(\frac{r^2}{R^2}+\frac{1}{4}-\frac{r}{R}\cos(\theta_{rR})\right)^{\frac{2-D}{4}}K_{\frac{D-2}{2}}\left(\sqrt{g(D)\left[\frac{r^2}{R^2}+\frac{1}{4}-\frac{r}{R}\cos(\theta_{rR})\right]}\right)\right\}$$

$$\Psi(r,R)=-\frac{R^{(6-3D)/2}}{(2\pi)^{\frac{D}{2}}}\frac{2\mu_B}{\hbar^2}g(D)^{\frac{D-2}{4}}K_{is_0}(\kappa_0 R)\times\left\{\left(\frac{r^2}{R^2}+\frac{1}{4}+\frac{r}{R}\cos(\theta_{rR})\right)^{\frac{2-D}{4}}K_{\frac{D-2}{2}}\left(\sqrt{g(D)\left[\frac{r^2}{R^2}+\frac{1}{4}+\frac{r}{R}\cos(\theta_{rR})\right]}\right)+\left(\frac{r^2}{R^2}+\frac{1}{4}-\frac{r}{R}\cos(\theta_{rR})\right)^{\frac{2-D}{4}}K_{\frac{D-2}{2}}\left(\sqrt{g(D)\left[\frac{r^2}{R^2}+\frac{1}{4}-\frac{r}{R}\cos(\theta_{rR})\right]}\right)\right\}$$

$$\kappa_0^{(n)}R_c=2e^{-\gamma}\exp\left(-\frac{n\pi}{s_0}\right)[1+\mathcal{O}(s)]$$

$$\frac{E_3^{(n)}}{E_3^{(n+1)}}=\exp\left(\frac{2\pi}{s_0}\right)\ n\to 0,1,2,\cdots.$$

CONCLUSIONES.

Resulta evidente que las métricas desarrolladas en este trabajo, abonan a la comprensión de las premisas nucleares de la Teoría Cuántica de Campos Relativistas o Curvos, en la medida en que:

Suponemos un campo cuántico indeterminado en el que, interactúan partículas subatómicas aglutinadas según su naturaleza, con distintos centros de masa y energía y con trayectorias multideterminantales. En condiciones gravitacionales, extremas o no, una partícula proyectil, sea oscura o estrella, según las definiciones recogidas por la TCCR, deforma el espacio – tiempo cuántico, curvándolo o en su defecto, generando un agujero negro cuántico. Las métricas recogidas en este trabajo, permiten explicar matemáticamente, los aspectos tensoriales del campo curvado, así como y en forma principal, el orbital de la partícula oscura o estrella, a propósito de la gravedad que la interfiere. Diseñamos mapas hipotéticos con la finalidad de trazar la trayectoria de la partícula deformante y, en consecuencia, de las partículas orbitales, lo que permite anticipar escenarios de colapso o aniquilación por colapso. En este punto es importante precisar, que el propulsor de la partícula deformante es en sí, su masa y energía, aunque no converjan al momento del colapso o de la aniquilación. Las condiciones de extrema gravedad o gravedad en condiciones no perturbativas, vuelven a la partícula deformante, un centro de gravedad en sí mismo, desplazándose por el campo, deformando su entorno e incidiendo en el comportamiento de las partículas vecinas en las relaciones de interacción. En la TCCR, usamos, no solamente tensores para explicar la curvatura, sino operadores, propagadores, osciladores e inyectores relativos no solamente a la partícula deformante sino a las partículas vecinas u orbitales las cuales se ven repercutidas por la gravedad generada por la partícula principal. El escenario de gravedad a escala cuántica, no se produce necesariamente por excitación de los estados cuánticos de una partícula específica, sino del momento mismo de su estado fundamental, provocado por la masa o la energía, que son extremadamente densas, sin embargo, cualquier partícula excitada, es capaz de generar condiciones gravitacionales, cuando se aniquila o colapsa. El momento angular y el spin de la partícula gravitacional y las partículas orbitales, es incierto, al igual que su conducta vectorial, sin embargo, este trabajo contribuye a precisar matemáticamente el instante exacto de la deformación del mapa cuántico, para cuyos efectos, hemos dise;ado planos divergentes de curvatura además de establecer modelos matriciales y superoperadores para describir, la acción gravitacional de la particula oscura o estrella en un momento espec'ifico en el plano cuántico. El trabajo aquí desarrolla, cuantiza estas dinámicas, calculando incluso, qubits de información que permitan registrar la gravedad intersecando el plano cuántico en el que se despliega.

REFERENCIAS BIBLIOGRÁFICAS.

Théotime Girardot, Derivation of the Hartree dynamics for a N-particles fermionic

2D system interacting via long-range electric and magnetic two-body singular potentials in a dilute regime, arXiv:2507.16300v1 [math-ph] 22 Jul 2025.

