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

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Investigador Independiente

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

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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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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 de multideterminantal 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 Hartree-Fock para campos cuánticos relativistas o curvos. Modelo Matemático.

$$\mathfrak{H}^{(N)} := \{ \Psi \in \mathfrak{H}^{\otimes N} \mid \forall \pi \in S_N: \Psi(\underline{x}_\pi) = (-1)^\pi \Psi(\underline{x}) \}$$

$$H_N(\underline{Z}, \underline{R}) := \sum_{n=1}^N \left\{ -\Delta_n - \sum_{k=1}^K \frac{Z_k}{|\vec{x}_n - \vec{R}_k|} \right\} + \sum_{1 \leq m < n \leq N} \frac{1}{|\vec{x}_m - \vec{x}_n|}.$$

$$\mathcal{S}^{\wedge N} := \mathcal{S}^{\otimes N} \cap \mathfrak{H}^{(N)}$$

$$E_{\text{gs}}(N) \equiv E_{\text{gs}}(N, \underline{Z}, \underline{R}) := \inf \sigma(H_N)$$

$$E_{\text{gs}}(N) = \inf \{ \langle \Psi \mid H_N \Psi \rangle \mid \Psi \in \mathfrak{H}^{(N)}, \|\Psi\| = 1 \}$$



$$f_1 \wedge f_2 \wedge \cdots \wedge f_N := \frac{1}{\sqrt{N!}} \sum_{\pi \in \mathcal{S}_N} (-1)^\pi f_{\pi(1)} \otimes f_{\pi(2)} \otimes \cdots \otimes f_{\pi(N)}$$

$$\mathfrak{h}=L^2(\mathbb{R}^3\times\{\uparrow,\downarrow\}),$$

$$E_{\mathrm{HF}}(N)\!:=\!\inf\Big\{\Big\langle\Phi(\underline{f})\mid H_N\Phi(\underline{f})\Big\rangle\mid f_1,\ldots,f_N\in\mathfrak{h},\langle f_i\mid f_j\rangle_{\mathfrak{h}}=\delta_{i,j}\Big\}$$

$$\begin{aligned}\mathcal{E}_{\mathrm{HF}}(\underline{f}) &:= \left\langle \Phi(\underline{f}) \mid H_N \Phi(\underline{f}) \right\rangle \\ &= \sum_{i=1}^N \langle f_i \mid h f_i \rangle_{\mathfrak{h}} + \frac{1}{2} \sum_{i,j=1}^N \langle f_i \wedge f_j \mid V(f_i \wedge f_j) \rangle_{\mathfrak{h} \otimes \mathfrak{h}},\end{aligned}$$

$$h\!:=\!-\Delta-\sum_{k=1}^K Z_k|\vec{x}-\vec{R}_k|^{-1}$$

$$\mathcal{E}_{\mathrm{HF}}(\underline{f})=T(\underline{f})-U\left(\rho_{\underline{f}}\right)+\frac{1}{2}D\left(\rho_{\underline{f}}\right)-\frac{1}{2}X\left(\gamma_{\underline{f}}\right)$$

$$T(\underline{f})\!:=\!\sum_{\tau=\uparrow,\downarrow}\sum_{i=1}^N\int\left|\vec{\nabla}f_i(\vec{x},\tau)\right|^2d^3x, U(\rho)\!:=\!\sum_{k=1}^K\int\frac{Z_k\rho(\vec{x})}{\left|\vec{x}-\vec{R}_k\right|}d^3x,$$

$$D(\rho)\!:=\!\iint\frac{\rho(\vec{x})\rho(\vec{y})d^3xd^3y}{\left|\vec{x}-\vec{y}\right|}, X(\gamma)\!:=\!\iint\frac{|\gamma(\vec{x},\vec{y})|^2d^3xd^3y}{\left|\vec{x}-\vec{y}\right|},$$

$$\gamma_{\underline{f}}(\vec{x},\vec{y})\!:=\!\sum_{\tau=\uparrow,\downarrow}\sum_{i=1}^Nf_i(\vec{x},\tau)\overline{f_i(\vec{y},\tau)}$$

$$\rho_{\underline{f}}(\vec{x})\!:=\!\gamma_{\underline{f}}(\vec{x},\vec{x})$$

$$E_{\mathrm{HF}}(Z)=E_{\mathrm{TF}}(Z,Z\underline{Z},\underline{R}(Z))+\frac{Z^2}{4}\sum_{k=1}^Kz_k^2+\mathcal{O}(Z^{5/3}),$$

$$\frac{Z^2}{4}\sum_{k=1}^Kz_k^2$$

$$\mathcal{E}_{\mathrm{HF}}\left(\underline{f}^{(\mathrm{HF})}\right)\leq E_{\mathrm{HF}}(N)+\varepsilon$$

$$\langle f_i \mid f_j \rangle_{\mathfrak{h}} = \delta_{i,j}$$

$$cZ^{7/3}\leq T\left(\underline{f}^{(\mathrm{HF})}\right), U(\rho_{\mathrm{HF}}), D(\rho_{\mathrm{HF}})\leq CZ^{7/3}\\ cZ^{5/3}\leq X(\gamma_{\mathrm{HF}})\leq CZ^{5/3}$$

$$\langle f_i \mid f_j \rangle_{\mathfrak{h}} = \delta_{i,j}$$

$$\underline{f}^{(\mathrm{HF})} = \left(f_1^{(\mathrm{HF})}, \ldots, f_N^{(\mathrm{HF})}\right)$$

$$h_{\mathrm{HF}}\left[\underline{f}^{(\mathrm{HF})}\right]f_i^{(\mathrm{HF})}=e_if_i^{(\mathrm{HF})},$$

$$\begin{aligned} & \left(h_{\mathrm{HF}}[\underline{f}]g\right)[\vec{x},\tau]:= \\ & (hg)[\vec{x},\tau]+\left(\int\frac{\rho_{\underline{f}}(\vec{y})d^3y}{|\vec{x}-\vec{y}|}\right)g(\vec{x},\tau)-\int\frac{\gamma_{\underline{f}}(\vec{x},\vec{y})g(\vec{y},\tau)d^3y}{|\vec{x}-\vec{y}|}. \end{aligned}$$

$$\mathfrak{H}^{(N)}\!:=\bigwedge^N\mathfrak{h}\!:=\overline{\mathrm{span}\{f_1\wedge\cdots\wedge f_N\mid f_1,\ldots,f_N\in\mathfrak{h}\}}^{\|\cdot\|}\subseteq\mathfrak{h}^{\otimes N},$$

$$\mathfrak{F}\equiv\mathfrak{F}[\mathfrak{h}]\!:=\bigoplus_{N=0}^{\infty}\mathfrak{H}^{(N)},$$

$$\begin{aligned}\Pi_k^{(N)}[f_1\otimes\cdots\otimes f_N]&:=f_k\otimes f_1\otimes\cdots\otimes f_{k-1}\otimes f_{k+1}\otimes\cdots\otimes f_N,\\ \Pi_{i,j}^{(N)}[f_1\otimes\cdots\otimes f_N]&:=\\ f_i\otimes f_j\otimes f_1\otimes\cdots\otimes f_{i-1}\otimes f_{i+1}\otimes\cdots\otimes f_{j-1}\otimes f_{j+1}\otimes\cdots\otimes f_N\end{aligned}$$

$$\mathfrak{H}^{(N)}h_0\!:=V_0\!=\!0, h_1\!=\!h, V_1\!=\!0$$

$$\begin{aligned} h_N &:= \sum_{i=1}^N \left(\Pi_i^{(N)}\right)^* \left(h \otimes \mathbf{1}^{\otimes (N-1)}\right) \Pi_i^{(N)} \\ V_N &:= 2 \sum_{1 \leq i < j \leq N} \left(\Pi_{i,j}^{(N)}\right)^* \left(V \otimes \mathbf{1}^{\otimes (N-2)}\right) \Pi_{i,j}^{(N)} \\ H_N &:= h_N + \frac{1}{2} V_N \end{aligned}$$

$$h=-\Delta_x-\sum_{k=1}^K\,Z_k\,|\,\vec{x}-\vec{R}_k|^{-1}\,\text{and}\,V=|\vec{x}-\vec{y}|^{-1}$$

$$\mathbb{h}\!:=\bigoplus_{N=0}^{\infty}h_N, \mathbb{V}\!:=\bigoplus_{N=0}^{\infty}V_N, \mathbb{H}\!:=\bigoplus_{N=0}^{\infty}H_N=\mathbb{h}+\frac{1}{2}\mathbb{V},$$

$$\mathbb{H}_{\mu}\!:=\mathbb{H}-\mu\mathbb{N}\geq\mu Z-\sum_{1\leq k<\ell\leq K}Z_kZ_{\ell}|R_k-R_{\ell}|^{-1}$$

$$\mathbb{N}\!:=\bigoplus_{N=0}^{\infty}N\cdot\mathbf{1}_{\mathfrak{H}^{(N)}}$$

$$\|Vf\|_{\mathfrak{h}}\leq \varepsilon\|hf\|_{\mathfrak{h}}+b_{\varepsilon}\|f\|_{\mathfrak{h}}$$

$$\psi_N\in\mathfrak{H}^{(N)}$$

$$\langle \Psi \mid \mathbb{H} \Psi \rangle = \mathrm{Tr}_{\mathfrak{F}}(\mathbb{H} \mid \Psi) \langle \Psi \mid \rangle$$

$$|\Psi\rangle\langle\Psi|\in\mathcal{B}(\mathfrak{F})$$

$$\mathfrak{DM}:=\{\rho\in\mathcal{L}^1(\mathfrak{F})\mid\rho\geq0,\mathrm{Tr}_{\mathfrak{F}}(\rho)=1,\rho\text{ is even}\},$$

$$\phi\in\mathfrak{H}^{(m)}\text{ and }\psi\in\mathfrak{H}^{(n)}$$

$$\rho\in\mathfrak{DM}$$

$$\rho=\sum_{\nu=1}^{\infty}r_{\nu}|\Psi_{\nu}\rangle\langle\Psi_{\nu}|$$

$$\mathfrak{DM}^{(N)}:=\{\rho\in\mathfrak{DM}\mid\rho\mathbb{N}=\mathbb{N}\rho=N\cdot\rho\},$$

$$\mathfrak{DM}\subseteq\mathcal{L}^1(\mathfrak{F})$$

$$|\Psi\rangle\langle\Psi|\in\mathfrak{DM}$$

$$E_{\mathrm{gs}}(N)=\inf\{\mathrm{Tr}_{\mathfrak{F}}(\rho\mathbb{H})\mid\rho\in\mathfrak{DM}^{(N)},\langle\mathbb{H}\rangle_{\rho}<\infty\},$$

$$\langle A\rangle_{\rho}:=\mathrm{Tr}_{\mathfrak{F}}(\rho^{1/2}A\rho^{1/2}).$$

$$E_{\mathrm{gs}}:=\inf_{N\in\mathbb{Z}^+}E_{\mathrm{gs}}(N)=\inf\{\mathrm{Tr}_{\mathfrak{F}}(\rho\mathbb{H}_{\mu})\mid\rho\in\mathfrak{DM},\langle\mathbb{H}\rangle_{\rho}<\infty\}$$

$$c^*(f)\colon\mathfrak{H}^{(0)}\rightarrow\mathfrak{H}^{(1)}$$

$$c^*(f)\Omega:=f$$

$$c^*(f)\colon\mathfrak{H}^{(N)}\rightarrow\mathfrak{H}^{(N+1)}$$

$$c^*(f)[f_1\wedge\cdots\wedge f_N]:=f\wedge f_1\wedge\cdots\wedge f_N$$

$$\mathfrak{F}\|c^*(f)\|_{\mathcal{B}(\mathfrak{F})}=\|f\|_{\mathfrak{h}}c^*(f)\in\mathcal{B}(\mathfrak{F})$$

$$\mathfrak{H}^{(N)}=\overline{\mathrm{span}\{c^*(f_1)\cdots c^*(f_N)\Omega\mid f_1,\ldots,f_N\in\mathfrak{h}\}^{\|\cdot\|}}\text{ and}\\ \mathfrak{F}=\overline{\mathrm{span}\{c^*(f_1)\cdots c^*(f_N)\Omega\mid N\in\mathbb{Z}_0^+,f_1,\ldots,f_N\in\mathfrak{h}\}^{\|\cdot\|}},$$

$$\mathfrak{F}_{\mathrm{fin}}[\mathfrak{s}]:=\mathrm{span}\{c^*(f_1)\cdots c^*(f_N)\Omega\mid N\in\mathbb{Z}_0^+,f_1,\ldots,f_N\in\mathfrak{s}\}\subseteq\mathfrak{F}[\mathfrak{h}]$$

$$c(f):=[c^*(f)]^*\in\mathcal{B}(\mathfrak{F})$$

$$\mathfrak{h}\ni f\mapsto c(f)\in\mathcal{B}(\mathfrak{F})$$

$$\{c^*(f),c(f)\}_{f\in\mathfrak{h}}\subseteq\mathcal{B}(\mathfrak{F})$$

$$\{c(f),c^*(g)\}=\langle f\mid g\rangle_{\mathfrak{h}}\cdot\mathbf{1}_{\mathfrak{F}}\text{ and }c(f)\Omega=0$$

$$\{f_j\}_{j=1}^\infty\subseteq\mathfrak{s}\subseteq\mathfrak{h}$$

$$\mathbb{N} = \sum_{j=1}^{\infty} c^*(f_j)c(f_j), \mathbb{H} = \sum_{j,k=1}^{\infty} \langle f_j \mid hf_k \rangle c^*(f_j)c(f_k)$$

$$\mathbb{V} = \sum_{i,j,k,\ell=1}^{\infty} \langle f_i \otimes f_j \mid V(f_k \otimes f_\ell) \rangle c^*(f_i)c^*(f_j)c(f_\ell)c(f_k)$$

$$\left\langle g \mid \gamma_\rho^{(1)} f \right\rangle_{\mathfrak{h}} := \mathrm{Tr}_{\mathfrak{F}}[\rho c^*(f)c(g)],$$

$$\left\langle g_1 \otimes g_2 \mid \gamma_\rho^{(2)}(f_1 \otimes f_2) \right\rangle_{\mathfrak{h} \otimes \mathfrak{h}} := \mathrm{Tr}_{\mathfrak{F}}[\rho c^*(f_1)c^*(f_2)c(g_2)c(g_2)],$$

$$\langle \mathbb{N}^2 \rangle_\rho := \mathrm{Tr}_{\mathfrak{F}}[\rho \mathbb{N}^2] < \infty$$

$$\gamma_\rho^{(1)} \in \mathcal{L}^1(\mathfrak{h}) \text{ and } \gamma_\rho^{(2)} \in \mathcal{L}^1(\mathfrak{h} \otimes \mathfrak{h})$$

$$\mathrm{Tr}_{\mathfrak{h}}\left[\gamma_\rho^{(1)}\right]=\langle \mathbb{N}\rangle_\rho \text{ and } \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left[\gamma_\rho^{(2)}\right]=\langle \mathbb{N}^2-\mathbb{N}\rangle_\rho.$$

$$0\leq \gamma_\rho^{(1)}\leq \mathbf{1}_{\mathfrak{h}} \text{ and } 0\leq \gamma_\rho^{(2)}\leq (N-1)\mathbf{1}_{\mathfrak{h}\otimes\mathfrak{h}}.$$

$$\langle \mathbb{H} \rangle_\rho = \varepsilon_Q \left(\gamma_\rho^{(1)}, \gamma_\rho^{(2)} \right) := \mathrm{Tr}_{\mathfrak{h}} \left[h \gamma_\rho^{(1)} \right] + \frac{1}{2} \mathrm{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} \left[V \gamma_\rho^{(2)} \right].$$

$$\left\langle g \mid \gamma_\rho^{(1)} f \right\rangle_{\mathfrak{h}} = \frac{1}{N-1} \sum_{j=1}^{\infty} \left\langle g \otimes f_j \mid \gamma_\rho^{(2)}(f \otimes f_j) \right\rangle_{\mathfrak{h} \otimes \mathfrak{h}},$$

$$\rho(\underline{f})=|\Phi(\underline{f})\rangle\langle\Phi(\underline{f})|\in\mathfrak{DM}^{(N)}$$

$$\Phi(\underline{f})=f_1\wedge\cdots\wedge f_N$$

$$\gamma_{\rho(\underline{f})}^{(1)}=\sum_{i=1}^N|f_i\rangle\langle f_i|$$

$$\gamma_{\rho(\underline{f})}^{(2)}=\sum_{i,j=1}^N|f_i\wedge f_j\rangle\langle f_i\wedge f_j|=(\mathbf{1}-\mathrm{Ex})\left(\gamma_{\rho(\underline{f})}^{(1)}\otimes\gamma_{\rho(\underline{f})}^{(1)}\right),$$

$$\begin{aligned}\left\langle \Phi(\underline{f}) \mid H_N \Phi(\underline{f}) \right\rangle &= \varepsilon_Q \left(\gamma_{\rho(\underline{f})}^{(1)} (\mathbf{1} - \mathrm{Ex}) \left(\gamma_{\rho(\underline{f})}^{(1)} \otimes \gamma_{\rho(\underline{f})}^{(1)} \right) \right) \\ &= \mathrm{Tr}_{\mathfrak{h}} \left[h \gamma_{\rho(\underline{f})}^{(1)} \right] + \frac{1}{2} \mathrm{Tr}_{\mathfrak{h} \otimes \mathfrak{h}} \left[V (\mathbf{1} - \mathrm{Ex}) \left(\gamma_{\rho(\underline{f})}^{(1)} \otimes \gamma_{\rho(\underline{f})}^{(1)} \right) \right]\end{aligned}$$

$$E_{\mathrm{HF}}(N)=\inf\{\mathcal{E}_{\mathrm{HF}}(\gamma)\mid \gamma=\gamma^*\in\mathcal{L}^1(\mathfrak{h}),\mathrm{Tr}(\gamma)=N,\gamma=\gamma^2\},$$

$$\mathcal{E}_{\mathrm{HF}}(\gamma)=\mathrm{Tr}_{\mathfrak{h}}[h\gamma]+\frac{1}{2}\mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}[V(\mathbf{1}-\mathrm{Ex})(\gamma\otimes\gamma)].$$

$$E_{\mathrm{HF}}(N)=\inf\{\mathcal{E}_{\mathrm{HF}}(\gamma)\mid \gamma\in\mathcal{L}^1(\mathfrak{h}),\mathrm{Tr}(\gamma)=N,0\leq\gamma\leq\mathbf{1}_{\mathfrak{h}}\}.$$



$$\gamma_0=\sum_{j=1}^J\lambda_j|f_j\rangle\langle f_j|\text{ and }\varepsilon_{\text{HF}}(\gamma_0)=\sum_{i=1}^J\lambda_ih_i+\frac{1}{2}\sum_{i,j=1}^J\lambda_i\lambda_jV_{i,j},$$

$$h_i\!:=\langle f_i\mid hf_i\rangle$$

$$V_{i,j}\!:=\langle f_i\wedge f_j\mid V(f_i\wedge f_j)\rangle>0$$

$$\sum_{j=1}^J\lambda_j=N$$

$$\gamma_\delta\!:= (\lambda_p+\delta)|f_p\rangle\langle f_p|+(\lambda_q-\delta)|f_q\rangle\langle f_q|+\sum_{j\in\mathbb{Z}^+\setminus\{p,q\}}\lambda_j|f_j\rangle\langle f_j|.$$

$$\min\{\mathcal{E}_{\text{HF}}(\gamma_r),\mathcal{E}_{\text{HF}}(\gamma_{-r})\}<\mathcal{E}_{\text{HF}}(\gamma_0)$$

$$\gamma(\tau_1,\ldots,\tau_J)=\sum_{j=1}^J\tau_j|f_j\rangle\langle f_j|$$

$$\sum_{j=1}^J\tau_j=N$$

$$\sum_{n=1}^N\left|G_j^{(n)}\right|^2=\lambda_j$$

$$g_n^{(\theta)}\!:=\sum_{j=1}^J e^{2\pi i\theta_j}G_j^{(n)}f_j\in\mathfrak{h},$$

$$\Phi\left(\underline{g}^{(\theta)}\right)=g_1^{(\theta)}\wedge\cdots\wedge g_N^{(\theta)}\in\mathfrak{H}^{(N)}$$

$$\begin{aligned} &\left\langle \Phi\left(\underline{g}^{(\theta)}\right)\mid H_N\Phi\left(\underline{g}^{(\theta)}\right)\right\rangle \\ &= \sum_{n=1}^N\left\langle g_n^{(\theta)}\mid hg_n^{(\theta)}\right\rangle_{\mathfrak{h}}+\frac{1}{2}\sum_{m,n=1}^N\left\langle g_m^{(\theta)}\wedge g_n^{(\theta)}\mid V\left(g_m^{(\theta)}\wedge g_n^{(\theta)}\right)\right\rangle_{\mathfrak{h}\otimes\mathfrak{h}}. \end{aligned}$$

$$\mathbb{E}_{\theta}[F]\!:=\int_0^1\cdots\int_0^1F(\theta)d\theta_1\cdots d\theta_J$$

$$\mathbb{E}_{\boldsymbol{\theta}}\left[e^{2\pi i(\boldsymbol{\Theta}_j-\boldsymbol{\Theta}_k)}\right]=\delta_{j,k}$$

$$\begin{aligned}\mathbb{E}_{\theta}\left[\sum_{n=1}^N\left\langle g_n^{(\Theta)}\mid hg_n^{(\Theta)}\right\rangle_{\mathfrak{h}}\right]&=\sum_{n=1}^N\sum_{j,k=1}^J\mathbb{E}_{\theta}\left[e^{2\pi i(\Theta_j-\Theta_k)}\right]G_j^{(n)}\overline{G_k^{(n)}}\langle f_j\mid hf_k\rangle_{\mathfrak{h}}\\&=\sum_{j=1}^J\left(\sum_{n=1}^N\left|G_j^{(n)}\right|^2\right)\langle f_j\mid hf_j\rangle_{\mathfrak{h}}=\sum_{j=1}^J\lambda_jh_j\end{aligned}$$

$$\mathbb{E}_{\theta}\left[e^{2\pi i(\Theta_i+\Theta_j-\Theta_k-\Theta_{\ell})}\right]=(\delta_{i,k}\delta_{j,\ell}+\delta_{i,\ell}\delta_{j,k})$$

$$\begin{aligned}\mathbb{E}_{\theta}\left[\sum_{m,n=1}^N\left\langle g_m^{(\Theta)}\wedge g_n^{(\Theta)}\mid V\left(g_m^{(\Theta)}\wedge g_n^{(\Theta)}\right)\right\rangle_{\mathfrak{h}\otimes\mathfrak{h}}\right]&\\&=\sum_{m,n=1}^N\sum_{i,j,k,\ell=1}^J\mathbb{E}_{\theta}\left[e^{2\pi i(\Theta_i+\Theta_j-\Theta_k-\Theta_{\ell})}\right] \\&\quad G_i^{(m)}G_j^{(n)}\overline{G_k^{(m)}G_{\ell}^{(n)}}\langle f_i\wedge f_j\mid V(f_k\wedge f_{\ell})\rangle_{\mathfrak{h}\otimes\mathfrak{h}}\\&=\sum_{m,n=1}^N\sum_{i,j=1}^J\left(\left|G_i^{(m)}\right|^2\left|G_j^{(n)}\right|^2-G_j^{(m)}G_i^{(n)}\overline{G_i^{(m)}G_j^{(n)}}\right)V_{i,j}\\&=\sum_{i,j=1}^J\lambda_i\lambda_jV_{i,j}-\sum_{i,j=1}^J\left|\sum_{n=1}^NG_i^{(n)}\overline{G_j^{(n)}}\right|^2V_{i,j}\leq\sum_{i,j=1}^J\lambda_i\lambda_jV_{i,j}\end{aligned}$$

$$\mathbb{E}_{\theta}\left[\left\langle\Phi\left(\underline{g}^{(\Theta)}\right)\mid H_N\Phi\left(\underline{g}^{(\Theta)}\right)\right\rangle\right]\leq\mathcal{E}_{\mathrm{aux}}\left(\gamma_0\right)$$

$$\left\langle\Phi\left(\underline{g}^{(\theta)}\right)\mid H_N\Phi\left(\underline{g}^{(\theta)}\right)\right\rangle\leq\mathcal{E}_{\mathrm{aux}}\left(\gamma_0\right)$$

$$E_{\mathrm{HF}}(N)\leq E_{\mathrm{aux}}\left(N\right)$$

$$\gamma\in\mathcal{L}^1(\mathfrak{h})\text{ that obeys }0\leq\gamma\leq\mathbf{1}_{\mathfrak{h}},$$

$$\begin{aligned}(h_{\mathrm{HF}}[\gamma]g)[\vec{x},\tau]&:=\\(hg)[\vec{x},\tau]&+\left(\int\frac{\rho_{\gamma}(\vec{y})d^3y}{|\vec{x}-\vec{y}|}\right)g(\vec{x},\tau)-\int\frac{\gamma(\vec{x},\vec{y})g(\vec{y},\tau)d^3y}{|\vec{x}-\vec{y}|}\end{aligned}$$

$$\rho_{\gamma}(\vec{x})\!:=\!\gamma(\vec{x},\vec{x})$$

$$\gamma(\vec{x},\vec{y})=\sum_{\tau=\uparrow,\downarrow}\gamma(\vec{x},\tau,\vec{y},\tau)$$

$$\gamma_{\underline{f}}\!:=\!\sum_{n=1}^N|f_n\rangle\langle f_n|$$

$$\overline{\mathrm{Tr}}_{\mathfrak{h}}\left[\gamma_{\underline{f}}\right]<N$$

$$\rho_{\text{av}}:=\mathbb{E}_{\theta}\left(\left|\Phi\left(\underline{g}^{(\theta)}\right)\right\rangle\left\langle\Phi\left(\underline{g}^{(\theta)}\right)\right|\right)\\=\int_0^1\cdots\int_0^1\left|\Phi\left(\underline{g}^{(\theta)}\right)\right\rangle\left\langle\Phi\left(\underline{g}^{(\theta)}\right)\right|d\theta_1\cdots d\theta_J\in\mathfrak{DM}^{(N)}$$

$$\gamma_{\rho_{\text{av}}}^{(2)}\leq (\mathbf{1}-\text{Ex})\left(\gamma_{\rho_{\text{av}}}^{(1)}\otimes\gamma_{\rho_{\text{av}}}^{(1)}\right),$$

$$\mathfrak{F}=\bigoplus_{N=0}^{\infty}\mathfrak{H}^{(N)}$$

$$\rho=\bigoplus_{N=0}^{\infty}\rho_N\in\mathfrak{DM}$$

$$A^*(f_1\oplus \mathfrak{j}f_2)\!:=\!c^*(f_1)+c(f_2)\in\mathcal{B}(\mathfrak{F}),$$

$$F=f_1\oplus \mathfrak{j}f_2\in\mathfrak{h}\oplus\mathfrak{h}$$

$$A(F)=A^*(\mathfrak{J}F) \text{ and } \{A(F),A^*(G)\}=\langle F\mid G\rangle_{\mathfrak{h}\oplus\mathfrak{h}}$$

$$\mathfrak{J}\colon \mathfrak{h}\oplus\mathfrak{h}\rightarrow \mathfrak{h}\oplus\mathfrak{h}$$

$$\mathfrak{I}(f_1\oplus \mathfrak{j}f_2)\!:=\!f_2\oplus \mathfrak{j}f_1$$

$$\mathfrak{h}\oplus\mathfrak{h}\ni F\mapsto A^*(F)$$

$$\mathfrak{h}\rightarrow\mathfrak{h}^*,|f\rangle\mapsto\langle f|$$

$$(\mathfrak{j}_1f)(x)\!:=\!\overline{f(x)} \text{ and } (\mathfrak{j}_2\hat{f})(\xi)\!:=\!\overline{\hat{f}(\xi)}$$

$$\mathrm{Tr}_{\mathfrak{F}}[\rho A^*(F_1)\cdots A^*(F_{2k-1})]=0$$

$$\mathrm{Tr}_{\mathfrak{F}}[\rho A^*(F_1)\cdots A^*(F_{2k})]$$

$$F_j=f_j\oplus 0$$

$$F\in\mathfrak{h}\oplus\mathfrak{h}$$

$$\mathcal{L}^1_{\mathbb{N}^k}(\mathfrak{F})\!:=\!\left\{\rho\in\mathcal{L}^1(\mathfrak{F})\mid\left(\mathbb{N}^{k/2}\rho\mathbb{N}^{k/2}\right)\in\mathcal{L}^1(\mathfrak{F})\right\}\subseteq\mathcal{L}^1(\mathfrak{F})$$

$$\|\rho\|_{\mathbb{N}^k}:=\mathrm{Tr}_{\mathfrak{F}}\mid (\mathbb{N}+\mathbf{1})^{k/2}\rho(\mathbb{N}+1)^{-k/2}\mid$$

$$\mathfrak{DM}_{\mathbb{N}^k}:=\mathfrak{DM}\cap\mathcal{L}^1_{\mathbb{N}^k}(\mathfrak{F})$$

$$(k-gRDM)\Gamma_{\rho}^{(k)}\in\mathcal{B}\big((\mathfrak{h}\oplus\mathfrak{h})^{\otimes k}\big)$$

$$\left\langle G_1\otimes\cdots\otimes G_k\left|\Gamma_{\rho}^{(k)}(F_1\otimes\cdots\otimes F_k)\right.\right\rangle\\:=\mathrm{Tr}_{\mathfrak{F}}[\rho A^*(F_1)\cdots A^*(F_k)A(G_k)\cdots A(G_1)]$$

$$(k-RDM)\gamma_\rho^{(k)}\in\mathcal{B}(\mathfrak{h}^{\otimes k})$$

$$\begin{aligned} & \left\langle g_1\otimes\cdots\otimes g_k\mid \gamma_\rho^{(k)}(f_1\otimes\cdots\otimes f_k)\right\rangle \\ &:=\left\langle \begin{pmatrix} g_1 \\ 0 \end{pmatrix}\otimes\cdots\otimes \begin{pmatrix} g_k \\ 0 \end{pmatrix}\middle|\Gamma_\rho^{(k)}\left[\begin{pmatrix} f_1 \\ 0 \end{pmatrix}\otimes\cdots\otimes \begin{pmatrix} f_k \\ 0 \end{pmatrix}\right]\right\rangle \end{aligned}$$

$$\langle g\mid \alpha_\rho(jf)\rangle\colon=\mathrm{Tr}_{\mathfrak{F}}[\rho c(f)c(g)]$$

$$\alpha_\rho^*=-\mathrm{j}\alpha_\rho\mathrm{j}$$

$$\Gamma_\rho^{(1)}:\mathfrak{h}\oplus\mathfrak{h}\rightarrow\mathfrak{h}\oplus\mathfrak{h}$$

$$\left\langle G\mid \Gamma_\rho^{(1)}F\right\rangle_{\mathfrak{h}\oplus\mathfrak{h}}=\mathrm{Tr}_{\mathfrak{F}}[\rho A^*(F)A(G)]$$

$$\Gamma_\rho^{(1)}=\begin{pmatrix} \gamma_\rho^{(1)} & \alpha_\rho \\ \alpha_\rho^* & \mathbf{1}-\mathrm{j}\gamma_\rho^{(1)}\mathrm{j} \end{pmatrix}=\begin{pmatrix} \gamma_\rho^{(1)} & \alpha_\rho \\ -\mathrm{j}\alpha_\rho\mathrm{j} & \mathbf{1}-\mathrm{j}\gamma_\rho^{(1)}\mathrm{j} \end{pmatrix}$$

$$\left\langle g\mid \gamma_\rho^{(1)}f\right\rangle=\mathrm{Tr}_{\mathfrak{F}}[\rho c^*(f)c(g)]$$

$$\mathrm{J}\Gamma_\rho^{(1)}\mathrm{J}=\mathbf{1}-\Gamma_\rho^{(1)}$$

$$\begin{pmatrix} \gamma_\rho^{(1)}-\left(\gamma_\rho^{(1)}\right)^2-\alpha_\rho\alpha_\rho^* & \gamma_\rho^{(1)}\alpha_\rho-\alpha_\rho\mathrm{j}\gamma_\rho^{(1)}\mathrm{j} \\ \left[\gamma_\rho^{(1)}\alpha_\rho-\alpha_\rho\mathrm{j}\gamma_\rho^{(1)}\mathrm{j}\right]^* & \mathrm{j}\left[\gamma_\rho^{(1)}-\left(\gamma_\rho^{(1)}\right)^2-\alpha_\rho\alpha_\rho^*\right]\mathrm{j} \end{pmatrix}=\Gamma_\rho^{(1)}-\left(\Gamma_\rho^{(1)}\right)^2\geq 0$$

$$\mathrm{Tr}_{\mathfrak{h}}[\alpha_\rho^*\alpha_\rho]\leq\mathrm{Tr}_{\mathfrak{h}}\Big[\gamma_\rho^{(1)}-\big(\gamma_\rho^{(1)}\big)^2\Big]$$

$$\Gamma_\rho^{(1)}-\left(\Gamma_\rho^{(1)}\right)^2\in\mathcal{L}^1(\mathfrak{h}\oplus\mathfrak{h})$$

$$\Gamma_{\rho\sim}^{(1)}-\left(\Gamma_\rho^{(1)}\right)^2$$

$$\Gamma_\rho^{(1)}=\sum_{i=1}^\infty \tilde{\lambda}_i|F_i\rangle\langle F_i|$$

$$\{F_i\}_{i=1}^\infty\subseteq\mathfrak{h}\oplus\mathfrak{h}$$

$$F_i=f_i'\oplus\mathrm{j}f_i''\Gamma_\rho^{(1)}$$

$$\mathrm{J}\Gamma_\rho^{(1)}\mathrm{J}=1-\Gamma_\rho^{(1)}$$

$$\Gamma_\rho^{(1)}=\sum_{\ell=1}^\infty\{\lambda_\ell|F_\ell\rangle\langle F_\ell|+(1-\lambda_\ell)|\mathrm{J}F_\ell\rangle\langle\mathrm{J}F_\ell|\}$$

$$F_\ell = f'_\ell \oplus \mathfrak{j} f''_\ell \text{ and } \{F_\ell, \mathfrak{J} F_\ell\}_{\ell=1}^\infty \subseteq \mathfrak{h} \oplus \mathfrak{h}$$

$$\begin{aligned} \Gamma_\rho^{(1)} &= \gamma_\rho^{(1)} \oplus \left(1 - \mathfrak{j} \gamma_\rho^{(1)} \mathfrak{j}\right) \\ &= \sum_{\ell=1}^\infty \{ \lambda_\ell |f_\ell \oplus 0\rangle \langle f_\ell \oplus 0| + (1 - \lambda_\ell) |0 \oplus \mathfrak{j} f_\ell\rangle \langle 0 \oplus \mathfrak{j} f_\ell| \} \end{aligned}$$

$$\sum_{\ell=1}^\infty \lambda_\ell = \mathrm{Tr}_{\mathfrak{h}} \left[\gamma_\rho^{(1)} \right] < \infty$$

$$\begin{aligned} A(WF) &= A^*(\mathfrak{J}WF) = A^*(W\mathfrak{J}F) \text{ and} \\ \{A(WF), A^*(WG)\} &= \langle WF \mid WG \rangle_{\mathfrak{h} \oplus \mathfrak{h}} = \langle F \mid G \rangle_{\mathfrak{h} \oplus \mathfrak{h}}, \end{aligned}$$

$$\mathrm{Bog}_{\mathfrak{h} \oplus \mathfrak{h}} := \{W \in U(\mathfrak{h} \oplus \mathfrak{h}) \mid \mathfrak{J}W = W\mathfrak{J}\}$$

$$\mathrm{Bog}_{\mathfrak{h} \oplus \mathfrak{h}} = \left\{ \begin{pmatrix} u & \mathfrak{j} v \mathfrak{j} \\ v & \mathfrak{j} u \mathfrak{j} \end{pmatrix} \in U(\mathfrak{h} \oplus \mathfrak{h}) \mid \mathrm{Tr}_{\mathfrak{h}}[v^* v] < \infty \right\},$$

$$\mathbb{U}_W A^*(F) \mathbb{U}_W^* = A^*(WF)$$

$$\begin{aligned} \mathrm{Bog}_{\mathfrak{F}} &:= \\ \{ \mathbb{U} \in U(\mathfrak{F}) \mid \exists V \in \mathcal{B}(\mathfrak{h} \oplus \mathfrak{h}) \forall F \in \mathfrak{h} \oplus \mathfrak{h}: \mathbb{U} A^*(F) \mathbb{U}^* &= A^*(VF) \} \end{aligned}$$

$$d^*(f) \mathrel{\mathop:}= \mathbb{U}_W c^*(f) \mathbb{U}_W^*$$

$$\{F_\ell, \mathfrak{J} F_\ell\} \subseteq \mathfrak{h} \oplus \mathfrak{h}$$

$$W^* \Gamma_\rho^{(1)} W = \sum_{\ell=1}^\infty \{ \lambda_\ell |f_\ell \oplus 0\rangle \langle f_\ell \oplus 0| + (1 - \lambda_\ell) |0 \oplus \mathfrak{j} f_\ell\rangle \langle 0 \oplus \mathfrak{j} f_\ell| \}$$

$$\mathrm{Tr}_{\mathfrak{F}}[\rho A^*(WF)A(WG)] = \mathrm{Tr}_{\mathfrak{F}}[\mathbb{U}_W^* \rho \mathbb{U}_W A^*(F)A(G)]$$

$$\begin{aligned} \Gamma_{\mathbb{U}_W^* \rho \mathbb{U}_W}^{(1)} &= W^* \Gamma_\rho^{(1)} W \\ &= \sum_{\ell=1}^\infty \{ \lambda_\ell |f_\ell \oplus 0\rangle \langle f_\ell \oplus 0| + (1 - \lambda_\ell) |0 \oplus \mathfrak{j} f_\ell\rangle \langle 0 \oplus \mathfrak{j} f_\ell| \} \end{aligned}$$

$$\gamma_{\mathbb{U}_W^* \rho \mathbb{U}_W}^{(1)} = \sum_{\ell=1}^\infty \lambda_\ell |f_\ell\rangle \langle f_\ell|$$

$$W = \begin{pmatrix} u \mathfrak{j} v \mathfrak{j} \\ v \mathfrak{j} u \mathfrak{j} \end{pmatrix} \in \mathrm{Bog}_{\mathfrak{h} \oplus \mathfrak{h}}$$

$$\begin{aligned} 0 \leq \gamma_{\mathbb{U}_W^* \rho \mathbb{U}_W}^{(1)} &= u^* \gamma_\rho^{(1)} u + v^* \left(\mathbf{1} - \mathfrak{j} \gamma_\rho^{(1)} \mathfrak{j} \right) v + v^* \alpha_\rho u + u^* \alpha_\rho v \\ &\leq u^* \gamma_\rho^{(1)} u + v^* v + v^* \alpha_\rho u + u^* \alpha_\rho v, \end{aligned}$$

$$\left\| \gamma_{\mathbb{U}_W^* \rho \mathbb{U}_W}^{(1)} \right\|_{\mathcal{L}^1} \leq \left\| \gamma_\rho^{(1)} \right\|_{\mathcal{L}^1} + \|v\|_{\mathcal{L}^2}^2 + 2 \|v\|_{\mathcal{L}^2} \|\alpha_\rho\|_{\mathcal{L}^2} < \infty.$$

$$\mathfrak{G}^{(1)}\!:=\left\{\Gamma^{(1)}=\begin{pmatrix}\gamma^{(1)} & \alpha \\ \alpha^* & 1-\mathrm{j}\gamma^{(1)}\mathrm{j}\end{pmatrix}\in\mathcal{B}(\mathfrak{h}\oplus\mathfrak{h})\left|\right.\Gamma^{(1)}=\mathrm{J}(1-\Gamma^{(1)})\mathrm{J}\geq 0,\gamma^{(1)}\in\mathcal{L}^1(\mathfrak{h})\right\}$$

$$\mathfrak{g}^{(1)}\!:=\{\gamma^{(1)}\in\mathcal{L}^1(\mathfrak{h})\mid 0\leq\gamma^{(1)}\leq 1\}$$

$$W^*\Gamma^{(1)}W=\begin{pmatrix}\gamma & 0 \\ 0 & \mathbf{1}-\mathrm{j}\gamma\mathrm{j}\end{pmatrix}\text{ and }\gamma=\sum_{\ell=1}^{\infty}\lambda_{\ell}|f_{\ell}\rangle\langle f_{\ell}|$$

$$\mathbb{1}_0\!:=\sum_{\ell=K}^L\mu_{\ell}n_{\ell}, Z_0\!:=\mathrm{Tr}_{\mathfrak{F}}[e^{-\mathbb{h}_0}], \text{ and } \rho_0\!:=\mathbb{P}_1Z_0^{-1}\exp\left[-\mathbb{h}_0\right]$$

$$\Psi_{\underline{v}}\!:=\prod_{\ell=1}^{\infty}\left[c^*(f_{\ell})\right]^{v_{\ell}}\Omega$$

$$\underline{v}=(v_{\ell})_{\ell=1}^{\infty}\in\{0,1\}^{\mathbb{Z}^+}$$

$$A(\underline{v})\!:=\{\ell\in\mathbb{Z}^+\mid v_{\ell}=1\}\subseteq\mathbb{Z}^+$$

$$n_k\Psi_{\underline{v}}=v_k\Psi_{\underline{v}}$$

$$Z_0=\sum_{\underline{v}:|A(\underline{v})|<\infty}\langle\Psi_{\underline{v}}\mid e^{-\mathfrak{h}_0}\Psi_{\underline{v}}\rangle=\prod_{\ell=K}^L(1+e^{-\mu_{\ell}})<\infty,$$

$$\sum_{\ell=1}^{\infty}e^{-\mu_{\ell}}=\sum_{\ell=K}^L(1-\lambda_{\ell})^{-1}\lambda_{\ell}\leq(1-\lambda_K)^{-1}\sum_{\ell=1}^{\infty}\lambda_{\ell}<\infty$$