Rabah Abdelmouheymen KHAMADJA, FROM VQE TO SQD : MODERN QUANTUM ALGORITHMS FOR ELECTRONIC STRUCTURE PROBLEMS, arXiv:2509.21555v1 [quant-ph] 25 Sep 2025.

Simon H. Hille y Attila Szabó, TeMFpy: a Python library for converting fermionic mean-field states into tensor networks, arXiv:2510.05227v1 [cond-mat.str-el] 6 Oct 2025.

Paul A. Johnson, Charles-Émile Fecteau, Samuel Nadeau, Mauricio Rodríguez-Mayorga y Pierre-François Loos, Connections between Richardson-Gaudin States, Perfect-Pairing, and Pair Coupled-Cluster Theory, arXiv:2510.06144v1 [physics.chem-ph] 7 Oct 2025.

Alfred Li, Ankit Mahajan y Sandeep Sharma, Fokker-Planck equation governing the distribution of walkers in AFQMC, arXiv:2510.19914v1 [physics.chem-ph] 22 Oct 2025.

Gerald V. Dunne, Slater Decomposition of Laughlin States, arXiv:cond-mat/9306022v1 8 Jun 1993.

Håkon Emil Kristiansen, Håkon Kvernmoen, Simen Kvaal y Thomas Bondo Pedersen, Configuration weights in coupled-cluster theory, arXiv:2411.00690v2 [physics.chem-ph] 27 Feb 2025.

Yuri Alexandre Aoto y Márcio Fabiano da Silva, Calculating the distance from an electronic wave function to the manifold of Slater determinants through the geometry of Grassmannians, arXiv:2012.05283v1 [quant-ph] 9 Dec 2020.

Bin Yan, Rachel E. Wooten, Kevin M. Daily y Chris H. Greene, Hyperspherical Slater determinant approach to few-body fractional quantum Hall states, arXiv:1611.05305v1 [cond-mat.str-el] 16 Nov 2016.

Clemens Giuliani, Jannes Nys, Rocco Martinazzo, Giuseppe Carleo y Riccardo Rossi, Precise Quantum Chemistry calculations with few Slater Determinants, arXiv:2503.14502v2 [physics.chem-ph] 2 May 2025.

Chong Hian Chee, Daniel Leykam, Adrian M. Mak y Dimitris G. Angelakis, Shallow quantum circuits for efficient preparation of Slater determinants and correlated states on a quantum computer, arXiv:2301.07477v5 [quant-ph] 26 Jul 2023.]

PIETRO SILVI, DAVIDE ROSSINI, ROSARIO FAZIO, GIUSEPPE E. SANTORO y VITTORIO GIOVANNETTI, Matrix Product State representation for Slater Determinants and Configuration Interaction States, arXiv:1205.4154v2 [quant-ph] 5 Nov 2012.

CHIARA BOCCATO, FRANCESCA PIERONI y DARIO TREVISAN, ON DISTANCES AMONG SLATER DETERMINANT STATES AND DETERMINANTAL POINT PROCESSES, arXiv:2504.08971v1 [math-ph] 11 Apr 2025.

John Kearney, Hojin Yoo y Kathryn M. Zurek, Is a Higgs Vacuum Instability Fatal for High-Scale Inflation, arXiv:1503.05193v1 [hep-th] 17 Mar 2015.

G. F. Bertsch y L. M. Robledo, Symmetry Restoration in Hartree-Fock-Bogoliubov Based

Theories, Phys. Rev. Lett. **108**, 042505 — Published 26 January 2012.

S.V. Molodtsov y G.M. Zinovjev, Bogolyubov-Hartree-Fock approach to studying the QCD ground state, arXiv:0811.4405v3 [hep-ph] 11 Aug 2009.

Marcel Griesemer y Fabian Hantsch, Unique Solutions to Hartree-Fock Equations for Closed Shell Atoms, arXiv:1012.5179v1 [math-ph] 23 Dec 2010.

Niels Benedikter, Effective Dynamics of Interacting Fermions from Semiclassical Theory to the Random Phase Approximation, arXiv:2203.11255v3 [math-ph] 5 Jul 2022.

P. A. M. Guichon, J. R. Stone y A. W. Thomas, Hartree-Fock Formulation of the QMC Model at Finite Temperature, arXiv:2310.19262v1 [nucl-th] 30 Oct 2023.

Ettore Vitali, Peter Rosenberg y Shiwei Zhang, Monte Carlo Methods in the Manifold of Hartree-Fock-Bogoliubov Wave Functions, arXiv:2409.11571v1 [cond-mat.str-el] 17 Sep 2024.

Stefan Vuckovic, John Kozlowski y Kieron Burke, Density functional analysis: The theory of density-corrected DFT, arXiv:1908.05721v1 [physics.chem-ph] 15 Aug 2019.

I. C. Danchev, A. N. Antonov, D. N. Kadrev, M. K. Gaidarov, P. Sarriguren y E. Moya de Guerra, Symmetry energy properties of neutron-rich nuclei from the coherent density fluctuation model applied to nuclear matter calculations with Bonn potentials, arXiv:2006.01471v1 [nucl-th] 2 Jun 2020.

CYRIL MALÉZÉ, SCATTERING FOR THE ONE DIMENSIONAL HARTREE FOCK EQUATION, arXiv:2406.17715v3 [math.AP] 10 Mar 2025.

Google AI Quantum and Collaborators, Hartree-Fock on a superconducting qubit quantum computer, arXiv:2004.04174v2 [quant-ph] 20 Apr 2020.

SOHEI ASHIDA, CONVERGENCE OF SCF SEQUENCES FOR THE HARTREE-FOCK EQUATION, arXiv:2205.10300v4 [math.AP] 25 Jan 2023.

Nikolai Kaschewski y Axel Pelster, The Weighted Hartree-Fock-Bogoliubov method for interacting fermions: An application to ultracold Fermi superfluids, arXiv:2508.18801v1 [cond-mat.quant-gas] 26 Aug 2025.

Andreas Erbs Hillers-Bendtsen y Todd J. Martinez, Accelerating Hartree-Fock and Density Functional Theory Calculations using Tensor Hypercontraction. (arXiv)

Federico Rossi y Henrik Koch, Convex Hartree-Fock theory: A simple framework for ground state conical intersections, arXiv:2508.21453v1 [physics.chem-ph] 29 Aug 2025.

Yaolong Zhang, Bin Jiang y Hua Guo, SchrödingerNet: A Universal Neural Network Solver for The Schrödinger Equation. (arXiv)

Jong-Kwon Ha y Ryan J. MacDonell, Supplemental Material for Analog Quantum Simulation of Coupled Electron-Nuclear Dynamics in Molecules. (arXiv)

Xuezhi Bian, Yanze Wu, Tian Qiu, Tao Zhen y Joseph E. Subotnik, A semiclassical non-adiabatic phase-space approach to molecular translations and rotations: A new picture of surface hopping and electronic inertial effects, arXiv:2410.01156v1 [physics.chem-ph] 2 Oct 2024.

Jan Biedermann y Lukas Janssen, Dirac quantum criticality in twisted double bilayer transition metal dichalcogenides, arXiv:2509.04561v1 [cond-mat.mes-hall] 4 Sep 2025.

Pujita Das, Parth Bahuguna, Tulika Maitra y Narayan Mohanta, Superconducting pairing symmetries in charge-ordered kagomé metals, arXiv:2509.04571v1 [cond-mat.supr-con] 4 Sep 2025.

Rahul Ghosh, Quantum Phases in a Two-Dimensional Generalized interacting SSH Model, arXiv:2509.05655v1 [cond-mat.str-el] 6 Sep 2025.

E. Rule, I. A. Chernyshev, I. Stetcu, J. Carlson y R. Weiss, Recursive algorithm for constructing antisymmetric fermionic states in first quantization mapping, arXiv:2509.07279v1 [quant-ph] 8 Sep 2025.

Giorgio Visentin y François Mauger, Configuration-interaction calculations with density-functional theory molecular orbitals for modeling valence- and core-excited states in molecules, arXiv:2509.08245v1 [physics.chem-ph] 10 Sep 2025.

M. Rothman, B. Johnson-Toth, G. Hagen, M. Heinz y T. Papenbrock, NuLattice: Ab initio computations of atomic nuclei on lattices, arXiv:2509.08771v1 [nucl-th] 10 Sep 2025.

Bilal Hawashin, Julian Kleeschulte, David Kurz y Michael M. Scherer, Relativistic Mott transition, high-order van Hove singularity, and mean-field phase diagram of twisted double bilayer WSe2, arXiv:2509.09398v1 [cond-mat.mes-hall] 11 Sep 2025.

Usuf Rahaman, Investigation of ground state properties and shape evolution in Hf isotopes using the CDFT approach, arXiv:2509.12565v1 [nucl-th] 16 Sep 2025.

Ibrahim E. Awad, Abd Al-Aziz A, Abu-Saleh, Gurleen Cheema, Joshua W. Hollett y Raymond A. Poirier, Atomic Radial Correlation Energy Density Components, arXiv:2509.12580v1 [physics.chem-ph] 16 Sep 2025.

Shi-jing, Suo Qiu, H. Sagawa y Xian-Rong Zhou, Charge symmetry breaking effect in mirror Λ hypernuclei with Skyrme-Hartree-Fock model, arXiv: 2509.13655v2 [nucl-th] 23 Oct 2025.

Félix Desrochers, Joe Huxford, Mark R. Hirsbrunner y Yong Baek Kim, Electronic Crystal Phases in the Presence of Non-Uniform Berry Curvature and Tunable Berry Flux : TheλN-Jellium model, isoarXiv: 2509.15300v1 [cond-mat.str-el] 18 Sep 2025.