$$\left\langle f_{\ell}\mid \gamma_{\rho_0}^{(1)}f_k\right\rangle=\frac{\mathrm{Tr}_{\mathfrak{F}}\big[e^{-\mathfrak{h}_0}c^*(f_k)c(f_{\ell})\big]}{Z_0}=\frac{\delta_{k,\ell}e^{-\mu_k}}{1+e^{-\mu_k}}=\delta_{k,\ell}\lambda_k$$

$$\left\langle f_{\ell}\mid \gamma_{\rho_0}^{(1)}f_k\right\rangle=\delta_{k,\ell}=\delta_{k,\ell}\lambda_k$$

$$W^*\Gamma^{(1)}W=\Gamma_{\rho_0}^{(1)}$$

$$\Gamma^{(1)}=W\Gamma_{\rho_0}^{(1)}W^*=\Gamma_{\mathbb{U}_W\rho_0\mathbb{U}_W^*}^{(1)}$$

$$\mathbb{U}_W\rho_0\mathbb{U}_W^*\in\mathfrak{DM}$$

$$\mathfrak{DM}_{\mathbb{N}}\rightarrow\mathfrak{G}^{(1)},\rho\mapsto\Gamma_{\rho}^{(1)}$$

$$\mathfrak{DM}^{(N)}\rightarrow\{\gamma\in\mathfrak{g}^{(1)}\mid\mathrm{Tr}[\gamma]=N\},\rho\mapsto\gamma_{\rho}^{(1)}$$

$$(\Gamma^{(1)},\Gamma^{(2)})\in\mathcal{B}(\mathfrak{h}^2)\times\mathcal{B}(\mathfrak{h}^2\otimes\mathfrak{h}^2)$$

$$\rho\in\mathfrak{DM}_{\langle\mathbb{N}^2\rangle<\infty}$$



$$\mathfrak{h}^2:=\mathfrak{h}\oplus\mathfrak{h}$$

$$\begin{array}{l} E_{\mathrm{gs}}=\inf\{\mathcal{E}_Q(\gamma^{(1)},\gamma^{(2)})\mid (h\gamma^{(1)})\in\mathcal{L}^1(\mathfrak{h}),\\ \qquad (\gamma^{(1)},\gamma^{(2)})\in\mathcal{B}(\mathfrak{h})\times\mathcal{B}(\mathfrak{h}\otimes\mathfrak{h})\,\mathfrak{R}\},\\ E_{\mathrm{gs}}(N)=\inf\{\mathcal{E}_Q(\gamma^{(1)},\gamma^{(2)})\mid (h\gamma^{(1)})\in\mathcal{L}^1(\mathfrak{h}),\\ \qquad (\gamma^{(1)},\gamma^{(2)})\in\mathcal{B}(\mathfrak{h})\times\mathcal{B}(\mathfrak{h}\otimes\mathfrak{h})\,\mathfrak{G}\}. \end{array}$$

$$(\Gamma^{(1)},\Gamma^{(2)})\in\mathcal{B}(\mathfrak{h}^2)\times\mathcal{B}(\mathfrak{h}^2\otimes\mathfrak{h}^2)$$

$$A\colon \mathcal{L}^1(\mathfrak{h})\times \mathcal{L}^1(\mathfrak{h}\otimes \mathfrak{h})\rightarrow A(\gamma^{(1)},\gamma^{(2)})=B\colon \mathcal{L}^1(\mathfrak{h})\times \mathcal{L}^1(\mathfrak{h}\otimes \mathfrak{h})\rightarrow B\left(\gamma^{(1)}_\rho,\gamma^{(2)}_\rho\right)=\rho\in \mathfrak{DM}$$

$$\begin{array}{l} E_{\mathrm{gs}}\geq \inf\{\mathcal{E}_Q(\gamma^{(1)},\gamma^{(2)})\mid\\ (h\gamma^{(1)})\in\mathcal{L}^1(\mathfrak{h}),B(\gamma^{(1)},\gamma^{(2)})=\text{ true }\},\\ E_{\mathrm{gs}}(N)\geq \inf\{\mathcal{E}_Q(\gamma^{(1)},\gamma^{(2)})\mid\\ (h\gamma^{(1)})\in\mathcal{L}^1(\mathfrak{h}),\mathrm{Tr}[\gamma^{(1)}]=N,B(\gamma^{(1)},\gamma^{(2)})=\text{ true }\}. \end{array}$$

$$\begin{array}{l} E_{\mathrm{GPQ}}(N)\!:=\!\inf\{\mathcal{E}_Q(\gamma^{(1)},\gamma^{(2)})\mid (h\gamma^{(1)})\in\mathcal{L}^1(\mathfrak{h})\\ \mathrm{Tr}[\gamma^{(1)}]=N, (\gamma^{(1)},\gamma^{(2)}) \text{ fulfills GPQ}\} \end{array}$$

$$\rho=\rho^*\in\mathcal{L}^1(\mathfrak{F})$$

$$\mathrm{Tr}_{\mathfrak{F}}(|\rho|^{1/2}\mathbb{N}^2|\rho|^{1/2})<\infty$$

$$\begin{array}{l} \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}[(P\otimes P)\gamma^{(2)}]\geq \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}[(P\otimes P)(1-\mathrm{Ex})(\gamma^{(1)}\otimes\gamma^{(1)})] \\ \qquad -\mathrm{Tr}_{\mathfrak{h}}[P\gamma^{(1)}]\min\Big\{1,9\mathrm{Tr}_{\mathfrak{h}}\Big[P\Big(\gamma^{(1)}-(\gamma^{(1)})^2\Big)^{1/2}\Big]\Big\}, \end{array}$$

$$0\leq E_{\mathrm{HF}}(Z)-E_{\mathrm{gs}}(N)\leq E_{\mathrm{HF}}(Z)-E_{\mathrm{GPQ}}(N)\leq o\big(Z^{(5/3)}\big)$$

$$\begin{array}{l} E_{\mathrm{GPQ:T}}(N)\!:=\!\inf\{\mathcal{E}_Q(\gamma^{(1)},\gamma^{(2)})\mid (h\gamma^{(1)})\in\mathcal{L}^1(\mathfrak{h}),\\ \mathrm{Tr}[\gamma^{(1)}]=N, (\gamma^{(1)},\gamma^{(2)}) \text{ fulfills GPQ and } T_{1;2}\} \end{array}$$

$$\forall F\in\mathfrak{h}\oplus\mathfrak{h}\colon \mathbb{U}_WA^*(F)\mathbb{U}_W^*=A^*(WF),$$

$$\mathrm{Bog}_{\mathfrak{h}\oplus\mathfrak{h}}\ni W\mapsto \mathbb{U}_W\in \mathrm{Bog}_{\mathfrak{F}}$$

$$\mathbb{Q}(T)\in\mathcal{B}(\mathcal{D}(N);\mathfrak{F}_f)$$

$$T=T^*=\begin{pmatrix} a & b \\ b^* & 0 \end{pmatrix}\in\mathcal{B}[\mathfrak{h}\oplus\mathfrak{h}]$$

$$\mathbb{Q}(T)\!:=\!\sum_{i,j=1}^{\infty}\left\langle F_i\mid TF_j\right\rangle A^*(F_i)A(F_j)$$

$$\{F_i\}_{i=1}^\infty\subseteq\mathfrak{h}\oplus\mathfrak{h}$$

$$[\mathbb{Q}(T),A^*(F)]=A^*(\hat{T}F)$$



$$e^{i\mathbb{Q}(T)}A^*(F)e^{-i\mathbb{Q}(T)}=A^*(e^{i\hat{T}}F)$$

$$\hat{T}=-\mathsf{J}\hat{T}\mathsf{J}:=\begin{pmatrix}a&2b\\2b^*&-a\end{pmatrix}\in\mathcal{B}[\mathfrak{h}\oplus\mathfrak{h}]$$

$$A_t^*(\tilde{F}):=e^{it\mathbb{Q}(T)}A^*(e^{-it\hat{T}}\tilde{F})e^{-it\mathbb{Q}(T)}$$

$$e^{i\mathbb{Q}(T)}A^*(e^{-i\hat{T}}\tilde{F})e^{-i\mathbb{Q}(T)}=A_1^*(\tilde{F})=A_0^*(\tilde{F})=A^*(\tilde{F})$$

$$\frac{1}{2}\mathbb{Q}(\hat{T})=\mathbb{Q}(T)+\frac{1}{2}\mathrm{Tr}[a]$$

$$[i\hat{T}]\mathsf{J}=-i\,\mathsf{J}T=\mathsf{J}[i\hat{T}]$$

$$\exp\left[i\mathbb{Q}(T)\right]=\mathbb{U}_{\exp\left[-i\hat{T}\right]}$$

$$\mathrm{Bog}_{\mathfrak{F}}=\overline{\left\{\exp\left[i\mathbb{Q}(T)\right]\,\middle|\,T=\begin{pmatrix}a&b\\b^*&0\end{pmatrix},a\in\mathcal{B}(\mathfrak{h}),a\geq0,b\in\mathcal{L}^2(\mathfrak{h})\right\}},$$

$$\rho_0=\mathbb{P}_1Z_0^{-1}\exp\left[-\mathfrak{h}_0\right]\in\mathfrak{DM}$$

$$\mathbb{1}_0=\sum_{\ell=K}^L\mu_\ell c^*(f_\ell)c(f_\ell)=\mathbb{Q}(H_0)$$

$$H_0\!:=\!\begin{pmatrix}h_0&0\\0&0\end{pmatrix}\text{ and }h_0\!:=\!\sum_{\ell=K}^L\mu_\ell|f_\ell\rangle\langle f_\ell|.$$

$$\rho_\varepsilon\in\mathfrak{QDM}\rightarrow\rho_0\mathfrak{DM}_{\mathbb{N}}$$

$$\tau_\ell(\varepsilon)\!:=\!\begin{cases}1-\varepsilon/K,&\ell<K\\ \mu_\ell,&K\leq\ell\leq L\\ \varepsilon e^{-\ell^2},&\ell>L\end{cases}$$

$$h_\varepsilon\!:=\!\sum_{\ell=1}^\infty\tau_\ell(\varepsilon)|f_\ell\rangle\langle f_\ell|$$

$$Z_\varepsilon:=\mathrm{Tr}_{\mathfrak{F}}(\exp\left[-\mathbb{Q}(H_\varepsilon)\right])$$

$$\rho_\varepsilon\!:=\!Z_\varepsilon^{-1}\exp\left[-\mathbb{Q}(H_\varepsilon)\right]$$

$$T_\varepsilon=\begin{pmatrix}a_\varepsilon b_\varepsilon\\b_\varepsilon^*\\0\end{pmatrix},a_\varepsilon\in\mathcal{B}(\mathfrak{h}),a_\varepsilon\geq0,b_\varepsilon\in\mathcal{L}^2(\mathfrak{h}),\mathbb{U}_W\Psi=\lim_{\varepsilon\rightarrow0}\exp\left[i\mathbb{Q}(T_\varepsilon)\right]\Psi\in\mathfrak{FDM}_{\mathbb{N}}$$

$$\tilde{\rho}_\varepsilon\!:=\!\exp\left[i\mathbb{Q}(T_\varepsilon)\right]\rho_\varepsilon\exp\left[-i\mathbb{Q}(T_\varepsilon)\right]\rightarrow\tilde{\rho}_0\;\varepsilon\rightarrow0$$

$$\tilde{\rho}_\varepsilon=Z^{-1}\exp\left[-\mathbb{Q}(\tilde{H}_\varepsilon)\right],\text{ where }\tilde{H}_\varepsilon=e^{-i\hat{T}}H_\varepsilon e^{i\hat{T}}$$



$$\mathfrak{QDM}:=\overline{\{Z^{-1}\exp\left[-\mathbb{Q}(H_0)\right]\mid H_0\in\mathrm{qh},Z:=\exp\left[-\mathbb{Q}(H_0)\right]<\infty\}},$$

$$\mathrm{qh}:=\left\{\left(\begin{smallmatrix}a&b\\b^*&0\end{smallmatrix}\right)\middle| \, a=a^*\geq 0, e^{-a}\in\mathcal{L}^1(\mathfrak{h}), b\in\mathcal{L}^2(\mathfrak{h})\right\},$$

$$\rho=\left|\Phi_{\underline{f}}\right\rangle\!\!\left\langle\Phi_{\underline{f}}\right|$$

$$\Phi_{\underline{f}}=f_1\wedge\cdots\wedge f_N$$

$$W=\begin{pmatrix}P^\perp&\mathfrak{j}P\mathfrak{j}\\P&\mathfrak{j}P^\perp\end{pmatrix}$$

$$P=\sum_{n=1}^N|f_n\rangle\langle f_n|$$

$$\rho=|\mathbb{U}_W\Omega\rangle\langle\mathbb{U}_W\Omega|$$

$$W\in\mathrm{Bog}_{\mathfrak{h}\oplus\mathfrak{h}}\exp\left[-i\mathbb{Q}(T)\right]$$

$$q\colon \mathfrak{DM}\rightarrow \mathfrak{QDM}, \rho\mapsto q(\rho)=\eta.$$

$$q(\rho)=\eta\in\mathfrak{QDM}$$

$$\langle M\rangle:=\mathrm{Tr}_{\mathfrak{F}}[\rho M]$$

$$M\in\mathcal{B}(\mathfrak{F})$$

$$\langle A_1A_2\cdots A_{2k}\rangle=\sum_{\pi\in\mathcal{P}_{2k}}(-1)^\pi\langle A_{\pi(1)}A_{\pi(2)}\rangle\langle A_{\pi(3)}A_{\pi(4)}\rangle\cdots\langle A_{\pi(2k-1)}A_{\pi(2k)}\rangle,$$

$$\langle A_1A_2A_3A_4\rangle=\langle A_1A_2\rangle\langle A_3A_4\rangle-\langle A_1A_3\rangle\langle A_2A_4\rangle+\langle A_1A_4\rangle\langle A_2A_3\rangle,$$

$$S[\rho,q(\rho)]:=\mathrm{Tr}_{\mathfrak{F}}\{\rho(\log\left[\rho\right]-\log\left[q(\rho)\right])\}<\infty$$

$$S[\rho,q(\rho)]=\inf_{\eta\in\mathfrak{QDM}}\{S[\rho,\eta]\}$$

$$S[\rho]:=-\mathrm{Tr}_{\mathfrak{F}}\{\rho\log\left[\rho\right]\},S[\eta]$$

$$-\log\left[q(\rho)\right]=\mathbb{Q}+\log\left(Z\right)$$

$$\begin{aligned} S[\rho,\eta]&=S[\rho]+\mathrm{Tr}_{\mathfrak{F}}\{\rho(-\log\left[\eta\right])\}=\log\left(Z\right)+S[\rho]+\mathrm{Tr}_{\mathfrak{F}}\{\rho\mathbb{Q}\}\\ &=\log\left(Z\right)+S[\rho]+\mathrm{Tr}_{\mathfrak{F}}\{q[\rho]\mathbb{Q}\}=S[\rho]-\mathrm{Tr}_{\mathfrak{F}}\{q[\rho]\log\left[\eta\right]\} \end{aligned}$$

$$S[\rho,\eta]-S[\rho,q(\rho)]=\mathrm{Tr}_{\mathfrak{F}}\{q(\rho)(\log\left[q(\rho)\right]-\log\left[\eta\right])\}=S[q(\rho),\eta]\geq 0,$$

$$S[\rho]:=-\mathrm{Tr}_{\mathfrak{F}}\{\rho\log\left[\rho\right]\}\text{ of }\rho\text{ and }q[\rho]$$

$$S[\rho]=-\mathrm{Tr}_{\mathfrak{F}}\{\rho\log\left[\rho\right]\}=S^{(1)}\left[\Gamma_{\rho}^{(1)}\right]:=-\mathrm{Tr}_{\mathfrak{h}\oplus\mathfrak{h}}\left\{\Gamma_{\rho}^{(1)}\log\left[\Gamma_{\rho}^{(1)}\right]\right\}.$$

$$\rho_0=\mathbb{P}_1Z_0^{-1}\exp\left[-\mathfrak{h}_0\right]$$



$$E_{\text{BHF}}:=\inf\{\text{Tr}_{\mathfrak{F}}(\rho\mathbb{H}_{\mu})\mid\rho\in\mathfrak{QDM},\langle\mathbb{H}\rangle_{\rho}<\infty\}$$

$$\text{Tr}_{\mathfrak{F}}(\rho\mathbb{H}_{\mu})=\mathcal{E}_{\text{BHF}}\left(\Gamma_{\rho}^{(1)}\right)$$

$$\Gamma_{\rho}^{(1)}=\begin{pmatrix}\gamma_{\rho}^{(1)} & \alpha_{\rho} \\ \alpha_{\rho}^* & 1-\mathrm{j}\gamma_{\rho}^{(1)}\mathrm{j}\end{pmatrix}\in\mathfrak{G}^{(1)}$$

$$\begin{aligned}\mathcal{E}_{\text{BHF}}\left(\Gamma_{\rho}^{(1)}\right):=&\text{Tr}_{\mathfrak{h}}\left[h_{\mu}\gamma_{\rho}^{(1)}\right]+\frac{1}{2}\text{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left[V(1-\text{Ex})\left(\gamma_{\rho}^{(1)}\otimes\gamma_{\rho}^{(1)}\right)\right] \\ &+\frac{1}{2}\text{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\left[V\text{Ex}(\alpha_{\rho}^*\otimes\alpha_{\rho})\right],\end{aligned}$$

$$\mathfrak{QDM}\ni\rho\mapsto\Gamma_{\rho}^{(1)}\in\mathfrak{G}^{(1)}$$

$$E_{\text{BHF}}=\inf\{\mathcal{E}_{\text{BHF}}(\Gamma^{(1)})\mid\Gamma^{(1)}\in\mathfrak{G}^{(1)}\}.$$

$$\Gamma_{\text{BHF}}^{(1)}=\mathbf{1}_{\text{neg}}\left(h_{\text{BHF}}\left[\Gamma_{\text{BHF}}^{(1)}\right]\right),$$

$$\mathbf{1}_{\text{neg}}\left(h_{\text{BHF}}\left[\Gamma_{\text{BHF}}^{(1)}\right]\right)h_{\text{BHF}}\left[\Gamma_{\text{BHF}}^{(1)}\right]\mathbf{1}\left(h_{\text{BHF}}\left[\Gamma_{\text{BHF}}^{(1)}\right]<0\right)\leq\mathbf{1}_{\text{neg}}\left(h_{\text{BHF}}\left[\Gamma_{\text{BHF}}^{(1)}\right]\right)\leq\mathbf{1}\left(h_{\text{BHF}}\left[\Gamma_{\text{BHF}}^{(1)}\right]\leq0\right)$$

$$\mathbf{1}-\Gamma_{\text{BHF}}^{(1)}=\text{J}\Gamma_{\text{BHF}}^{(1)}\text{J}\Gamma_{\text{BHF}}^{(1)}\mathbf{1}_{\text{neg}}\left(h_{\text{BHF}}\left[\Gamma_{\text{BHF}}^{(1)}\right]\right)\left(\Gamma_{\beta}^{(1)}\right)_{\beta\in\mathbb{R}^+}$$

$$\Gamma_{\beta}^{(1)}=F_{\beta}\left(h_{\beta}\left[\Gamma_{\beta}^{(1)}\right]\right),$$

$$F_{\beta}(x)=\left(1+e^{\beta x}\right)^{-1}$$

$$-\mathcal{P}_{\beta}(\Gamma^{(1)}):=\mathcal{E}_{\text{BHF}}(\Gamma^{(1)})-\beta^{-1}S^{(1)}(\Gamma^{(1)}).$$

$$\mathcal{P}_{\beta}(\Gamma^{(1)})\leq\beta^{-1}\log\left[\text{Tr}_{\mathfrak{F}}\{\exp\left[-\beta\mathbb{H}_{\mu}\right]\}_{\mathfrak{j}}\right],$$

$$\text{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}[V\text{Ex}(\alpha_{\rho}^*\otimes\alpha_{\rho})]=\int\;V(x,y)|\alpha_{\rho}(x,y)|^2\,d\nu(x)d\nu(y)\geq0$$

$$\Gamma^{(1)}=\begin{pmatrix}\gamma^{(1)} & \alpha \\ \alpha^* & 1-\mathrm{j}\gamma^{(1)}\mathrm{j}\end{pmatrix}\in\mathfrak{G}^{(1)}$$

$$\tilde{\Gamma}^{(1)}:=\begin{pmatrix}\mathbf{1} & 0 \\ 0 & -\mathbf{1}\end{pmatrix}\Gamma^{(1)}\begin{pmatrix}\mathbf{1} & 0 \\ 0 & -\mathbf{1}\end{pmatrix}=\begin{pmatrix}\gamma^{(1)} & -\alpha \\ -\alpha^* & \mathbf{1}-\mathrm{j}\gamma^{(1)}\mathrm{j}\end{pmatrix}\in\mathfrak{G}^{(1)}$$

$$\hat{\Gamma}^{(1)}=\frac{1}{2}(\Gamma^{(1)}+\tilde{\Gamma}^{(1)})=\begin{pmatrix}\gamma^{(1)} & 0 \\ 0 & 1-\mathrm{j}\gamma^{(1)}\mathrm{j}\end{pmatrix}\in\mathfrak{G}^{(1)}$$

$$\begin{aligned}\mathcal{E}_{\text{BHF}}(\hat{\Gamma}^{(1)})=&\text{Tr}_{\mathfrak{h}}[h_{\mu}\gamma^{(1)}]+\frac{1}{2}\text{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}[V(1-\text{Ex})(\gamma^{(1)}\otimes\gamma^{(1)})] \\ &\leq\mathcal{E}_{\text{BHF}}(\Gamma^{(1)})\end{aligned}$$

$$E_{\text{BHF}}=E_{\text{HF}}=\inf\{\mathcal{E}_{\text{HF}}(\gamma)\mid\gamma\in\mathcal{L}^1(\mathfrak{h}),0\leq\gamma\leq\mathbf{1}\},$$



$$E_{\mathrm{HF}}\!:=\inf_{N\in\mathbb{Z}^+}\{E_{\mathrm{HF}}(N)\}$$

$$\Gamma^{(1)}=\begin{pmatrix} \gamma^{(1)} & \alpha \\ \alpha^* & 1-\mathrm{j}\gamma^{(1)}\mathrm{j} \end{pmatrix}\in\mathfrak{G}^{(1)}$$

$$\mathfrak{h}=\hat{\mathfrak{h}}\otimes\mathbb{C}^2\text{ with }\hat{\mathfrak{h}}=L^2(M,d\nu)$$

$$h=\hat{h}\otimes 1\text{ and }V=(-\hat{V})\otimes (1\otimes 1)$$

$$(\mathfrak{j}\otimes \mathfrak{j})\hat{V}=\hat{V}(\mathfrak{j}\otimes \mathfrak{j})$$

$$\Gamma^{(1)}\equiv\Gamma^{(1)}[\hat{\gamma}]\!:=\begin{pmatrix} \hat{\gamma} & 0 & 0 & \sqrt{\hat{\gamma}-\hat{\gamma}^2} \\ 0 & \hat{\gamma} & -\sqrt{\hat{\gamma}-\hat{\gamma}^2} & 0 \\ 0 & -\sqrt{\hat{\gamma}-\hat{\gamma}^2} & \mathbf{1}-\hat{\gamma} & 0 \\ \sqrt{\hat{\gamma}-\hat{\gamma}^2} & 0 & 0 & \mathbf{1}-\hat{\gamma} \end{pmatrix},$$

$$\mathcal{E}_{\mathrm{aux}}(\hat{\gamma})\!:=\frac{1}{2}\mathcal{E}_{\mathrm{BHF}}(\Gamma^{(1)}[\hat{\gamma}])=\mathrm{Tr}_{\hat{h}}[\hat{h}\hat{\gamma}]\\ -\frac{1}{2}\iint\hat{V}(x,y)\Big\{\rho_{\hat{\gamma}}(x)\rho_{\hat{\gamma}}(y)-|\hat{\gamma}(x,y)|^2+\Big|\sqrt{\hat{\gamma}-\hat{\gamma}^2}(x,y)\Big|^2\Big\}d\nu(x)d\nu(y)$$

$$\alpha=\sqrt{\hat{\gamma}-\hat{\gamma}^2}\otimes\begin{pmatrix}0&1\\-1&0\end{pmatrix}$$

$$\left|\Phi\left(\underline{g}^{(\theta)}\right)\right\rangle\left\langle\Phi\left(\underline{g}^{(\theta)}\right)\right|\left\langle\Phi\left(\underline{g}^{(\theta)}\right)\right|\mathbb{H}\Phi\left(\underline{g}^{(\theta)}\right)\Big\rangle\mathrm{Tr}_{\mathfrak{F}}[\rho_{\mathrm{av}}\mathbb{H}]\rho_{\mathrm{av}}$$

$$\hat{E}_{\mathrm{BHF}}\!:=\inf\{\langle\Omega\mid\mathbb{U}^*\mathbb{H}_\mu\mathbb{U}\Omega\rangle\mid\mathbb{U}\in\mathrm{Bog}_{\widetilde{\mathfrak{F}}}\}.$$

$$\mathrm{Tr}_{\mathfrak{F}}[\rho_{\mathrm{BHF}}\mathbb{H}_\mu]=E_{\mathrm{BHF}}$$

$$E_{\mathrm{BHF}}=\langle\Omega\mid\mathbb{U}^*\mathbb{H}_\mu\mathbb{U}\Omega\rangle$$

$$\rho_{\mathrm{BHF}}\in\mathfrak{QDM}\cap\mathfrak{DM}_{\mathbb{N}}$$

$$\mathrm{Tr}_{\mathfrak{F}}[\rho_{\mathrm{BHF}}\mathbb{H}_\mu]=E_{\mathrm{BHF}}$$

$$\langle \mathbb{N} \rangle_{\rho_{\mathrm{BHF}}} \rho_{\mathrm{BHF}} = \widetilde{\mathbb{U}}^* \rho_0 \widetilde{\mathbb{U}}$$

$$\rho_0=\mathbb{P}_1Z^{-1}\exp\left[-\mathbb{Q}(H_0)\right]$$

$$\mathbb{Q}(H_0)=\sum_{\ell=K}^L\mu_\ell c^*(f_\ell)c(f_\ell)$$

$$\widetilde{\mathbb{H}}\!:=\mathbb{H}_\mu-E_{\mathrm{gs}}\geq 0$$

$$\tilde{E}_{\mathrm{BHF}}\!:=E_{\mathrm{BHF}}-E_{\mathrm{gs}}\geq 0$$

$$\tilde{E}_{\mathrm{BHF}}=\mathrm{Tr}_{\mathfrak{F}}[\rho_{\mathrm{BHF}}\widetilde{\mathbb{H}}]=\mathrm{Tr}_{\mathfrak{F}}\left[\rho_{\mathrm{BHF}}^{1/2}\widetilde{\mathbb{H}}\rho_{\mathrm{BHF}}^{1/2}\right]$$

$$\begin{aligned}\tilde{E}_{\text{BHF}} &= \text{Tr}_{\mathfrak{F}} \left[\rho_{\text{BHF}}^{1/2} \tilde{\mathbb{H}} \rho_{\text{BHF}}^{1/2} \right] = \sum_{\underline{\nu}: |A(\underline{\nu})| < \infty} \left\langle \rho_{\text{BHF}}^{1/2} \tilde{\mathbb{U}}^* \Psi_{\underline{\nu}} \mid \tilde{\mathbb{H}} \rho_{\text{BHF}}^{1/2} \tilde{\mathbb{U}}^* \Psi_{\underline{\nu}} \right\rangle \\ &= \sum_{\underline{\nu}: |A(\underline{\nu})| < \infty} \left\langle \rho_0^{1/2} \Psi_{\underline{\nu}} \mid \tilde{\mathbb{U}}^* \tilde{\mathbb{H}} \tilde{\mathbb{U}} \rho_0^{1/2} \Psi_{\underline{\nu}} \right\rangle = \sum_{\underline{\nu} \in \mathcal{A}} \left\langle \rho_0^{1/2} \Psi_{\underline{\nu}} \mid \tilde{\mathbb{U}}^* \tilde{\mathbb{H}} \tilde{\mathbb{U}} \rho_0^{1/2} \Psi_{\underline{\nu}} \right\rangle,\end{aligned}$$

$$\{\Psi_{\underline{\nu}} | \underline{\nu} \in \{0,1\}^{\mathbb{Z}^+}, |A(\underline{\nu})| < \infty\} \subseteq \mathfrak{F}$$

$$\mathcal{A} \!:=\! \left\{ \underline{\nu} \in \{0,1\}^{\mathbb{Z}^+} \, | \, |A(\underline{\nu})| < \infty, \rho_0^{1/2} \Psi_{\underline{\nu}} \neq 0 \right\}$$

$$\begin{aligned}\rho_0^{1/2}\Psi_{\underline{\nu}} &= c_1^* \cdots c_{K-1}^* \prod_{\ell \in A(\underline{\nu}) \cap \{K, \dots, L\}} \left(\sqrt{\lambda_\ell (1-\lambda_\ell)^{-1}} c_\ell^* \right) \Omega \\ &= \left\| \rho_0^{1/2} \Psi_{\underline{\nu}} \right\| \prod_{\ell \in A(\underline{\nu}) \cap \{1, \dots, L\}} c_\ell^* \Omega\end{aligned}$$

$$\mathcal{A}\!:=\!\left\{\underline{\nu}\in\{0,1\}^{\mathbb{Z}^+}\,|\,|A(\underline{\nu})|<\infty, A(\underline{\nu})\subseteq\{1,\dots,L\}\right\}$$

$$\tilde{E}_{\text{BHF}} = \sum_{\underline{\nu} \in \mathcal{A}} \left\| \rho_0^{1/2} \Psi_{\underline{\nu}} \right\|^2 \langle \tilde{\mathbb{U}} \Psi_{\underline{\nu}} \mid \tilde{\mathbb{H}} \tilde{\mathbb{U}} \Psi_{\underline{\nu}} \rangle$$

$$|\tilde{\mathbb{U}}\Psi_{\underline{\nu}}\rangle\langle\tilde{\mathbb{U}}\Psi_{\underline{\nu}}|\in\mathfrak{QDM}$$

$$\langle \tilde{\mathbb{U}} \Psi_{\underline{\nu}} \mid \tilde{\mathbb{H}} \tilde{\mathbb{U}} \Psi_{\underline{\nu}} \rangle \geq \tilde{E}_{\text{BHF}}$$

$$\left\|\rho_0^{1/2}\Psi_{\underline{\nu}}\right\|^2>0$$

$$\sum_{\underline{\nu} \in \mathcal{A}} \left\| \rho_0^{1/2} \Psi_{\underline{\nu}} \right\|^2 = \text{Tr}_{\mathfrak{F}}[\rho_0]$$

$$\forall \underline{\nu} \in \mathcal{A}: \langle \tilde{\mathbb{U}} \Psi_{\underline{\nu}} \mid \tilde{\mathbb{H}} \tilde{\mathbb{U}} \Psi_{\underline{\nu}} \rangle = \tilde{E}_{\text{BHF}}$$

$$\mathbb{H}=\mathbb{h}+\frac{1}{2}\mathbb{V}$$

$$\mathbb{H}_\mu\colon\Leftrightarrow\,\forall U\in\mathcal{S}\colon U\big(\mathbb{H}_\mu+E_0\big)^{-1}=\big(\mathbb{H}_\mu+E_0\big)^{-1}U.$$

$$E_{\text{BHF}}(\mathcal{S})\!:=\!\inf\{\text{Tr}_{\mathfrak{F}}(\rho\mathbb{H}_{\mu})\mid\rho\in\mathfrak{QDM},\langle\mathbb{H}\rangle_{\rho}<\infty,\forall U\in\mathcal{S}\colon U\rho=\rho U\}.$$

$$e_{N+1}\!:=\!\inf\{\sigma(h_{\text{HF}}[\gamma_{\text{HF}}])\setminus\{e_1,e_2,\ldots,e_N\}\}>e_N$$

$$\Lambda\!:=\!(\mathbb{R}/L\mathbb{Z})^3$$

$$U_{\vec{a}} = \exp\left[-i\vec{a}\cdot\vec{\mathbb{p}}\right]$$

$$\mathcal{T}_{\Lambda}\!:=\!\{U_{\vec{a}}\mid \vec{a}\in\Lambda\}$$

$$e_{\text{gs}}\!:=\!\lim_{L\rightarrow\infty}\{L^{-3}E_{\text{gs}}\}$$

$$e_{\mathrm{BHF}}:=\lim_{L\rightarrow\infty}\{L^{-3}E_{\mathrm{BHF}}\}e_{\mathrm{BHF}}(\mathcal{T}_\Lambda)\!:=\lim_{L\rightarrow\infty}\{L^{-3}E_{\mathrm{BHF}}(\mathcal{T}_\Lambda)\}$$

$$\Gamma^{(1)}(k,k')=\delta_{k,k'}\begin{pmatrix} \hat{\gamma}(k)\otimes\begin{pmatrix}1&0\\0&1\end{pmatrix} & \hat{\alpha}(k)\otimes\begin{pmatrix}0&1\\-1&0\end{pmatrix} \\ \hat{\alpha}(k)^*\otimes\begin{pmatrix}0&1\\-1&0\end{pmatrix} & [\mathbf{1}-\hat{\gamma}(k)]\otimes\begin{pmatrix}1&0\\0&1\end{pmatrix}\end{pmatrix},$$

$$\hat{\gamma}\in L^1(\Lambda^*;\overline{\mathbb{R}^+_0})$$

$$\Lambda^*=\frac{2\pi}{L}\mathbb{Z}^3$$

$$\begin{aligned}\mathcal{E}_{\text{BCS}}(\Gamma^{(1)})&= \sum_{k\in\Lambda^*}(\omega(k)-\mu)\hat{\gamma}(k)+\frac{1}{2}\|\hat{\mathcal{V}}\|_1\|\hat{\gamma}\|_1^2\\ &\quad -\frac{1}{2}\int_{\Lambda}V(x)|\gamma(x)|^2d^3x+\frac{1}{2}\int_{\Lambda}V(x)|\alpha(x)|^2d^3x\end{aligned}$$

$$\mathfrak{h}=\ell^2(\Lambda)\otimes\mathbb{C}^2$$

$$\Lambda\colon=(\mathbb{Z}/L\mathbb{Z})^d$$

$$T=t\otimes \mathbb{1}$$

$$\vec{v}_{\mathrm{HF}}(x)\!:=\mathrm{Tr}_{\mathbb{C}^2}[\gamma_{\mathrm{HF}}(x,x)\vec{\sigma}]=(-1)^x\Delta\vec{e}$$

$$\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_z)\in\mathbb{C}^{2\times 2}$$

$$S_z=\sum_{x\in\Lambda}\sigma_z$$

$$\vec{v}_{\mathrm{HF}}(x)=\pm\eta\vec{e}_3$$

$$\Lambda_L\colon=(\mathbb{R}/L\mathbb{Z})^3$$

$$\mathbb{Z}_L^3=(\mathbb{Z}/L\mathbb{Z})^3\subset\Lambda$$

$$\mathbb{H}=\mathbb{h}+\frac{1}{2}\mathbb{V}$$

$$H=H_0+U\sum_{\mathbf{x}}\left(n_{\mathbf{x},\uparrow}-\frac{1}{2}\right)\left(n_{\mathbf{x},\downarrow}-\frac{1}{2}\right),$$

$$H_0=\sum_{\mathbf{x},\mathbf{y}}\sum_{\sigma=\uparrow,\downarrow}t_{\mathbf{x},\mathbf{y}}c_{\mathbf{x},\sigma}^\dagger c_{\mathbf{y},\sigma}-\mu\sum_{\mathbf{x}}(n_{\mathbf{x}}-1)$$

$$n_{\mathbf{x},\sigma}=c_{\mathbf{x},\sigma}^\dagger c_{\mathbf{x},\sigma}$$

$$n_{\mathbf{x}}=n_{\mathbf{x},\uparrow}+n_{\mathbf{x},\downarrow}$$

$$\varepsilon_0(\mathbf{k}) = -2t \sum_{i=1}^n \cos(k_i)$$

$$\varepsilon_1(\mathbf{k}) = -4t' \sum_{1 \leq i < j \leq n} \cos(k_i) \cos(k_j),$$

$$\varepsilon_2(\mathbf{k}) = -4t' \delta \sum_{1 \leq i < j \leq n} \sin(k_i) \sin(k_j)$$

$$H_0 = \sum_{\mathbf{k}, \sigma} \left([\varepsilon(\mathbf{k}) - \mu] \left[c_{\sigma}^{\dagger}(\mathbf{k}) c_{\sigma}(\mathbf{k}) - \frac{1}{2} \right] \right. \\ \left. + \varepsilon_2(\mathbf{k}) c_{\sigma}^{\dagger}(\mathbf{k}) c_{\sigma}(\mathbf{k} + \mathbf{Q}) \right)$$

$$\varepsilon(\mathbf{k}) = \varepsilon_0(\mathbf{k}) + \varepsilon_1(\mathbf{k})$$

$$c_{\sigma}^{\dagger}(\mathbf{k})c_{\sigma}(\mathbf{k})-\frac{1}{2}$$

$$c_{\sigma}^{\dagger}(\mathbf{k})c_{\sigma}(\mathbf{k})$$

$$(t,t',\delta,U,\mu,\nu)\rightarrow (t,-t',\delta,U,-\mu,-\nu)$$

$$\vec{s}_{\mathbf{x}} = (s_{\mathbf{x}}^x, s_{\mathbf{x}}^y, s_{\mathbf{x}}^z)$$

$$s_{\mathbf{x}}^x = c_{\mathbf{x},\uparrow}^{\dagger}c_{\mathbf{x},\downarrow} + c_{\mathbf{x},\downarrow}^{\dagger}c_{\mathbf{x},\uparrow} \\ s_{\mathbf{x}}^y = -\mathrm{i}c_{\mathbf{x},\uparrow}^{\dagger}c_{\mathbf{x},\downarrow} + \mathrm{i}c_{\mathbf{x},\downarrow}^{\dagger}c_{\mathbf{x},\uparrow} \\ s_{\mathbf{x}}^z = n_{\mathbf{x},\uparrow} - n_{\mathbf{x},\downarrow}$$

$$N_n(\epsilon) = \int_{[-\pi,\pi]^n} \frac{d^n \mathbf{k}}{(2\pi)^n} \delta(\epsilon - \varepsilon_0(\mathbf{k}))$$

$$d(\mathbf{x})\overrightarrow{m}(\mathbf{x})=(m^x(\mathbf{x}),m^y(\mathbf{x}),m^z(\mathbf{x}))$$

$$d(\mathbf{x})=\langle n_{\mathbf{x}}-1\rangle, \overrightarrow{m}(\mathbf{x})=\langle \vec{s}_{\mathbf{x}}\rangle$$

$$H_{\mathrm{HF}}=H_0+\frac{U}{2}\sum_{\mathbf{x}}\left(d(\mathbf{x})(n_{\mathbf{x}}-1)-\overrightarrow{m}(\mathbf{x})\cdot\vec{s}_{\mathbf{x}}\right)$$

$$v = \frac{\sum_{\mathbf{x}} \langle n_{\mathbf{x}} - 1 \rangle}{\sum_{\mathbf{x}} 1}$$

$$\sum_{\mathbf{x}}1=L^n$$

$$d(\mathbf{x})=d_0+(-1)^{\mathbf{x}}d_1\\ \overrightarrow{m}(\mathbf{x})=m_0\vec{e}+(-1)^{\mathbf{x}}m_1\vec{e}$$

$$(-1)^{\mathbf{x}} = (-1)^{x_1+\cdots+x_n}$$

$$\mathcal{G}=\mathcal{G}(\boldsymbol{d},\overrightarrow{\boldsymbol{m}};\mu)$$

$$\frac{\partial \mathcal{G}}{\partial d(\mathbf{x})} = 0, \frac{\partial \mathcal{G}}{\partial \vec{m}(\mathbf{x})} = \vec{0}$$

$$\frac{\partial}{\partial \vec{m}} = \left(\frac{\partial}{\partial m^x}, \frac{\partial}{\partial m^y}, \frac{\partial}{\partial m^z} \right)$$

$$v=-\frac{\partial \mathcal{G}}{\partial \mu}$$

$$\mathcal{F}(\mu)=\mathcal{G}(\boldsymbol{d}^*,\overrightarrow{\boldsymbol{m}}^*;\mu)$$

$$\mathcal{G}=\frac{U}{4L^n}\sum_{\mathbf{x}}\left(\vec{m}(\mathbf{x})^2-d(\mathbf{x})^2\right)\\-\frac{1}{L^n}\sum_I\frac{1}{\beta}\ln\left(2\mathrm{cosh}\left(\frac{\beta E_I}{2}\right)\right)$$

$$H_{\mathrm{HF}}=\sum_{I,J}h_{I,J}\Big(c_I^\dagger c_J-\frac{1}{2}\delta_{I,J}\Big)$$

$$\mathcal{G}(\boldsymbol{d}^*,\overrightarrow{\boldsymbol{m}}^*;\mu)=\min_{\overrightarrow{\boldsymbol{m}}}\max_{\boldsymbol{d}}\mathcal{G}(\boldsymbol{d},\overrightarrow{\boldsymbol{m}};\mu)$$

$$\mathrm{Ln}_{\beta}(\epsilon)=\frac{1}{\beta}\ln\left(2\mathrm{cosh}\left(\frac{\beta\epsilon}{2}\right)\right)\,(\epsilon\in\mathbb{R})$$

$$\mathcal{G}(d_0,d_1,m_0,m_1;\mu)=\frac{U}{4}(m_0^2+m_1^2-d_0^2-d_1^2)\\-\frac{1}{2}\int_{[-\pi,\pi]^n}\frac{d^nk}{(2\pi)^n}\sum_{r,r'=\pm}\mathrm{Ln}_{\beta}(E_{r,r'}(\mathbf{k}))$$

$$E_{r,r'}(\mathbf{k})\!=\!\varepsilon_1(\mathbf{k})-\mu+\frac{Ud_0}{2}-r\frac{Um_0}{2}\\+r'\sqrt{\varepsilon_0(\mathbf{k})^2+\left(\varepsilon_2(\mathbf{k})+\frac{Ud_1}{2}-r\frac{Um_1}{2}\right)^2}$$

$$f_{\beta}(\epsilon)=-\frac{1}{2}\tanh\left(\frac{\beta\epsilon}{2}\right)=\frac{1}{\mathrm{e}^{\beta\epsilon}+1}-\frac{1}{2}$$

$$f_{\beta}(\epsilon)=-\frac{\partial}{\partial \epsilon}\mathrm{Ln}_{\beta}(\epsilon)$$

$$1/\beta\downarrow 0, \, \mathrm{Ln}_{\beta}(\epsilon)\rightarrow \frac{1}{2}|\epsilon| \, \text{and} \, f_{\beta}(\epsilon)\rightarrow -\frac{1}{2}\mathrm{sgn}(\epsilon)=\theta(-\epsilon)-\frac{1}{2}$$

$$\frac{\partial \mathcal{G}}{\partial d_i}=0, \frac{\partial \mathcal{G}}{\partial m_i}=0\,(i=0,1),$$

$$v=-\frac{\partial \mathcal{G}}{\partial \mu}$$



$$\tilde{\mu} = \mu - \frac{U}{2}d_0 = \mu - \frac{U}{2}v$$

$$\text{AF}:(d_0,d_1,m_0,m_1)=(d_{\text{AF}},0,0,m_{\text{AF}})$$

$$\text{F}:(d_0,d_1,m_0,m_1)=(d_{\text{F}},0,m_{\text{F}},0)$$

$$\text{P}:(d_0,d_1,m_0,m_1)=(d_{\text{P}},0,0,0)$$

$$d(\mathbf{x})=d_0,\overrightarrow{m}(\mathbf{x})=(-1)^{\mathbf{x}}m_1\vec{e}$$

$$\mathcal{G}(d_0,m_1;\mu)=\frac{U}{4}(m_1^2-d_0^2)\\ -\int_{[-\pi,\pi]^n}\frac{d^n\mathbf{k}}{(2\pi)^n}\Big(\text{Ln}_{\beta}(E_+(\mathbf{k}))+\text{Ln}_{\beta}(E_-(\mathbf{k}))\Big)$$

$$E_{\pm}(\mathbf{k})=\frac{U}{2}d_0-\mu\pm\sqrt{\varepsilon_0(\mathbf{k})^2+\left(\frac{U}{2}m_1\right)^2}$$

$$\mathcal{G}(d_0^*,m_1^*;\mu)=\min_{m_1}\max_{d_0}\mathcal{G}(d_0,m_1;\mu).$$

$$\frac{\partial \mathcal{G}}{\partial d_0}=0,\frac{\partial \mathcal{G}}{\partial m_1}=0$$

$$d_0=\int\frac{d^n\mathbf{k}}{(2\pi)^n}\big(f_{\beta}(E_+(\mathbf{k}))+f_{\beta}(E_-(\mathbf{k}))\big),\\ m_1=-\frac{U}{2}\int\frac{d^n\mathbf{k}}{(2\pi)^n}\frac{f_{\beta}(E_+(\mathbf{k}))-f_{\beta}(E_-(\mathbf{k}))}{\sqrt{\varepsilon_0(\mathbf{k})^2+\left(\frac{U}{2}m_1\right)^2}}m_1,$$

$$f_{\beta}(\epsilon)\int\int_{[-\pi,\pi]^n}$$

$$v=\int\frac{d^n\mathbf{k}}{(2\pi)^n}\big(f_{\beta}(E_+(\mathbf{k}))+f_{\beta}(E_-(\mathbf{k}))\big)$$

$$(d_0^*,m_1^*)=(d_{\text{AF}},m_{\text{AF}})$$

$$(d_0^*,m_1^*)=(d_{\text{P}},0)$$

$$\left(d_0^{(i)},m_1^{(i)}\right)\text{ with }m_1^{(i)}>0$$

$$\mathcal{G}\left(d_0^{(i)},m_1^{(i)};\mu\right),\text{ i.e., }\mathcal{G}(d_{\text{AF}},m_{\text{AF}};\mu)=\min_i\mathcal{G}\left(d_0^{(i)},m_1^{(i)};\mu\right)$$

$$\mathcal{F}_{\text{AF}}(\mu)=\mathcal{G}(d_{\text{AF}},m_{\text{AF}};\mu),\mathcal{F}_{\text{P}}(\mu)=\mathcal{G}(d_{\text{P}},0;\mu),$$

$$\mathcal{G}(d_0^*,m_1^*;\mu)=\min(\mathcal{F}_{\text{AF}}(\mu),\mathcal{F}_{\text{P}}(\mu));$$



$$v = -\frac{\partial \mathcal{G}(d_0^*, m_1^*; \mu)}{\partial \mu}.$$

$$v_{\text{AF}}^{\text{max}} = -\frac{\partial \mathcal{F}_{\text{AF}}(\mu)}{\partial \mu} \Big|_{\mu=\mu_c}$$

$$v_{\text{P}}^{\text{min}} = -\frac{\partial \mathcal{F}_{\text{P}}(\mu)}{\partial \mu} \Big|_{\mu=\mu_c}.$$

$$v_{\text{AF}}^{\text{max}} < v < v_{\text{P}}^{\text{min}}$$

$$\max_{d_0} \mathcal{G} = \max_{d_0} \mathcal{G}(d_0, m_1; \mu)$$

$$\max_{d_0} \mathcal{G} = \mathcal{G}(d_0^*(m_1, \mu), m_1; \mu)$$

$$v_{\text{P}}^{\text{min}} = -\frac{\partial \mathcal{F}_{\text{P}}(\mu)}{\partial \mu} \Big|_{\mu=\mu_c} > -\frac{\partial \mathcal{F}_{\text{AF}}(\mu)}{\partial \mu} \Big|_{\mu=\mu_c} = v_{\text{AF}}^{\text{max}}.$$

$$\mathcal{G}_{\text{mixed}} = w\mathcal{G}(d_0, m_1; \mu) + (1-w)\mathcal{G}(\tilde{d}_0, 0; \mu)$$