Xuan Zeng, Ru-You Zheng, Zhi-Wei Liu, Li-Sheng Geng y Xian-Rong Zhou, Hypernuclear structure with the new leading order covariant chiral hyperon-nucleon force, arXiv:2509.16878v1 [nucl-th] 21 Sep 2025.

Xin Lu, Yuanfan Yang, Zhongqing Guo y Jianpeng Liu, General Many-Body Perturbation Framework for Moiré Systems, arXiv:2509.19764v3 [cond-mat.str-el] 22 Oct 2025.

Jian Kang, Minxuan Wang y Oskar Vafek, Orbital magnetization and magnetic susceptibility of interacting electrons, therearXiv: 2509.20626v1 [cond-mat.str-el] 25 Sep 2025.

Alan A. Dzhioev y N. V. Antonenko, Isoenergetic description of induced fission pathways within energy-density functional theory, arXiv:2509.22006v1 [nucl-th] 26 Sep 2025.

Hopersky A.N, Nadolinsky A.M, Novikov S.A y Koneev R.V, Two-photon ionization of the *K-shell* of a heavy beryllium-like atomic ion. (arXiv)

Peyman Najafi, Aaron Villanueva y Hilbert Kappen, Path Integral Quantum Control for Quantum Chemistry Applications, arXiv:2509.24104v1 [quant-ph] 28 Sep 2025.

R. Folprecht, Knapp,1 G. De Gregorio, R. Mancino, P. Vesely y N. Lo Iudice, Bulk and spectroscopic nuclear properties within an ab initio renormalized random-phase approximation framework, arXiv:2510.00878v1 [nucl-th] 1 Oct 2025.

Xiaoyu Liu, Chong Wang, Xiao-Wei Zhang, Ting Cao y Di Xiao, Orbital Magnetization in Correlated States of Twisted Bilayer Transition Metal Dichalcogenides, efarXiv: 2510.01727v1 [cond-mat.mes-hall] 2 Oct 2025.

Yanek Verghis, Denis Sedov, Jakob Weßling, Prathyush P. Poduval y Mathias S. Scheurer, Vestigial pairing from fluctuating magnetism and triplet superconductivity, arXiv:2510.02474v1 [cond-mat.supr-con] 2 Oct 2025.

Nicolau Sobrosa, Miguel Goncalvez, Eduardo V. Castro, Pedro Ribeiro y Bruno Amorim, Ground state and excitations of quasiperiodic 1D narrow-band moiré systems – a mean field approach, inarXiv: 2510.04132v1 [cond-mat.str-el] 5 Oct 2025.

Claudia D. Alvarado, Eduardo Chiumiento, Homogeneous spaces in Hartree-Fock-Bogoliubov theory, arXiv:2402.15606v1 [math.FA] 23 Feb 2024.

A. I.Komech, On the Hartree-Fock dynamics in wave-matrix picture, arXiv:1407.5208v4 [math-ph] 4 Jun 2015.

Sahil Gulania, Stephen K. Gray, Yuri Alexeev, Bo Peng y Niranjan Govind, Hybrid algorithm for the time-dependent Hartree–Fock method using the Yang–Baxter equation on quantum computers, arXiv:2309.00737v1 [quant-ph] 1 Sep 2023.

James Daniel Whitfield y Zoltán Zimborás, On the NP-completeness of the Hartree-Fock method for translationally invariant systems, arXiv:1408.3459v2 [quant-ph] 30 Dec 2014.

B. R. Quea, J. M. Zhang, H. F. Song y Y. Liu, Hartree-Fock approximation for bosons with symmetry-adapted variational wave functions, arXiv:2502.15863v1 [cond-mat.quant-gas] 21 Feb 2025.

Jia Liu, Yi Fei Niu y Wen Hui Long, Configuration-interaction relativistic Hartree-Fock model, arXiv:2411.05370v3 [nucl-th] 11 Apr 2025.

CHARLES COLLOT, ELENA DANESI, ANNE-SOPHIE DE SUZZONI y CYRIL MALEZE, STABILITY OF HOMOGENEOUS EQUILIBRIA OF THE HARTREE-FOCK EQUATION, FOR ITS EQUIVALENT FORMULATION FOR RANDOM FIELDS, arXiv:2310.03442v2 [math.AP] 15 Oct 2024.

Ichio Kikuchi y Akihito Kikuchi, Symbolic, numeric and quantum computation of Hartree-Fock equation, arXiv:2401.00019v2 [quant-ph] 18 Jun 2024.

Amir Ayati, Hugh G. A. Burton y Stijn De Baerdemacker, Spin-Symmetry Projected constrained Unrestricted Hartree–Fock, arXiv:2412.16458v1 [quant-ph] 21 Dec 2024.

Alexis Ralli, Tim Weaving, Peter V. Coveney y Peter J. Love, Bridging Quantum Chemistry and MaxCut: Classical Performance Guarantees and Quantum Algorithms for the Hartree-Fock Method, arXiv:2506.04223v1 [quant-ph] 4 Jun 2025.

Vlad-Mihai Ene, Ilinca Lianu y Ioan Grosu, Hartree-Fock approximation for non-Coulomb interactions in three and two-dimensional systems, arXiv:2408.14967v1 [cond-mat.quant-gas] 27 Aug 2024.

Matteo Castagnola, Rosario R. Riso, Yassir El Moutaoukal y Enrico Ronca, Strong coupling quantum electrodynamics Hartree-Fock response theory, arXiv:2502.14511v1 [physics.chem-ph] 20 Feb 2025.

Klaas Giesbertz, Hartree–Fock & Density Functional Theory, arXiv:2010.10243v2 [physics.ed-ph] 7 Feb 2023.

Fei Xu, Multilevel correction type of adaptive finite element method for Hartree–Fock equation, arXiv:2510.10879v1 [math.NA] 13 Oct 2025.

Sunilkumar V. Rajat, Sandeep Gautam y Arko Roy, Finite-temperature phase diagram and collective modes of coherently coupled Bose mixtures, arXiv:2510.11671v1 [cond-mat.quant-gas] 13 Oct 2025.

N. Ebrahimian, Absorbed power in ultracold polarized Fermi mixtures at normal-superfluid separation phase: Mass-imbalanced effect. (arXiv).

Yasuhiro Tanaka y Hitoshi Seo, Photoinduced melting dynamics and collective mode in a correlated charge-order system, arXiv:2510.16855v1 [cond-mat.str-el] 19 Oct 2025.

Yulong Pan y Michael Lindsey, Fast adaptive discontinuous basis sets for electronic structure, arXiv:2510.21213v1 [physics.comp-ph] 24 Oct 2025.

Xuepeng Wang, Johannes S. Hofmann y Debanjan Chowdhury, Intertwined Orders, Quantum Criticality and Skyrmions in Tunable Topological Bands, arXiv:2510.21913v1 [cond-mat.str-el] 24 Oct 2025.

Fei Xu, Effective approximations for Hartree–Fock exchange potential, arXiv:2509.00733v1 [physics.chem-ph] 31 Aug 2025.

Paul Haubenwallner y Matthias Heller, Fully numerical Hartree-Fock calculations for atoms and small molecules with quantics tensor trains, arXiv:2503.08430v2 [physics.chem-ph] 11 Jun 2025.

Ericka Roy Miller y Shane M. Parker, Numerically Stable Resonating Hartree-Fock, arXiv:2411.00712v2 [physics.chem-ph] 13 Mar 2025.

E. Langmann y J. Lenells, Update of Hartree–Fock theory for Hubbard-like models, arXiv:2506.16525v1 [cond-mat.str-el] 19 Jun 2025.

Volker Bach, Hartree–Fock Theory, Lieb's Variational Principle and their Generalizations, arXiv:2209.10189v1 [quant-ph] 21 Sep 2022.

D. S. Rosa, T. Frederico, R. M. Francisco y G. Krein, Reliability of the Born-Oppenheimer

approximation in noninteger dimensions, arXiv:2408.01776v1 [cond-mat.quant-gas] 3 Aug 2024.

X. L. Huang, S. L. Wu, L. C. Wang y X. X. Yi, Born-Oppenheimer approximation for open quantum systems within the quantum trajectory approach, arXiv:1003.1177v2 [quant-ph] 17 Apr 2010.

Haci Akbas y O. Teoman Turgut, Born-Oppenheimer Approximation for a Singular System, arXiv:1602.02811v2 [math-ph] 29 Mar 2016.

John Bonini, Iman Ahmadabadi y Johannes Flick, Cavity-Born Oppenheimer Approximation for Molecules and Materials via Electric Field Response, reasonarXiv: 2407.14613v1 [physics.chem-ph] 19 Jul 2024.

Marit R. Fiechter y Jeremy O. Richardson, Understanding the Cavity Born–Oppenheimer Approximation, arXiv:2401.03532v1 [physics.chem-ph] 7 Jan 2024.

Haowu Duan, Alex Kovner y Michael Lublinsky, Born-Oppenheimer Renormalization group for High Energy Scattering: the Setup and the Wave Function, arXiv:2412.05085v1 [hep-ph] 6 Dec 2024.

Haowu Duan, Alex Kovner y Michael Lublinsky, Born-Oppenheimer Renormalization group for High Energy Scattering: CSS, DGLAP and all that, arXiv:2412.05097v1 [hep-ph] 6 Dec 2024.

Anjiao Gu y Shi Jin, Quantum simulation of a class of highly-oscillatory transport equations via Schrödingerisation, arXiv:2501.10176v2 [math.NA] 4 Sep 2025.

D. Germani, B. Grinstein y A.D. Polosa, Tetraquarks in the Born-Oppenheimer approximation, arXiv:2501.13249v2 [hep-ph] 3 Apr 2025.

Jakob Hoffmann, Lasse Müller y Marc Wagner, arXiv:2501.16188v1 [hep-lat] 27 Jan 2025.