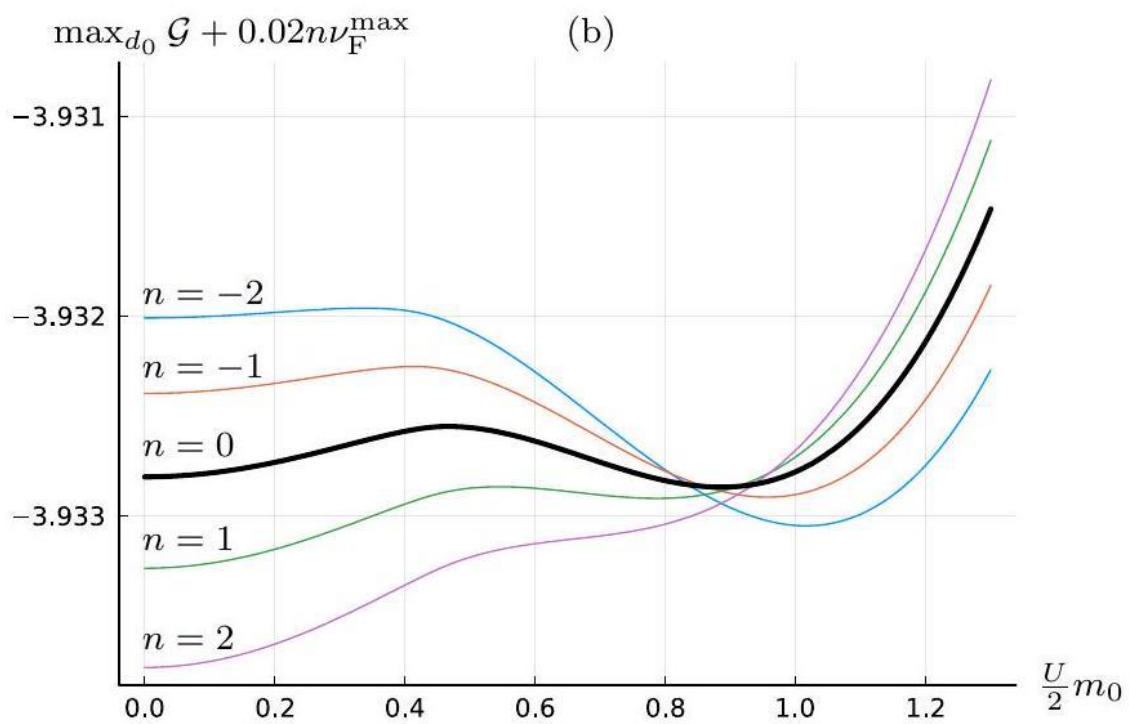
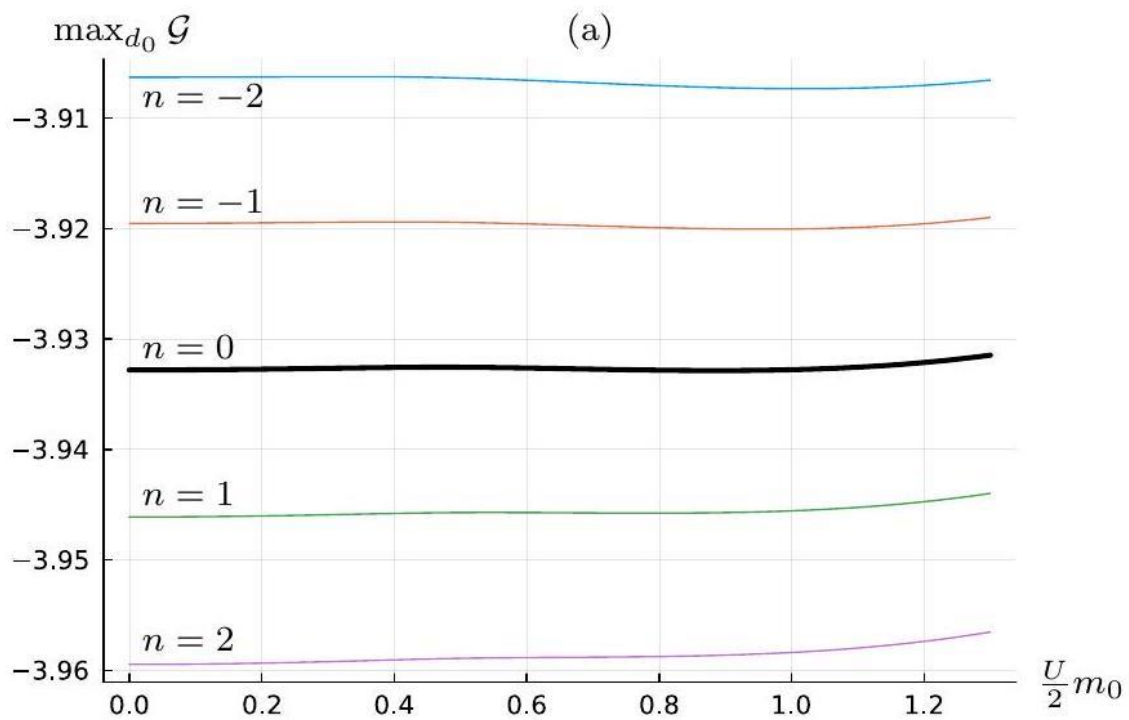
$$v = wv_{\text{AF}}^{\text{max}} + (1-w)v_{\text{P}}^{\text{min}}$$

$$w = \frac{v_{\text{P}}^{\text{min}} - v}{v_{\text{P}}^{\text{min}} - v_{\text{AF}}^{\text{max}}}$$

$$(d(\mathbf{x}), \vec{m}(\mathbf{x})) = \begin{cases} (d_0, m_1 \vec{e}(-1)^{\mathbf{x}}) & (\mathbf{x}/L \in R_w) \\ (\tilde{d}_0, \vec{0}) & (\mathbf{x}/L \notin R_w) \end{cases}$$

$$\frac{\partial \mathcal{G}_{\text{mixed}}}{\partial w} = \mathcal{G}(d_{\text{AF}}, m_{\text{AF}}; \mu) - \mathcal{G}(d_{\text{P}}, 0; \mu) = 0$$





$$\max_{d_0} \mathcal{G} = \mathcal{G}(d_0, m_0; \mu)$$

$$\Delta_F = \frac{U}{2} m_0$$

$$\max_{d_0} \mathcal{F}(d_0, m_0; \mu) + 0.02 n v_F^{\max}$$

$$d(\mathbf{x}) = d_0, \vec{m}(\mathbf{x}) = m_0 \vec{e}$$

$$\mathcal{G}(d_0, m_0; \mu) = \frac{U}{4}(m_0^2 - d_0^2) - \int_{[-\pi, \pi]^n} \frac{d^n \mathbf{k}}{(2\pi)^n} (\text{Ln}_\beta(E_+(\mathbf{k})) + \text{Ln}_\beta(E_-(\mathbf{k})))$$

$$E_\pm(\mathbf{k}) = \frac{U}{2}d_0 - \mu + \varepsilon_0(\mathbf{k}) \pm \frac{U}{2}m_0$$

$$\mathcal{G}(d_0^*, m_0^*; \mu) = \min_{m_0} \max_{d_0} \mathcal{G}(d_0, m_0; \mu)$$

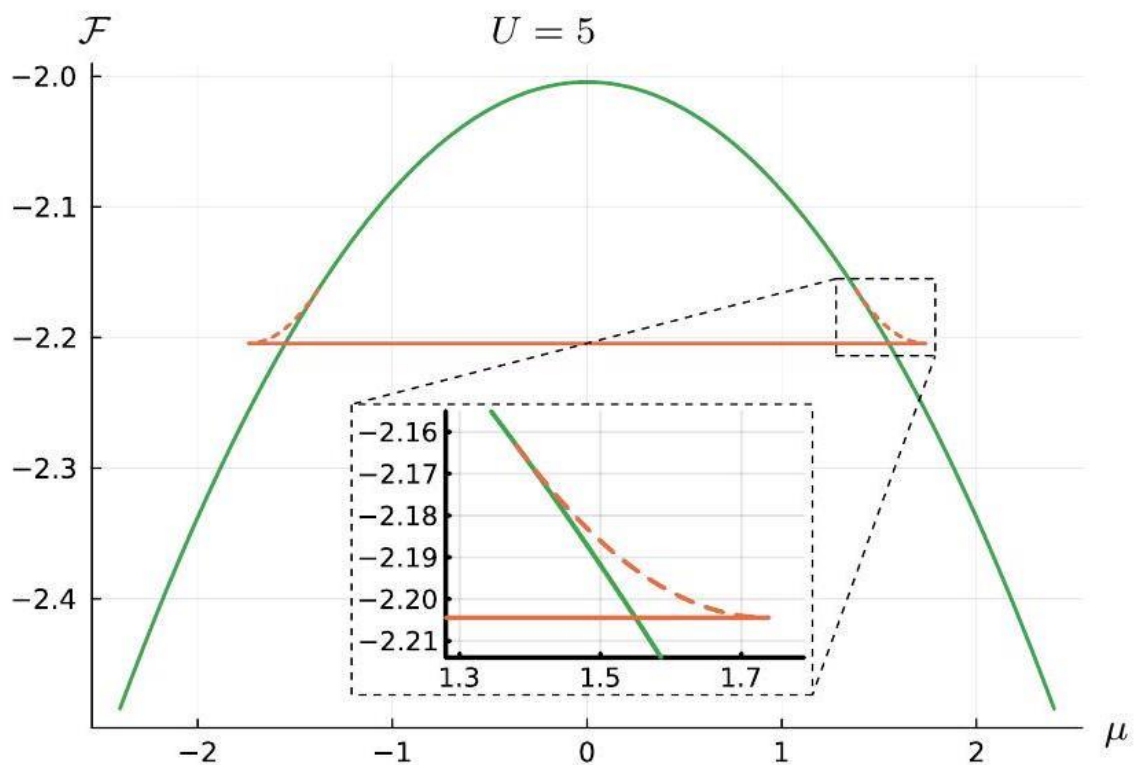
$$\mathcal{F}_F(\mu) = \mathcal{G}(d_F, m_F; \mu)$$

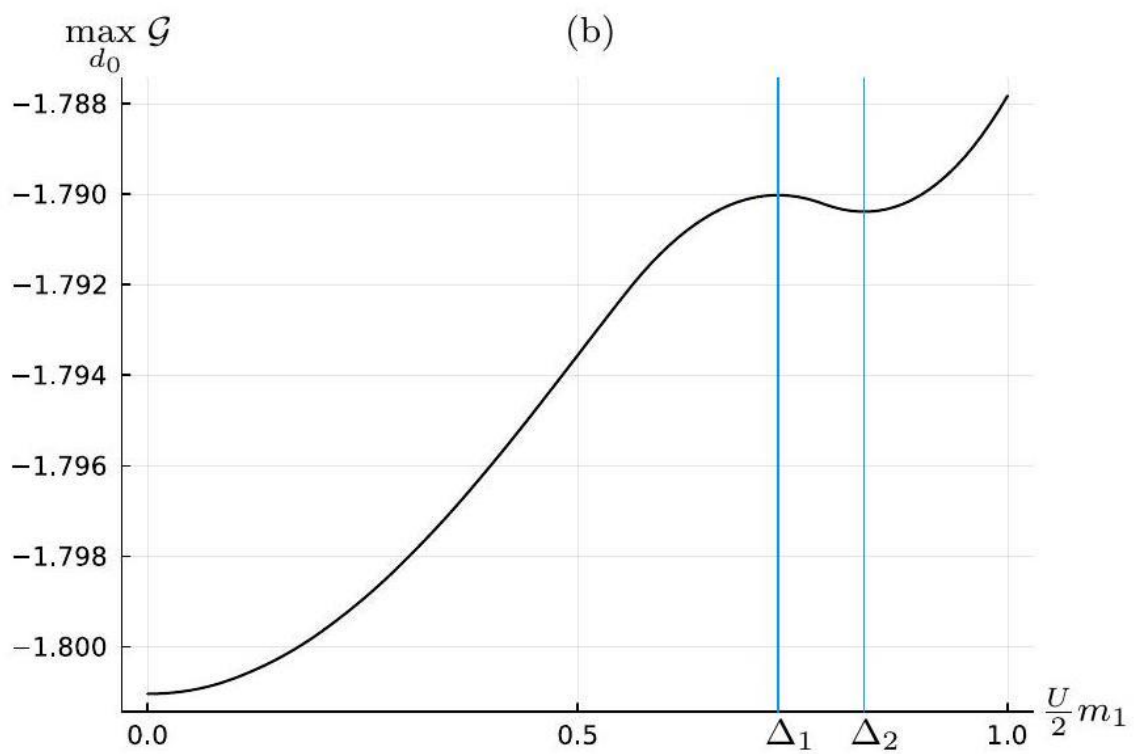
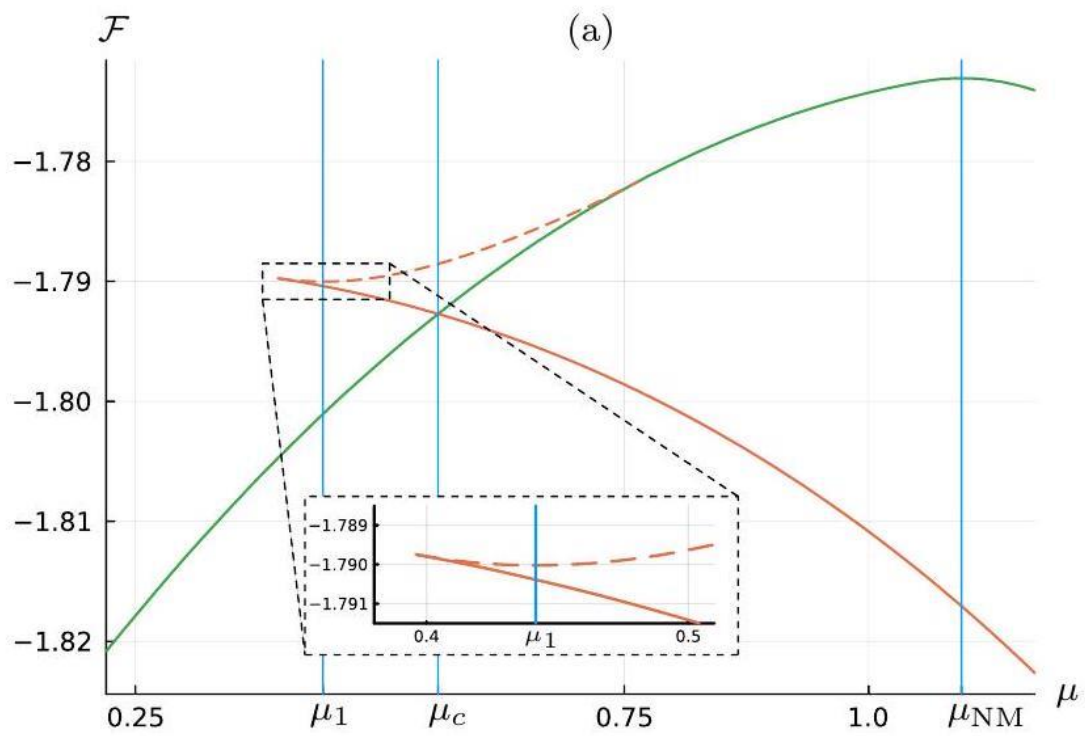
$$(d_0^{(i)}, m_0^{(i)}) \text{ with } m_0^{(i)} > 0 \text{ for } i = 1, 2, \dots$$

$$\mathcal{G}(d_F, m_F; \mu) = \min_i \mathcal{G}(d_0^{(i)}, m_0^{(i)}; \mu)$$

$$\min(\mathcal{F}_{AF}(\mu), \mathcal{F}_F(\mu), \mathcal{F}_P(\mu)),$$

$$v_P^{\min} = -\left. \frac{\partial \mathcal{F}_P(\mu)}{\partial \mu} \right|_{\mu=\mu_c}, v_F^{\max} = -\left. \frac{\partial \mathcal{F}_F(\mu)}{\partial \mu} \right|_{\mu=\mu_c}$$





$$\rho_G = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})}$$

$$\begin{aligned} \langle c_I^\dagger c_J c_K^\dagger c_L \rangle &= \langle c_I^\dagger c_K^\dagger c_L c_J \rangle + \delta_{J,K} \langle c_I^\dagger c_L \rangle \\ &= \langle c_I^\dagger c_J \rangle \langle c_K^\dagger c_L \rangle - \langle c_I^\dagger c_L \rangle \langle c_K^\dagger c_J \rangle + \delta_{J,K} \langle c_I^\dagger c_L \rangle \end{aligned}$$

$$\Omega(\rho) = \text{Tr}(\rho H) + \frac{1}{\beta} \text{Tr}(\rho \ln(\rho)),$$

$$\Omega(\rho_G) = \min_{\rho \in \mathcal{S}} \Omega(\rho),$$

$$\Omega(\rho_{\text{HF}}^*) = \min_{\rho \in \mathcal{S}_{\text{qf}}} \Omega(\rho)$$

$$\Omega(\rho_{\text{HF,rst}}^*) = \min_{\rho \in \mathcal{S}_{\text{qf,rst}}} \Omega(\rho).$$

$$\rho_{\text{qf}} = \frac{e^{-\beta H_{\text{qf}}}}{Z_{\text{qf}}}, Z_{\text{qf}} = \text{Tr}(e^{-\beta H_{\text{qf}}}),$$

$$H_{\text{qf}} = \sum_{\mathbf{x}, \sigma, \mathbf{y}, \sigma'} h_{\mathbf{x}, \sigma; \mathbf{y}, \sigma'} \left(c_{\mathbf{x}, \sigma}^\dagger c_{\mathbf{y}, \sigma'} - \frac{1}{2} \delta_{\mathbf{x}, \mathbf{y}} \delta_{\sigma, \sigma'} \right)$$

$$-\frac{1}{2} \sum_{\mathbf{x}, \sigma} h_{\mathbf{x}, \sigma; \mathbf{x} \sigma} = -\frac{1}{2} \text{tr}(h)$$

$$\rho_{\text{HF}} = \frac{e^{-\beta H_{\text{HF}}}}{Z_{\text{HF}}}, Z_{\text{HF}} = \text{Tr}(e^{-\beta H_{\text{HF}}}),$$

$$\langle A \rangle = \text{Tr}(\rho_{\text{qf}} A)$$

$$\begin{aligned} \Omega(\rho_{\text{qf}}) &= \left\langle H + \frac{1}{\beta} \ln(\rho_{\text{qf}}) \right\rangle \\ &= \langle H \rangle - \langle H_{\text{qf}} \rangle - \frac{1}{\beta} \ln(Z_{\text{qf}}). \end{aligned}$$

$$\begin{aligned} \langle n_{\mathbf{x},\uparrow} n_{\mathbf{x},\downarrow} \rangle &= \langle c_{\mathbf{x},\uparrow}^\dagger c_{\mathbf{x},\uparrow} \rangle \langle c_{\mathbf{x},\downarrow}^\dagger c_{\mathbf{x},\downarrow} \rangle - \langle c_{\mathbf{x},\uparrow}^\dagger c_{\mathbf{x},\downarrow} \rangle \langle c_{\mathbf{x},\downarrow}^\dagger c_{\mathbf{x},\uparrow} \rangle \\ &= \langle n_{\mathbf{x},\uparrow} \rangle \langle n_{\mathbf{x},\downarrow} \rangle - \langle s_{\mathbf{x}}^+ \rangle \langle s_{\mathbf{x}}^- \rangle = \frac{1}{4} (\langle n_{\mathbf{x}} \rangle^2 - \langle \vec{s}_{\mathbf{x}} \rangle^2) \end{aligned}$$

$$s_{\mathbf{x}}^+ := c_{\mathbf{x},\uparrow}^\dagger c_{\mathbf{x},\downarrow} = \frac{1}{2} (s_{\mathbf{x}}^x + i s_{\mathbf{x}}^y), s_{\mathbf{x}}^- = (s_{\mathbf{x}}^+)^{\dagger}$$

$$\langle \vec{s}_{\mathbf{x}} \rangle (\langle s_{\mathbf{x}}^x \rangle, \langle s_{\mathbf{x}}^y \rangle, \langle s_{\mathbf{x}}^z \rangle)$$

$$\langle H \rangle = \langle H_0 \rangle + \frac{U}{4} \sum_{\mathbf{x}} (\langle n_{\mathbf{x}} - 1 \rangle^2 - \langle \vec{s}_{\mathbf{x}} \rangle^2).$$

$$\frac{1}{\beta} \ln(Z_{\text{qf}}) = \text{tr}(\text{Ln}_{\beta}(h))$$

$$\text{tr}(\text{Ln}_{\beta}(h)) = \sum_I \text{Ln}_{\beta}(E_I)$$

$$n_{\mathbf{x},\uparrow,\downarrow} - \frac{1}{2} = \frac{1}{2} (n_{\mathbf{x}} - 1 \pm s_{\mathbf{x}}^z)$$

$$\left(n_{\mathbf{x},\uparrow} - \frac{1}{2}\right)\left(n_{\mathbf{x},\downarrow} - \frac{1}{2}\right) = \frac{1}{2}(n_{\mathbf{x}} - 1)^2 - \frac{1}{4}$$

$$H = H_0 + U \sum_{\mathbf{x}} v_{\mathbf{x},\uparrow} v_{\mathbf{x},\downarrow}$$

$$v_{\mathbf{x},\uparrow,\downarrow} = \frac{1}{2}(n_{\mathbf{x}} - 1 \pm \vec{e}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{x}})$$

$$\delta v_{\mathbf{x},\sigma} = v_{\mathbf{x},\sigma} - \langle v_{\mathbf{x},\sigma} \rangle$$

$$v_{\mathbf{x},\uparrow} v_{\mathbf{x},\downarrow} \approx \langle v_{\mathbf{x},\uparrow} \rangle v_{\mathbf{x},\downarrow} + v_{\mathbf{x},\uparrow} \langle v_{\mathbf{x},\downarrow} \rangle - \langle v_{\mathbf{x},\uparrow} \rangle \langle v_{\mathbf{x},\downarrow} \rangle.$$

$$\begin{aligned} H_{\text{HF}} &= H_0 + U \sum_{\mathbf{x}} (\langle v_{\mathbf{x},\uparrow} \rangle v_{\mathbf{x},\downarrow} + v_{\mathbf{x},\uparrow} \langle v_{\mathbf{x},\downarrow} \rangle) \\ &= H_0 + \frac{U}{2} \sum_{\mathbf{x}} ((n_{\mathbf{x}} - 1)(n_{\mathbf{x}} - 1) - \langle \vec{e}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{x}} \rangle \vec{e}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{x}}) \end{aligned}$$

$$E_{\text{pot}} = U \sum_{\mathbf{x}} \langle v_{\mathbf{x},\uparrow} \rangle \langle v_{\mathbf{x},\downarrow} \rangle = \frac{U}{4} \sum_{\mathbf{x}} ((n_{\mathbf{x}} - 1)^2 - \langle \vec{e}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{x}} \rangle^2)$$

$$\langle H \rangle = \langle H_{\text{HF}} - E_{\text{pot}} \rangle$$

$$\langle H_{\text{HF}} - E_{\text{pot}} \rangle = \langle H_0 \rangle + E_{\text{pot}},$$

$$\langle \vec{e}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{x}} \rangle^2 = \langle \vec{s}_{\mathbf{x}} \rangle^2$$

$$H_{\text{HF}} = H_0 + \frac{U}{2} \sum_{\mathbf{x}} ((n_{\mathbf{x}} - 1)(n_{\mathbf{x}} - 1) - \langle \vec{s}_{\mathbf{x}} \rangle \cdot \vec{s}_{\mathbf{x}})$$

$$\begin{aligned} h_{\mathbf{x},\sigma;\mathbf{y},\sigma'} &= (t_{\mathbf{x},\mathbf{y}} - \mu \delta_{\mathbf{x},\mathbf{y}}) \delta_{\sigma,\sigma'} \\ &\quad + \frac{U}{2} \delta_{\mathbf{x},\mathbf{y}} (d(\mathbf{x}) \delta_{\sigma,\sigma'} - \vec{m}(\mathbf{x}) \cdot \vec{\sigma}_{\sigma,\sigma'}) \end{aligned}$$

$$\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$$

$$\vec{s}_{\mathbf{x}} = \sum_{\sigma,\sigma'} c_{\mathbf{x},\sigma}^{\dagger} \vec{\sigma}_{\sigma,\sigma'} c_{\mathbf{x},\sigma'}$$

$$-\frac{1}{2} \sum_{\mathbf{x},\sigma} h_{\mathbf{x},\sigma;\mathbf{x},\sigma} = \sum_{\mathbf{x}} (\mu - (U/2)d(\mathbf{x}))$$

$$\frac{\partial}{\partial d(\mathbf{x})} H_{\text{HF}} = (U/2)(n_{\mathbf{x}} - 1)$$

$$\begin{aligned}\frac{U}{2}\langle n_{\mathbf{x}} - 1 \rangle &= \frac{\text{Tr}(e^{-\beta H_{\text{HF}}}(U/2)(n_{\mathbf{x}} - 1))}{\text{Tr}(e^{-\beta H_{\text{HF}}})} \\ &= -\frac{1}{\beta} \frac{\partial}{\partial d(\mathbf{x})} \ln(\text{Tr}(e^{-\beta H_{\text{HF}}})) \\ &= -\frac{1}{\beta} \frac{\partial}{\partial d(\mathbf{x})} \ln(Z_{\text{HF}})\end{aligned}$$

$$\frac{U}{2}\langle \vec{s}_{\mathbf{x}} \rangle = \frac{1}{\beta} \frac{\partial}{\partial \vec{m}(\mathbf{x})} \ln(Z_{\text{HF}})$$

$$G = \frac{U}{4} \sum_{\mathbf{x}} (\vec{m}(\mathbf{x})^2 - d(\mathbf{x})^2) - \frac{1}{\beta} \ln(Z_{\text{HF}})$$

$$\begin{aligned}\frac{\partial G}{\partial d(\mathbf{x})} &= -\frac{U}{2} d(\mathbf{x}) + \frac{U}{2} \langle n_{\mathbf{x}} - 1 \rangle, \\ \frac{\partial G}{\partial \vec{m}(\mathbf{x})} &= \frac{U}{2} \vec{m}(\mathbf{x}) - \frac{U}{2} \langle \vec{s}_{\mathbf{x}} \rangle,\end{aligned}$$

$$\frac{\partial}{\partial d(\mathbf{x})} G = 0, \frac{\partial}{\partial \vec{m}(\mathbf{x})} G = \vec{0}$$

$$\sum_{\mathbf{x}} \langle n_{\mathbf{x}} - 1 \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln(Z_{\text{HF}})$$

$$\sum_{\mathbf{x}} (n_{\mathbf{x}} - 1) = -\frac{\partial}{\partial \mu} H_{\text{HF}}$$

$$v = -\frac{1}{L^n} \frac{\partial G}{\partial \mu}.$$

$$\mathcal{G} = \frac{1}{L^n} \left(\frac{U}{4} \sum_{\mathbf{x}} (\vec{m}(\mathbf{x})^2 - d(\mathbf{x})^2) - \text{tr}(\text{Ln}_{\beta}(h)) \right)$$

$$\begin{aligned}\langle H \rangle - \langle H_{\text{HF}} \rangle &= \frac{U}{4} \sum_{\mathbf{x}} (\langle n_{\mathbf{x}} - 1 \rangle^2 - \langle \vec{s}_{\mathbf{x}} \rangle^2) \\ &\quad - \frac{U}{2} \sum_{\mathbf{x}} (d(\mathbf{x}) \langle n_{\mathbf{x}} - 1 \rangle - \vec{m}(\mathbf{x}) \cdot \langle \vec{s}_{\mathbf{x}} \rangle)\end{aligned}$$

$$\langle H \rangle - \langle H_{\text{HF}} \rangle = \frac{U}{4} \sum_{\mathbf{x}} (\vec{m}(\mathbf{x})^2 - d(\mathbf{x})^2) + \mathcal{C}$$

$$\mathcal{C} = \frac{U}{4} \sum_{\mathbf{x}} ([d(\mathbf{x}) - \langle n_{\mathbf{x}} - 1 \rangle]^2 - [\vec{m}(\mathbf{x}) - \langle \vec{s}_{\mathbf{x}} \rangle]^2).$$

$$\Omega = \frac{U}{4} \sum_{\mathbf{x}} (\vec{m}(\mathbf{x})^2 - d(\mathbf{x})^2) - \text{tr}(\text{Ln}_{\beta}(h)) + \mathcal{C}$$

$$\Omega(\boldsymbol{d}^*, \overline{\boldsymbol{m}}^*; \mu) = \min_{\overline{\boldsymbol{m}}, \boldsymbol{d}} \Omega(\boldsymbol{d}, \overline{\boldsymbol{m}}; \mu)$$

$$\Omega = G + \mathcal{C},$$

$$\frac{\partial \Omega}{\partial d(\mathbf{x})} = -\frac{U}{2}d(\mathbf{x}) + \frac{U}{2}\langle n_{\mathbf{x}} - 1 \rangle + \frac{\partial \mathcal{C}}{\partial d(\mathbf{x})}$$

$$\frac{\partial \Omega}{\partial \vec{m}(\mathbf{x})} = \frac{U}{2}\vec{m}(\mathbf{x}) - \frac{U}{2}\langle \vec{s}_{\mathbf{x}} \rangle + \frac{\partial \mathcal{C}}{\partial \vec{m}(\mathbf{x})}$$

$$v=-\frac{1}{L^n}\frac{\partial \Omega}{\partial \mu}+\frac{1}{L^n}\frac{\partial \mathcal{C}}{\partial \mu},$$

$$\mathcal{C} = \frac{1}{U} \sum_{\mathbf{x}} \left(\left(\frac{\partial G}{\partial d(\mathbf{x})} \right)^2 - \left(\frac{\partial G}{\partial \vec{m}(\mathbf{x})} \right)^2 \right)$$

$$\frac{\partial G}{\partial d(\mathbf{x})}=0, \frac{\partial G}{\partial \vec{m}(\mathbf{x})}=\vec{0}$$

$$\frac{\partial \Omega}{\partial d(\mathbf{x})}=0, \frac{\partial \Omega}{\partial \vec{m}(\mathbf{x})}=\vec{0}$$

$$v=-\frac{1}{L^n}\frac{\partial \Omega}{\partial \mu}$$

$$\mathcal{F}=\Omega/L^n=G/L^n=\mathcal{G}$$

$$d(\mathbf{x})\!=\!d_0+(-1)^{\mathbf{x}}d_1$$

$$\vec{m}(\mathbf{x})=m_0\vec{e}_0+(-1)^{\mathbf{x}}m_1\vec{e}_1$$

$$\vec{e}_0=(0,0,1) \text{ and } \vec{e}_1=(\sin{(\theta)},0,\cos{(\theta)})$$

$$\vec{e}_0\cdot\vec{\sigma}_{\sigma,\sigma'}=\sigma\delta_{\sigma,\sigma'},\vec{e}_1\cdot\vec{\sigma}_{\sigma,\sigma'}=\cos{(\theta)}\sigma\delta_{\sigma,\sigma'}+\sin{(\theta)}\delta_{\sigma,-\sigma'}$$

$$\phi_i=\frac{U}{2}d_i, B_i=-\frac{U}{2}m_i\,(i=0,1),$$

$$H_{\rm HF}=\sum_{\mathbf{k},\sigma}\left([\varepsilon(\mathbf{k})-\mu+\phi_0+B_0\sigma]c_{\sigma}^{\dagger}(\mathbf{k})c_{\sigma}(\mathbf{k})\right.\\ \left.+[\varepsilon_2(\mathbf{k})+\phi_1+B_1\cos{(\theta)}\sigma]c_{\sigma}^{\dagger}(\mathbf{k})c_{\sigma}(\mathbf{k}+\mathbf{Q})\right.\\ \left.+B_1\sin{(\theta)}c_{\sigma}^{\dagger}(\mathbf{k})c_{-\sigma}(\mathbf{k}+\mathbf{Q})\right)-E_0$$

$$C(\mathbf{k}) = \left(c_{\uparrow}^{\dagger}(\mathbf{k}), c_{\uparrow}^{\dagger}(\mathbf{k}+\mathbf{Q}), c_{\downarrow}^{\dagger}(\mathbf{k}), c_{\downarrow}^{\dagger}(\mathbf{k}+\mathbf{Q})\right)^{\dagger},$$

$$H_{\rm HF}=\sum_{\mathbf{k}\in\Lambda_{L,\,\mathrm{half}}^*}C(\mathbf{k})^{\dagger}h(\mathbf{k})C(\mathbf{k})-E_0,$$



$$h(\mathbf{k})$$

$$= \begin{pmatrix} \varepsilon(\mathbf{k}) - \mu + \phi_0 + B_0 & \varepsilon_2(\mathbf{k}) + \phi_1 + B_1 \cos(\theta) & 0 & B_1 \sin(\theta) \\ \varepsilon_2(\mathbf{k}) + \phi_1 + B_1 \cos(\theta) & \varepsilon(\mathbf{k} + \mathbf{Q}) - \mu + \phi_0 + B_0 & B_1 \sin(\theta) & 0 \\ 0 & B_1 \sin(\theta) & \varepsilon(\mathbf{k}) - \mu + \phi_0 - B_0 & \varepsilon_2(\mathbf{k}) + \phi_1 - B_1 \cos(\theta) \\ B_1 \sin(\theta) & 0 & \varepsilon_2(\mathbf{k}) + \phi_1 - B_1 \cos(\theta) & \varepsilon(\mathbf{k} + \mathbf{Q}) - \mu + \phi_0 - B_0 \end{pmatrix}.$$

$$\frac{1}{L^n} \sum_I \text{Ln}_\beta(E_I) = \frac{1}{L^n} \sum_{\mathbf{k} \in \Lambda_{L, \text{half}}^*} \sum_{r, r' = \pm} \text{Ln}_\beta(E_{r, r'}(\mathbf{k})) = \frac{1}{2} \frac{1}{L^n} \sum_{\mathbf{k}} \sum_{r, r' = \pm} \text{Ln}_\beta(E_{r, r'}(\mathbf{k})),$$

$$E_{r,r'}(\mathbf{k})=E_{r,r'}(\mathbf{k}+\mathbf{Q})$$

$$\frac{U}{4L^n}\sum_{\mathbf{x}}\left(\vec{m}(\mathbf{x})^2-d(\mathbf{x})^2\right)=\frac{U}{4L^n}\sum_{\mathbf{x}}\left(m_0^2+m_1^2+2m_0m_1\cos\left(\theta\right)(-1)^{\mathbf{x}}-d_0^2-d_1^2-2d_0d_1(-1)^{\mathbf{x}}\right)$$

$$=\frac{U}{4}(m_0^2+m_1^2-d_0^2-d_1^2)$$

$$\mathcal{G}=\frac{U}{4}(m_0^2+m_1^2-d_0^2-d_1^2)-\frac{1}{2}\frac{1}{L^n}\sum_{\mathbf{k}}\sum_{r,r'=\pm}\text{Ln}_\beta(E_{r,r'}(\mathbf{k}))$$

$$E_{r,r'}(\mathbf{k})=\frac{\varepsilon(\mathbf{k})+\varepsilon(\mathbf{k}+\mathbf{Q})}{2}+\phi_0+rB_0+r'\sqrt{\left(\frac{\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}+\mathbf{Q})}{2}\right)^2+(\varepsilon_2(\mathbf{k})+\phi_1+rB_1)^2}$$

$$d_0=\frac{1}{2}\int_{[-\pi,\pi]^n}\frac{d^nk}{(2\pi)^n}\sum_{r,r'=\pm}f_\beta(E_{r,r'}(\mathbf{k}))$$

$$m_0=\frac{1}{2}\int_{[-\pi,\pi]^n}\frac{d^nk}{(2\pi)^n}\sum_{r,r'=\pm}rf_\beta(E_{r,r'}(\mathbf{k}))$$

$$d_1=\frac{1}{2}\int_{[-\pi,\pi]^n}\frac{d^nk}{(2\pi)^n}\sum_{r,r'=\pm}r'f_\beta(E_{r,r'}(\mathbf{k}))\frac{\varepsilon_2(\mathbf{k})+\frac{Ud_1}{2}-r\frac{Um_1}{2}}{\sqrt{\varepsilon_0(\mathbf{k})^2+\left(\varepsilon_2(\mathbf{k})+\frac{Ud_1}{2}-r\frac{Um_1}{2}\right)^2}}$$

$$m_1=\frac{1}{2}\int_{[-\pi,\pi]^n}\frac{d^nk}{(2\pi)^n}\sum_{r,r'=\pm}rr'f_\beta(E_{r,r'}(\mathbf{k}))\frac{\varepsilon_2(\mathbf{k})+\frac{Ud_1}{2}-r\frac{Um_1}{2}}{\sqrt{\varepsilon_0(\mathbf{k})^2+\left(\varepsilon_2(\mathbf{k})+\frac{Ud_1}{2}-r\frac{Um_1}{2}\right)^2}}$$

$$v=\frac{1}{2}\int_{[-\pi,\pi]^n}\frac{d^nk}{(2\pi)^n}\sum_{r,r'=\pm}f_\beta(E_{r,r'}(\mathbf{k}))$$

$$\Omega(H;\rho)=\mathrm{Tr}(\rho H)+\frac{1}{\beta}\mathrm{Tr}(\rho\ln\left(\rho\right)),$$

$$\Omega(H;\rho_{\mathrm{HF}}^*)=\min_{\rho_{\mathrm{qf}}}\Omega(H;\rho_{\mathrm{qf}})$$

$$\mathrm{Tr}(\rho_{\mathrm{qf}}H)=\langle H\rangle$$

$$\Omega(H; \rho_{\text{qf}}) = \langle H_0 \rangle + \frac{U}{4} \sum_{\mathbf{x}} (\langle n_{\mathbf{x}} - 1 \rangle^2 - \langle \vec{s}_{\mathbf{x}} \rangle^2) + \frac{1}{\beta} \text{Tr}(\rho_{\text{qf}} \ln(\rho_{\text{qf}}))$$

$$0 = \min_{d(\mathbf{x})} (\langle n_{\mathbf{x}} - 1 \rangle - d(\mathbf{x}))^2 = \langle n_{\mathbf{x}} - 1 \rangle^2 + \min_{d(\mathbf{x})} (d(\mathbf{x})^2 - 2d(\mathbf{x})\langle n_{\mathbf{x}} - 1 \rangle)$$

$$\langle n_{\mathbf{x}} - 1 \rangle^2 = \max_{d(\mathbf{x})} (-d(\mathbf{x})^2 + 2d(\mathbf{x})\langle n_{\mathbf{x}} - 1 \rangle)$$

$$-\langle \vec{s}_{\mathbf{x}} \rangle^2 = \min_{\vec{m}(\mathbf{x})} (\vec{m}(\mathbf{x})^2 - 2\vec{m}(\mathbf{x}) \cdot \langle \vec{s}_{\mathbf{x}} \rangle)$$

$$\Omega(H; \rho_{\text{qf}}) = \min_{\vec{m}} \max_d \left(\langle H_0 \rangle + \frac{U}{4} \sum_{\mathbf{x}} (\vec{m}(\mathbf{x})^2 - 2\vec{m}(\mathbf{x}) \cdot \langle \vec{s}_{\mathbf{x}} \rangle - d(\mathbf{x})^2 + 2d(\mathbf{x})\langle n_{\mathbf{x}} - 1 \rangle) + \frac{1}{\beta} \text{Tr}(\rho_{\text{qf}} \ln(\rho_{\text{qf}})) \right)$$

$$\langle H_0 \rangle + \frac{U}{4} \sum_{\mathbf{x}} (-2\vec{m}(\mathbf{x}) \cdot \langle \vec{s}_{\mathbf{x}} \rangle + 2d(\mathbf{x})\langle n_{\mathbf{x}} - 1 \rangle)$$

$$\langle H_{\text{HF}} \rangle + \frac{1}{\beta} \text{Tr}(\rho_{\text{qf}} \ln(\rho_{\text{qf}})) = \Omega(H_{\text{HF}}; \rho_{\text{qf}})$$

$$\Omega(H; \rho_{\text{qf}}) = \min_{\vec{m}} \max_d \left(\frac{U}{4} \sum_{\mathbf{x}} (\vec{m}(\mathbf{x})^2 - d(\mathbf{x})^2) + \Omega(H_{\text{HF}}, \rho_{\text{qf}}) \right)$$

$$\Omega(H; \rho_{\text{HF}}^*) = \min_d \max_{\vec{m}} \left(\frac{U}{4} \sum_{\mathbf{x}} (\vec{m}(\mathbf{x})^2 - d(\mathbf{x})^2) + \min_{\rho_{\text{qf}}} \Omega(H_{\text{HF}}; \rho_{\text{qf}}) \right)$$

$$\min_{\rho_{\text{qf}}} \Omega(H_{\text{HF}}; \rho_{\text{qf}}) = \Omega(H_{\text{HF}}; \rho_{\text{HF}}).$$

$$\Omega(H_{\text{HF}}; \rho_{\text{HF}}) = \text{Tr}(\rho_{\text{HF}} H_{\text{HF}}) + \frac{1}{\beta} \text{Tr}(\rho_{\text{HF}} (-\beta H_{\text{HF}} - \ln(Z_{\text{HF}}))) = -\frac{1}{\beta} \ln(Z_{\text{HF}})$$

$$\Omega(H; \rho_{\text{HF}}^*) = \min_{\vec{m}} \max_d G(\mathbf{d}, \vec{m}; \mu)$$

$$H_{\text{AF}} = H_0 + \frac{U}{2} \sum_{\mathbf{x}} (d_0(n_{\mathbf{x}} - 1) - (-1)^{\mathbf{x}} m_1 \vec{e} \cdot \vec{s}_{\mathbf{x}})$$

$$\rho_{\text{AF}} = \frac{e^{-\beta H_{\text{AF}}}}{\text{Tr}(e^{-\beta H_{\text{AF}}})}$$

$$\Omega(H; \rho_{\text{AF}}^*) = \min_{\rho_{\text{AF}}} \Omega(H; \rho_{\text{AF}})$$

$$\min_{d_0, m_1, \vec{e}} \Omega(H, \rho_{\text{AF}}(d_0, m_1, \vec{e}; \mu))$$

$$\begin{aligned} \sum_{\mathbf{x}} \langle n_{\mathbf{x}} - 1 \rangle^2 &= L^n a^2 = L^n \max_{\tilde{d}_0} (-\tilde{d}_0^2 + 2\tilde{d}_0 a) \\ &= \max_{\tilde{d}_0} \left(-L^n \tilde{d}_0^2 + 2 \sum_{\mathbf{x}} \tilde{d}_0 \langle n_{\mathbf{x}} - 1 \rangle \right) \end{aligned}$$

$$\begin{aligned} - \sum_{\mathbf{x}} \langle \vec{s}_{\mathbf{x}} \rangle^2 &= -L^n b^2 = L^n \min_{\tilde{m}_1} (\tilde{m}_1^2 - 2\tilde{m}_1 b) \\ &= \min_{\tilde{m}_1} \left(L^n \tilde{m}_1^2 - 2 \sum_{\mathbf{x}} (-1)^{\mathbf{x}} \tilde{m}_1 \vec{e} \cdot \langle \vec{s}_{\mathbf{x}} \rangle \right) \end{aligned}$$

$$\begin{aligned} \Omega(H; \rho_{\text{AF}}) &= \min_{\tilde{m}_1} \max_{\tilde{d}_0} \left(L^n \frac{U}{4} (\tilde{m}_1^2 - \tilde{d}_0^2) \right. \\ &\quad \left. + \langle \tilde{H}_{\text{AF}} \rangle + \frac{1}{\beta} \text{Tr}(\rho_{\text{AF}} \ln(\rho_{\text{AF}})) \right) \\ &= \min_{\tilde{m}_1} \max_{\tilde{d}_0} \left(L^n \frac{U}{4} (\tilde{m}_1^2 - \tilde{d}_0^2) + \Omega(\tilde{H}_{\text{AF}}; \rho_{\text{AF}}) \right) \end{aligned}$$

$$\tilde{H}_{\text{AF}} = H_{\text{AF}}(\tilde{d}_0, \tilde{m}_1, \vec{e}; \mu)$$

$$\begin{aligned} \Omega(H; \rho_{\text{AF}}^*) &= \min_{\tilde{m}_1} \max_{\tilde{d}_0} \left(L^n \frac{U}{4} (\tilde{m}_1^2 - \tilde{d}_0^2) \right. \\ &\quad \left. + \min_{\rho_{\text{AF}}} \Omega(\tilde{H}_{\text{AF}}; \rho_{\text{AF}}) \right) \end{aligned}$$

$$\rho = \tilde{\rho}_{\text{AF}} = \rho_{\text{AF}}(\tilde{d}_0, \tilde{m}_1, \vec{e}; \mu)$$

$$\min_{\rho_{\text{AF}}} \Omega(\tilde{H}_{\text{AF}}; \rho_{\text{AF}}) = \Omega(\tilde{H}_{\text{AF}}; \tilde{\rho}_{\text{AF}}) = -\frac{1}{\beta} \ln \left(\text{Tr}(e^{-\beta \tilde{H}_{\text{AF}}}) \right)$$

$$\Omega(H; \rho_{\text{AF}}^*) = \min_{m_1} \max_{d_0} G_{\text{AF}}(d_0, m_1; \mu)$$

$$G_{\text{AF}}(d_0, m_1; \mu) = L^n \frac{U}{4} (m_1^2 - d_0^2) - \frac{1}{\beta} \ln \left(\text{Tr}(e^{-\beta H_{\text{AF}}}) \right)$$

$$\lim_{L \rightarrow \infty} L^{-n} G_{\text{AF}}(d_0, m_1; \mu) = \mathcal{G}(d_0, m_1; \mu)$$

$$\Omega(H; \rho_{\text{mixed}}) = w \Omega(H; \rho_{\text{AF}}) + (1 - w) \Omega(H; \rho_{\text{AF}}) + \Delta \Omega$$

$$\{c_l, c_j^\dagger\} = \delta_{l,j}, \{c_l, c_j\} = 0$$

$$|n_1,\ldots,n_{\mathcal{N}}\rangle:=(c_1^\dagger)^{n_1}\cdots(c_{\mathcal{N}}^\dagger)^{n_{\mathcal{N}}}|0\rangle$$

$$H=H_0+\sum_{I,J,K,L}v_{I,J,K,L}c_I^\dagger c_Jc_K^\dagger c_L$$

$$H_0=\sum_{I,J}t_{I,J}c_I^\dagger c_J$$

$$t_{I,J}=\overline{t_{J,I}},v_{I,J,K,L}=\overline{v_{L,K,J,I}}$$

$$k_i\in (2\pi/L)\mathbb{Z}, -\pi\leq k_i<\pi\;(i=1,\ldots,n).$$

$$c_{\sigma}(\mathbf{k})=\frac{1}{L^{n/2}}\sum_{\mathbf{x}}c_{\mathbf{x},\sigma}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$\sum_{\mathbf{x}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}=L^n\delta_{\mathbf{k},\mathbf{0}}$$

$$\delta_{\mathbf{k},\mathbf{0}}=\prod_{i=1}^n\delta_{k_i,0}$$

$$c_{\mathbf{x},\sigma}=\frac{1}{L^{n/2}}\sum_{\mathbf{k}}c_{\sigma}(\mathbf{k})\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$\sum_{\mathbf{k}}\sum_{\mathbf{k}\in\Lambda_L^*}$$

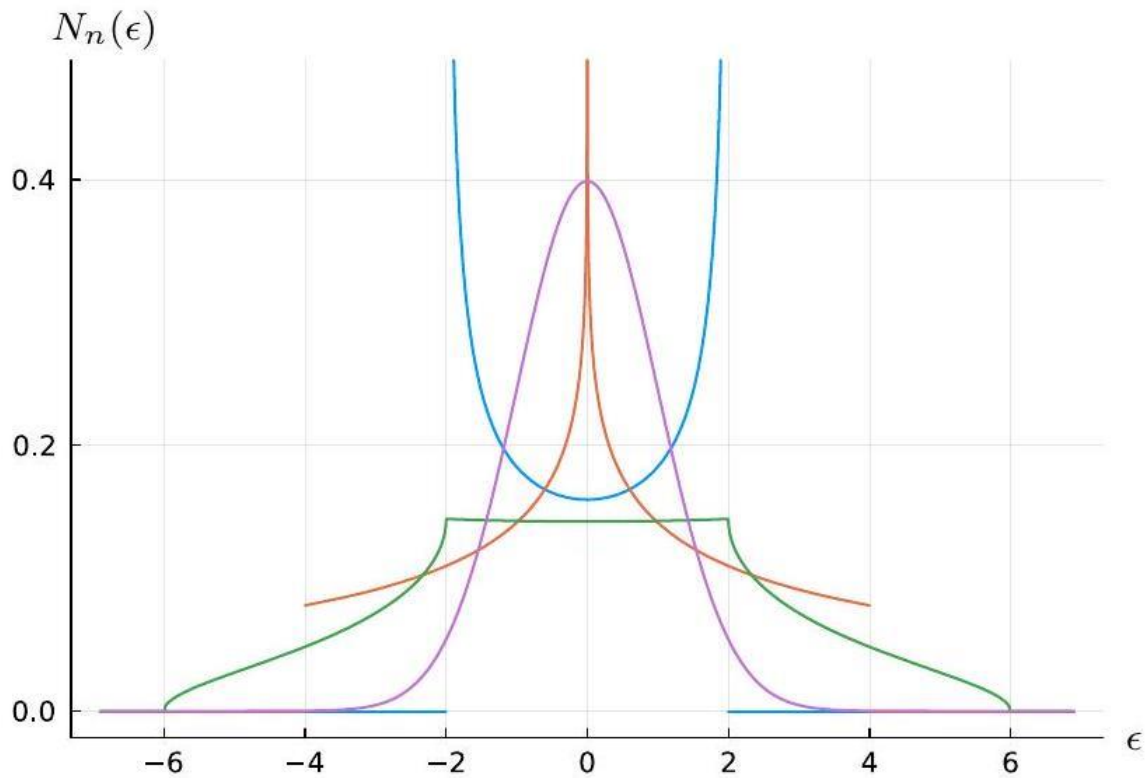
$$\lim_{L\rightarrow\infty}\frac{1}{L^n}\sum_{\mathbf{k}}g(\mathbf{k})=\int_{[-\pi,\pi]^n}\frac{d^n\mathbf{k}}{(2\pi)^n}g(\mathbf{k})$$

$$\int_{[-\pi,\pi]^n}\frac{d^n\mathbf{k}}{(2\pi)^n}g(\varepsilon_0(\mathbf{k}))=\int N_n(\epsilon)g(\epsilon)d\epsilon$$

$$c_{\mathbf{x},\sigma}\rightarrow (-1)^{\mathbf{x}}c_{\mathbf{x},\sigma}^\dagger,c_{\mathbf{x},\sigma}^\dagger\rightarrow (-1)^{\mathbf{x}}c_{\mathbf{x},\sigma}$$

$$n_{\mathbf{x},\sigma}-\frac{1}{2}\rightarrow -\Big(n_{\mathbf{x},\sigma}-\frac{1}{2}\Big)$$

$$c_{\mathbf{x},\sigma}^\dagger c_{\mathbf{y},\sigma}\rightarrow \pm c_{\mathbf{x},\sigma}^\dagger c_{\mathbf{y},\sigma}$$



$$N_1(\epsilon) = \frac{\theta(1 - |\epsilon/2t|)}{2t\pi\sqrt{1 - (\epsilon/2t)^2}}$$

$$N_{\infty}(\epsilon) = \frac{1}{\sqrt{2\pi}t^*}e^{-\frac{1}{2}(\epsilon/t^*)^2}.$$

$$\Omega(\alpha\rho_1+(1-\alpha)\rho_2)<\alpha\Omega(\rho_1)+(1-\alpha)\Omega(\rho_2)$$

$$\delta_v\Omega(\rho)=\left.\frac{d}{d\alpha}\Omega(\rho+\alpha v)\right|_{\alpha=0}$$

$$\delta_v\Omega(\rho)=\delta_v\mathrm{Tr}(f(\rho))=\mathrm{Tr}(f'(\rho)v)$$

$$f(x)=x\ln\left(x\right)\text{ of }x\in\left(0,1\right)$$

$$\rho=\sum_k\rho_k|k\rangle\langle k|\text{ with }\langle k\mid k'\rangle=\delta_{k,k'}$$

$$\rho_k=\langle k|\rho|k\rangle\approx\rho_k+\alpha\langle k|v|k\rangle$$

$$\begin{aligned}\mathrm{Tr}(f(\rho+\alpha v)-f(\rho))&\approx\sum_k[f(\rho_k+\alpha\langle k|v|k\rangle)-f(\rho_k)]\\&\approx\sum_k\alpha f'(\rho_k)\langle k|v|k\rangle=\alpha\sum_k\langle k|f'(\rho)v|k\rangle=\alpha\mathrm{Tr}(f'(\rho)v);\end{aligned}$$

$$\delta_v\Omega(\rho)=\mathrm{Tr}([H+(1/\beta)(\ln{(\rho)}+I)]v)$$

$$\delta_v\Omega(\rho)=0$$

$$H+(1/\beta)(\ln{(\rho)}+I)=cI$$

$$\rho = \mathrm{e}^{\beta c-1} \mathrm{e}^{-\beta H}$$

$$\rho^* = \mathrm{e}^{-\beta H}/\mathrm{Tr}(\mathrm{e}^{-\beta H}),$$

$$\begin{aligned} & \Omega(\rho^* + \alpha(\rho - \rho^*)) - \Omega(\rho^*) \\ &= \Omega(\alpha\rho + (1-\alpha)\rho^*) - \Omega(\rho^*) \\ &< \alpha\Omega(\rho) + (1-\alpha)\Omega(\rho^*) - \Omega(\rho^*) \\ &= \alpha[\Omega(\rho) - \Omega(\rho^*)] \end{aligned}$$

$$\delta_v\Omega(\rho^*) < \Omega(\rho) - \Omega(\rho^*)$$

$$\Omega(\alpha\rho_1+(1-\alpha)\rho_2)\leq \alpha\Omega(\rho_1)+(1-\alpha)\Omega(\rho_2)$$

$$\Omega(\rho^*)=\min_{\rho\in\mathcal{S}_c}\Omega(\rho)$$

$$\rho = w\rho_{\mathrm{AF}} + (1-w)\rho_{\mathrm{P}}$$

$$\Omega(\rho) = w\Omega(\rho_{\mathrm{AF}}) + (1-w)\Omega(\rho_{\mathrm{P}})$$

$$\rho = \sum_{i=1}^K \alpha_i \rho_i$$

$$\Omega(\rho) = \sum_{i=1}^K \alpha_i \Omega(\rho_i)$$

$$\alpha_K = 1 - \sum_{i=1}^{K-1} \alpha_i \frac{\partial \Omega}{\partial \alpha_i}$$

$$\Omega(\rho_i)=\Omega(\rho_j)\,(1\leq i<j\leq K).$$

$$h_{I,J}=\sum_K\left(U^\dagger\right)_{I,K}E_KU_{K,J},\left(U^\dagger\right)_{I,K}=\overline{U_{K,I}}$$

$$\tilde{c}_I = \sum_J U_{I,J} c_J$$

$$\begin{aligned} H_{\text{qf}} &= \sum_{I,J,K} \overline{U_{K,I}} E_K U_{K,J} \left(c_I^\dagger c_J - \frac{1}{2} \delta_{I,J} \right) \\ &= \sum_K E_K \left(\tilde{c}_K^\dagger \tilde{c}_K - \frac{1}{2} \right) \end{aligned}$$

$$(\tilde{c}_1^\dagger)^{n_1}\cdots(\tilde{c}_{\mathcal{N}}^\dagger)^{n_{\mathcal{N}}}|0\rangle$$

$$\begin{aligned}
\text{Tr}(e^{-\beta H_{\text{qf}}}) &= \sum_{n_1=0,1} \cdots \sum_{n_{\mathcal{N}}=0,1} \langle 0 | (\tilde{c}_{\mathcal{N}})^{n_{\mathcal{N}}} \cdots (\tilde{c}_1)^{n_1} \\
&\times \prod_K e^{-\beta E_K (\tilde{c}_K^\dagger \tilde{c}_K - \frac{1}{2})} (\tilde{c}_1^\dagger)^{n_1} \cdots (\tilde{c}_{\mathcal{N}}^\dagger)^{n_{\mathcal{N}}} | 0 \rangle \\
&= \prod_K \sum_{n_K=0,1} e^{-\beta E_K (n_K - \frac{1}{2})} \\
&= \prod_K (e^{\beta E_K/2} + e^{-\beta E_K/2})
\end{aligned}$$

$$\frac{1}{\beta} \ln Z_{\text{qf}} = \frac{1}{\beta} \ln \prod_K (e^{\beta E_K/2} + e^{-\beta E_K/2}) = \sum_K \text{Ln}_{\beta}(E_K)$$

$$\frac{\text{Tr}(e^{(A+\alpha B)B})}{\text{Tr}(e^{(A+\alpha B)})} = \frac{\partial}{\partial \alpha} \ln \text{Tr}(e^{(A+\alpha B)})$$

$$\frac{\partial}{\partial \alpha} \ln \text{Tr}(e^{(A+\alpha B)}) = \frac{1}{\text{Tr}(e^{(A+\alpha B)})} \frac{\partial}{\partial \alpha} \text{Tr}(e^{(A+\alpha B)})$$

$$\begin{aligned}
\frac{\partial}{\partial \alpha} \text{Tr}(e^{(A+\alpha B)}) &= \sum_{k=0}^{\infty} \frac{\text{Tr}\left(\frac{\partial}{\partial \alpha} (A + \alpha B)^k\right)}{k!} \\
&= \sum_{k=1}^{\infty} \frac{\text{Tr}((A + \alpha B)^{k-1} B)}{(k-1)!} \\
&= \text{Tr}\left(\sum_{k=0}^{\infty} \frac{(A + \alpha B)^k}{k!} B\right) = \text{Tr}(e^{(A+\alpha B)} B)
\end{aligned}$$

$$\gamma_{I,J} = \langle c_J^\dagger c_I \rangle$$

$$\gamma = \frac{1}{e^{\beta h} + 1} \Leftrightarrow h = \frac{1}{\beta} \ln (\gamma^{-1} - 1),$$

$$\gamma_{I,J} = \sum_K (U^\dagger)_{I,K} \gamma_K U_{K,J}$$

$$\gamma_K = 1/(e^{\beta E_K} + 1)$$

$$H_{\text{qf}} = \sum_K E_K (\tilde{c}_K^\dagger \tilde{c}_K - 1/2)$$

$$\text{Tr}(e^{-\beta H_{\text{qf}}}) = \prod_K \sum_{n_K=0,1} e^{-\beta E_K (n_K - \frac{1}{2})}$$

$$\begin{aligned}
& \text{Tr} \left(e^{-\beta H_{\text{q}}} \tilde{c}_I^\dagger \tilde{c}_J \right) = \sum_{n_1=0,1} \cdots \sum_{n_{\mathcal{N}}=0,1} \langle 0 | (\tilde{c}_{\mathcal{N}})^{n_{\mathcal{N}}} \cdots (\tilde{c}_1)^{n_1} \\
& \times \prod_K e^{-\beta E_K (\tilde{c}_K^\dagger \tilde{c}_K - \frac{1}{2})} \cdot \tilde{c}_I^\dagger \tilde{c}_J \cdot (\tilde{c}_1^\dagger)^{n_1} \cdots (\tilde{c}_{\mathcal{N}}^\dagger)^{n_{\mathcal{N}}} | 0 \rangle \\
& = \delta_{I,J} \prod_{K \neq I} \sum_{n_K=0,1} e^{-\beta E_K (n_K - \frac{1}{2})} \cdot \sum_{n_I=0,1} n_I e^{-\beta E_I (n_I - \frac{1}{2})} \\
& = \delta_{I,J} \text{Tr} (e^{-\beta H_{\text{HF}}}) \frac{\sum_{n_I=0,1} n_I e^{-\beta E_I (n_I - \frac{1}{2})}}{\sum_{n_I=0,1} e^{-\beta E_I (n_I - \frac{1}{2})}}
\end{aligned}$$

$$\begin{aligned}
\langle \tilde{c}_I^\dagger \tilde{c}_J \rangle &= \frac{\text{Tr} (e^{-\beta H_{\text{qf}}} \tilde{c}_I^\dagger \tilde{c}_J)}{\text{Tr} (e^{-\beta H_{\text{qf}}})} \\
&= \delta_{I,J} \frac{e^{-\beta E_I/2}}{e^{\beta E_I/2} + e^{-\beta E_I/2}} = \delta_{I,J} \frac{1}{e^{\beta E_I} + 1}
\end{aligned}$$

$$c_I = \sum_J (U^\dagger)_{I,J} \tilde{c}_J$$

$$\begin{aligned}
\gamma_{I,J} = \langle c_J^\dagger c_I \rangle &= \sum_{K,L} \overline{\underbrace{U_{J,K}^\dagger}_{U_{K,J}}} (U^\dagger)_{I,L} \frac{\langle \tilde{c}_K^\dagger \tilde{c}_L \rangle}{\delta_{K,L}/(e^{\beta E_K} + 1)} \\
&= \sum_K (U^\dagger)_{I,K} \frac{1}{e^{\beta E_K} + 1} U_{K,J}
\end{aligned}$$

$$\begin{aligned}
\langle \tilde{c}_I^\dagger \tilde{c}_K^\dagger \tilde{c}_L \tilde{c}_J \rangle &= \frac{\text{Tr} (e^{-\beta H_{\text{qf}}} \tilde{c}_I^\dagger \tilde{c}_K^\dagger \tilde{c}_J \tilde{c}_L)}{\text{Tr} (e^{-\beta H_{\text{qf}}})} \\
&= (\delta_{I,J} \delta_{K,L} - \delta_{I,L} \delta_{K,J}) \frac{1}{e^{\beta E_I} + 1} \frac{1}{e^{\beta E_K} + 1},
\end{aligned}$$

$$\text{Tr}(\rho_{\text{qf}} c_J^\dagger c_I) = \gamma_{I,J} = \text{Tr}(\rho c_J^\dagger c_I)$$

$$\gamma = \sum_k \gamma_k |k\rangle \langle k|$$

$$\langle k | k' \rangle = \delta_{k,k'}$$

$$\gamma_k = \langle k | \gamma | k \rangle \text{ for } k, k' = 1, \dots, \mathcal{N}$$

$$\gamma^{(\epsilon)} = \gamma + \epsilon \sum_{k: \gamma_k=0} |k\rangle \langle k|$$

$$\langle H_{\text{qf}} \rangle = \sum_{I,J} h_{I,J} \left(\gamma_{J,I} - \frac{1}{2} \delta_{I,J} \right) = \text{tr} \left(h \left(\gamma - \frac{1}{2} \right) \right)$$

$$\left(n_{\uparrow}-\frac{1}{2}\right)\left(n_{\downarrow}-\frac{1}{2}\right)=\frac{1}{4}(n+\vec{e}\cdot\vec{s}-1)(n-\vec{e}\cdot\vec{s}-1)$$

$$n_{\uparrow,\downarrow}=\frac{1}{2}(n\pm s^z)$$

$$(n+s^z-1)(n-s^z-1)=(n+\vec{e}\cdot\vec{s}-1)(n-\vec{e}\cdot\vec{s}-1)$$

$$(\vec{e}\cdot\vec{s})^2=(s^z)^2$$

$$(s^x)^2=(s^z)^2,(s^y)^2=(s^z)^2\\ \{s^x,s^y\}=\{s^y,s^z\}=\{s^z,s^x\}=0$$

$$(\vec{e}\cdot\vec{s})^2=(e^xs^x+e^ys^y+e^zs^z)^2$$

$$H_{\rm HF}=H_0+\frac{U}{2}\sum_{\bf k}\left(\tilde{d}_0(-{\bf k})(\tilde{n}_{\bf k}-L^{n/2}\delta_{{\bf k},0})-\tilde{\vec{m}}(-{\bf k})\cdot\tilde{\vec{s}}_{\bf k}\right)$$

$$\tilde{n}_{\mathbf{k}}=\frac{1}{L^{n/2}}\sum_{\mathbf{x}}n_{\mathbf{x}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}},\tilde{d}(\mathbf{k})=\frac{1}{L^{n/2}}\sum_{\mathbf{x}}d(\mathbf{x})\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$\frac{U}{2}\langle\tilde{n}_{\mathbf{k}}\rangle=-\frac{1}{\beta}\frac{\partial}{\partial\tilde{d}(-\mathbf{k})}\ln Z_{\rm HF}\;(\mathbf{k}\neq\mathbf{0})\\ \frac{U}{2}\langle\tilde{s}_{\mathbf{k}}\rangle=\frac{1}{\beta}\frac{\partial}{\partial\tilde{\vec{m}}(-\mathbf{k})}\ln Z_{\rm HF}$$

$$Z_{\rm HF}=\mathrm{Tr}(\mathrm{e}^{-\beta H_{\rm HF}})$$

$$\tilde{d}(\mathbf{k})=d_0L^{n/2}\delta_{\mathbf{k},0}$$

$$\tilde{\vec{m}}(\mathbf{k})=m_1\vec{e}L^{n/2}\delta_{\mathbf{k},\mathbf{Q}}$$

$$\langle \tilde{n}_{\mathbf{k}} \rangle = \delta_{\mathbf{k},0} \langle \tilde{n}_0 \rangle, \langle \tilde{s}_{\mathbf{k}} \rangle = \delta_{\mathbf{k},\mathbf{Q}} \vec{e} \langle \vec{e} \cdot \tilde{\vec{s}}_{\mathbf{Q}} \rangle$$

$$\langle n_{\mathbf{x}} \rangle = a \text{ and } \langle \vec{s}_{\mathbf{x}} \rangle = (-1)^{\mathbf{x}} \vec{e} b$$

$$f(x,y)=\sin{(x+y)}\colon \min_{x\in\mathbb{R}}\max_{y\in\mathbb{R}}\sin{(x+y)}=1$$

$$\max_{y\in\mathbb{R}}\min_{x\in\mathbb{R}}\sin{(x+y)}=-1$$

$$\min_{\rho_{\mathrm{qf}}}\min_{\overline{\boldsymbol{m}}}\max_{\boldsymbol{d}}A(\boldsymbol{d},\overline{\boldsymbol{m}},\rho_{\mathrm{qf}})=\min_{\overline{\boldsymbol{m}}}\max_{\boldsymbol{d}}\min_{\rho_{\mathrm{qf}}}A(\boldsymbol{d},\overline{\boldsymbol{m}},\rho_{\mathrm{qf}})$$

$$A(\boldsymbol{d},\overline{\boldsymbol{m}},\rho_{\mathrm{qf}})\!=\!\frac{U}{4}\sum_{\mathbf{x}}\left(\overline{\boldsymbol{m}}(\mathbf{x})^2-d(\mathbf{x})^2\right)+\Omega(H_{\mathrm{HF}},\rho_{\mathrm{qf}})\\ \!=\!\frac{U}{4}\sum_{\mathbf{x}}\left(\overline{\boldsymbol{m}}(\mathbf{x})^2-d(\mathbf{x})^2\right)\\ \!+\!\mathrm{Tr}\!\left(\rho_{\mathrm{qf}}\!\left(H_0\!+\!\frac{U}{2}\sum_{\mathbf{x}}\left(d(\mathbf{x})(n_{\mathbf{x}}-1)-\overline{\boldsymbol{m}}(\mathbf{x})\cdot\vec{s}_{\mathbf{x}}\right)\right)\right)\\ \!+\!\frac{1}{\beta}\mathrm{Tr}\left(\rho_{\mathrm{qf}}\ln\left(\rho_{\mathrm{qf}}\right)\right),$$

$$H_{\text{HF}} = H_{\text{HF}}(\mathbf{d}, \overline{\mathbf{m}})$$

$$\mathbf{d} = (d(\mathbf{x})) \in \mathbb{R}^{L^n}$$

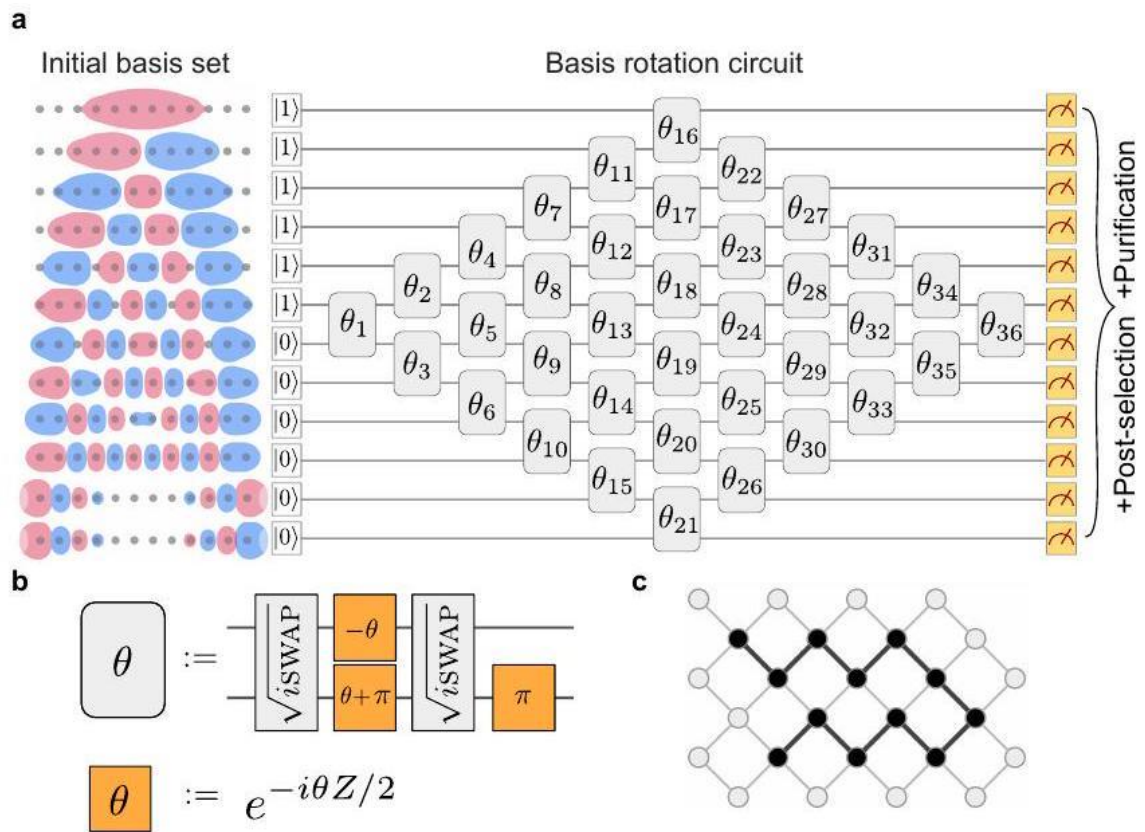
$$\overline{\mathbf{m}} = (\overline{m}(\mathbf{x})) \in \mathbb{R}^{3L^n}$$

$$\min_{\rho_{\text{qf}}} \max_{\mathbf{d}} A(\mathbf{d}, \overline{\mathbf{m}}, \rho_{\text{qf}}) \geq \max_{\mathbf{d}} \min_{\rho_{\text{qf}}} A(\mathbf{d}, \overline{\mathbf{m}}, \rho_{\text{qf}}),$$

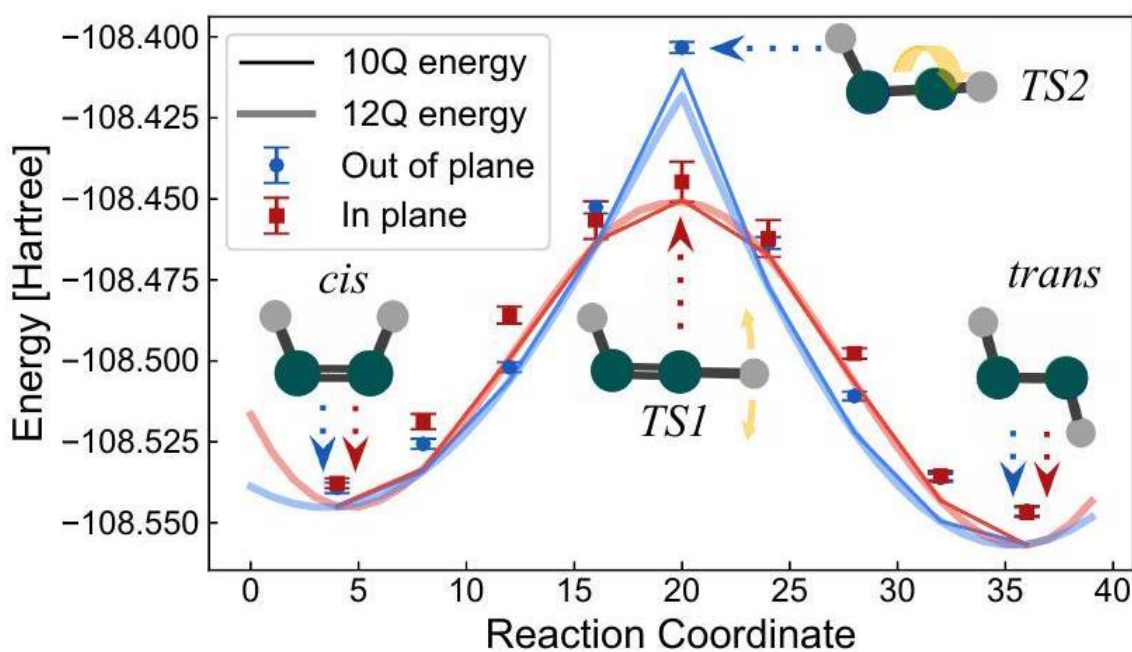
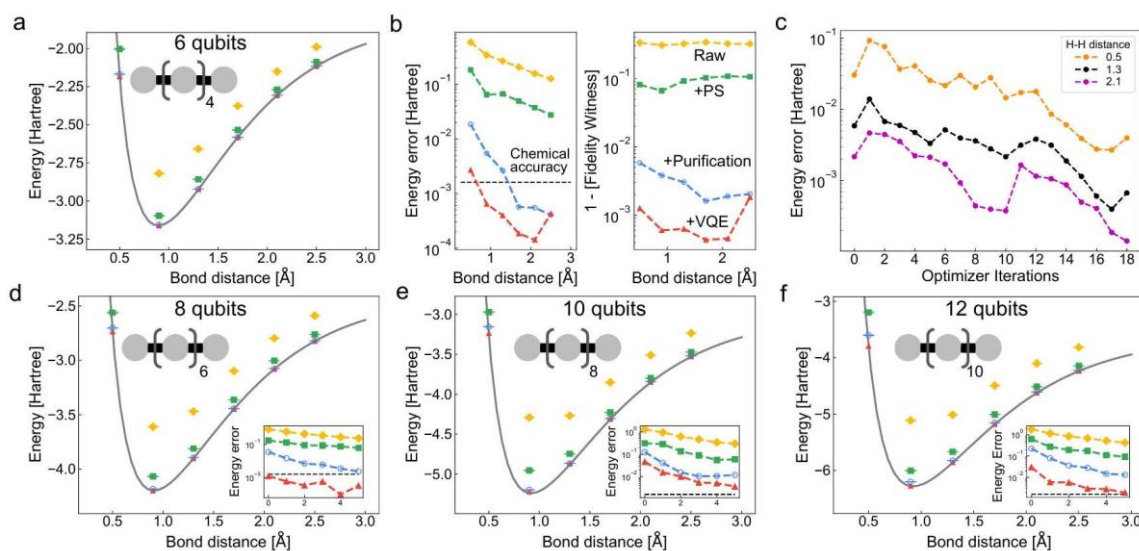
$$\mathcal{S} = \cap_{\{v \in \mathbb{C}^N : \langle v | v \rangle = 1\}} \mathcal{S}_v$$

$$\rho_{\text{HF}} = \text{e}^{-\beta H_{\text{HF}}} / \text{Tr}(\text{e}^{-\beta H_{\text{HF}}}) \in \mathcal{S}_{\text{qF}}$$

$$\tilde{\varphi}_p(r) = \sum_{q=1}^N [e^{\kappa}]_{pq} \varphi_q(r),$$



$$|\psi_{\text{HF}}\rangle = |\psi_{\kappa^*}\rangle \; \kappa^* = \text{argmin}_{\kappa} \langle \psi_{\kappa} | H | \psi_{\kappa} \rangle. \tag{3}$$



$$\langle a_p^\dagger a_q^\dagger a_r a_s \rangle = \langle a_p^\dagger a_s \rangle \langle a_q^\dagger a_r \rangle - \langle a_q^\dagger a_s \rangle \langle a_p^\dagger a_r \rangle.$$

$$\langle \psi | [[H, G], G] | \psi \rangle$$

$$|\psi(r_1, \dots, r_n)\rangle = (n!)^{-1/2} A_n(\chi_1(r_1) \dots \chi_n(r_n))$$

$$\chi_i(r) = \sum_j c_i^j \phi_j(r)$$

$$\langle \delta \psi | H | \psi \rangle = 0$$

$$\langle r \mid \psi \rangle = \langle r \mid \prod_{i=1}^n a_i^\dagger \mid 0 \rangle = \frac{1}{\sqrt{n!}} \text{Det} \left[\begin{pmatrix} \chi_1(r_1) & \cdots & \chi_1(r_n) \\ \vdots & \ddots & \vdots \\ \chi_n(r_1) & \cdots & \chi_n(r_n) \end{pmatrix} \right]$$

$$\langle \delta \psi | = \langle \psi | a_i^\dagger a_a \zeta$$

$$\langle \psi | a_i^\dagger a_a H | \psi \rangle = 0$$

$$[a_p^\dagger a_q, a_r^\dagger a_s] = \delta_{q,r} a_p^\dagger a_s - \delta_{p,s} a_r^\dagger a_s$$

$$\kappa=\sum_{p,q}\kappa_{p,q}a_p^\dagger a_q$$

$$[\kappa,a_p^\dagger]=a_q^\dagger\kappa_{p,q}\,,\,[\kappa,a_p]=a_q\kappa_{p,q}^*$$

$$e^K a_p^\dagger e^{-K} = \sum_q a_q^\dagger u_{q,p}, \, e^K a_p e^{-K} = \sum_q a_q u_{q,p}^*$$

$$u=e^{\kappa}$$

$$|\phi(\kappa)\rangle=e^K a_1^\dagger e^{-K} \ldots e^K a_n^\dagger e^{-K} |0\rangle=e^K |\psi\rangle.$$

$$E(\kappa)=\langle\phi(\kappa)|H|\phi(\kappa)\rangle=\langle\psi|e^KHe^{-K}|\psi\rangle.$$

$$^1D_i^j=\langle\phi|a_j^\dagger a_i|\phi\rangle$$

$$^2D_{ij}^{pq}=\langle\phi|a_p^\dagger a_q^\dagger a_j a_i|\phi\rangle=\,^1D_i^p\,^1D_j^q-\,^1D_i^q\,^1D_j^p.$$

$$E(\kappa)=\sum_{ij}h_{ij}\langle\phi(\kappa)|a_i^\dagger a_j|\phi(\kappa)\rangle+\sum_{ijkl}V_{ijkl}\langle\phi(\kappa)|a_i^\dagger a_j^\dagger a_k a_l|\phi(\kappa)\rangle=\sum_{ij}h_{ij}\,^1D_j^i+\sum_{ijkl}V_{ijkl}\,^2D_{lk}^{ij}$$

$$h_{i,j}=\int dr\chi_i^*(r)\left(-\nabla^2(r)+\sum_A\frac{Z_A}{|r-R_A|}\right)\chi_j(r)\\ V_{l,k}^{i,j}=\frac{1}{2}\iint dr_1dr_2\chi_i^*(r_1)\chi_j^*(r_2)(|r_1-r_2|^{-1})\chi_k(r_2)\chi_l(r_1)$$

$$^1\tilde{D}_q^p=\langle\phi|e^{-K}a_p^\dagger e^K e^{-K}a_p e^K|\phi\rangle=\langle\phi|\sum_ju_{p,i}a_i^\dagger\sum_{q,j}u_{q,j}^*a_j|\phi\rangle=\sum_{ij}u_{p,i}u_{q,j}^*\langle\phi|a_i^\dagger a_j|\phi\rangle.$$

$$U(e^\kappa)=e^K\,K=\sum_{i,j}\kappa_{i,j}a_i^\dagger a_j\,\kappa^\dagger=-\kappa$$

$$R(u)_{pq}=e^{\log|u|_{pq}(a_p^\dagger a_q-a_q^\dagger a_p)}$$

$$U(e^\kappa)\cdot U(e^{\kappa'})=U(e^\kappa\cdot e^{\kappa'})$$

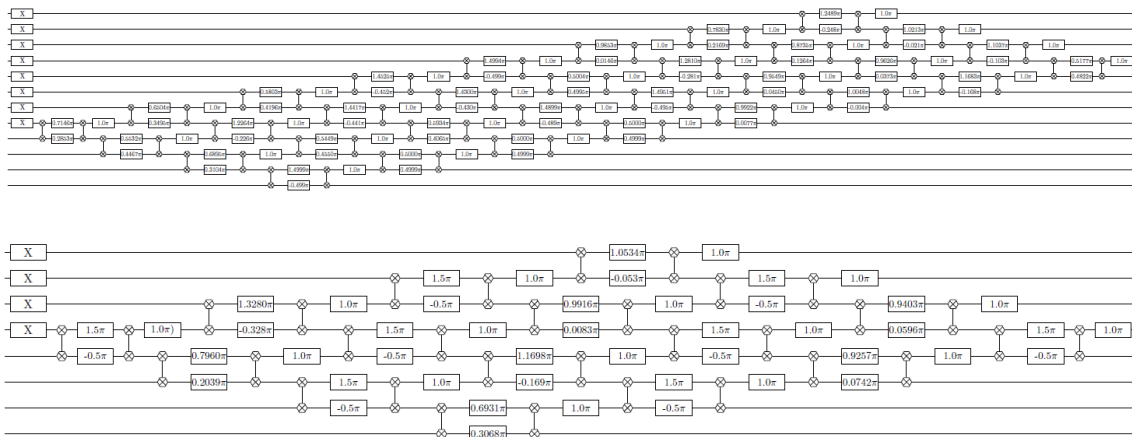
$$R_{pq}(\theta)U(u)=U(r_{pq}(\theta)u)$$

$$r(\theta)_{p,q} = \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \dots & \cos(\theta) & \dots & -\sin(\theta) & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & \sin(\theta) & \dots & \cos(\theta) & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix}$$

$$\prod_k R_k(\theta_k) U(u) = \sum_p e^{-i\phi_p a_p^\dagger a_p} = \sum_p e^{-i\phi_p |p\rangle\langle p|}$$

$$|\psi(\kappa)\rangle = \prod_{i=1}^{\eta} \tilde{a}_i^\dagger |\text{vac}\rangle = \prod_{i=1}^{\eta} e^{-K} \tilde{a}_i^\dagger e^K |\text{vac}\rangle = \prod_{i=1}^{\eta} \sum_p [e^\kappa]_{i,p} a_p^\dagger |\text{vac}\rangle$$