Galit Cohen, Rachel Steinitz-Eliyahu, E. K. U. Gross, Sivan Refaely-Abramson y Ryan Requist, Non-adiabaticity from first principles: the exact-factorization approach for solids, arXiv:2502.07439v1 [cond-mat.mtrl-sci] 11 Feb 2025.

Robert Stanton, Mehmet Cagri Kaymak y Anders M. N. Niklasson, Shadow Molecular Dynamics for a Charge-Potential Equilibration Model, arXiv:2502.09602v1 [physics.chem-ph] 13 Feb 2025.

Max Hays, Junghyun Kim y William D. Oliver, Non-degenerate noise-resilient superconducting qubit, arXiv:2502.15459v1 [quant-ph] 21 Feb 2025.

Kamran Behnia, Phonon thermal Hall as a lattice Aharonov-Bohm effect, arXiv:2502.18236v5 [cond-mat.mes-hall] 29 Sep 2025.

Muhammad Naeem Anwar, arXiv:2502.20329v1 [hep-ph] 27 Feb 2025.

Richard F. Lebed y Steven R. Martinez, Meson-Meson Molecular Binding Potentials in the Diabatic Dynamical Diquark Model, arXiv:2502.20567v2 [hep-ph] 15 Apr 2025.

Ville J Harkonen, Beyond Born-Oppenheimer Green's function theories: absolute and relational, arXiv:2503.01417v1 [cond-mat.other] 3 Mar 2025.

Aleksander P. Wozniak, Ludwik Adamowicz, Thomas Bondo Pedersen y Simen Kvaal, Rothe Time Propagation for Coupled Electronic and Rovibrational Quantum Dynamics, arXiv:2503.09813v1 [physics.chem-ph] 12 Mar 2025.

A. Becker, G. M. Koutentakis y P. Schmelcher, Dynamical probe of the pseudo Jahn-Teller effect in one-dimensional confined fermions, arXiv:2503.09835v2 [cond-mat.quant-gas] 24 Jun 2025.

Hervé Bergeron, Przemysław Małkiewicz y Patrick Peter, Non-Gaussianities as a Signature of Quantumness of Quantum Cosmology, arXiv:2503.14570v1 [gr-qc] 18 Mar 2025.

Bowen Kang, Xi Xia y Tao Guo, Hidden heavy flavor tetraquarks in the Born-Oppenheimer approximation, arXiv:2503.10173v2 [hep-ph] 6 Apr 2025.

Kiyoharu Kawana, Phases and propagation of closed p-brane, arXiv:2503.14902v1 [hep-th] 19 Mar 2025.

Mirko Daumann y Thomas Dahm, Particle pairing causes subdiffusion of heavy particles in the imbalanced Hubbard model, arXiv:2503.15409v2 [cond-mat.stat-mech] 22 Jul 2025.

Thomas Schnappinger y Markus Kowalewski, Molecular Polarizability under Vibrational Strong Coupling, arXiv:2503.17102v1 [physics.chem-ph] 21 Mar 2025.

Nadine C. Bradbury, Titouan Duston, Zhen Tao, Jonathan I. Rawlinson, Robert Littlejohn y Joseph Subotnik, Symmetry Breaking as Predicted by a Phase Space Hamiltonian with a Spin Coriolis Potential, arXiv:2504.03100v2 [physics.chem-ph] 28 May 2025.

Rhiannon A. Zarotiadis, Joseph E. Lawrence y Jeremy O. Richardson, Nonadiabatic ring-polymer instanton rate theory: a generalized dividing-surface approach, arXiv:2505.04770v1 [physics.chem-ph] 7 May 2025.

David Linteau, Saverio Moroni, Giuseppe Carleo y Markus Holzmann, Universal neural wave functions for high-pressure hydrogen, arXiv:2504.07062v1 [cond-mat.str-el] 9 Apr 2025.

Yaser Tavakoli, Ahad Khaleghi Ardabili y Sara Mosaddegh, Fermions in a loop quantum cosmological spacetime, arXiv:2505.06695v2 [gr-qc] 30 Sep 2025.

S. GHERGHE, I. MOYANO y I.M. SIGAL, ON THE TIME-DEPENDENT BORN-OPPENHEIMER APPROXIMATION, arXiv:2505.18701v1 [quant-ph] 24 May 2025.

Lei Liu, Yanmei Xiao y Tao Guo, Hydrogen-like structures in the strong interaction, arXiv:2505.22177v1 [hep-ph] 28 May 2025.

Simon Euchner y Igor Lesanovsky, Rydberg atom arrays as quantum simulators for molecular dynamics, arXiv:2506.09865v1 [quant-ph] 11 Jun 2025.

Titouan Duston, Nadine Bradbury, Zhen Tao y Joseph E. Subotnik, Conical Intersections and Electronic Momentum As Viewed From Phase Space Electronic Structure Theory, arXiv:2506.11963v1 [physics.chem-ph] 13 Jun 2025.