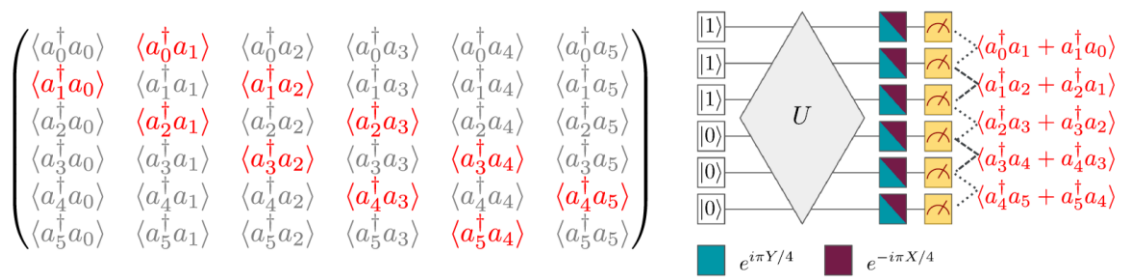
$$\prod_{i=1}^{\eta} \sum_{j=1}^{\eta} V_{i,j} \tilde{a}_i^\dagger |\text{vac}\rangle = \det[V] \prod_{i=1}^{\eta} \tilde{a}_i^\dagger |\text{vac}\rangle$$



$$\langle a_i^\dagger a_i \rangle = \frac{I - \langle Z_i \rangle}{2} = \langle M_i \rangle$$

$$\begin{pmatrix} \langle a_0^\dagger a_0 \rangle & \langle a_0^\dagger a_1 \rangle & \langle a_0^\dagger a_2 \rangle & \langle a_0^\dagger a_3 \rangle & \langle a_0^\dagger a_4 \rangle & \langle a_0^\dagger a_5 \rangle \\ \langle a_1^\dagger a_0 \rangle & \langle a_1^\dagger a_1 \rangle & \langle a_1^\dagger a_2 \rangle & \langle a_1^\dagger a_3 \rangle & \langle a_1^\dagger a_4 \rangle & \langle a_1^\dagger a_5 \rangle \\ \langle a_2^\dagger a_0 \rangle & \langle a_2^\dagger a_1 \rangle & \langle a_2^\dagger a_2 \rangle & \langle a_2^\dagger a_3 \rangle & \langle a_2^\dagger a_4 \rangle & \langle a_2^\dagger a_5 \rangle \\ \langle a_3^\dagger a_0 \rangle & \langle a_3^\dagger a_1 \rangle & \langle a_3^\dagger a_2 \rangle & \langle a_3^\dagger a_3 \rangle & \langle a_3^\dagger a_4 \rangle & \langle a_3^\dagger a_5 \rangle \\ \langle a_4^\dagger a_0 \rangle & \langle a_4^\dagger a_1 \rangle & \langle a_4^\dagger a_2 \rangle & \langle a_4^\dagger a_3 \rangle & \langle a_4^\dagger a_4 \rangle & \langle a_4^\dagger a_5 \rangle \\ \langle a_5^\dagger a_0 \rangle & \langle a_5^\dagger a_1 \rangle & \langle a_5^\dagger a_2 \rangle & \langle a_5^\dagger a_3 \rangle & \langle a_5^\dagger a_4 \rangle & \langle a_5^\dagger a_5 \rangle \end{pmatrix} \begin{matrix} |0\rangle \\ |0\rangle \end{matrix} = \begin{matrix} x & \langle a_0^\dagger a_0 \rangle \\ -x & \langle a_1^\dagger a_1 \rangle \\ -|x| & \langle a_2^\dagger a_2 \rangle \\ -|0\rangle & \langle a_3^\dagger a_3 \rangle \end{matrix}$$

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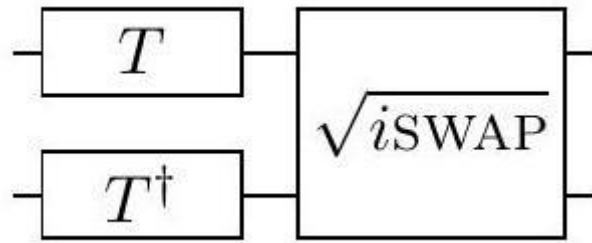


$$\langle a_i^\dagger a_{i+1} \rangle = \langle a_{i+1}^\dagger a_i \rangle^*$$

$$a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i 2\Re \langle a_i^\dagger a_{i+1} \rangle$$

$$\langle a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i \rangle = \frac{1}{2} (\langle X_i X_{i+1} \rangle + \langle Y_i Y_{i+1} \rangle) = 2\Re \langle a_i^\dagger a_{i+1} \rangle$$

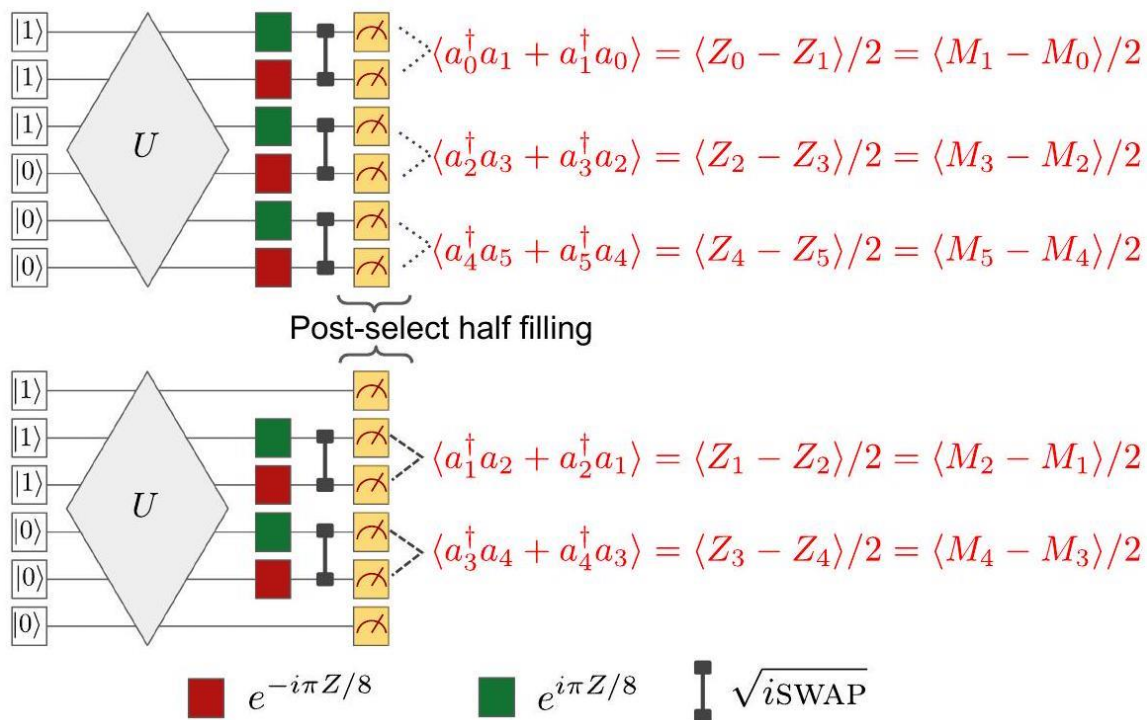
$$\{\Re(a_1^\dagger a_3 + a_3^\dagger a_1), \Re(a_3^\dagger a_0 + a_0^\dagger a_3), \Re(a_0^\dagger a_5 + a_5^\dagger a_0), \Re(a_5^\dagger a_2 + a_2^\dagger a_5), \Re(a_2^\dagger a_4 + a_4^\dagger a_2)\}.$$



$$\text{FSWAP} = a_p^\dagger a_q + a_q^\dagger a_p - a_p^\dagger a_p - a_q^\dagger a_q.$$

$$U_M \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} U_M^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\langle U_m(a_a^\dagger a_{a+1} + a_{a+1}^\dagger a_a)U_m^\dagger \rangle = \left\langle U_m \frac{1}{2} (X_a X_{a+1} + Y_a Y_{a+1}) U_m^\dagger \right\rangle = \frac{1}{2} \langle Z_a - Z_{a+1} \rangle = \frac{1}{2} (M_{a+1} - M_a).$$



$$\text{Cov}\left[\frac{1}{2}(Z_a - Z_b), \frac{1}{2}(Z_p - Z_q)\right] = \frac{1}{4}(\text{Cov}[Z_a, Z_p] - \text{Cov}[Z_a, Z_q] - \text{Cov}[Z_b, Z_p] + \text{Cov}[Z_b, Z_q])$$

$$\text{Cov}[a_i^\dagger a_j + a_j^\dagger a_i, a_p^\dagger a_q + a_q^\dagger a_p]_\psi = D_q^i \delta_p^j - D_q^i D_j^p + D_p^i \delta_q^j - D_p^i D_j^q + D_q^j \delta_p^i - D_q^j D_i^p + D_p^j \delta_q^i - D_p^j D_i^q.$$

$$\left\langle a_{\sigma(i)}^\dagger a_{\sigma(i+1)} \right\rangle$$

$$n^{(\omega)} = \sum_{j=1}^L \left[(1-\omega_j)n_j + \omega_j(\mathbb{I} - n_j) \right] = \sum_{j=1}^L \left[n_j - \omega_j n_j + \omega_j \mathbb{I} - \omega_j n_j \right] = \sum_{j=1}^L \left[n_j + \omega_j \mathbb{I} - 2\omega_j n_j \right]$$

$$\mathcal{W} = U(\mathbb{I} - n^{\omega})U^{\dagger}$$

$$\text{Tr}[U\rho_pU^\dagger a_i^\dagger a_j] = [\mathbf{u}D\mathbf{u}^\dagger]_{i,j}$$

$$F_{\mathcal{W}}(\rho_p) = 1 - \sum_{j=1}^L \left([\mathbf{u}^\dagger D \mathbf{u}]_{j,j} + \omega_j - 2\omega_j [\mathbf{u}^\dagger D \mathbf{u}]_{j,j} \right)$$

$$|\langle \psi_u \mid \psi_v \rangle|^2 = |\det(v^\dagger u)|^2$$

$$\min_{\text{Tr}[D]=\eta, D\geq 0, D^2=D} \|D-\tilde{D}\|$$

$$D_{n+1}=3D_n^2-2D_n^3$$

$$P_k=1+\Delta$$

$$\mu_k = \mathbb{E}(\Delta^k)$$

$$\mathbb{E}(P_{k+1}) = \mathbb{E}(3P_k^2 - 2P_k^3) = 1 - 3\sigma^2 - 2\mu^3$$

$$\mathbb{E}(P_{k+1}^2) = 1 - 6\sigma^2 - 4\mu_3 + 9\mu_4 + 12\mu_5 + 4\mu_6$$

$$\mathbb{V}(P_{k+1}) = \mathbb{E}(P_{k+1}^2) - \mathbb{E}(P_{k+1})^2 = 9(\mu_4 - \sigma^4) + 12(\mu_5 - \sigma^2\mu_3) + 4(\mu_6 - \mu_3^2)$$

$$\mathbb{V}(P_{k+1}) \leq 9\sigma^4(\alpha_4 - 1) + 12|\sigma|^5(\alpha_5 + \alpha_3) + 4|\sigma|^6\alpha_6$$

$$\mathbb{V}(P_{k+1}) \leq 9\sigma^4(\alpha_4 - 1) + 4|\sigma|^5(\alpha_6 + 3\alpha_5 + 3\alpha_3)$$

$$9\sigma^4(\alpha_4 - 1) + 4|\sigma|^5(\alpha_6 + 3\alpha_5 + 3\alpha_3) \leq \sigma^2$$

$$\sigma^2 \leq \frac{1}{9(\alpha_4 - 1)} \left(1 - \frac{\beta(-\beta + \sqrt{\beta^2 + 36\alpha_4 - 36})}{18(\alpha_4 - 1)} \right)$$

$$\beta = 4(\alpha_6 + 3\alpha_5 + 3\alpha_3)$$

$$\alpha_{2j+1} = 0 \forall j, \alpha_4 = 3, \alpha_6 = 15$$

$$\mathbb{V}(P_{k+1}) \leq 18\sigma^4 + 12\sigma^6$$

$$\sigma^2 \leq \frac{-3}{20} + \frac{\sqrt{564}}{120} \approx 0.048$$

$$|\lambda(\rho) - \lambda(\rho + sE)| \leq s\|E\|$$

$$\mathbb{E}((\lambda(\rho) - \lambda(\rho + E))^2) \leq \mathbb{E}\left(\sum_{i,j} [E^2]_{i,j}\right) \leq M\sigma_M^2$$

$$\mathbb{V}(\lambda(\rho + E)) \leq M\sigma_M^2$$

$$\sigma_M^2 \leq \frac{1}{M} \left(\frac{-3}{20} + \frac{\sqrt{564}}{120} \right)$$

$$\langle \nu(j-1) | \lambda(j) \rangle = \frac{1}{R} \frac{\langle \nu(j-1) | E | \lambda(j-1) \rangle}{\nu(j-1) - \lambda(j-1)} + O(1/R^2)$$

$$\begin{aligned}
\sum_{\nu \neq \lambda} |\langle \nu(j-1) | \lambda(j) \rangle|^2 &\leq \sum_{\nu \neq \lambda} \frac{1}{R^2} \frac{|\langle \nu(j-1) | E | \lambda(j-1) \rangle|^2}{(\lambda(j-1) - \nu(j-1))^2} + O(1/R^3) \\
&\leq \sum_{\nu \neq \lambda} \frac{1}{\gamma^2(j-1)R^2} |\langle \nu(j-1) | E | \lambda(j-1) \rangle|^2 + O(1/R^3) \\
&= \sum_{\nu \neq \lambda} \frac{1}{\gamma^2(j-1)R^2} \langle \lambda(j-1) | E | \nu(j-1) \rangle \langle \nu(j-1) | E | \lambda(j-1) \rangle + O(1/R^3) \\
&= \frac{1}{\gamma^2(j-1)R^2} (\langle \lambda(j-1) | E^2 | \lambda(j-1) \rangle - (\langle \lambda(j-1) | E | \lambda(j-1) \rangle)^2) + O(1/R^3) \\
&\leq \frac{\|E^2\|}{\gamma^2(j-1)R^2} + O(1/R^3)
\end{aligned}$$

$$|\langle \lambda(j-1) | \lambda(j) \rangle - 1|^2 \leq \frac{\|E^2\|}{\gamma^2(j-1)R^2} + O(1/R^3)$$

$$\left| |\lambda(j)\rangle - |\lambda(j-1)\rangle \right| \leq \frac{\sqrt{2\|E^2\|}}{\gamma(j-1)R} + O(1/R^2)$$

$$\left| |\lambda(R)\rangle - |\lambda(0)\rangle \right| \leq \sum_{j=1}^R \left| |\lambda(j)\rangle - |\lambda(j-1)\rangle \right| \leq \sum_{j=1}^R \frac{\sqrt{2\|E^2\|}}{\gamma(j-1)R} + O(1/R)$$

$$\lim_{R \rightarrow \infty} \sum_{j=1}^R \frac{\sqrt{2\|E^2\|}}{\gamma(j-1)R} + O(1/R) \leq \frac{\sqrt{2\|E^2\|}}{\gamma_{\min}} = \frac{\sqrt{2}\|E\|}{\gamma_{\min}}.$$

$$\gamma_{\min} \geq 1 - 2\|E\|$$

$$\| |\lambda(\rho)\rangle - |\lambda(\rho + E)\rangle \| \leq \sqrt{2}\|E\|(1 + 4\|E\|) \leq 2\sqrt{2}\|E\|$$

$$\mathbb{V}(|\lambda(\rho)\rangle - |\lambda(\rho + E)\rangle) \leq 8M\sigma_M^2$$

$$\sigma_M^2 = \frac{\epsilon^2}{8M}$$

$$N_{\text{samp}} \geq \frac{\epsilon}{2\sqrt{2M}}$$

$$\mathbb{V}(\|E\|) \leq M\sigma_M^2$$

$$P \leq 16M\sigma_M^2 \sim 2\epsilon^2$$

$$\sqrt{i\text{SWAP}} \approx \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & e^{i\pi/24} \end{pmatrix} = \text{CPHASE}(\pi/24)\sqrt{i\text{SWAP}}$$

$$U_1 = \text{diag}(1,1,1,e^{-i\phi})\sqrt{i\text{SWAP}}$$

$$U_2 = \text{diag}(1, e^{i\phi/2}, e^{i\phi/2}, 1) \sqrt{i\text{SWAP}}.$$

$$\text{diag}(1, 1, 1, e^{-i\phi}) \approx e^{-i\phi} \times \left(II + \frac{i\phi}{4} IZ + \frac{i\phi}{4} ZI - \frac{i\phi}{4} ZZ \right),$$

$$\text{Err}_1 \approx 3 \left(\frac{\phi}{4} \right)^2 = \frac{3}{16} \phi^2.$$

$$\text{diag}(1, e^{i\phi/2}, e^{i\phi/2}, 1) \approx e^{i\phi/4} \left(II - \frac{i\phi}{4} ZZ \right)$$

$$\text{Err}_2 \approx \frac{1}{16} \phi^2.$$

$$\text{Rz}(\theta, \delta\alpha) = e^{-iZ\theta(1+\delta\alpha)/2}$$

$$G(\theta, \delta\alpha) = e^{\theta(1+\delta\alpha)(a_i^\dagger a_j - a_j^\dagger a_i)}$$

$$G(\theta) = \sqrt{i\text{SWAP}_{i,j}}^\dagger e^{-i\theta(1+\delta\alpha)Z_i/2} e^{i\theta(1+\delta\alpha)Z_j/2} \sqrt{i\text{SWAP}_{i,j}}$$

$$G(-\theta, \delta\alpha, i, j) a_r^\dagger G(\theta, \delta\alpha, i, j) = \begin{cases} a_i^\dagger \cos(\theta(1+\delta\alpha)) + a_j^\dagger \sin(\theta(1+\delta\alpha)) & \text{if } r = i \\ a_j^\dagger \cos(\theta(1+\delta\alpha)) - a_i^\dagger \sin(\theta(1+\delta\alpha)) & \text{if } r = j \\ a_r^\dagger & \text{if } r \neq i \& r \neq j \end{cases}$$

$$G(-\theta, \delta\alpha, i, j) a_s G(\theta, \delta\alpha, i, j) = \begin{cases} a_i \cos(\theta(1+\delta\alpha)) + a_j \sin(\theta(1+\delta\alpha)) & \text{if } s = i \\ a_j \cos(\theta(1+\delta\alpha)) - a_i \sin(\theta(1+\delta\alpha)) & \text{if } s = j \\ a_s & \text{if } s \neq i \& s \neq j \end{cases}$$

$$\rho(\delta\alpha) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\delta\alpha)^2}{2\sigma^2}}$$

$$\int_{-\infty}^{\infty} \rho(\delta\alpha, \sigma) G(-\theta, \delta\alpha, i, j) a_r^\dagger G(\theta, \delta\alpha, i, j) d\delta\alpha = \begin{cases} a_i^\dagger \cos(\theta) e^{-\frac{\theta^2\sigma^2}{2}} + a_j^\dagger \sin(\theta) e^{-\frac{\theta^2\sigma^2}{2}} & \text{if } r = i \\ a_j^\dagger \cos(\theta) e^{-\frac{\theta^2\sigma^2}{2}} - a_i^\dagger \sin(\theta) e^{-\frac{\theta^2\sigma^2}{2}} & \text{if } r = j \\ a_r^\dagger & \text{if } r \neq i \& r \neq j \end{cases}$$

$$\int_{-\infty}^{\infty} \rho(\delta\alpha, \sigma) G(-\theta, \delta\alpha, i, j) a_s G(\theta, \delta\alpha, i, j) d\delta\alpha = \begin{cases} a_i \cos(\theta) e^{-\frac{\theta^2\sigma^2}{2}} + a_j \sin(\theta) e^{-\frac{\theta^2\sigma^2}{2}} & \text{if } s = i \\ a_j \cos(\theta) e^{-\frac{\theta^2\sigma^2}{2}} - a_i \sin(\theta) e^{-\frac{\theta^2\sigma^2}{2}} & \text{if } s = j \\ a_s & \text{if } s \neq i \& s \neq j \end{cases}$$

$$Z = \sum_{i < b} c_{b,i} (a_b^\dagger a_i - a_i^\dagger a_b)$$

$$\frac{dE}{dc_{b,i}} = \langle \phi_0 | \frac{de^{-Z}}{dc_{b,i}} H e^Z | \phi_0 \rangle + \langle \phi_0 | e^{-Z} H \frac{de^Z}{dc_{b,i}} | \phi_0 \rangle$$



$$\frac{dE}{dc_{b,i}} = \langle \phi_0 | e^{-Z} [H, \nabla f(Z)_{c_{b,i}}] e^Z | \phi_0 \rangle$$

$$U(c_{b,i}) = e^{\sum_{b,i} c_{b,i} E_{b,i}^-} = e^{\sum_{b,i} c_{b,i} (a_b^\dagger a_i - a_i^\dagger a_b)}$$

$$\frac{dU(\mathbf{c})}{dc_{b,i}} = \left[\int_0^1 dx e^{x \sum_{b,i} c_{b,i} E_{b,i}^-} E_{b,i}^- e^{-x \sum_{b,i} c_{b,i} E_{b,i}^-} \right] e^{\sum_{b,i} c_{b,i} E_{b,i}^-}$$

$$\mathrm{ad}\left(\sum_{b',i'} c_{b',i'} E_{b',i'}^- \right) (E_{b,i}^-)$$

$$\sum_{b',i'} c_{b',i'} E_{b',i'}^-$$

$$i\mathbf{C} = i\sum_r \lambda_r \tilde{a}_r^\dagger \tilde{a}_r$$

$$\tilde{a}_p = \sum_q u_{p,q}^* a_q, \tilde{a}_p^\dagger = \sum_q u_{p,q} a_q^\dagger$$

$$\mathbf{Y} = \sum_{k,l} Y_{kl} \tilde{a}_k^\dagger \tilde{a}_l$$

$$Y_{kl} = (U^\dagger E_{b,i}^- U)_{k,l}$$

$$\begin{aligned} \mathrm{ad}\left(\sum_{b',i'} c_{b',i'} E_{b',i'}^- \right) (E_{b,i}^-) &= \sum_{rkl} i\lambda_r Y_{kl} [\tilde{a}_r^\dagger \tilde{a}_r, \tilde{a}_k^\dagger \tilde{a}_l] \\ &= \sum_{rkl} i\lambda_r Y_{kl} (\tilde{a}_r^\dagger \tilde{a}_l \delta_k^r - \tilde{a}_k^\dagger \tilde{a}_r \delta_r^l) \\ &= i \sum_{kl} (\lambda_k - \lambda_l) Y_{kl} \tilde{a}_k^\dagger \tilde{a}_l \end{aligned}$$

$$\mathrm{ad}\left(\sum_{b',i'} c_{b',i'} E_{b',i'}^- \right) (E_{b,i}^-) = i^n \sum_{kl} (\lambda_k - \lambda_l)^n Y_{kl} \tilde{a}_k^\dagger \tilde{a}_l$$

$$\begin{aligned} \frac{dU(\mathbf{c})}{dc_{b,i}} &= \left[\sum_{kl} Y_{kl} \frac{e^{i(\lambda_k - \lambda_l)} - 1}{i(\lambda_k - \lambda_l)} \tilde{a}_k^\dagger \tilde{a}_l \right] e^{\sum_{b,i} c_{b,i} E_{b,i}^-} \\ &= \left(\sum_{k,l} [UMU^\dagger]_{kl} a_k^\dagger a_l \right) e^{\sum_{b,i} c_{b,i} E_{b,i}^-} \end{aligned}$$

$$M_{kl} = Y_{kl} \frac{e^{i(\lambda_k - \lambda_l)} - 1}{i(\lambda_k - \lambda_l)}$$

$$\delta \tilde{E} = \delta \langle \tilde{\psi} | H | \tilde{\psi} \rangle = 0$$

$$U=e^R\,R=-R^\dagger$$

$$\tilde{E}\rightarrow\tilde{E}'=\tilde{E}+\langle\tilde{\psi}|[H,R]|\tilde{\psi}\rangle+\frac{1}{2}\langle\tilde{\psi}|[[H,R],R]|\tilde{\psi}\rangle+\cdots$$

$$\langle\tilde{\psi}|[H,R]|\tilde{\psi}\rangle=0\,\forall R=-R^\dagger$$

$$A_R=\langle\phi|[H,R]|\phi\rangle\neq 0$$

$$\psi=e^{-f_RR}\phi$$

$$E_{f_R}=\langle\phi|e^{f_RR}He^{-f_RR}|\phi\rangle\approx\langle\phi|H+f_R[H,R]+\frac{f_R^2}{2}[[H,R],R]|\phi\rangle$$

$$\frac{dE_{f_R}}{df_R}=\langle\phi|[H,R]+\frac{f_R}{2}[[H,R],R]|\phi\rangle=0\;f_R=-A_R/B_{R,R}\;B_{R,R}=\langle\phi|[[H,R],R]|\phi\rangle$$

$$0=\langle\phi|e^{f_RR}[H,R]e^{-f_RR}|\phi\rangle=\langle\phi|[H,R]+f_R[[H,R],R]+\frac{f_R^2}{2}[[[H,R],R],R]+\cdots|\phi\rangle$$

$$f_R=-A_R/B_{R,R}$$

$$R=\sum_kc_kX, X\subset\mathcal{L}$$

$$0\approx\langle\phi|[H,X_k]+\sum_l\left[[H,X_k],X_l\right]c_l|\phi\rangle$$

$$A_{p,q}=\langle\psi|[H,a_p^\dagger a_q]|\psi\rangle\;B_{p,q;r,s}=\langle\psi|\left[[H,a_p^\dagger a_q],a_r^\dagger a_s\right]|\psi\rangle.$$

$$\begin{pmatrix} 0 & \mathbf{A} \\ \mathbf{A}^\dagger & \mathbf{B} \end{pmatrix} \begin{pmatrix} 1 \\ f_{p,q} \end{pmatrix} = \epsilon \begin{pmatrix} 1 \\ f_{p,q} \end{pmatrix}$$

$$\mathbf{A}+(\mathbf{B}-\epsilon)f_{p,q}=0$$

$$\begin{cases} f_{p,q} & \max(f_{p,q})<\gamma \\ \frac{\gamma}{\max(f_{p,q})}f_{p,q} & \max(f_{p,q})\geq\gamma \end{cases}$$

$$|\Psi_I\rangle=\sum_A c_{AI}|\Phi_A\rangle$$

$$\phi_p^A(x)=\sum_{\mu}\chi_{\mu}(x)C_{\mu p}^A$$

$$E_I=\langle\Psi_I|\hat{H}|\Psi_I\rangle=\sum_{AB}c_{AI}^*\langle\Phi_A|\hat{H}|\Phi_B\rangle c_{BI}$$

$$\hat{H}=\sum_{\mu\nu}h_{\mu\nu}\hat{a}_{\mu}^{\dagger}\hat{a}_{\nu}+\frac{1}{2}\sum_{\mu\nu\lambda\sigma}[\mu\lambda\mid\nu\sigma]\hat{a}_{\mu}^{\dagger}\hat{a}_{\nu}^{\dagger}\hat{a}_{\sigma}\hat{a}_{\lambda}$$

$$[\mu\lambda \mid v\sigma] = \iint d\mathbf{x}_1\mathbf{x}_2\chi_\mu^*(\mathbf{x}_1)\chi_\lambda(\mathbf{x}_1)\hat{r}_{12}^{-1}\chi_v^*(\mathbf{x}_2)\chi_\sigma(\mathbf{x}_2)$$

$$s_{AB} \equiv \langle \Phi_A \mid \Phi_B \rangle$$

$$s_{AB} = |{\bf S}_{00}^{AB}|$$

$$\mathbf{S}_{00}^{AB} = \mathbf{C}_0^{A,\dagger} \mathbf{S} \mathbf{C}_0^B$$

$$\mathbf{S}^{AB} = \mathbf{C}^{A,\dagger} \mathbf{S} \mathbf{C}^B = \begin{bmatrix} \mathbf{S}_{\mathrm{oo}}^{AB} & \mathbf{S}_{\mathrm{ou}}^{AB} \\ \mathbf{S}_{\mathrm{uo}}^{AB} & \mathbf{S}_{\mathrm{uu}}^{AB} \end{bmatrix}$$

$$\gamma_{\mu\nu}^{AB} \equiv \langle \Phi_A | \hat{a}_\mu^\dagger \hat{a}_\nu | \Phi_B \rangle$$

$$\gamma^{AB} = s_{AB} \mathbf{C}_o^B (\mathbf{S}_{00}^{AB})^{-1} \mathbf{C}_o^{A,\dagger} = s_{AB} \mathbf{Q}^{AB}$$

$$\begin{aligned}\Gamma_{\lambda\mu\sigma\nu}^{AB} &= \langle \Phi_A | \hat{a}_\mu^\dagger \hat{a}_\nu^\dagger \hat{a}_\sigma \hat{a}_\lambda | \Phi_B \rangle \\ &= s_{AB} [Q_{\lambda\mu}^{AB} Q_{\sigma\nu}^{AB} - Q_{\sigma\mu}^{AB} Q_{\lambda\nu}^{AB}]\end{aligned}$$

$$H_{AB} \equiv \langle \Phi_A | \hat{H} | \Phi_B \rangle$$

$$H_{AB} = \langle \mathbf{h} \gamma^{AB} \rangle + \frac{1}{2} \langle \mathbf{V} \Gamma^{AB} \rangle = \langle \mathbf{h} \gamma^{AB} \rangle + \frac{1}{2} \langle \mathbf{G}^{AB} \gamma^{AB} \rangle,$$

$$V_{\mu\lambda v\sigma}=[\mu\lambda \mid v\sigma]$$

$$\begin{aligned}G_{\mu\nu}^{AB} &= \sum_{\lambda\sigma} [\mu\nu||\lambda\sigma]Q_{\sigma\lambda}^{AB} \\ [\mu\nu||\lambda\sigma] &= [\mu\nu\mid\lambda\sigma] - [\mu\sigma\mid\lambda\nu].\end{aligned}$$

$$\mathcal{L} = E^{\text{ResHF}} - \sum_{IJ} N_{IJ} [\langle \Psi_I \mid \Psi_J \rangle - \delta_{IJ}],$$

$$N_{IJ} = \delta_{IJ} E_I w_I$$

$$\mathbf{Hc} = \mathbf{scE}$$

$$\begin{aligned}\mathbf{F}^A &= \sum_I w_I \mathbf{F}_I^A \\ \mathbf{F}_I^A &= \mathbf{F}^{AA} |c_{AI}|^2 + \sum_{B \neq A} c_{AI}^* [\mathbf{K}^{AB} + (\mathbf{K}^{AB})^\dagger] c_{BI},\end{aligned}$$

$$\mathbf{F}^{AB} = \mathbf{h} + \mathbf{G}^{AB}$$

$$\begin{aligned}\mathbf{K}^{AB} &= s_{AB} (\mathbf{1} - \mathbf{S} \mathbf{Q}^{AB}) \mathbf{F}^{AB} \mathbf{Q}^{AB} \mathbf{S} \\ &\quad + (H_{AB} - s_{AB} E_I) \mathbf{S} \mathbf{Q}^{AB} \mathbf{S}\end{aligned}$$

$$\mathbf{Q}^{AB} \mathbf{S} \mathbf{Q}^{AB} = \mathbf{Q}^{AB}$$

$$\mathbf{S}_{00}^{AB} = \mathbf{U}^{AB} \mathbf{\Sigma}^{AB} \mathbf{V}^{AB,\dagger}$$

$$\text{adj}(\mathbf{M}) \equiv |\mathbf{M}|(\mathbf{M})^{-1}$$

$$s_{AB} = |\mathbf{S}_{\text{o o}}^{AB}|$$

$$\gamma^{AB} = \mathbf{C}_{\text{o}}^B \text{adj}(\mathbf{S}_{\text{o o}}^{AB}) \mathbf{C}_{\text{o}}^{A,\dagger}$$

$$\text{adj}(\mathbf{S}_{\text{o o}}^{AB}) = \eta \mathbf{V}^{AB} \mathbf{\Xi} \mathbf{U}^{AB,\dagger}$$

$$\xi_i = \prod_{j \neq i} \sigma_j$$

$$\eta = |\mathbf{U}^{AB}(\mathbf{V}^{AB})^\dagger| = \pm 1$$

$$\gamma^{AB} = \eta \mathbf{B}_{\text{o}} \mathbf{\Xi}^{AB} \mathbf{A}_{\text{o}}^\dagger$$

$$\mathbf{A}_{\text{o}} = \mathbf{C}_{\text{o}}^A \mathbf{U}^{AB}$$

$$\mathbf{B}_{\text{o}} = \mathbf{C}_{\text{o}}^B \mathbf{V}^{AB}$$

$$\frac{1}{2} \langle \mathbf{G}^{AB} \gamma^{AB} \rangle = \eta \frac{1}{2} \sum_{ij} [i_A i_B || j_A j_B] \xi_{ij}$$

$$\xi_{ij} = \frac{1}{\sigma_i} \frac{1}{\sigma_j} \prod_m \sigma_m$$

$$\xi_{ij} = \begin{cases} \prod_{m \neq i,j} \sigma_m & \text{if } i \neq j \\ \tau & \text{if } i = j \end{cases}$$

$$\mathbf{A}^\dagger \mathbf{K}^{AB} \mathbf{A} = \begin{bmatrix} \mathbf{A}_{\text{o}}^\dagger \mathbf{K}^{AB} \mathbf{A}_{\text{o}} & \mathbf{A}_{\text{o}}^\dagger \mathbf{K}^{AB} \mathbf{A}_{\text{u}} \\ \mathbf{A}_{\text{u}}^\dagger \mathbf{K}^{AB} \mathbf{A}_{\text{o}} & \mathbf{A}_{\text{u}}^\dagger \mathbf{K}^{AB} \mathbf{A}_{\text{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{K}_{\text{o}}^{AB} & \mathbf{K}_{\text{o u}}^{AB} \\ \mathbf{K}_{\text{u o}}^{AB} & \mathbf{K}_{\text{u u}}^{AB} \end{bmatrix}$$

$$\mathbf{A}_{\text{o}} = \mathbf{C}_{\text{o}}^A \mathbf{U}^{AB}$$

$$\mathbf{Q}^{AB} \mathbf{S} \mathbf{A}_{\text{u}} = \mathbf{B}_{\text{o}} (\mathbf{\Sigma}^{AB})^{-1} \mathbf{A}_{\text{o}}^\dagger \mathbf{S} \mathbf{A}_{\text{u}} = 0.$$

$$\mathbf{A}_{\text{o}}^\dagger (\mathbf{1} - \mathbf{S} \mathbf{Q}^{AB}) = \mathbf{A}_{\text{o}}^\dagger - \mathbf{\Sigma}^{AB} (\mathbf{\Sigma}^{AB})^{-1} \mathbf{A}_{\text{o}}^\dagger = 0$$

$$\mathbf{A}_{\text{o}}^\dagger \mathbf{S} \mathbf{Q}^{AB} \mathbf{S} \mathbf{A}_{\text{o}} = \mathbf{\Sigma}^{AB} (\mathbf{\Sigma}^{AB})^{-1} \mathbf{A}_{\text{o}}^\dagger \mathbf{S} \mathbf{A}_{\text{o}} = \mathbf{1}$$

$$\mathbf{K}_{\text{o o}}^{AB} = (H_{AB} - s_{AB} E_I) \mathbf{1}$$

$$\begin{aligned} \mathbf{K}_{\text{u o}}^{AB} = s_{AB} \mathbf{A}_{\text{u}}^\dagger (\mathbf{1} - \mathbf{S} \mathbf{Q}^{AB}) \mathbf{F}^{AB} \mathbf{Q}^{AB} \mathbf{S} \mathbf{A}_{\text{o}} \\ + (H_{AB} - s_{AB} E_I) \mathbf{A}_{\text{u}}^\dagger \mathbf{S} \mathbf{Q}^{AB} \mathbf{S} \mathbf{A}_{\text{o}} \end{aligned}$$

$$\begin{aligned}
K_{ai}^{AB} = & \eta (\bar{h}_{ai}^{AB} - E_I \bar{S}_{ai}^{AB}) \xi_i \\
& + \eta \sum_j (\bar{S}_{ai}^{AB} \bar{h}_{jj}^{AB} - \bar{S}_{aj}^{AB} \bar{h}_{ji}^{AB} + [a_A i_B \| j_A j_B]) \xi_{ij} \\
& + \eta \sum_{jk} \left(\frac{1}{2} \bar{S}_{ai}^{AB} [j_A j_B \| k_A k_B] - \bar{S}_{aj}^{AB} [j_A i_B \| k_A k_B] \right) \xi_{ijk}
\end{aligned}$$

$$\bar{h}_{pq}^{AB} = \sum_{\mu\nu} A_{\mu p}^* h_{\mu\nu} B_{\nu q}$$

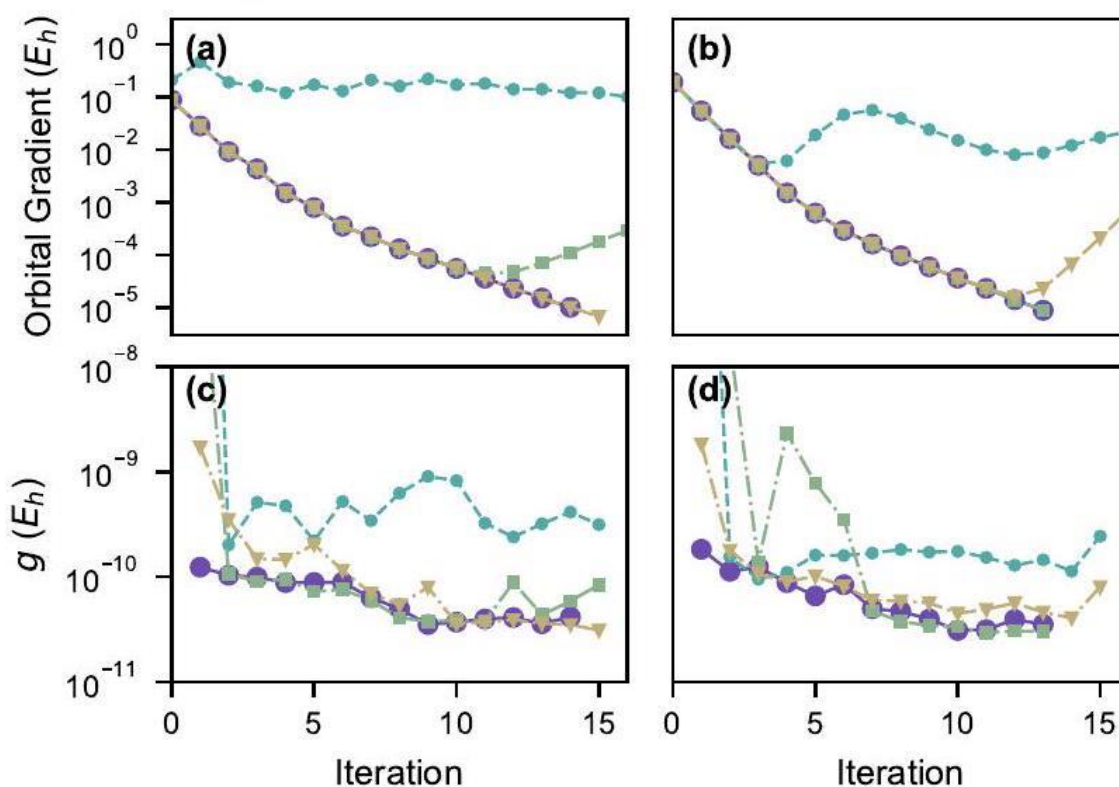
$$\bar{S}_{pq}^{AB} = \sum_{\mu\nu} A_{\mu p}^* S_{\mu\nu} B_{\nu q}$$

$$\xi_{ijk} = \frac{1}{\sigma_i} \frac{1}{\sigma_j} \frac{1}{\sigma_k} \prod_m \sigma_m$$

$$\begin{aligned}
& \sum_{j < k} (\bar{S}_{ai}^{AB} [j_A j_B \| k_A k_B] \\
& - \bar{S}_{aj}^{AB} [j_A i_B \| k_A k_B] - \bar{S}_{ak}^{AB} [k_A i_B \| j_A j_B]) \xi_{ijk}
\end{aligned}$$