Maxime Labat, Guillaume Jeanmairet y Emmanuel Giner, Prediction of the aqueous redox properties of functionalized quinones using a new QM/MM variational formulation, arXiv:2506.12448v1 [physics.chem-ph] 14 Jun 2025.

CLAUDIO CACCIAPUOTI, ANDREA POSILICANO y HAMIDREZA SABERBAGHI, THE BORN-OPPENHEIMER APPROXIMATION FOR A 1D 2+1 PARTICLE SYSTEM WITH ZERO-RANGE INTERACTIONS, arXiv:2506.21457v1 [math-ph] 26 Jun 2025.

Eric W. Fischer, Cavity Born-Oppenheimer Coupled Cluster Theory: Towards Electron Correlation in the Vibrational Strong Light-Matter Coupling Regime, arXiv:2507.10100v2 [physics.chem-ph] 4 Sep 2025.

Olimpia Lombardi, Sebastian Fortin, Juan Camilo Martínez González y Hernán Accorinti, What are we talking about when we discuss the Born-Oppenheimer approximation. (arXiv)

LINO BENEDETTO, QUANTUM ERGODICITY FOR CONTACT METRIC STRUCTURES, arXiv:2507.18216v3 [math.AP] 18 Sep 2025.

O. Jonathan Fajen, Oscar Granas, Todd J. Martinez y Anders M. N. Niklasson, Shadow excited state molecular dynamics with the ΔSCF method, arXiv:2507.21461v1 [physics.chem-ph] 29 Jul 2025.

Kratika Mazde, Lisa Mickel y Patrick Peter, Quantum cosmological background superposition and perturbation predictions, arXiv:2508.06231v1 [gr-qc] 8 Aug 2025.

Dil K. Limbu, Sandip Bhusal, Diana M. Castaneda-Bagatella y Farnaz A. Shakib, Diagonal Born–Oppenheimer Corrections in Condensed-Phase Ring Polymer Surface Hopping, arXiv:2509.10629v1 [physics.chem-ph] 12 Sep 2025.

Morris Brooks y David Mitrouskas, Adiabatic Klein–Gordon Dynamics for the Renormalized Nelson Model, arXiv:2509.14226v1 [math-ph] 17 Sep 2025.

Xiaohan Dan, Zhuoran Long, Tianyin Qiu, Jan Paul Menzel, Qiang Shi y Victor Batista, Nonadiabatic H-Atom Scattering Channels on Ge(111) Elucidated by the Hierarchical Equations of Motion, arXiv:2509.16916v1 [cond-mat.mtrl-sci] 21 Sep 2025.

Julian Stetzler, Sophya Garashchuk y Vitaly Rassolov, Factorized electron-nuclear dynamics with effective complex potential: on-the-fly implementation for H+2 in a laser field, arXiv:2510.07483v1 [physics.chem-ph] 8 Oct 2025.

Nora Brambilla, Gast~ao Krein, Jaume Tarrus Castella y Antonio Vairo, The Born-Oppenheimer approximation in an e_ective _eld theory language, arXiv:1707.09647v2 [hep-ph] 22 Jan 2018.

Bernardo Barrera, Daniel P. Arovas, Anushya Chandran y Anatoli Polkovnikov, The Moving Born-Oppenheimer Approximation, arXiv:2502.17557v2 [quant-ph] 7 Apr 2025.

Jakob Gunther, Alberto Baiardi, Markus Reiher y Matthias Christandl, More quantum chemistry with fewer qubits, arXiv:2308.16873v4 [quant-ph] 3 Nov 2024.

Ludwig Nutzel, Alexander Gresch, Lukas Hehn, Lucas Marti,1 Robert Freund, Alex Steiner, Christian D. Marciniak, Timo Eckstein, Nina Stockinger, Stefan Wolf, Thomas Monz, Michael Kuhn y Michael J. Hartmann, Solving an Industrially Relevant Quantum Chemistry Problem on Quantum Hardware, alarXiv: 2408.10801v1 [quant-ph] 20 Aug 2024.

Dominic W. Berry, M_aria Kieferov, Artur Scherer, Yuval R. Sanders, Guang Hao Low, Nathan Wiebe, Craig Gidney y Ryan Babbush, Improved Techniques for Preparing Eigenstates of Fermionic Hamiltonians, arXiv:1711.10460v2 [quant-ph] 21 Dec 2017.

Dave Wecker, Bela Bauer, Bryan K. Clark, Matthew B. Hastings y Matthias Troyer, Can quantum chemistry be performed on a small quantum computer?, arXiv:1312.1695v2 [quant-ph] 6 Jan 2014.

Yangjun Wu, Xiansong Xu, Dario Poletti, Yi Fan, Chu Guo y Honghui Shang, A real neural network state for quantum chemistry, afarXiv: 2301.03755v1 [quant-ph] 10 Jan 2023.

Ka-Wa Yip, Kubra Yeter-Aydeniz y Sijia S. Dong, Variational Quantum Annealing for Quantum Chemistry, arXiv:2503.15473v1 [quant-ph] 19 Mar 2025.