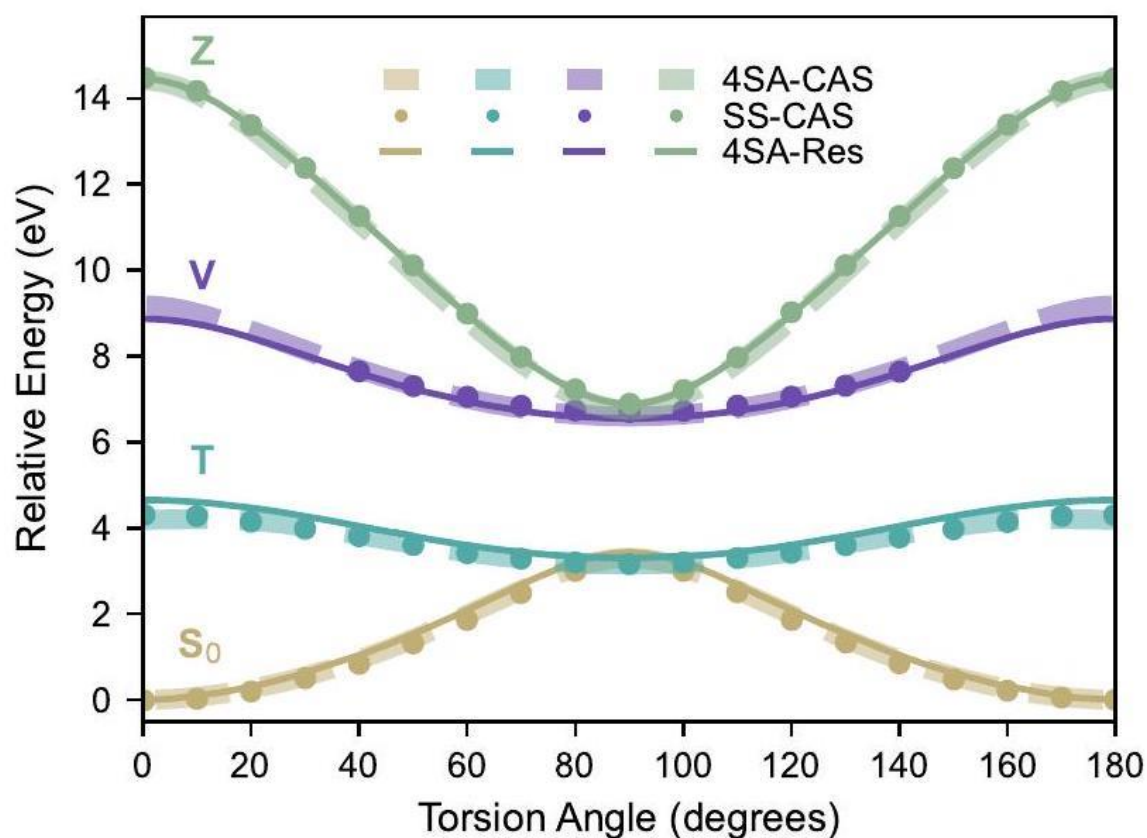
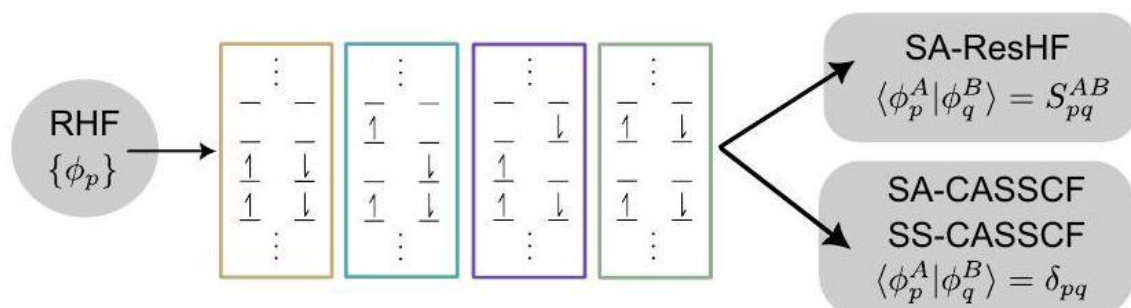
$$\xi_{ijk} = \begin{cases} \prod_{m \neq i,j,k} \sigma_m & \text{if } i \neq j \neq k \\ \tau & \text{otherwise} \end{cases}$$

$$(pq \mid rs) \approx \sum_{PQ} (pq \mid P)(P \mid Q)^{-1}(Q \mid rs),$$



$$g_{err}(h) = \sqrt{\sum_{Aia} \left| F_{ia}^A - \frac{dE^{SA}}{d\kappa_{ai}^A}(h) \right|^2},$$

$$|\Psi_I\rangle = c_{AI}|\Phi_A\rangle + c_{BI}|\Phi_B\rangle + c_{CI}|\Phi_C\rangle + c_{DI}|\Phi_D\rangle$$



$$\mathbf{K}_{uo}^{AB} = \mathbf{A}_u^\dagger (\mathbf{K1} + \mathbf{K2} + \mathbf{K3} + \mathbf{K4}) \mathbf{A}_o$$

$$\mathbf{K1} = s_{AB} \mathbf{F}^{AB} \mathbf{Q}^{AB} \mathbf{S}$$

$$\mathbf{K2} = -s_{AB} \mathbf{S} \mathbf{Q}^{AB} \mathbf{F}^{AB} \mathbf{Q}^{AB} \mathbf{S}$$

$$\mathbf{K3} = H_{AB} \mathbf{S} \mathbf{Q}^{AB} \mathbf{S}$$

$$\mathbf{K4} = -s_{AB} E_I \mathbf{S} \mathbf{Q}^{AB} \mathbf{S}$$

$$(pq | rs) \approx (pq | \tilde{P})(\tilde{P} | rs),$$

$$(pq | \tilde{P}) = (pq | Q)(L^{-1})_{QP}$$

$$\begin{aligned}
(K^{AB,\alpha})_{ai}^{2e-} &= (K1^\alpha)_{ai}^{2e-} + (K2^\alpha)_{ai}^{2e-} + (K3^\alpha)_{ai}^{2e-} \\
(K1^\alpha)_{ai}^{2e-} &= \eta \left(a_A^\alpha i_B^\alpha \mid j_A^\beta j_B^\beta \right) \xi_i^\alpha \xi_j^\beta \\
&\quad + \eta \left| \Sigma^{AB,\beta} \right| (a_A^\alpha i_B^\alpha \mid j_A^\alpha j_B^\alpha) \xi_{ij}^\alpha \\
(K2^\alpha)_{ai}^{2e-} &= -\eta \bar{S}_{aj}^{AB,\alpha} \left(j_A^\alpha i_B^\alpha \mid k_A^\beta k_B^\beta \right) \xi_{ij}^\alpha \xi_k^\beta \\
&\quad - \eta \left| \Sigma^{AB,\beta} \right| \bar{S}_{aj}^{AB,\alpha} (j_A^\alpha i_B^\alpha \mid k_A^\alpha k_B^\alpha) \xi_{ijk}^\alpha \\
(K3^\alpha)_{ai}^{2e-} &= \eta \bar{S}_{ai}^{AB,\alpha} \left(j_A^\beta j_B^\beta \mid k_A^\beta k_B^\beta \right) \xi_{ij}^\alpha \xi_k^\beta \\
&\quad + \frac{1}{2} \eta \bar{S}_{ai}^{AB,\alpha} \left(j_A^\beta j_B^\beta \mid k_A^\beta k_B^\beta \right) \xi_i^\alpha \xi_{jk}^\beta \\
&\quad + \frac{1}{2} \eta \left| \Sigma^{AB,\beta} \right| \bar{S}_{ai}^{AB,\alpha} (j_A^\beta j_B^\beta \mid k_A^\alpha k_B^\alpha) \xi_{ijk}^\alpha
\end{aligned}$$

$$\begin{aligned}
(K1^\alpha)_{ai}^{2e-} &= \eta (a_A^\alpha i_B^\alpha \mid \tilde{P}) \left(\tilde{P} \mid j_A^\beta j_B^\beta \right) \xi_i^\alpha \xi_j^\beta \\
&\quad + \eta \left| \Sigma^{AB,\beta} \right| (a_A^\alpha i_B^\alpha \mid \tilde{P}) (\tilde{P} \mid j_A^\alpha j_B^\alpha) \xi_{ij}^\alpha \\
&\quad - \eta \left| \Sigma^{AB,\beta} \right| (a_A^\alpha j_B^\alpha \mid \tilde{P}) (\tilde{P} \mid j_A^\alpha i_B^\alpha) \xi_{ij}^\alpha
\end{aligned}$$

$$\begin{aligned}
T_{aiP} &\leftarrow \xi_i^\alpha (a_A^\alpha i_B^\alpha \mid \tilde{P}) \\
T_P &\leftarrow (\tilde{P} \mid j_A^\beta j_B^\beta) \xi_j^\beta \\
(K1^\alpha)_{ai}^{2e-} &+= \eta T_{aiP} T_P.
\end{aligned}$$

$$\begin{aligned}
T_{Pi} &\leftarrow (\tilde{P} \mid j_A^\alpha j_B^\alpha) \xi_{ij}^\alpha \\
(K1^\alpha)_{ai}^{2e-} &+= \eta (a_A^\alpha i_B^\alpha \mid \tilde{P}) T_{Pi}
\end{aligned}$$

$$\begin{aligned}
T_{Pji} &\leftarrow (\tilde{P} \mid j_A^\alpha i_B^\alpha) \xi_{ij}^\alpha \\
(K1^\alpha)_{ai}^{2e-} &-= \eta (a_A^\alpha j_B^\alpha \mid \tilde{P}) T_{Pji}
\end{aligned}$$

$$\begin{aligned}
(K2^\alpha)_{ai}^{2e-} &= -\eta \bar{S}_{aj}^{AB,\alpha} (j_A^\alpha i_B^\alpha \mid \tilde{P}) (\tilde{P} \mid k_A^\beta k_B^\beta) \xi_{ij}^\alpha \xi_k^\beta \\
&\quad - \eta \left| \Sigma^{AB,\beta} \right| \bar{S}_{aj}^{AB,\alpha} (j_A^\alpha i_B^\alpha \mid \tilde{P}) (\tilde{P} \mid k_A^\alpha k_B^\alpha) \xi_{ijk}^\alpha \\
&\quad + \eta \left| \Sigma^{AB,\beta} \right| \bar{S}_{aj}^{AB,\alpha} (j_A^\alpha k_B^\alpha \mid \tilde{P}) (\tilde{P} \mid k_A^\alpha i_B^\alpha) \xi_{ijk}^\alpha
\end{aligned}$$

$$\begin{aligned}
T_{aji} &\leftarrow \bar{S}_{aj}^{AB,\alpha} \xi_{ij}^\alpha \\
T_{aiP} &\leftarrow T_{aji} (j_A^\alpha i_B^\alpha \mid \tilde{P}) \\
T_P &\leftarrow (\tilde{P} \mid k_A^\beta k_B^\beta) \xi_k^\beta \\
(K2^\alpha)_{ai}^{2e-} &-= \eta T_{aiP} T_P.
\end{aligned}$$

$$\begin{aligned}
T_{ajiP} &\leftarrow \bar{S}_{aj}^{AB,\alpha} (j_A^\alpha i_B^\alpha \mid \tilde{P}) \\
T_{Pij} &\leftarrow (\tilde{P} \mid k_A^\alpha k_B^\alpha) \xi_{ijk}^\alpha \\
(K2^\alpha)_{ai}^{2e-} &-= \eta \left| \Sigma^{AB,\beta} \right| T_{ajiP} T_{Pij}.
\end{aligned}$$

$$\begin{aligned}
T_{ajkP} &\leftarrow \bar{S}_{aj}^{AB,\alpha} (j_A^\alpha k_B^\alpha \mid \tilde{P}) \\
T_{Pkij} &\leftarrow (\tilde{P} \mid k_A^\alpha i_B^\alpha) \xi_{ijk}^\alpha \\
(K2^\alpha)_{ai}^{2e-} &+= \eta \left| \Sigma^{AB,\beta} \right| T_{ajkP} T_{Pkij},
\end{aligned}$$

$$\begin{aligned}
(K3^\alpha)_{ai}^{2e-} &= \eta \bar{S}_{ai}^{AB,\alpha} (j_A^\alpha j_B^\alpha | \tilde{P}) (\tilde{P} | k_A^\beta k_B^\beta) \xi_{ij}^\alpha \xi_k^\beta \\
&+ \frac{1}{2} \eta \bar{S}_{ai}^{AB,\alpha} \xi_i^\alpha (j_A^\beta j_B^\beta | \tilde{P}) (\tilde{P} | k_A^\beta k_B^\beta) \xi_{jk}^\beta \\
&- \frac{1}{2} \eta \bar{S}_{ai}^{AB,\alpha} \xi_i^\alpha (j_A^\beta k_B^\beta | \tilde{P}) (\tilde{P} | k_A^\beta j_B^\beta) \xi_{jk}^\beta \\
&+ \frac{1}{2} \eta |\Sigma^{AB,\beta}| \bar{S}_{ai}^{AB,\alpha} (j_A^\alpha j_B^\alpha | \tilde{P}) (\tilde{P} | k_A^\alpha k_B^\alpha) \xi_{ijk}^\alpha \\
&- \frac{1}{2} \eta |\Sigma^{AB,\beta}| \bar{S}_{ai}^{AB,\alpha} (j_A^\alpha k_B^\alpha | \tilde{P}) (\tilde{P} | k_A^\alpha j_B^\alpha) \xi_{ijk}^\alpha
\end{aligned}$$

$$\begin{aligned}
T_{iP} &\leftarrow \xi_{ij}^\alpha (j_A^\alpha j_B^\alpha | \tilde{P}) \\
T_P &\leftarrow (\tilde{P} | k_A^\beta k_B^\beta) \xi_k^\beta \\
(K3^\alpha)_{ai}^{2e-} &+= \eta \bar{S}_{ai}^{AB,\alpha} T_{iP} T_P.
\end{aligned}$$

$$\begin{aligned}
T_{jP} &\leftarrow (j_A^\alpha j_B^\alpha | \tilde{P}) \\
T_{Pk} &\leftarrow (\tilde{P} | k_A^\alpha k_B^\alpha) \\
T_{jk} &\leftarrow T_{jP} T_{Pk} \\
T &\leftarrow T_{jk} \xi_{jk}^\beta \\
(K3^\alpha)_{ai}^{2e-} &+= \frac{1}{2} \eta \bar{S}_{ai}^{AB,\alpha} \xi_i^\alpha T.
\end{aligned}$$

$$\begin{aligned}
T_{Pkj} &\leftarrow (\tilde{P} | k_A^\beta j_B^\beta) \xi_{jk}^\beta \\
T &\leftarrow (j_A^\beta k_B^\beta | \tilde{P}) T_{Pkj} \\
(K3^\alpha)_{ai}^{2e-} &-= \frac{1}{2} \eta \bar{S}_{ai}^{AB,\alpha} \xi_i^\alpha T.
\end{aligned}$$

$$\begin{aligned}
T_{jP} &\leftarrow (j_A^\alpha j_B^\alpha | \tilde{P}) \\
T_{Pk} &\leftarrow (\tilde{P} | k_A^\alpha k_B^\alpha) \\
T_{jk} &\leftarrow T_{jP} T_{Pk} \\
T_i &\leftarrow \xi_{ijk}^\alpha T_{jk} \\
(K3^\alpha)_{ai}^{2e-} &+= \frac{1}{2} \eta |\Sigma^{AB,\beta}| \bar{S}_{ai}^{AB,\alpha} T_i.
\end{aligned}$$

$$\begin{aligned}
T_{Pijk} &\leftarrow (\tilde{P} | k_A^\alpha j_B^\alpha) \xi_{ijk}^\alpha \\
T_i &\leftarrow (j_A^\alpha k_B^\alpha | \tilde{P}) T_{Pijk} \\
(K3^\alpha)_{ai}^{2e-} &-= \frac{1}{2} \eta |\Sigma^{AB,\beta}| \bar{S}_{ai}^{AB,\alpha} T_i.
\end{aligned}$$

$$\phi_p^{A,\omega}(\mathbf{x}_1) = s(\omega) \psi_p^{A,\omega}(\mathbf{r}_1)$$

$$\mathbf{S}^{AB,\omega} = \mathbf{C}^{A,\omega,\dagger} \mathbf{S} \mathbf{C}^{B,\omega}$$

$$s_{AB} = |\mathbf{s}_{00}^{AB,\alpha}| |\mathbf{s}_{00}^{AB,\beta}| = \eta \left[\prod_i^{N_\alpha} \sigma_i^\alpha \right] \left[\prod_j^{N_\beta} \sigma_j^\beta \right],$$

$$\eta = \left| \mathbf{U}^{AB,\alpha} (\mathbf{V}^{AB,\alpha})^\dagger \right| \left| \mathbf{U}^{AB,\beta} (\mathbf{V}^{AB,\beta})^\dagger \right| = \pm 1$$



$$\gamma^{AB,\omega} = s_{AB} \mathbf{Q}^{AB,\omega}$$

$$H_{AB} = s_{AB} \sum_{\omega} \left[\langle \mathbf{h} \mathbf{Q}^{AB,\omega} \rangle + \frac{1}{2} \langle \mathbf{G}^{AB,\omega} \mathbf{Q}^{AB,\omega} \rangle \right],$$

$$G_{\mu\nu}^{AB,\omega} = \sum_{\lambda\sigma} (\mu\nu||\lambda\sigma) Q_{\sigma\lambda}^{AB,\omega} + \sum_{\lambda\sigma} (\mu\nu|\lambda\sigma) Q_{\sigma\lambda}^{AB,\omega'}$$

$$(\mu\nu|\lambda\sigma)=\iint d\mathbf{r}_1\mathbf{r}_2\chi_{\mu}^*(\mathbf{r}_1)\chi_{\nu}(\mathbf{r}_1)\hat{r}_{12}^{-1}\chi_{\lambda}^*(\mathbf{r}_2)\chi_{\sigma}(\mathbf{r}_2)$$

$$\mathbf{K}^{AB,\omega} = s_{AB}(\mathbf{1} - \mathbf{S}\mathbf{Q}^{AB,\omega})\mathbf{F}^{AB,\omega}\mathbf{Q}^{AB,\omega}\mathbf{S} \\ + (H_{AB} - s_{AB}E_I) \\ \mathbf{S}\mathbf{Q}^{AB,\omega}\mathbf{S}$$

$$\mathbf{F}^{AB,\omega} = \mathbf{h} + \mathbf{G}^{AB,\omega}$$

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_e})=\frac{1}{\sqrt{N_e!}}\begin{vmatrix}\phi_1(\mathbf{r}_1)&\phi_1(\mathbf{r}_2)&\cdots&\phi_1(\mathbf{r}_{N_e})\\ \phi_2(\mathbf{r}_1)&\phi_2(\mathbf{r}_2)&\cdots&\phi_2(\mathbf{r}_{N_e})\\ \vdots&\vdots&\ddots&\vdots\\ \phi_{N_e}(\mathbf{r}_1)&\phi_{N_e}(\mathbf{r}_2)&\cdots&\phi_{N_e}(\mathbf{r}_{N_e})\end{vmatrix},$$

$$H_e=T_e+V_{ne}+V_{ee}+V_{nn}$$

$$T_e\!=\!\sum_{i=1}^{N_e}\!-\frac{1}{2}\Delta_i$$

$$V_{ne}=\sum_{A=1}^{N_n}\sum_{i=1}^{N_e}\frac{-Z_A}{|\mathbf{r}_i-\mathbf{R}_A|}$$

$$V_{ee}=\sum_{i=1}^{N_e}\sum_{j>i}^{N_e}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}\equiv\sum_{i=1}^{N_e}\sum_{j>1}^{N_e}g_{ij}$$

$$V_{nn}=\sum_{A=1}^{N_n}\sum_{B>A}^{N_n}\frac{Z_AZ_B}{|\mathbf{R}_A-\mathbf{R}_B|}$$

$$h=-\frac{1}{2}\Delta+\sum_{A=1}^{N_n}\frac{-Z_A}{|\mathbf{r}-\mathbf{R}_A|}$$

$$J_a=\int\frac{\phi_a(\mathbf{r}')\phi_a(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'$$

$$K_a|\phi_b\rangle=\phi_a(\mathbf{r})\int\frac{\phi_a(\mathbf{r}')\phi_b(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'$$

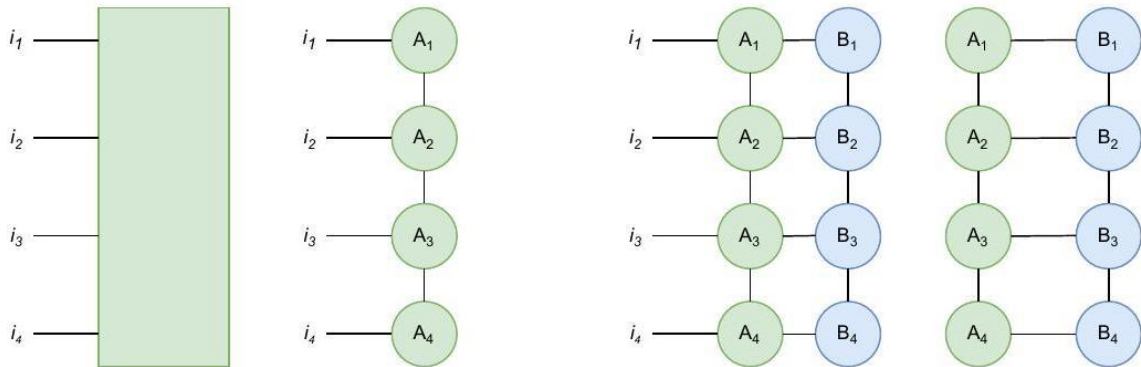
$$E(\phi_1,\ldots\phi_n)=\sum_{a=1}^{N_e}\langle\phi_a|h|\phi_a\rangle+\frac{1}{2}\sum_{a=1,b=1}^{N_e}\langle\phi_a|U_b|\phi_a\rangle-\langle\phi_a|K_b|\phi_a\rangle+V_{nn}$$

$$F\phi'_a=\epsilon_a\phi'_a,$$

$$F = h + \sum_{b=1}^{N_e} J_b - K_b.$$

$$T^{i_1 \cdots i_n} \approx A_{r_1}^{i_1} \cdot A_{r_1 r_2}^{i_2} \cdot \ldots \cdot A_{r_{n-1} r_n}^{i_{n-1}} \cdot A_{r_n}^{i_n} \equiv \prod_{a=1}^n A_a^{i_a},$$

$$\sum_i dr_i r_{i+1}$$



$$\mathcal{T}^{i_1 j_1 \cdots i_n j_n} \approx A_{r_1}^{i_1 j_1} \cdot A_{r_1 r_2}^{i_2 j_2} \cdot \ldots \cdot A_{r_{n-1} r_n}^{i_{n-1} j_{n-1}} \cdot A_{r_n}^{i_n j_n} \equiv \prod_{a=1}^n A_a^{i_a j_a},$$

$$\text{TTM} \cdot \text{TT} = \sum_{(j_1, \ldots, j_n)} \left(A_1^{i_1 j_1} \cdot A_2^{i_2 j_2} \cdots A_n^{i_n j_n} \right) \left(B_1^{j_1} \cdot B_2^{j_2} \cdots B_n^{j_n} \right).$$

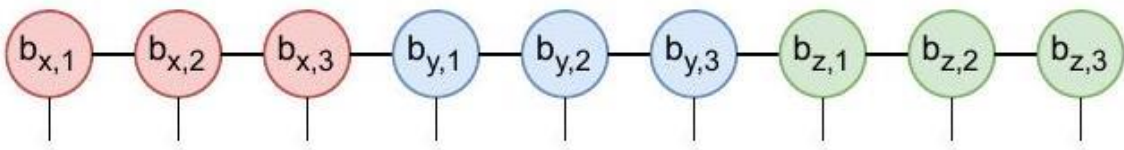
$$\text{TTM} \cdot \text{TT} = C_1^{i_1} \cdot C_2^{i_2} \cdots C_n^{i_n},$$

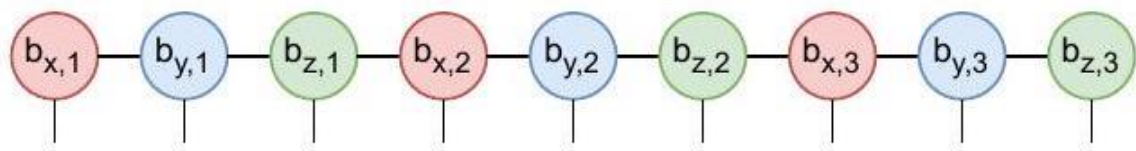
$$C_k^{i_k} = \sum_{j_k} A_k^{i_k j_k} B_k^{j_k}$$

$$C_k = \begin{pmatrix} A_k & 0 \\ 0 & B_k \end{pmatrix},$$

$$\text{TT}_a \cdot \text{TT}_b = \sum_{(j_1, \ldots, j_n)} \left(A_1^{j_1} \cdot A_2^{j_2} \cdots A_n^{j_n} \right) \left(B_1^{j_1} \cdot B_2^{j_2} \cdots B_n^{j_n} \right),$$

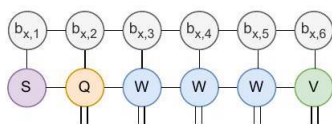
$$x_i(b_{x_i,1},b_{x_i,2},\ldots,b_{x_i,p_i})=\sum_{j=1}^{p_i}\frac{b_{x_i,j}}{2^j}(x_{i,\max}-x_{i,\min})+x_{i,\min},$$





$$\begin{pmatrix} 2 & 0 & 3 & 0 \\ 1 & 2 & 0 & 3 \\ 0 & 1 & 2 & 0 \\ 0 & 0 & 1 & 2 \end{pmatrix}.$$

$$\textbf{a)} \begin{pmatrix} v_n & v_{n-1} & \cdots & v_3 & v_2 \\ v_{n+1} & \ddots & \ddots & \ddots & v_3 \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ v_{2n-1} & \ddots & \ddots & \ddots & v_{n-1} \\ v_{2n} & v_{2n-1} & \cdots & v_{n+1} & v_n \end{pmatrix}$$



$$S_+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$S_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$R_0 = [0 \ S_+]$$

$$R_1 = [S_+ \ I]$$

$$Q_0 = [I \ S_-]$$

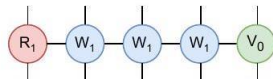
$$Q_1 = [S_- \ 0]$$

$$W_0 = \begin{bmatrix} I & S_- \\ 0 & S_+ \end{bmatrix} \quad W_1 = \begin{bmatrix} S_- & 0 \\ S_+ & I \end{bmatrix}$$

$$V_0 = \begin{bmatrix} I \\ 0 \end{bmatrix} \quad V_1 = \begin{bmatrix} S_- \\ S_+ \end{bmatrix}$$

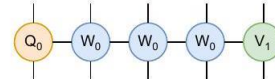
$$\textbf{b)} \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & 1 & \ddots & \vdots \\ \vdots & & \ddots & 1 & 0 \\ \vdots & & & \ddots & 1 \\ 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix} \quad \left. \vphantom{\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & 1 & \ddots & \vdots \\ \vdots & & \ddots & 1 & 0 \\ \vdots & & & \ddots & 1 \\ 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix}} \right\} i$$

i: 11110



$$\textbf{c)} \quad i \left\{ \begin{pmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ 1 & \ddots & & & \vdots \\ \vdots & \ddots & \ddots & & \vdots \\ 0 & 1 & \ddots & & \vdots \\ \vdots & \ddots & 1 & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix} \right.$$

i: 00001



$$f''(x_n) = \frac{f(x_{n-1}) - 2f(x_n) + f(x_{n+1}))}{h^2},$$

$$\begin{pmatrix} f''(x_0) \\ f''(x_1) \\ \cdots \\ \cdots \\ f''(x_n) \end{pmatrix} = \begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \cdots & -2 \end{pmatrix} \cdot \begin{pmatrix} f(x_0) \\ f(x_1) \\ \cdots \\ \cdots \\ f(x_n) \end{pmatrix}.$$

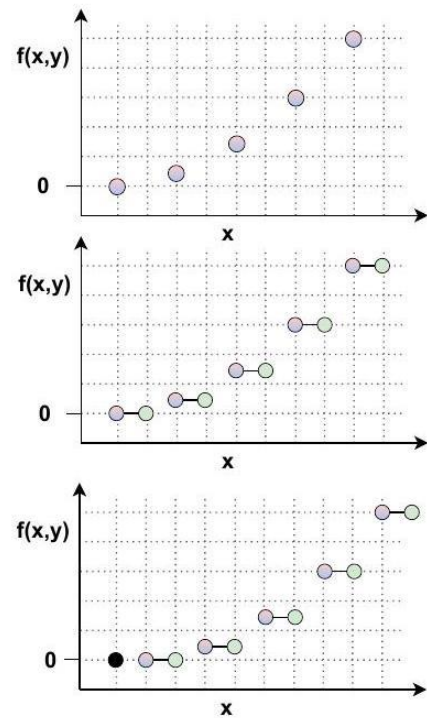
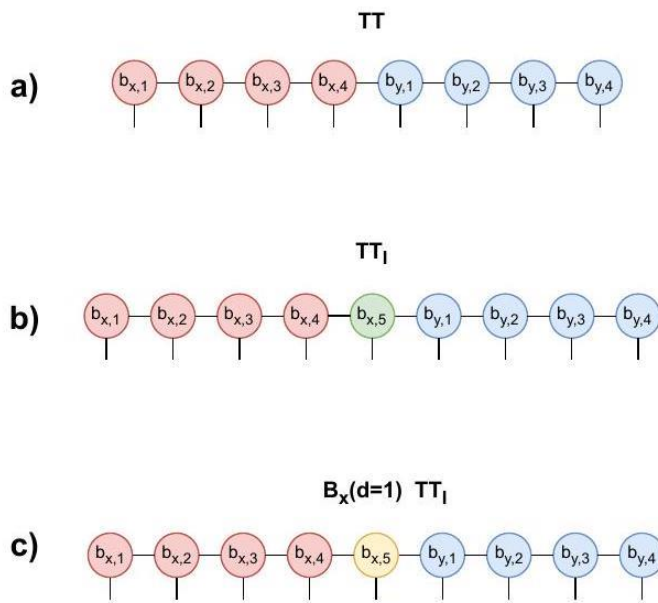
$$\mathrm{TT}_{\mathrm{disp}} = B(d)\mathrm{TT},$$

$$\mathrm{TT}_{\mathrm{disp}} = \prod_i^n B_{x_i}(d_{x_i})\mathrm{TT}.$$

$$\prod_i^n B_{x_i}(d_{x_i})$$

$$f(x_1,x_2,\ldots,x_{i,j},\ldots,x_n)=\frac{f(x_1,x_2,\ldots,x_{i,j-1},\ldots,x_n)+f(x_1,x_2,\ldots,x_{i,j+1},\ldots,x_n)}{2}.$$

$$\mathrm{TT}_{\mathrm{intpl.}} = \frac{\mathrm{TT}_I + B_{x_i}(d_{x_i} = 1)\mathrm{TT}_I}{2}.$$



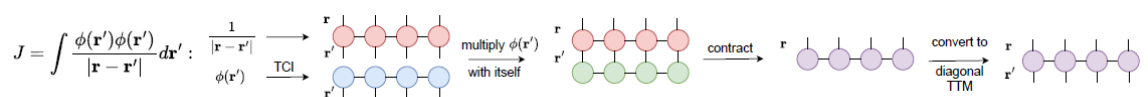
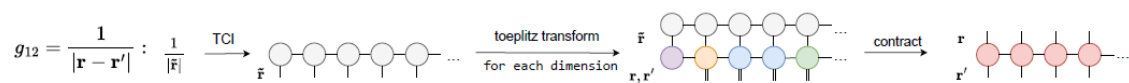
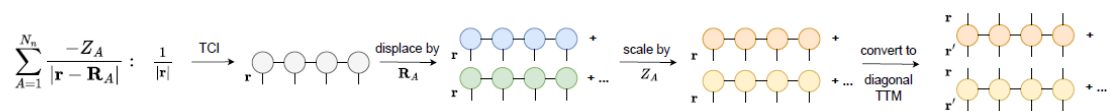
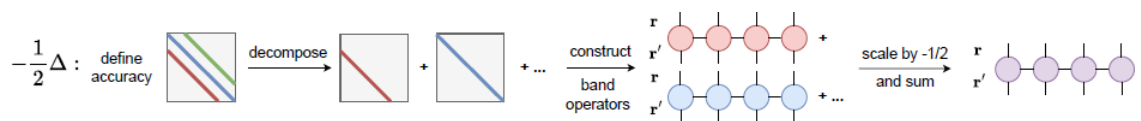
$$A_{ij}^{aa'} = A_{ij}^a \cdot I^{aa'}$$

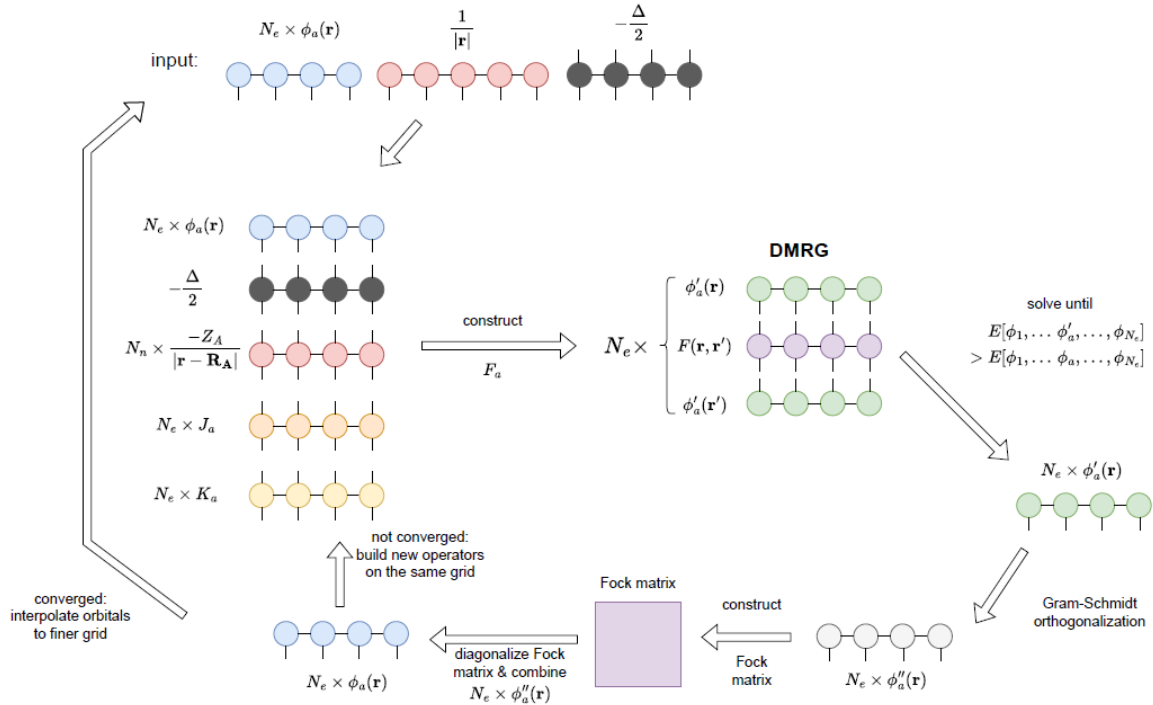
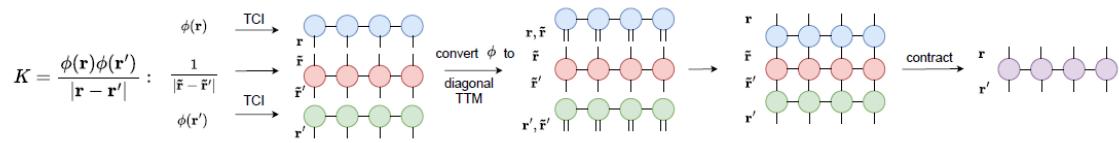
$$A_{ij}^{aa'b} = A_{ij}^{ab} \cdot I^{aa'}$$

$$\mathbf{r}_i = \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix}.$$

$$V_{ne} = \sum_{A=1}^{N_n} \frac{-Z_A}{\sqrt{(x - X_A)^2 + (y - Y_A)^2 + (z - Z_A)^2}}.$$

$$g_{12} = \frac{1}{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}}$$





$$E_{HF}(\phi_1, \dots, \phi'_a, \dots, \phi_{N_e}) > E_{HF}(\phi_1, \dots, \phi_a, \dots, \phi_{N_e}).$$

$$\epsilon_{\text{kin}} = \sum_i^{N_e} \left| \langle \phi_i | -\frac{1}{2} \Delta | \phi_i \rangle_{\text{QTT}} - \langle \phi_i | -\frac{1}{2} \Delta | \phi_i \rangle_{\text{LCAO}} \right|,$$

$$\epsilon_{\text{nuc}} = \sum_i^{N_e} \left| \langle \phi_i | \sum_j^{N_n} \frac{Z_n}{|\mathbf{r} - \mathbf{R}_n|} | \phi_i \rangle_{\text{QTT}} - \langle \phi_i | \sum_j^{N_n} \frac{Z_n}{|\mathbf{r} - \mathbf{R}_n|} | \phi_i \rangle_{\text{LCAO}} \right|,$$

$$\epsilon_{\text{coul}} = \sum_{i,j}^{N_e} \left| \langle \phi_i(1)\phi_i(1) | \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} | \phi_j(2)\phi_j(2) \rangle_{\text{QTT}} - \langle \phi_i(1)\phi_i(1) | \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} | \phi_j(2)\phi_j(2) \rangle_{\text{LCAO}} \right|,$$

$$\epsilon_{\text{exch}} = \sum_{i,j}^{N_e} \left| \langle \phi_i(1)\phi_j(1) | \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} | \phi_j(2)\phi_i(2) \rangle_{\text{QTT}} - \langle \phi_i(1)\phi_j(1) | \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} | \phi_j(2)\phi_i(2) \rangle_{\text{LCAO}} \right|.$$

$$\langle \phi_i(1)\phi_i(1) | g_{12} | \phi_j(2)\phi_j(2) \rangle \text{ or } \langle \phi_i(1)\phi_j(1) | g_{12} | \phi_j(2)\phi_i(2) \rangle$$

$$\phi_i^{\text{LCAO}}(\mathbf{r}) = \sum_j^{N_e} c_{ij} \phi_j^{\text{QTT}}(\mathbf{r})$$

$$c_{ij} = \langle \phi_i^{\text{LCAO}}(\mathbf{r}) | \phi_j^{\text{QTT}}(\mathbf{r}) \rangle$$

$$f(c'_{ij}) = |c_{ij} - c'_{ij}|_F + |\det(c'_{ij}) - 1|,$$

$$|\det(c'_{ij})| = 1$$

$$\|\phi^{\text{LCAO}} - \phi^{\text{QTT}}\| \equiv \sqrt{\langle \phi_i^{\text{LCAO}}(\mathbf{r}) - \phi_j^{\text{QTT}}(\mathbf{r}) | \phi_i^{\text{LCAO}}(\mathbf{r}) - \phi_j^{\text{QTT}}(\mathbf{r}) \rangle}$$

$$\|\phi^{\text{LCAO}} - \phi^{\text{QTT}}\| = \sum_{i,j,k=1}^{2_d^p} \left| \phi(x_i, y_j, z_k)^{\text{LCAO}} - \phi(x_i, y_j, z_k)^{\text{QTT}} \right|.$$

	rank dependency on p_d	efficient QTT approximation	error source
ϕ_i	const.	yes	no
$\phi_i \phi_j$	const. $< r_{\max}(\phi_i) + r_{\max}(\phi_j)$	yes	no
Δ	const. < 20	yes	yes
$\frac{1}{ \mathbf{r} }$	const. ≈ 170	yes	no
$\frac{1}{ \mathbf{r}_1 - \mathbf{r}_2 }$	const. ≈ 340	yes	no
$\frac{\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_1)}{ \mathbf{r}_1 - \mathbf{r}_2 }$	const. $< r_{\max}(\phi_i) + r_{\max}(\phi_j)$	yes	no
$\frac{\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_2)}{ \mathbf{r}_1 - \mathbf{r}_2 }$	linear with slight slope	no	yes

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 0 & 0 & 2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \end{pmatrix}.$$

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, S_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

$$|\langle \Psi | \hat{O} | \Psi \rangle - \langle \Phi | \hat{O} | \Phi \rangle| \leq 2 \| \hat{O} \| \cdot \| \Phi - \Psi \|.$$

$$\| \mathbf{u} + \mathbf{v} \| \leq \| \mathbf{u} \| + \| \mathbf{v} \|$$

$$| \langle \mathbf{u} | \mathbf{v} \rangle | \leq \| \mathbf{u} \| \cdot \| \mathbf{v} \|$$

$$\langle \Phi | \hat{O} | \Phi \rangle = \langle \Psi + \Delta | \hat{O} | \Psi + \Delta \rangle.$$

$$|\langle \Phi | \hat{O} | \Phi \rangle - \langle \Psi | \hat{O} | \Psi \rangle| = |\langle \Psi | \hat{O} | \Delta \rangle + \langle \Delta | \hat{O} | \Psi \rangle + \langle \Delta | \hat{O} | \Delta \rangle|,$$

$$|\langle \Phi | \hat{O} | \Phi \rangle - \langle \Psi | \hat{O} | \Psi \rangle| \leq |\langle \Psi | \hat{O} | \Delta \rangle| + |\langle \Delta | \hat{O} | \Psi \rangle| + |\langle \Delta | \hat{O} | \Delta \rangle| = 2 |\langle \Psi | \hat{O} | \Delta \rangle| + |\langle \Delta | \hat{O} | \Delta \rangle|.$$

$$|\langle \Psi | \hat{O} | \Delta \rangle| \leq \| \hat{O} \Delta \|$$

$$|\langle \Delta | \hat{O} | \Delta \rangle| \leq \| \Delta \| \cdot \| \hat{O} | \Delta \|$$

$$\| \hat{O} | \Delta \| = \| \hat{O} \| \cdot \| \Delta \|$$

$$|\langle \Psi | \hat{O} | \Psi \rangle - \langle \Phi | \hat{O} | \Phi \rangle| \leq \| \hat{O} \| \cdot (2 \| \Phi - \Psi \| + \| \Phi - \Psi \|^2).$$

$$\| \Delta \| = \| \Phi - \Psi \|$$

$$|\langle \Psi | \hat{O} | \Psi \rangle - \langle \Phi | \hat{O} | \Phi \rangle| \leq 2 \| \hat{O} \| \cdot \| \Phi - \Psi \|.$$

$$\langle \hat{O} \rangle = \sum_i^{N_e} \langle \phi_i(\mathbf{r}_1) | \hat{O}_1(\mathbf{r}_1) | \phi_i(\mathbf{r}_1) \rangle + \sum_{ij}^{N_e} \langle \phi_i(\mathbf{r}_1) \phi_j(\mathbf{r}_2) | \hat{O}_2(\mathbf{r}_1, \mathbf{r}_2) | \phi_k(\mathbf{r}_1) \phi_l(\mathbf{r}_2) \rangle + \dots,$$

$$\hat{O} = \sum_i^N \hat{O}_i(\dots \mathbf{r}_i)$$

$$\begin{aligned} \langle \Psi | \hat{O} | \Psi \rangle - \langle \Psi' | \hat{O} | \Psi' \rangle &= \sum_i^{N_e} \langle \phi_i | \hat{O}_1 | \phi \rangle - \langle \phi'_i | \hat{O}_1 | \phi'_i \rangle + \\ &\quad \sum_{ij}^{N_e} \langle \phi_i \phi_j | \hat{O}_2 | \phi_k \phi_l \rangle - \langle \phi'_i \phi'_j | \hat{O}_2 | \phi'_k \phi'_l \rangle + \dots \\ &\leq \sum_i^{N_e} 2 \| \hat{O}_1 \| \cdot \| \phi_i - \phi'_i \| + \sum_{ij}^{N_e} 2 \| \hat{O}_2 \| \cdot \| \phi_i \phi_j - \phi'_i \phi'_j \| + \dots \end{aligned}$$

$$\left\| \prod_i^N \phi_i(\mathbf{r}_i) - \prod_i^N \phi'_i(\mathbf{r}_i) \right\| \| \phi_i(\mathbf{r}) - \phi'_i(\mathbf{r}) \|$$

$$\left\| \prod_i^N \phi_i(\mathbf{r}_i) - \prod_i^N \phi'_i(\mathbf{r}_i) \right\| \leq \sum_i^N \| \phi_i(\mathbf{r}_i) - \phi'_i(\mathbf{r}_i) \|$$

$$\prod_i^N \phi_i(\mathbf{r}_i) - \prod_i^N \phi'_i(\mathbf{r}_i) = \sum_i^N \left(\prod_j^{i-1} \phi_j(\mathbf{r}_i) \right) (\phi_i(\mathbf{r}_i) - \phi'_i(\mathbf{r}_i)) \left(\prod_{j=i+1}^N \phi'_j(\mathbf{r}_j) \right)$$



$$\left\| \prod_i^N \phi_i(\mathbf{r}_i) - \prod_i^N \phi'_i(\mathbf{r}_i) \right\| = \sum_i^N \|\phi_i(\mathbf{r}_i) - \phi'_i(\mathbf{r}_i)\|.$$

$$H[\rho(\mathbf{r}), P(\mathbf{r}, \mathbf{r}')] \phi_\ell := \left(-\frac{1}{2} \Delta + V_{\text{ext}} + V_{\text{Har}}[\rho](\mathbf{r}) + V_{\text{x}}[P](\mathbf{r}, \mathbf{r}') \right) \phi_\ell = \lambda_\ell \phi_\ell, \ell = 1, \dots, N_e,$$

$$P(\mathbf{r},\mathbf{r}')\!:=\!\sum_{\ell=1}^{N_e}\phi_\ell(\mathbf{r})\phi_\ell^*(\mathbf{r}')$$

$$V_{\text{Har}}[\rho](\mathbf{r})=\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'$$

$$(V_{\text{x}}[P]\phi_\ell)(\mathbf{r})=-\int\frac{P(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\phi_\ell(\mathbf{r}')d\mathbf{r}'$$

$$\iint \frac{\psi_i(\mathbf{r})\psi_j^*(\mathbf{r})\psi_m(\mathbf{r}')\psi_n^*(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}', i,j,m,n=1,\dots,N$$

$$\left(-\frac{1}{2}\Delta+V_{\text{ext}}+V_{\text{Har}}[\rho^{\text{old}}](\mathbf{r})+V_{\text{x}}[P^{\text{old}}](\mathbf{r},\mathbf{r}')\right)\phi_\ell=\lambda_\ell\phi_\ell,\ell=1,\cdots,N_e.$$

$$E_{\text{xc}}^{\text{PBEO}} = \frac{1}{4} E_{\text{x}}^{\text{HF}} + \frac{3}{4} E_{\text{x}}^{\text{PBE}} + E_{\text{c}}^{\text{PBE}}$$

$$\tilde{V}_{\rm x}(\mathbf{r},\mathbf{r}')=\tilde{V}_{\rm x}^*(\mathbf{r}',\mathbf{r})$$

$$(\tilde{V}_{\rm x}\phi_\ell)(\mathbf{r})=(V_{\rm x}\phi_\ell)(\mathbf{r})$$

$$w_\ell(\mathbf{r})=(V_{\rm x}\phi_\ell)(\mathbf{r}), \ell=1,\dots,N_e$$

$$\tilde{V}_{\rm x}(\mathbf{r},\mathbf{r}')=[W(\mathbf{r}),\Phi(\mathbf{r})]A[W(\mathbf{r}'),\Phi(\mathbf{r}')]^*$$

$$W=(w_1,\cdots,w_{N_e}),\Phi=(\phi_1,\cdots,\phi_{N_e}),[W,\Phi]$$

$$\tilde{V}_{\rm x}\Phi=[W(\mathbf{r}),\Phi(\mathbf{r})]A\left[\begin{array}{ccc}\left(w_1^*(\mathbf{r}'),\phi_1(\mathbf{r}')\right) & \cdots & \left(w_1^*(\mathbf{r}'),\phi_{N_e}(\mathbf{r}')\right) \\ \vdots & \vdots & \vdots \\ \left(w_{N_e}^*(\mathbf{r}'),\phi_1(\mathbf{r}')\right) & \cdots & \left(w_{N_e}^*(\mathbf{r}'),\phi_{N_e}(\mathbf{r}')\right) \\ 1 & \cdots & 0 \\ \vdots & \vdots & \vdots \\ 0 & \cdots & 1\end{array}\right]$$

$$\left(\phi_i^*(\mathbf{r}'),\phi_j(\mathbf{r}')\right):=\int\phi_i^*(\mathbf{r}')\phi_j(\mathbf{r}')d\mathbf{r}'=\delta_{ij}$$

$$M=\left[\begin{array}{ccc}\left(w_1^*(\mathbf{r}'),\phi_1(\mathbf{r}')\right) & \cdots & \left(w_1^*(\mathbf{r}'),\phi_{N_e}(\mathbf{r}')\right) \\ \vdots & \vdots & \vdots \\ \left(w_{N_e}^*(\mathbf{r}'),\phi_1(\mathbf{r}')\right) & \cdots & \left(w_{N_e}^*(\mathbf{r}'),\phi_{N_e}(\mathbf{r}')\right)\end{array}\right]$$

$$[W(\mathbf{r}), \Phi(\mathbf{r})]A \begin{bmatrix} M \\ I \end{bmatrix} = W(\mathbf{r})$$

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{bmatrix}$$

$$[W(\mathbf{r}), \Phi(\mathbf{r})] \begin{bmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{bmatrix} \begin{bmatrix} M \\ I \end{bmatrix} = W(\mathbf{r})$$

$$W(\mathbf{r})(A_{11}M + A_{12}) + \Phi(\mathbf{r})(A_{12}^*M + A_{22}) = W(\mathbf{r}).$$

$$\begin{cases} A_{11}M + A_{12} &= I \\ A_{12}^*M + A_{22} &= 0 \end{cases}$$

$$A_{12} = I - A_{11}M$$

$$A_{22} = -(I - A_{11}M)^*M = MA_{11}M - M$$

$$\begin{aligned} \tilde{V}_x(\mathbf{r}, \mathbf{r}') = & W(\mathbf{r})A_{11}W^*(\mathbf{r}') + W(\mathbf{r})(I - A_{11}M)\Phi^*(\mathbf{r}') \\ & + \Phi(\mathbf{r})(I - MA_{11})W^*(\mathbf{r}') + \Phi(\mathbf{r})(MA_{11}M - M)\Phi^*(\mathbf{r}'), \end{aligned}$$

$$\tilde{V}_x(\mathbf{r}, \mathbf{r}') = W(\mathbf{r})\Phi^*(\mathbf{r}') + \Phi(\mathbf{r})W^*(\mathbf{r}') - \Phi(\mathbf{r})M\Phi^*(\mathbf{r}').$$

$$\tilde{V}_x(\mathbf{r}, \mathbf{r}') = W(\mathbf{r})W^*(\mathbf{r}') + W(\mathbf{r})(I - M)\Phi^*(\mathbf{r}') + \Phi(\mathbf{r})(I - M)W^*(\mathbf{r}') + \Phi(\mathbf{r})(M^2 - M)\Phi^*(\mathbf{r}')$$

$$\tilde{V}_x(\mathbf{r}, \mathbf{r}') = W(\mathbf{r})M^{-1}W^*(\mathbf{r}')$$

$$M = U^*\Lambda U$$

$$\Lambda = \text{diag}(\lambda_1, \dots, \lambda_{N_e})\Lambda^+$$

$$\Lambda^+ = \text{diag}(\lambda_1^+, \dots, \lambda_{N_e}^+), \text{ with } \lambda_i^+ = \begin{cases} \lambda_i^{-1} & \text{if } \lambda_i \neq 0 \\ 0 & \text{if } \lambda_i = 0 \end{cases}$$

$$A_{11} = U^*\Lambda^+U$$

$$\tilde{U} = (I - \Lambda\Lambda^+)U$$

$$I - A_{11}M = I - MA_{11} = \tilde{U}^*\tilde{U}$$

$$\tilde{V}_x(\mathbf{r}, \mathbf{r}') = W(\mathbf{r})U^*\Lambda^+UW^*(\mathbf{r}') + W(\mathbf{r})\tilde{U}^*\tilde{U}\Phi^*(\mathbf{r}') + \Phi(\mathbf{r})\tilde{U}^*\tilde{U}W^*(\mathbf{r}')$$

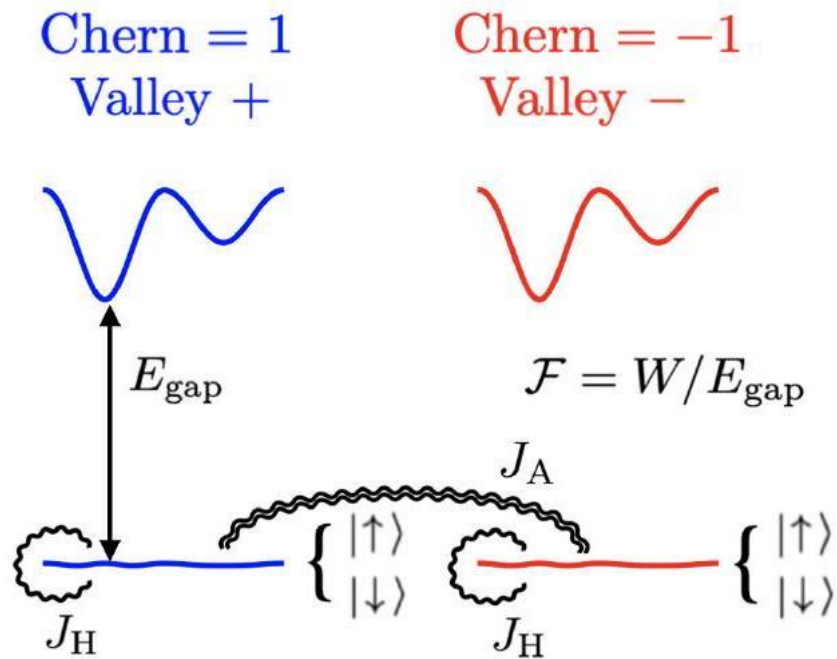
$$H_{\text{kin}}^{(\tau)} = \sum_{\mathbf{k}} \psi_{\mathbf{k},\tau}^\dagger [B_{\mathbf{k},\tau}^0 \eta_0 + \mathbf{B}_{\mathbf{k},\tau} \cdot \boldsymbol{\eta}] \sigma_0 \psi_{\mathbf{k},\tau},$$

$$\psi_{\mathbf{k},\tau}^\dagger = (c_{\mathbf{k},A,\tau,\uparrow}^\dagger, c_{\mathbf{k},B,\tau,\uparrow}^\dagger, c_{\mathbf{k},A,\tau,\downarrow}^\dagger, c_{\mathbf{k},B,\tau,\downarrow}^\dagger) c_{\mathbf{k},\eta,\tau,\sigma}^\dagger$$

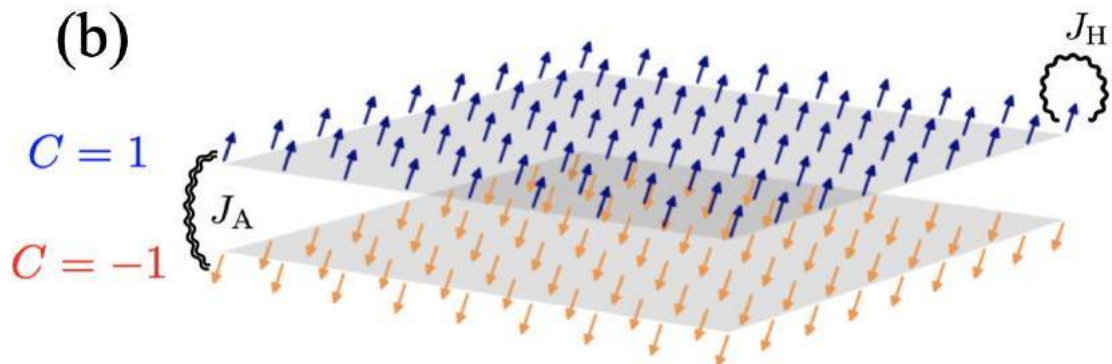
$$H_{\text{interaction}} = H_{\text{intra-valley}} + H_{\text{inter-valley}}$$

$$\begin{aligned}
 H_{\text{intra-valley}} &= J_H \sum_{\mathbf{r}, \tau=\pm} \mathbf{S}_{\mathbf{r}}^{\tau} \cdot \mathbf{S}_{\mathbf{r}}^{\tau} \\
 H_{\text{inter-valley}} &= J_A \sum_{\mathbf{r}} \mathbf{S}_{\mathbf{r}}^{+} \cdot \mathbf{S}_{\mathbf{r}}^{-}, \\
 \mathbf{S}_{\mathbf{r}}^{\tau} &= \sum_{\alpha, \beta=\uparrow, \downarrow} c_{\mathbf{r}, \tau, \alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha \beta} c_{\mathbf{r}, \tau, \beta}
 \end{aligned}$$

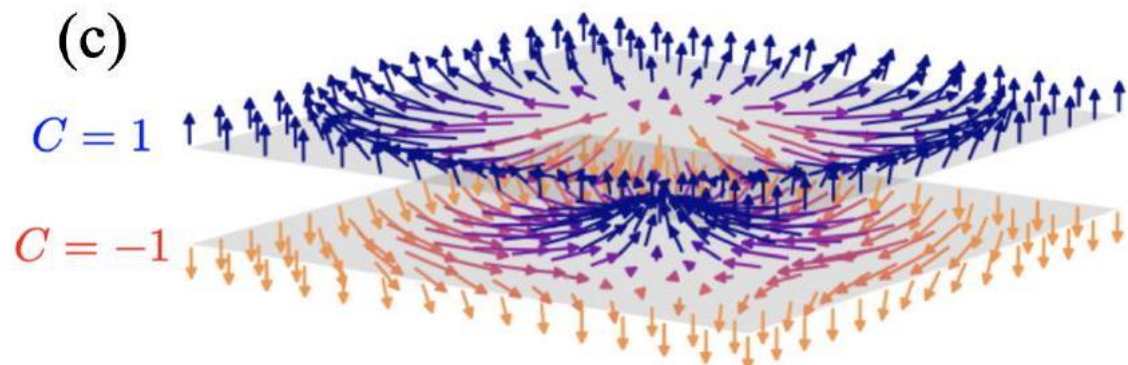
(a)



(b)



(c)



$$H_{\text{HF}}[P,Q] = \sum_{\tau} H_{\text{kin}}^{\tau} + \sum_{i;\alpha\beta} [H_{\text{ph}}[P_{mn}]_i c_{im}^{\dagger} c_{in} + H_{\text{SC}}[Q_{mn}]_i c_{im} c_{in} + \text{h.c.}]$$

Order Parameter	Density Matrix
Spin order	$c_{\tau\alpha}^{\dagger}\sigma_{\alpha\beta}^{\mu}c_{\tau\beta}$
Valley order	$c_{\alpha\sigma}^{\dagger}\tau_{\alpha\beta}^{\mu}c_{\beta\sigma}$
Spin-polarized inter-valley coherence	$c_{+\sigma}^{\dagger}c_{-\sigma} \pm c_{-\sigma}^{\dagger}c_{+\sigma}$
Spin-mixed inter-valley coherence	$c_{+\sigma}^{\dagger}c_{-\bar{\sigma}} \pm c_{-\sigma}^{\dagger}c_{+\bar{\sigma}}$
Spin-singlet SC ($\tau_z = 0$)	$c_{-\alpha}(i\sigma_y)_{\alpha\beta}c_{+\beta}$
Spin-triplet SC	$c_{-\alpha}(i\sigma_y\sigma_{\mu})_{\alpha\beta}c_{+\beta}$

$$P_{\text{CAF}}^{\mu} \equiv c_{\gamma\alpha}^{\dagger}\sigma_{\alpha\beta}^{\mu}\tau_{\gamma\gamma'}^z c_{\gamma'\beta}$$

(a)

$$\tilde{W}_{\Sigma} = \left(\begin{array}{c} \rightarrow \\ \rightarrow \\ \leftarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \right)$$

(b)

$$\tilde{K}_{BS} = \begin{pmatrix} \text{diagram 1} + \text{diagram 2} & \text{diagram 3} + \text{diagram 4} \\ \text{diagram 5} + \text{diagram 6} & \text{diagram 7} + \text{diagram 8} + \text{diagram 9} \end{pmatrix}$$

$$b_{\mathbf{k},\mathbf{q};+}^{\dagger} \equiv c_{\mathbf{k}+\mathbf{q},+\uparrow}^{\dagger} c_{\mathbf{k},+\downarrow}$$

$$b_{\mathbf{k},\mathbf{q};-}^{\dagger} \equiv c_{\mathbf{k}+\mathbf{q},-\downarrow}^{\dagger} c_{\mathbf{k},-\uparrow}$$

$$b_{\mathbf{k},\mathbf{q};+}^{\dagger}, b_{\mathbf{k},\mathbf{q};-}^{\dagger} \det(W_{\Sigma}^{-1} - K_{BS}) = 0.$$

$$W_{\Sigma}^{(0,0)} = \sum_{k_0} \frac{1}{ik_0 - E_{\mathbf{k}}^{+\uparrow}} \frac{1}{i(k_0 - \Omega) - E_{\mathbf{k}-\mathbf{q}}^{+\downarrow}}$$

$$= \frac{1}{i\Omega - (E_{\mathbf{k}}^{+\uparrow} - E_{\mathbf{k}-\mathbf{q}}^{+\downarrow})}$$

$$W_{\Sigma}^{(1,1)} = \sum_{k_0} \frac{1}{ik_0 + E_{-\mathbf{k}}^{-\downarrow}} \frac{1}{i(k_0 - \Omega) + E_{-\mathbf{k}+\mathbf{q}}^{-\uparrow}}$$

$$= \frac{1}{-i\Omega - (E_{-\mathbf{k}}^{-\downarrow} - E_{-\mathbf{k}+\mathbf{q}}^{-\uparrow})}$$

$$A_{\text{CAF}}(\mathbf{k}, \omega) = \text{Im} \langle P_{\text{CAF}}^{\dagger}(\mathbf{k}, \omega) P_{\text{CAF}}(\mathbf{k}, \omega) \rangle \Big|_{\omega \rightarrow \omega + i0^{+}}$$

$$SU(2)_{\text{spin}} \otimes U(1)_{\text{charge}} \otimes U(1)_{\text{valley}}$$

$$s_+^{\dagger} \equiv c_{\mathbf{k}_{e1},+\uparrow}^{\dagger} b_{\mathbf{k}_{e2},\mathbf{q};+}^{\dagger}$$

$$s_-^{\dagger} \equiv c_{\mathbf{k}_{e1},+\uparrow}^{\dagger} b_{\mathbf{k}_{e2},\mathbf{q};-}^{\dagger}$$

(a)

$$\tilde{W}_{\Sigma} = \left(\begin{array}{c} \rightarrow \\ \rightarrow \\ \leftarrow \\ \\ \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \right)$$

(b)

$$\tilde{K}_{BS} = \left(\begin{array}{cc} \text{diagram 1} + \text{diagram 2} & \text{diagram 3} + \text{diagram 4} \\ \text{diagram 5} + \text{diagram 6} & \text{diagram 7} + \text{diagram 8} + \text{diagram 9} \end{array} \right)$$

$$\det(\tilde{W}_{\Sigma}^{-1} - \tilde{K}_{BS}) = 0.$$

$$\begin{aligned} \tilde{W}_{\Sigma}^{(0,0)} &= \sum_{\Omega} \frac{1}{i(\Omega_{\text{tot}} - \Omega) - E_{\mathbf{k}_{e1}}^{+\uparrow}} \frac{1}{i\Omega - (E_{\mathbf{k}_{e2}}^{+\uparrow} - E_{\mathbf{k}_{e1}+\mathbf{k}_{e2}-\mathbf{q}}^{+\downarrow})} \\ &= \frac{-1}{i\Omega_{\text{tot}} - (E_{\mathbf{k}_{e1}}^{+\uparrow} + E_{\mathbf{k}_{e2}}^{+\uparrow} - E_{\mathbf{k}_{e1}+\mathbf{k}_{e2}-\mathbf{q}}^{+\downarrow})} \end{aligned}$$

$$\tilde{W}_{\Sigma}^{(1,1)} = \frac{1}{i\Omega_{\text{tot}} - (E_{\mathbf{k}_{e1}}^{+\uparrow} - E_{-\mathbf{k}_{e2}}^{+\downarrow} + E_{\mathbf{q}-\mathbf{k}_{e1}-\mathbf{k}_{e2}}^{+\uparrow})}.$$

$$\text{SU}(2)_{\text{spin}}^{\tau=+} \otimes \text{SU}(2)_{\text{spin}}^{\tau=-}$$

$$\chi^{\tau}(\mathbf{q}) = \frac{1}{L^2} \sum_{\mathbf{r}, \mathbf{r}'} e^{-i(\mathbf{r}-\mathbf{r}') \cdot \mathbf{q}} \langle \mathbf{S}^{\tau}(\mathbf{r}') \cdot \mathbf{S}^{\tau}(\mathbf{r}) \rangle,$$

$$\chi^{\tau}(\mathbf{q}=0) = S_{\text{tot}}^{\tau}(S_{\text{tot}}^{\tau}+1)/L^2$$

$$|\Psi_{\text{HF}}^{\delta\nu=0}\rangle S_{\text{tot}}^{\tau}(\delta\nu=0) = N/2 (N=L^2)$$

$$|\Psi_{\text{HF}}^{\delta\nu=1}\rangle \equiv s_+^{\dagger} |\Psi_{\text{HF}}^{\delta\nu=0}\rangle S_{\text{tot}}^{\tau=+}(\delta\nu=1) = (N-1)/2 \text{ or } (N-3)/2$$

$$\Delta S_{\tau=+} \equiv S_{\text{tot}}^{\tau=+}(\delta\nu=0) - S_{\text{tot}}^{\tau=+}(\delta\nu=1)$$

$$O_{\text{CAF}}^{\alpha} \equiv \psi_r^{\dagger} \sigma^{\alpha} \tau^z \psi_r, \alpha = 1, 2, 3$$

$$O_{\text{SC}} \equiv c_{\mathbf{r}+\uparrow}^{\dagger} c_{\mathbf{r}-\downarrow}^{\dagger} - c_{\mathbf{r}+\downarrow}^{\dagger} c_{\mathbf{r}-\uparrow}^{\dagger}$$

$$\Psi_{\mathbf{k}}^{\dagger} \equiv [d_{+\uparrow}^{\dagger}(\mathbf{k}), d_{+\downarrow}^{\dagger}(\mathbf{k}), d_{-\uparrow}(-\mathbf{k}), d_{-\downarrow}(-\mathbf{k})]$$

$$c_{\eta\tau\alpha}(\mathbf{k}) = u_{\eta\tau}(\mathbf{k})d_{\tau\alpha}(\mathbf{k})$$

$$\mathbf{N} \equiv (\text{Re}[O_{\text{SC}}], O_{\text{CAF}}^{\alpha}, \text{Im}[O_{\text{SC}}])$$

$$N_1 = \text{Re}[\Delta_S] = \frac{1}{2} \Psi^{\dagger} \sigma_y \mu_y \Psi$$

$$N_2 = S_x \tau_z = \frac{1}{2} \Psi^{\dagger} \sigma_x \Psi$$

$$N_3 = S_y \tau_z = \frac{1}{2} \Psi^{\dagger} \sigma_y \mu_z \Psi$$

$$N_4 = S_z \tau_z = \frac{1}{2} \Psi^{\dagger} \sigma_z \Psi$$

$$N_5 = -\text{Im}[\Delta_S] = \frac{1}{2} \Psi^{\dagger} \sigma_y \mu_x \Psi.$$

$$iL_{\alpha\beta} \equiv [N_{\alpha}, N_{\beta}]$$

$$L_{15} = -(n_{\text{tot}} - 2)/2 = -\mu_z/2$$

$$L_{23} = S_z = \sigma_z \mu_z/2$$

$$L_{24} = -S_y = -\sigma_y/2$$

$$L_{34} = S_x = \sigma_x \mu_z/2$$

$$L_{45} = -\text{Re}[\Delta_{\text{Tz}}] = -\sigma_x \mu_x/2, L_{14} = \text{Im}[\Delta_{\text{Tz}}] = \sigma_x \mu_y/2$$

$$L_{25} = \text{Re}[\Delta_{\text{Tx}}] = -\sigma_z \mu_x/2, L_{12} = \text{Im}[\Delta_{\text{Tx}}] = \sigma_z \mu_y/2$$

$$L_{35} = \text{Re}[\Delta_{\text{Ty}}] = \mu_y/2, L_{13} = \text{Im}[\Delta_{\text{Ty}}] = \mu_x/2$$

$$\begin{aligned} H_{\text{rotor}} = & \sum_{\mathbf{k}, \mathbf{p}, \mathbf{q}} F_{\mathbf{k}, \mathbf{p}, \mathbf{q}} \left[U_0 \Psi_{\mathbf{k}+\mathbf{q}}^{\dagger} \Psi_{\mathbf{k}} \Psi_{\mathbf{p}-\mathbf{q}}^{\dagger} \Psi_{\mathbf{p}} \right. \\ & + \sum_{\alpha\beta} U_{\alpha\beta} \Psi_{\mathbf{k}+\mathbf{q}}^{\dagger} L_{\alpha\beta} \Psi_{\mathbf{k}} \Psi_{\mathbf{p}-\mathbf{q}}^{\dagger} L_{\alpha\beta} \Psi_{\mathbf{p}} \\ & + \sum_{\mu} V_{\mu} \Psi_{\mathbf{k}+\mathbf{q}}^{\dagger} N_{\mu} \Psi_{\mathbf{k}} \Psi_{\mathbf{p}-\mathbf{q}}^{\dagger} N_{\mu} \Psi_{\mathbf{p}} \left. \right] \\ & + \frac{3|U_{\text{H}}|}{16} \sum_{\alpha\eta; \mathbf{k}\mathbf{p}} [|u_{\eta+}(\mathbf{k})|^2 |u_{\eta+}(\mathbf{p})|^2 d_{\mathbf{p};+\alpha}^{\dagger} d_{\mathbf{p};+\alpha}] \end{aligned}$$

$$F_{\mathbf{k}, \mathbf{p}, \mathbf{q}} \equiv \sum_{\eta} u_{\eta+}^*(\mathbf{k} + \mathbf{q}) u_{\eta+}(\mathbf{k}) u_{\eta+}^*(\mathbf{p} - \mathbf{q}) u_{\eta+}(\mathbf{p})$$

$$U_0=U_{15}=\frac{3|J_{\rm H}|}{8}, U_{23}=U_{34}=U_{24}=\frac{J_{\rm A}-3|J_{\rm H}|}{8}$$

$$U_{25}=U_{35}=U_{45}=U_{12}=U_{13}=U_{14}=\frac{J_{\rm A}}{16}$$

$$V_1=V_5=-\frac{3J_{\rm A}}{16}, V_2=V_3=V_4=-\frac{J_{\rm A}+3|J_{\rm H}|}{8}$$

$$S_{\rm WZW} = 2\pi i W[N_a]$$

$$W[N_a]=\frac{3}{8\pi^2}\int_u\int_{\mathbf{r},\tau}\varepsilon_{abcde}N^a\partial_xN^b\partial_yN^c\partial_\tau N^d\partial_uN^e$$

$$\pi_4\left(\frac{\mathrm{SO}(5)}{\mathrm{SO}(4)}\right)=\mathcal{Z}$$

$$|\Psi_{\rm G}^{\Theta}\rangle \equiv e^{-\Theta H} |\Psi_{\rm trial}\rangle$$

$$\nu \equiv \sum_{\mathbf{r}} \langle n_{\mathbf{r}} \rangle / L^2 = 2$$

$$U(1)_{\rm charge} \times U(1)_{\rm valley} \times SU(2)_{\rm spin}$$

$$\Delta \tau = \Theta / N_{\rm Trotter}$$

$$\xi_o \equiv \frac{1}{2\sin{(\pi/L)}}\sqrt{\frac{S_o(\boldsymbol{q}=\boldsymbol{0})}{S_o(\boldsymbol{q}=(2\pi/L,0))}}-1$$

$$S_o(\boldsymbol{q})=\frac{1}{L^2}\sum_{\mathbf{r},\mathbf{r}'}e^{-i(\mathbf{r}-\mathbf{r}')\cdot\boldsymbol{q}}\langle O^\dagger(\mathbf{r}')O(\mathbf{r})\rangle$$

$$\frac{\xi_o(J_{\rm H},L)}{L}=f_{\xi}(J_{\rm O})+L^{-\omega}g_{\xi}(J_{\rm O})\\ J_{\rm O}=[(J_{\rm H}-J_{\rm H}^c)/J_{\rm H}^c]L^{1/\nu_0}$$

$$S_O(\boldsymbol{q}=0;J_{\rm H},L)=L^{1-\eta_O}h_{S,\xi}(\xi_O/L)$$

$$\begin{aligned}\Delta_{\rm Tx}&=c_{\mathbf{r}+\uparrow}c_{\mathbf{r}-\uparrow}-c_{\mathbf{r}+\downarrow}c_{\mathbf{r}-\downarrow}\\\Delta_{\rm Ty}&=-i(c_{\mathbf{r}+\uparrow}c_{\mathbf{r}-\uparrow}+c_{\mathbf{r}+\downarrow}c_{\mathbf{r}-\downarrow})\\\Delta_{\rm Tz}&=c_{\mathbf{r}+\uparrow}c_{\mathbf{r}-\downarrow}+c_{\mathbf{r}+\downarrow}c_{\mathbf{r}-\uparrow}.\end{aligned}$$

$$\chi_{\Delta_{\rm T}}(\tau)\equiv\sum_{\alpha}\frac{\langle\Psi_{\rm G}^{\Theta}|e^{\tau H}\Delta_{T\alpha}^{\dagger}e^{-\tau H}\Delta_{T\alpha}|\Psi_{\rm G}^{\Theta}\rangle}{\langle\Psi_{\rm G}^{\Theta}|\Psi_{\rm G}^{\Theta}\rangle}$$

$$\frac{\xi_o(\mathcal{F},L)}{L}=\tilde{f}_{\xi}(\mathcal{F}_O)+L^{-\omega}\tilde{g}_{\xi}(\mathcal{F}_O)\\ \mathcal{F}_O=[(\mathcal{F}-\mathcal{F}^c)/\mathcal{F}^c]L^{1/\nu_0}$$



$$S_o(\boldsymbol{q}=0;\mathcal{F},L)=L^{1-\eta_o}\tilde{h}_{S,\xi}(\xi_o/L).$$

$$|{\boldsymbol{k}}_{e1}^+,{\boldsymbol{k}}_{e2}^+,{\boldsymbol{k}}_h^+\rangle\equiv c_{\boldsymbol{k}_{e1};+\uparrow}^\dagger c_{\boldsymbol{k}_{e2};+\uparrow}^\dagger c_{\boldsymbol{k}_h;+\downarrow}|\text{GS}\rangle$$

$$\boldsymbol{q}=\boldsymbol{k}_{e1}^+ + \boldsymbol{k}_{e2}^+ - \boldsymbol{k}_h^+$$

$$\boldsymbol{k}_{e(h)}^\tau c_{\boldsymbol{k}_{e1};+\uparrow}^\dagger c_{\boldsymbol{k}_{e2};+\uparrow}^\dagger |{\boldsymbol{k}}_{e1}^+,{\boldsymbol{k}}_{e2}^+,{\boldsymbol{k}}_h^+\rangle$$

$$|{\boldsymbol{k}}_{e1}^+,-{\boldsymbol{k}}_{e2}^-,-{\boldsymbol{k}}_h^-\rangle$$

$$\boldsymbol{q}=\boldsymbol{k}_{e1}^+ + \boldsymbol{k}_{e2}^- - \boldsymbol{k}_h^-$$

$$\begin{array}{ccc} \text{(a)} & \text{(b)} & \text{(c)} \\ \begin{array}{c} \rightarrow \boldsymbol{k}_{e1}^+ \\ \rightarrow \boldsymbol{k}_{e2}^+ \\ \leftarrow \boldsymbol{k}_h^+ \end{array} & \begin{array}{c} \rightarrow \boldsymbol{k}_{e1}^+ \\ \textcolor{red}{\leftarrow} -\boldsymbol{k}_{e2}^- \\ \textcolor{red}{\rightarrow} -\boldsymbol{k}_h^- \end{array} & \begin{array}{c} \boldsymbol{k}_{e1}^+ \text{---} \boldsymbol{k}_{e1}^+ \\ \boldsymbol{k}_{e2}^+ \text{---} \textcolor{red}{\rightarrow} -(p^- + \boldsymbol{k}_{e2}^+ - \boldsymbol{k}_h^+) \\ \boldsymbol{k}_h^+ \text{---} \textcolor{red}{\rightarrow} -p^- \end{array} \end{array}$$

$$|\text{GS}\rangle \equiv |+\downarrow\rangle \otimes |-\uparrow\rangle$$

$$\tilde{K}_{BS}^{\text{rep}}=J_{\text{A}}\sum_{p^-}u_+^*(\boldsymbol{k}_h^+)u_+(\boldsymbol{k}_{e2}^+)u_+^*(\boldsymbol{p}^-+\boldsymbol{k}_{e2}^+-\boldsymbol{k}_h^+)u_+(\boldsymbol{p}^-)|\boldsymbol{k}_{e1}^+,\boldsymbol{k}_{e2}^+,\boldsymbol{k}_h^+\rangle\langle\boldsymbol{k}_{e1}^+,-(\boldsymbol{p}^-+\boldsymbol{k}_{e2}^+-\boldsymbol{k}_h^+),-\boldsymbol{p}^-|,$$

$$u_{-}^{*}(-\boldsymbol{k})=u_{+}(\boldsymbol{k})$$

$$K\equiv\begin{bmatrix}K_{n\times n}^{(0,0)}&K_{n\times m}^{(0,1)}\\K_{m\times n}^{(1,0)}&K_{m\times m}^{(1,1)}\end{bmatrix};\;\Lambda_z\equiv\begin{bmatrix}\mathbb{I}_{n\times n}&\\&-\mathbb{I}_{m\times m}\end{bmatrix}.$$

$$\det[\Omega\Lambda_z-K]=0.$$

$$\langle\alpha|\Lambda_z|\alpha\rangle=1$$

$$\Psi_{\boldsymbol{k}}^\dagger\equiv\left[d_{+\uparrow}^\dagger(\boldsymbol{k}),d_{+\downarrow}^\dagger(\boldsymbol{k}),d_{-\uparrow}^\dagger(-\boldsymbol{k}),d_{-\downarrow}^\dagger(-\boldsymbol{k})\right]$$

$$d_{+\alpha}^\dagger(\boldsymbol{k}),d_{-\alpha}(-\boldsymbol{k})$$

$$u_+(\boldsymbol{k})=[u_-(-\boldsymbol{k})]^*$$

$$F_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}\equiv u_+^*(\boldsymbol{k}+\boldsymbol{q})u_+(\boldsymbol{k})u_+^*(\boldsymbol{p}-\boldsymbol{q})u_+(\boldsymbol{p}).$$

$$H_{J_{\text{H};+}}=-\frac{3J_{\text{H}}}{2}F_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}\left[d_{\boldsymbol{k}+\boldsymbol{q};+\uparrow}^\dagger d_{\boldsymbol{p}-\boldsymbol{q};+\downarrow}^\dagger d_{\boldsymbol{k};+\downarrow}d_{\boldsymbol{p};+\uparrow}\right]$$

$$H_{J_{\text{H};-}}=-\frac{3J_{\text{H}}}{2}F_{\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}}\left[d_{-\boldsymbol{k};-\uparrow}^\dagger d_{-\boldsymbol{p};-\downarrow}^\dagger d_{-\boldsymbol{k}-\boldsymbol{q};+\downarrow}d_{-\boldsymbol{p}+\boldsymbol{q};+\uparrow}\right].$$