Jonathan Romero, Ryan Babbush, Jarrod R. McClean, Cornelius Hempel, Peter Love y Alan Aspuru-Guzik, Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz, arXiv:1701.02691v2 [quant-ph] 10 Feb 2018.

Mario Motta y Julia E. Rice, Emerging quantum computing algorithms for quantum chemistry, arXiv:2109.02873v2 [quant-ph] 13 Nov 2021.

Matthew Otten, Matthew R. Hermes, Riddhish Pandharkar, Yuri Alexeev, Stephen K. Gray y Laura Gagliardi, Localized Quantum Chemistry on Quantum Computers, arXiv: 2203.02012v1 [quant-ph] 3 Mar 2022.

Mohammad Haidar, Hugo D. Nogueira y Jean-Philippe Karr, Quantum Computing Approach to Atomic and Molecular Three-Body Systems, arXiv:2510.18005v1 [quant-ph] 20 Oct 2025.

Zhong-Xia Shang, Han-Sen Zhong, Yu-Kun Zhang, Cheng-Cheng Yu, Xiao Yuan, Chao-Yang Lu, Jian-Wei Pan y Ming-Cheng Chen, Boson sampling enhanced quantum chemistry, arXiv: 2403.16698v2 [quant-ph] 18 Apr 2024.

Juan Miguel Arrazola, Olivia Di Matteo, Nicolas Quesada, Soran Jahangiri, Alain Delgado y Nathan Killoran, Universal quantum circuits for quantum chemistry, arXiv:2106.13839v2 [quant-ph] 10 Jun 2022.

Tian Xue, Jacob P. Covey y Matthew Otten, Efficient algorithms for quantum chemistry on modular quantum processors, arXiv:2506.13332v1 [quant-ph] 16 Jun 2025.

Seunghoon Lee, Joonho Lee, Huanchen Zhai, Yu Tong, Alexander M. Dalzell, Ashutosh Kumar, Phillip Helms, Johnnie Gray, Zhi-Hao Cui, Wen-Yuan Liu, Michael Kastoryano, Ryan Babbush, John Preskill, David R. Reichman, Earl T. Campbell, Edward F. Valeev, Lin Lin y Garnet Kin-Lic Chan, Is there evidence for exponential quantum advantage in quantum chemistry?, arXiv:2208.02199v3 [physics.chem-ph] 14 Nov 2022.

Ingrid von Glehn, James S. Spencer y David Pfau, A Self-Attention Ansatz for Ab-initio Quantum Chemistry, arXiv:2211.13672v2 [physics.chem-ph] 19 Apr 2023.

Yudong Cao, Jonathan Romero, Jonathan P. Olson, Matthias Degroote, Peter D. Johnson, Maria Kieferova, Ian D. Kivlichan, Tim Menke, Borja Peropadre, Nicolas P. D. Sawaya, Sukin Sim, Libor Veis y Alan Aspuru-Guzik, Quantum Chemistry in the Age of Quantum Computing, arXiv:1812.09976v2 [quant-ph] 28 Dec 2018.

Smik Patel, Praveen Jayakumar, Tzu-Ching Yen y Artur F. Izmaylov, Quantum Measurement for Quantum Chemistry on a Quantum Computer, arXiv:2501.14968v2 [quant-ph] 29 May 2025.

Stepan Fomichev, Kasra Hejazi, Modjtaba Shokrian Zini, Matthew Kiser, Joana Fraxanet, Pablo Antonio Moreno Casares, Alain Delgado, Joonsuk Huh, Arne-Christian Voigt, Jonathan E. Mueller y Juan Miguel Arrazola, Initial state preparation for quantum chemistry on quantum computers, arXiv:2310.18410v2 [quant-ph] 9 Feb 2024.

Samuele Piccinelli, Alberto Baiardi, Max Rossmannek, Almudena Carrera Vazquez, Francesco Tacchino, Stefano Mensa, Edoardo Altamura, Ali Alavi, Mario Motta, Javier Robledo-Moreno, William Kirby, Kunal Sharma, Antonio Mezzacapo y Ivano Tavernell.

Quantum chemistry with provable convergence via randomized sample-based quantum diagonalization, arXiv:2508.02578v1 [quant-ph] 4 Aug 2025.

Sam McArdle, Suguru Endo, Alan Aspuru-Guzik, Simon C. Benjamin y Xiao Yuan, Quantum computational chemistry, arXiv:1808.10402v3 [quant-ph] 27 Jan 2020.

Garnet Kin-Lic Chan, Quantum chemistry, classical heuristics, and quantum advantage, arXiv:2407.11235v1 [quant-ph] 15 Jul 2024.

Michael A. Jones, Harish J. Vallury, Charles D. Hill y Lloyd C. L. Hollenberg, Chemistry beyond the Hartree–Fock energy via quantum computed moments, www.nature.com/scientificreports.