$$H_{J_H} = \frac{3|J_H|}{8} \sum_{kpq} F_{k,p,q} \left[\Psi_{k+q}^\dagger \Psi_k \Psi_{p-q}^\dagger \Psi_p + \Psi_{k+q}^\dagger L_{15} \Psi_k \Psi_{p-q}^\dagger L_{15} \Psi_p - \sum_{(\alpha\beta)=(23),(34),(24)} \Psi_{k+q}^\dagger L_{\alpha\beta} \Psi_k \Psi_{p-q}^\dagger L_{\alpha\beta} \Psi_p \right. \\ \left. + \sum_{\mu=2,3,4} \Psi_{k+q}^\dagger N_\mu \Psi_k \Psi_{p-q}^\dagger N_\mu \Psi_p \right] + \frac{3|J_H|}{16} \sum_{\alpha;kp} [|u_+(\mathbf{k})|^2 |u_+(\mathbf{p})|^2 d_{p,+\alpha}^\dagger d_{p,+\alpha}]$$

$$H_{J_A} = \frac{J_A}{16} F_{k,p,q} \left[\sum_{(\alpha\beta)=(25),(35),(45),(12),(13),(14)} \Psi_{k+q}^\dagger L_{\alpha\beta} \Psi_k \Psi_{p-q}^\dagger L_{\alpha\beta} \Psi_p - 3 \sum_{\mu=1,5} \Psi_{k+q}^\dagger N_\mu \Psi_k \Psi_{p-q}^\dagger N_\mu \Psi_p \right] \\ - \frac{J_A}{8} F_{k,p,q} \left[- \sum_{(\alpha\beta)=(23),(34),(24)} \Psi_{k+q}^\dagger L_{\alpha\beta} \Psi_k \Psi_{p-q}^\dagger L_{\alpha\beta} \Psi_p + \sum_{\mu=2,3,4} \Psi_{k+q}^\dagger N_\mu \Psi_k \Psi_{p-q}^\dagger N_\mu \Psi_p \right]$$

$$\mathcal{L} = \sum_{\tau,\alpha} d_{\tau\alpha}^\dagger \frac{\partial d_{\tau\alpha}}{\partial \tau} - \lambda \sum_{q\mathbf{k};a} N_q^a \Lambda(\mathbf{k},\mathbf{q}) \Psi_{k+q}^\dagger \Gamma_a \Psi_{\mathbf{k}}$$

$$\Lambda(\mathbf{k},\mathbf{q})\equiv \langle u_{\mathbf{k}+\mathbf{q}}\mid u_{\mathbf{k}}\rangle$$

$$\Gamma_1=\sigma_y\mu_y, \Gamma_2=\sigma_x, \Gamma_3=\sigma_y\mu_z$$

$$\Gamma_4=\sigma_z, \Gamma_5=\sigma_y\mu_x$$

$$\Psi_{\mathbf{k}}^\dagger \equiv [d_{+\uparrow}^\dagger(\mathbf{k}), d_{+\downarrow}^\dagger(\mathbf{k}), d_{-\uparrow}(-\mathbf{k}), d_{-\downarrow}(-\mathbf{k})]$$

$$\langle u_{\mathbf{k}+\mathbf{q}}\mid u_{\mathbf{k}}\rangle$$

$$S_{\rm WZW}[N^a]=K\int_{\tau,r,u}\varepsilon_{abcde}N^a\partial_xN^b\partial_yN^c\partial_\tau N^d\partial_uN^e$$

$$S^{(4)} = \begin{array}{c} \begin{array}{ccc} \pi_i & & \pi_j \\ & \begin{array}{c} \xrightarrow{k} \end{array} & \\ \begin{array}{c} \downarrow k+p_1+p_2+p_3 \end{array} & \begin{array}{c} \square \end{array} & \begin{array}{c} \downarrow k+p_1 \end{array} \\ \begin{array}{c} \uparrow k+p_1+p_2 \end{array} & & \pi_l \\ \pi_m & & \end{array} \end{array}$$

$$= \frac{\lambda^4}{4} \pi_i \pi_j \pi_l \pi_m \sum_{\mathbf{k}, i\omega} \Lambda_{\mathbf{k}, \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3}^{\rm box} \text{Tr} \Big[G \Gamma^i G \Gamma^j G \Gamma^l G \Gamma^m \Big],$$

$$G_\omega=(i\omega+\lambda\Gamma_4)^{-1},$$

$$\sum_k \Lambda_{\mathbf{k}, \mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3}^{\text{box}} = \sum_k \text{tr}[\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3} \hat{P}_{\mathbf{k}+\mathbf{p}_1+\mathbf{p}_2} \hat{P}_{\mathbf{k}+\mathbf{p}_1}],$$

$$\hat{P}_{\mathbf{k}} \equiv |u_{\mathbf{k}}\rangle\langle u_{\mathbf{k}}|$$

$$\Lambda(\mathbf{k},\mathbf{p})\simeq 1+i a_{\mu}(\mathbf{k})p^{\mu}-\frac{1}{2}\gamma_{\mu\nu}(\mathbf{k})p^{\mu}p^{\nu}$$

$$\Lambda(\mathbf{k}+\mathbf{p},\mathbf{q})\simeq 1+i a_{\mu}(\mathbf{k})q^{\mu}-i\frac{F_{\mu\nu}(\mathbf{k})}{2}p^{\mu}q^{\nu}-\frac{1}{2}\gamma_{\mu\nu}(\mathbf{k})q^{\mu}q^{\nu},$$

$$\begin{aligned} S^{(4)} &= \frac{\lambda^4}{4} \pi_i \pi_j \pi_l \pi_m (p_1^\mu p_2^\nu + p_1^\mu p_3^\nu + p_2^\mu p_3^\nu) \int \frac{d^2 \mathbf{k}}{(2\pi)^2} \frac{F_{\mu\nu}(\mathbf{k})}{2} \sum_{i\omega} \text{Tr}[G\Gamma^i G\Gamma^j G\Gamma^l G\Gamma^m] \\ &= \frac{\lambda^4 C}{16\pi} \varepsilon_{\mu\nu} (p_1^\mu p_2^\nu + p_1^\mu p_3^\nu + p_2^\mu p_3^\nu) \pi_i \pi_j \pi_l \pi_m \sum_{i\omega} \text{Tr}[G\Gamma^i G\Gamma^j G\Gamma^l G\Gamma^m] \end{aligned}$$

$$\begin{aligned} \partial_{\Omega_3} S^{(4)} &= \pi_i \pi_j \pi_l \pi_m \frac{\lambda^4 C}{16\pi} \varepsilon_{\mu\nu} p_1^\mu p_2^\nu \Omega_3 \sum_{\omega_n} \text{Tr}[G_{\omega_n} \Gamma_i G_{\omega_n+\Omega_1} \Gamma_j G_{\omega_n+\Omega_1+\Omega_2} \Gamma_l \partial_{\Omega_3} G_{\omega_n+\Omega_1+\Omega_2+\Omega_3} \Gamma_m] \Bigg|_{\Omega_\alpha=0} \\ &= \frac{C}{16\pi} \varepsilon_{\mu\nu} p_1^\mu p_2^\nu \Omega_3 \pi_i \pi_j \pi_l \pi_m \text{Tr}[\Gamma_i \Gamma_j \Gamma_l \Gamma_m \Gamma_4] \sum_{\omega_n} \frac{\lambda^5}{(\omega_n^2 + \lambda^2)^3} \\ &= \frac{3C}{64\pi} \varepsilon_{\mu\nu} p_1^\mu p_2^\nu \Omega_3 (\pi_i \pi_j \pi_l \pi_m \varepsilon^{ijlm}) \end{aligned}$$

$$\partial_{\Omega_2} S^{(4)} = \pi_i \pi_j \pi_l \pi_m \frac{\lambda^4 C}{16\pi} \varepsilon_{\mu\nu} p_1^\mu p_3^\nu \Omega_2 \sum_{\omega_n} \text{Tr}[G_{\omega_n} \Gamma_i G_{\omega_n+\Omega_1} \Gamma_j \partial_{\Omega_2} G_{\omega_n+\Omega_1+\Omega_2} \Gamma_l G_{\omega_n+\Omega_1+\Omega_2+\Omega_3} \Gamma_m] \Bigg|_{\Omega_\alpha=0} + \partial_{\Omega_3} S^{(4)} = 0$$

$$\begin{aligned} \partial_{\Omega_1} S^{(4)} &= \pi_i \pi_j \pi_l \pi_m \frac{\lambda^4 C}{16\pi} \varepsilon_{\mu\nu} p_2^\mu p_3^\nu \Omega_1 \sum_{\omega_n} \text{Tr}[G_{\omega_n} \Gamma_i \partial_{\Omega_1} G_{\omega_n+\Omega_1} \Gamma_j G_{\omega_n+\Omega_1+\Omega_2} \Gamma_l G_{\omega_n+\Omega_1+\Omega_2+\Omega_3} \Gamma_m] \Bigg|_{\Omega_\alpha=0} + \partial_{\Omega_2} S^{(4)} \\ &= \frac{3C}{64\pi} \varepsilon_{\mu\nu} p_2^\mu p_3^\nu \Omega_1 (\pi_i \pi_j \pi_l \pi_m \varepsilon^{ijlm}) \end{aligned}$$

$$S_{\text{WZW}}[\pi^a]=i\frac{3C}{16\pi}\varepsilon^{ijklm}\int_{x,y,\tau}\pi_i\partial_x\pi_j\partial_y\pi_l\partial_\tau\pi_m$$

$$\begin{aligned} S_{\text{WZW}} &= 2\pi i C W[N_a] \\ W[N_a] &= \frac{3}{8\pi^2} \int_{\mathbf{r}, \tau, u} \varepsilon_{abcde} N^a \partial_x N^b \partial_y N^c \partial_\tau N^d \partial_u N^{\text{B}}. \end{aligned}$$

$$\eta_o(L)\equiv \frac{1}{\log\left[L/(L+2)\right]}\log\left.\frac{S_o(L+2)}{S_o(L)}\right|_{J_{\rm H}=J_{\rm H}^{\rm c}}-1.$$

$$\frac{1}{v_o(L)}\equiv \frac{1}{\log\left[(L+2)/L\right]}\log\left.\frac{\partial_{J_{\rm H}}R_o(L+2)}{\partial_{J_{\rm H}}R_o(L)}\right|_{J_{\rm H}=J_{\rm H}^{\rm c}},$$

$$-\sum_{i=1}^{N_e}\Delta_i+\sum_{i=1}^{N_e}\sum_I\frac{Z_I}{|\mathbf{r}_i-\mathbf{R}_I|}-\sum_{1\leq i< j\leq N_e}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|},$$

$$\sum_{i,j=1}^{N_\phi} (T_{ij} + U_{ij}) a_i^\dagger a_j + \sum_{i,j,k,l=1}^{N_\phi} V_{ijkl} a_i^\dagger a_k^\dagger a_j a_l.$$

$$T_{ij}=-\int_{\mathbb{R}^3}\phi_i(\mathbf{r})\Delta\phi_j(\mathbf{r})d\mathbf{r},U_{ij}=\sum_I\int_{\mathbb{R}^3}\phi_i(\mathbf{r})\frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|}\phi_j(\mathbf{r})d\mathbf{r}$$

$$V_{ijkl}=\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\phi_i(\mathbf{r}_1)\phi_j(\mathbf{r}_1)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_k(\mathbf{r}_2)\phi_l(\mathbf{r}_2)d\mathbf{r}_1d\mathbf{r}_2$$

$$\left(-\Delta+\sum_I\frac{1}{|\mathbf{r}-\mathbf{R}_I|}+V_{\mathrm{H}}[\rho]+V_{\mathrm{X}}[\{\psi_j\}]\right)\psi_k=\varepsilon_k\psi_k,k=1,\ldots,N_e$$

$$\rho(\mathbf{r})=\sum_{k=1}^{N_e}|\psi_k(\mathbf{r})|^2$$

$$V_{\mathrm{H}}[\rho](\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')\int_{\mathbb{R}^3}\frac{\rho(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}'$$

$$V_{\mathrm{X}}[\{\psi_j\}](\mathbf{r},\mathbf{r}')=-\sum_{k=1}^{N_e}\frac{\psi_k(\mathbf{r})\psi_k(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$E_{\mathrm{HF}}=\sum_{i=1}^{N_e}\langle\psi_i|T+U|\psi_i\rangle+\frac{1}{2}\langle\psi_i|V_{\mathrm{H}}[\rho]-V_{\mathrm{X}}[\{\psi_j\}]|\psi_i\rangle+E_{\mathrm{nuc}}$$

$$E_{\mathrm{nuc}}=\frac{1}{2}\sum_{I\neq J}\frac{1}{|\mathbf{R}_I-\mathbf{R}_J|}$$

$$\left(-\Delta+\sum_I\frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|}+V_{\mathrm{H}}[\rho]+V_{\mathrm{XC}}[\rho]\right)\psi_k=\varepsilon_k\psi_k,k=1,\ldots,N_e$$

$$\rho(\mathbf{r})=\sum_{k=1}^{N_e}|\psi_k(\mathbf{r})|^2,$$

$$E_{\mathrm{DFT}}=-\frac{1}{2}\sum_{i=1}^{N_e}\langle\psi_i|T|\psi_i\rangle+\int_{\mathbb{R}^3}\rho(\mathbf{r})[U+\epsilon_{\mathrm{XC}}(\rho)]d\mathbf{r}+\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'d\mathbf{r}+E_{\mathrm{nuc}}$$

$$V_{\mathrm{DG}}=\{v_h\colon v_h|_{K_m}\in V_m(K_m),m=1,\ldots,M\}$$

$$f(x_0)^-:=\lim_{x\rightarrow x_0,x\in K_m}f(x),f(x_0)^+:=\lim_{x\rightarrow x_0,x\in K_{m'}}f(x)$$

$$[[f]]=f^-\mathbf{n}^-+f^+\mathbf{n}^+$$

$$\{f\}:=\frac{1}{2}(f^-+f^+)$$

$$a_x=\min\{R_{I,x}\}-B, b_x=\max\{R_{I,x}\}+B,$$

$$S_{ij}=\int_{\mathbb{R}^3}\phi_i(\mathbf{r})\phi_j(\mathbf{r})d\mathbf{r}$$

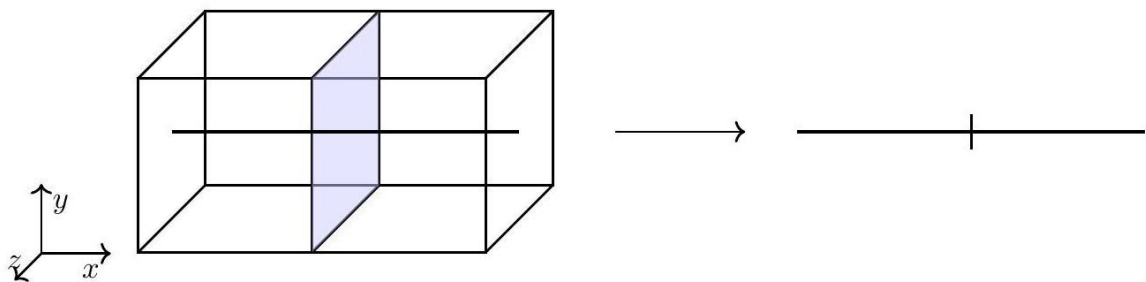
$$T_{ij}=\sum_{m=1}^M\int_{K_m}\nabla\phi_i(\mathbf{r})\cdot\nabla\phi_j(\mathbf{r})d\mathbf{r}+\int_{\Gamma}-\left[[\phi_i]\right]\cdot\left\{\nabla\phi_j\right\}-\left\{\nabla\phi_i\right\}\cdot\left[[\phi_j]\right]+\sigma\left[[\phi_i]\right]\cdot\left[[\phi_j]\right]ds$$

$$\sigma\geq\frac{C^2}{\epsilon h}, h=\min(x_k-x_{k-1},x_{k+1}-x_k)$$

$$\left|\frac{d}{dx}v^{\pm}(x_j)\right|^2\leq C^2\left\|\frac{d}{dx}v(x)\right\|_{L^2(K^{\pm})}^2$$

$$C^2\!:=\!\max\!\left\{\sum_i\left[\frac{d}{dx}\phi_i^-(x_k)\right]^2,\sum_i\left[\frac{d}{dx}\phi_i^+(x_k)\right]^2\right\}.$$

$$C^2=\frac{(p+1)^2}{h}$$

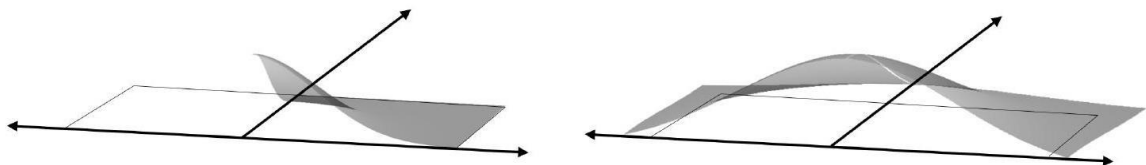


$$f(x,y,z)=f(x)f(y)f(z).$$

$$f(x,y,z)=x^{p_x}y^{p_y}z^{p_z}, p_x,p_y,p_z\leq p,$$

$$[a_x,b_x]\times[a_y,b_y]\times[a_z,b_z]$$

$$g(\mathbf{r})=x^{l_x}y^{l_y}z^{l_z}\exp\left(-\alpha|\mathbf{r}-\mathbf{R}|_2^2\right), l_x+l_y+l_z\leq l,$$



$$f(\mathbf{r})=g(\mathbf{r})\cdot\chi_m(\mathbf{r}), \chi_m(\mathbf{r})=\begin{cases}1, & \mathbf{r}\in K_m\\0, & \text{otherwise}\end{cases}$$

$$B_{\alpha}(\mathbf{R})=\{\mathbf{r}\colon |\mathbf{r}-\mathbf{R}|\leq 3/\sqrt{4\alpha}\}.$$

$$\left(\Delta+\sum_l\frac{Z_l}{|\mathbf{r}-\mathbf{R}_l|}\right)\tilde{\psi}_k=\varepsilon_k\tilde{\psi}_k,k=0,\ldots,N_{\text{init}}-1$$

$$[S_m]_{ij} = \int_{K_m} \left. \tilde{\psi}_i \right|_{K_m}(\mathbf{r}) \left. \tilde{\psi}_j \right|_{K_m}(\mathbf{r}) d(\mathbf{r})$$

$$S_m = U_m \Sigma_m V_m^T$$

$$N_{\rm init} = C N_{\rm filt} N_e,$$

$$\begin{aligned}\tilde{U}_{ij} &= \sum_I \int_{\mathbb{R}^3} \eta_i(\mathbf{r}) \frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|} \eta_j(\mathbf{r}) d\mathbf{r} \\ \tilde{V}_{ijkl} &= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \eta_i(\mathbf{r}_1) \eta_j(\mathbf{r}_1) \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} \eta_k(\mathbf{r}_2) \eta_l(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2\end{aligned}$$

$$\phi_i = \sum_{j=1}^{N_\eta} C_{ij} \eta_j$$

$$\begin{aligned}U_{ij} &= \sum_{k=1}^{N_\eta} \sum_{l=1}^{N_\eta} C_{ki} \tilde{U}_{kl} C_{lj} \\ V_{ijkl} &= \sum_{k=1}^{N_\eta} \sum_{l=1}^{N_\eta} C_{ai} C_{bj} \tilde{V}_{abcd} C_{ck} C_{dl}\end{aligned}$$

$$I_1 = \int_D \frac{f(\mathbf{r})}{\|\mathbf{r}\|} \, d\mathbf{r}$$

$$\frac{1}{\|\mathbf{r}\|} \approx \sum_{k=1}^{N_G} c_k \exp\left(-\alpha_k \|\mathbf{r}\|^2\right)$$

$$D = [a_x, b_x] \times [a_y, b_y] \times [a_z, b_z]$$

$$I_1 \approx \sum_{k=1}^{N_G} c_k \prod_{w \in \{x,y,z\}} \int_{a_w}^{b_w} \exp\left(-\alpha_k w^2\right) f_w(w) dw$$

$$I_2 = \int_D \int_{D'} \frac{f(\mathbf{r}) g(\mathbf{r}')}{\|\mathbf{r}-\mathbf{r}'\|} d\mathbf{r}' d\mathbf{r}$$

$$f(\mathbf{r}) = f_x(x)f_y(y)f_z(z) \text{ and } g(\mathbf{r}) = g_x(x)g_y(y)g_z(z)$$

$$D' = [a'_x, b'_x] \times [a'_y, b'_y] \times [a'_z, b'_z]$$

$$I_2 \approx \sum_{k=1}^{N_G} c_k \prod_{w \in \{x,y,z\}} \int_{a_w}^{b_w} \int_{a'_w}^{b'_w} \exp\left(-\alpha_k (w-w')^2\right) f_w(w) g_w(w') dw' dw$$

$$g_{\alpha}(x)=\exp\left(-\alpha x^2\right)\approx\sum_{k=0}^{N_F}a_{\alpha}^{(k)}\cos\left(\frac{k\pi x}{L_{\alpha}}\right)$$

$$\begin{aligned}
I_2 &\approx \sum_{n=1}^{N_G} c_n \prod_{w \in \{x,y,z\}} \sum_{k=0}^{N_F} a_{\alpha_n}^{(k)} \int_{a_w}^{b_w} \int_{a'_w}^{b'_w} \cos \left(\frac{k\pi(w-w')}{L_{\alpha_n}} \right) f_w(w) g_w(w') dw' dw \\
&= \sum_{n=1}^{N_G} c_n \prod_{w \in \{x,y,z\}} \sum_{k=0}^{N_F} a_{\alpha_n}^{(k)} \left(\int_{a_w}^{b_w} \cos \left(\frac{k\pi w}{L_{\alpha_n}} \right) f_w(w) dw \cdot \int_{a'_w}^{b'_w} \cos \left(\frac{k\pi w'}{L_{\alpha_n}} \right) g_w(w') dw' \right. \\
&\quad \left. + \int_{a_w}^{b_w} \sin \left(\frac{k\pi w}{L_{\alpha_n}} \right) f_w(w) dw \cdot \int_{a'_w}^{b'_w} \sin \left(\frac{k\pi w'}{L_{\alpha_n}} \right) g_w(w') dw' \right)
\end{aligned}$$

$$\{\phi_j\}_{j=1}^{N_\phi} u(\mathbf{r}) = \sum_{j=1}^{N_\phi} u_j \phi_j(\mathbf{r})$$

$$\begin{aligned}
J_{ij} &= \int_{\mathbb{R}^3} \phi_i(\mathbf{r}) \phi_j(\mathbf{r}) \cdot \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' d\mathbf{r} \\
&= \int_{\mathbb{R}^3} \phi_i(\mathbf{r}) \phi_j(\mathbf{r}) \cdot v_H(\mathbf{r}) d\mathbf{r}
\end{aligned}$$

$$-\Delta v_H(\mathbf{r}) = 4\pi\rho(\mathbf{r})$$

$$u(\mathbf{r}) = \sum_{j=1}^{N_\phi} u_j \phi_j(\mathbf{r})$$

$$\sum_{j=1}^{N_\phi} J_{ij} u_j = \int_{\mathbb{R}^3} \phi_i(\mathbf{r}) \cdot u(\mathbf{r}) v_H(\mathbf{r}) d\mathbf{r}$$

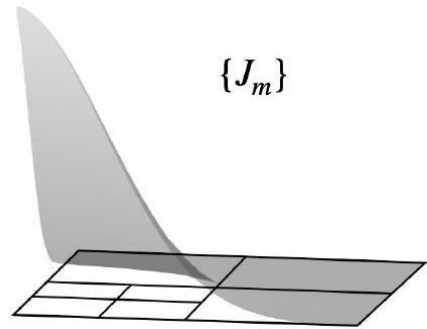
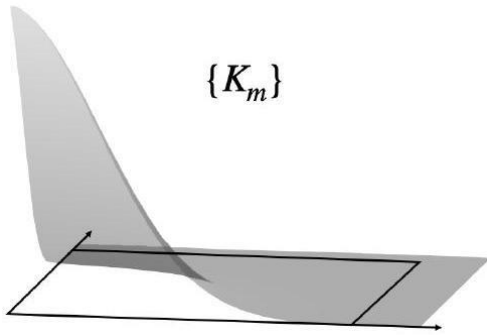
$$K_{ij} = \int_{\mathbb{R}^3} \phi_i(\mathbf{r}) \cdot \sum_{s=1}^{N_e} \psi_s(\mathbf{r}) \int_{\mathbb{R}^3} \frac{\phi_j(\mathbf{r}') \psi_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' d\mathbf{r}$$

$$u(\mathbf{r}) = \sum_{j=1}^{N_\phi} u_j \phi_j(\mathbf{r})$$

$$\begin{aligned}
\sum_j K_{ij} u_j &= \int_{\mathbb{R}^3} \phi_i(\mathbf{r}) \cdot \sum_{s=1}^{N_e} \psi_s(\mathbf{r}) \int_{\mathbb{R}^3} \frac{u(\mathbf{r}') \psi_s(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' d\mathbf{r} \\
&= \int_{\mathbb{R}^3} \phi_i(\mathbf{r}) \cdot \sum_{s=1}^{N_e} \psi_s(\mathbf{r}) v_s(\mathbf{r}) d\mathbf{r}
\end{aligned}$$

$$-\Delta v_s(\mathbf{r}) = 4\pi u(\mathbf{r}) \psi_s(\mathbf{r})$$

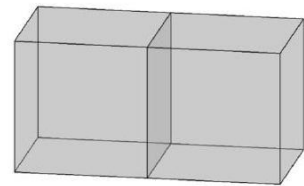
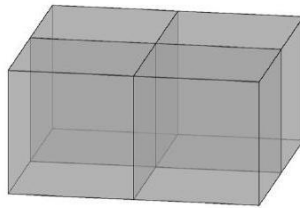
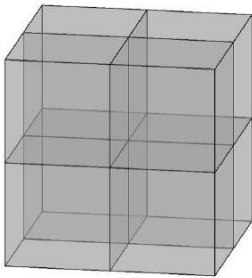
$$[\tilde{a}_x, \tilde{b}_x] = \bigcup_i \{x: |\eta_i^x(x)| > 10^{-9}\}$$



$$\sum_{i=1}^{(q+1)^3} \rho(\mathbf{x}_{im}) P_i(\mathbf{r}) \{\mathbf{x}_{im}\}_{i=1}^{(q+1)^3}$$

$$\{H_j\}_{j=1}^{n_{\text{ref}}} \{\tilde{\mathbf{x}}_{ij}\}_{i=1}^{(q+1)^3}$$

$$Q_m = \left| \sum_{i=1}^{(q+1)^3} \rho(\mathbf{x}_{im}) w_i - \sum_{j=1}^{n_{\text{ref}}} \sum_{i=1}^{(q+1)^3} \rho(\tilde{\mathbf{x}}_{ij}) \tilde{w}_i \right|,$$



$$\Omega\colon=\bigcup_{m=1}^{M_{\text{aux}}}J_m$$

$$-\Delta u=4\pi f$$

$$f(\mathbf{r})=\sum_{i=1}^{N_\phi} f_{ij}\phi_i(\mathbf{r})\phi_j(\mathbf{r})$$

$$-\Delta u=4\pi f \text{ in } \Omega; \; u(\mathbf{r})=\int_{\Omega} \frac{f(\mathbf{r}')}{\|\mathbf{r}-\mathbf{r}'\|} d\mathbf{r}', \mathbf{r}\in\partial\Omega$$

$$T+U-2\tilde{\varepsilon}_0I$$

$$(T+U)\tilde{\psi}_k=\varepsilon_k\tilde{\psi}_k, k=1,\ldots,N_{\text{init}}$$

$$O\big(MN_{\text{prim}}^2\,N_{\text{init}}+MN_{\text{prim}}\,N_{\text{init}}^2\,\big)$$

$$g(x) = \exp(-\alpha(x - x_0))$$

$$g(x) \approx \sum_{k=1}^{N_F} a_k \cos\left(\frac{k\pi x}{L_\alpha}\right),$$

$$L_\alpha = \sqrt{\frac{9}{\alpha} \log(10)}$$

$$a_k = \frac{1}{L_\alpha} \sqrt{\frac{\pi}{\alpha}} \exp\left(\frac{-\pi^2 k^2}{4\alpha L_\alpha^2}\right)$$

$$I_{\text{gp}} = \int_a^b g(x)p(x)dx$$

$$I_{\text{gp}} \approx \sum_{k=1}^{N_F} a_k \int_a^b \cos\left(\frac{k\pi x}{L_\alpha}\right) p(x) dx$$

$$\int_a^b \cos(\beta x) f(x) dx$$

$$\int_a^b \cos(\beta x) g(x) dx \approx \sum_{k=1}^{N_F} a_k \int_a^b \cos(\beta x) \cos\left(\frac{k\pi x}{L_\alpha}\right) dx$$

$$\int \cos(\beta x) \cos(\gamma x) dx = \begin{cases} \frac{1}{2} \left[\frac{\sin((\beta - \gamma)x)}{\beta - \gamma} + \frac{\sin((\beta + \gamma)x)}{\beta + \gamma} \right] + C, & \beta \neq \gamma \\ \frac{x}{2} + \frac{\sin(2\beta x)}{4\beta} + C, & \beta = \gamma \end{cases}$$

$$p(x) = \sum_{k=0}^q c_k P_k(x),$$

$$I_k = \int_{-1}^1 \cos(\beta x) P_k(x) dx, J_k = \int_{-1}^1 \sin(\beta x) P_k(x) dx, k = 0, \dots, q$$

$$P_k(x) = \frac{1}{2k+1} \frac{d}{dx} [P_{k+1}(x) - P_{k-1}(x)]$$

$$I_k = \frac{1}{2k+1} [(P_{k+1}(x) - P_{k-1}(x)) \cos(\beta x)]_a^b - \frac{\beta}{2k-1} [J_{k+1} - J_{k-1}]$$

$$J_k = \frac{1}{2k+1} [(P_{k+1}(x) - P_{k-1}(x)) \sin(\beta x)]_a^b + \frac{\beta}{2k-1} [I_{k+1} - I_{k-1}]$$

$$I_0 = \frac{2\sin(\beta)}{\beta}, I_1 = 0, J_0 = 0, J_1 = \frac{2\sin(\beta) - 2\beta\cos(\beta)}{\beta^2}.$$



$$\mathcal{H} = \sum_i \left(t e^{iA(\tau)} c_i^\dagger c_{i+1} + \text{H.c.} \right) + V \sum_i n_i n_{i+1},$$

$$A(\tau) = \frac{A_p}{\sqrt{2\pi}\tau_p} \exp\left(-\frac{\tau^2}{2\tau_p^2}\right) \cos(\omega_p \tau),$$

$$n_i n_{i+1} \rightarrow n_i \langle n_{i+1} \rangle + n_{i+1} \langle n_i \rangle - \langle n_i \rangle \langle n_{i+1} \rangle - \langle c_i^\dagger c_{i+1} \rangle c_{i+1}^\dagger c_i - \langle c_{i+1}^\dagger c_i \rangle c_i^\dagger c_{i+1} + \langle c_i^\dagger c_{i+1} \rangle \langle c_{i+1}^\dagger c_i \rangle$$

$$\phi = \frac{(-1)^i}{2} (\langle n_{i+1} \rangle - \langle n_i \rangle).$$

$$|\psi_{k,\nu}(\tau+\Delta\tau)\rangle = \exp\left[-i\Delta\tau\mathcal{H}_k^{\text{HF}}\left(\tau+\frac{\Delta\tau}{2}\right)\right]|\psi_{k,\nu}(\tau)\rangle,$$

$$\mathcal{H}_k^{\text{HF}}(\tau)\tau, |\psi_{k,\nu}(\tau)\rangle |\psi_{k,\nu}(\tau+\Delta\tau)\rangle (\Delta\tau)^3$$

$$\mathcal{H}_{\text{sp}} = \delta_{\text{sp}} \sum_i n_i (-1)^i,$$

$$|\Psi(\tau+\Delta\tau)\rangle = \exp\left[-i\Delta\tau\mathcal{H}_{\text{tot}}\left(\tau+\frac{\Delta\tau}{2}\right)\right]|\Psi(\tau)\rangle,$$

$$A_k(\varepsilon,\tau_{\text{pr}}) = A_k^<(\varepsilon,\tau_{\text{pr}}) + A_k^>(\varepsilon,\tau_{\text{pr}})$$

$$A_k^<(\varepsilon,\tau_{\text{pr}}) = \text{Im} \sum_{\alpha} \int d\tau_1 d\tau_2 s(\tau_1 - \tau_{\text{pr}}) s(\tau_2 - \tau_{\text{pr}}) \\ \times e^{i\varepsilon(\tau_1 - \tau_2)} G_{k,\alpha\alpha}^<(\tau_1,\tau_2)$$

$$A_k^>(\varepsilon,\tau_{\text{pr}}) = -\text{Im} \sum_{\alpha} \int d\tau_1 d\tau_2 s(\tau_1 - \tau_{\text{pr}}) s(\tau_2 - \tau_{\text{pr}}) \\ \times e^{i\varepsilon(\tau_1 - \tau_2)} G_{k,\alpha\alpha}^>(\tau_1,\tau_2)$$

$$G_{k,\alpha\beta}^<(\tau_1,\tau_2) = i \left\langle c_{k,\beta}^\dagger(\tau_2) c_{k,\alpha}(\tau_1) \right\rangle$$

$$G_{k,\alpha\beta}^>(\tau_1,\tau_2) = -i \left\langle c_{k,\alpha}(\tau_1) c_{k,\beta}^\dagger(\tau_2) \right\rangle$$

$$s(\tau) = \frac{1}{\sqrt{2\pi}\sigma_{\text{pr}}} \exp\left(-\frac{\tau^2}{2\sigma_{\text{pr}}^2}\right)$$

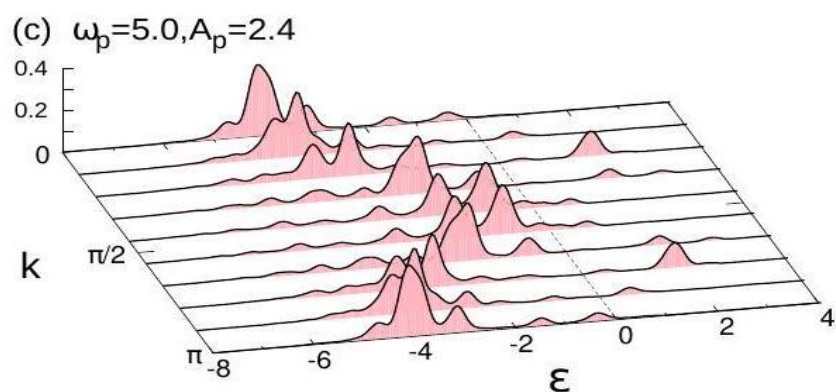
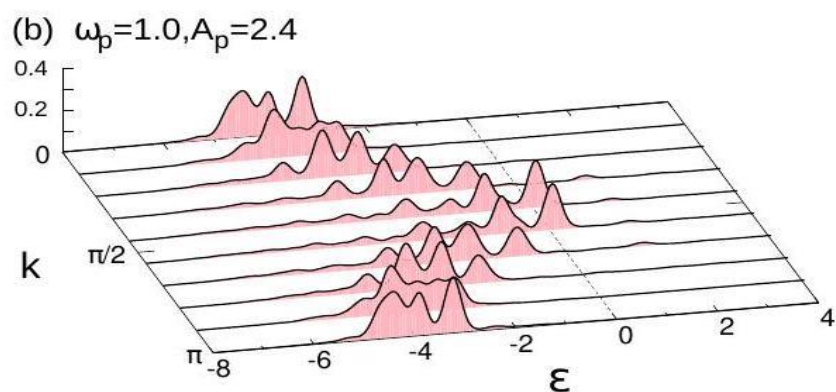
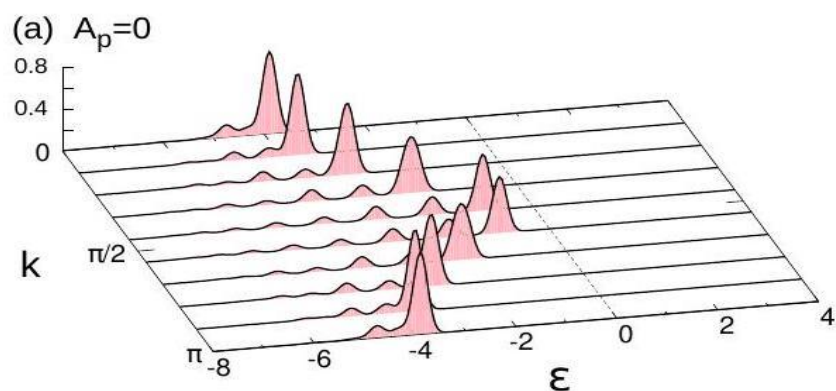
$$A(\tau) = A_{\text{cw}}\theta(\tau)e^{-\gamma\tau}\sin\omega\tau,$$

$$\mathcal{H}_{\text{imp}} = \delta_{\text{imp}} n_{i_p},$$

$$\Delta_{\text{CO}} = \mu_+ - \mu_-$$

$$\mu_+ = (E_0(N,N_e+2) - E_0(N,N_e))/2$$

$$\mu_- = (E_0(N,N_e) - E_0(N,N_e-2))/2$$



$$\hat{H} = \int d^3x \sum_i [\hat{\psi}^\dagger(\vec{r}i) H(\vec{r}i) \hat{\psi}(\vec{r}i) + U(\vec{r}i) \hat{\psi}^\dagger(\vec{r}i) \hat{\psi}(\vec{r}i) \\ + \Delta(\vec{r}) \hat{\psi}^\dagger(\vec{r} \uparrow) \hat{\psi}^\dagger(\vec{r} \downarrow) + \Delta^*(\vec{r}) \hat{\psi}(\vec{r} \downarrow) \hat{\psi}(\vec{r} \uparrow)]$$

$$H(\vec{r}i) = -(1/2m_i)(\vec{\nabla} - (ie\vec{A}/c))^2 - \mu_i$$

$$\Delta(\vec{r}) = \Delta^*(\vec{r}) = \Delta \cdot U(\vec{r}i)$$

$$U(\vec{r} \downarrow) = V \langle \psi^\dagger(\vec{r} \uparrow) \psi(\vec{r} \uparrow) \rangle$$

$$U(\vec{r} \uparrow) = V \langle \psi^\dagger(\vec{r} \downarrow) \psi(\vec{r} \downarrow) \rangle$$

$$V = -4\pi a/m_+ \text{ with } m_+ = 2m_\uparrow m_\downarrow / (m_\uparrow + m_\downarrow)$$

$$U(\vec{\textbf{r}}\downarrow)=U(\vec{\textbf{r}}\uparrow)\equiv U_s$$

$$U(\vec{\textbf{r}}\downarrow)\neq U(\vec{\textbf{r}}\uparrow)$$

$$a_{k,\sigma}^{\dagger}(a_{k,\sigma})\psi_{\sigma}^{\dagger}(\vec{r})=\sum_{\vec{k}}e^{i\vec{k}.\vec{r}}a_{k,\sigma}^{\dagger}\left(\psi_{\sigma}(\vec{r})=\sum_{\vec{k}}e^{i\vec{k}.\vec{r}}a_{k,\sigma}\right)$$

$$H=\sum_{\vec{k},\sigma}\left(\frac{k^2}{2m}-\mu_{\sigma}+U_{\sigma}\right)a_{\vec{k},\sigma}^{\dagger}a_{\vec{k},\sigma}+\sum_{\vec{k}}\Delta\left(a_{\vec{k},\uparrow}^{\dagger}a_{-\vec{k},\downarrow}^{\dagger}+a_{-\vec{k},\downarrow}a_{\vec{k},\uparrow}\right)$$

$$\psi_{\sigma}(\vec{r})=\sum_{\vec{k}}u_{\vec{k},\sigma}(\vec{r})\gamma_{\vec{k},\sigma}-v_{\vec{k},\sigma}(\vec{r})\gamma_{k,-\sigma}^{\dagger}$$

$$u_{\vec{k},\sigma}(\vec{r})\;v_{\vec{k},\sigma}(\vec{r})$$

$$H=\sum_{\vec{k},\sigma}E_{\vec{k}\alpha,\beta}\gamma_{\vec{k},\sigma}^{\dagger}\gamma_{\vec{k},\sigma}$$

$$E_{\vec{k}\alpha,\beta}\mu_s=((\mu_{\uparrow}+\mu_{\downarrow})/2)-U_s$$

$$h_s=(\mu_{\uparrow}-\mu_{\downarrow})/E_{\vec{k}\alpha\beta}$$

$$E_{\alpha,\beta}=\mp h_s\pm\frac{k^2}{2m_-}+\sqrt{\varepsilon_{p_{\alpha,\beta}}^2+\Delta^2}$$

$$\varepsilon_{\vec{k}_{\alpha}}=\varepsilon_{\vec{k}_{\beta}}\equiv(k^2/2m_+-\mu_s)$$

$$m_-=2m_{\uparrow}m_{\downarrow}/(m_{\downarrow}-m_{\uparrow})$$

$$\Delta-\sqrt{2\pi T\overline{\Delta}}(1-(T/8\overline{\Delta}))e^{-\Delta/T}$$

$$v_{\vec{k}}=\frac{1}{\sqrt{2}}\sqrt{1-\frac{k^2/2m_+-\mu_s}{E_{\vec{k}_{\alpha}}+h_s-k^2/2m_-}}\;u_{\vec{k}}=\frac{1}{\sqrt{2}}\sqrt{1+\frac{k^2/2m_+-\mu_s}{E_{\vec{k}_{\alpha}}+h_s-k^2/2m_-}}$$

$$1=\frac{-V}{2}\int\frac{d^3k}{(2\pi)^3}\left(\frac{1}{\sqrt{\left(\frac{k^2}{2m_+}-\mu_s\right)^2+\Delta^2}}-\frac{1}{\frac{k^2}{2m_+}}\right)$$

$$(k^2/2m_+\mu_s\rightarrow z,\Delta/\mu_s\rightarrow X)$$

$$\varsigma=-[1+X^2]^{-1/2}$$

$$\int_0^\infty \frac{z^\delta dz}{\sqrt{(z-1)^2+X^2}}=\frac{-\pi}{\sin \pi \delta^{-\delta}}\zeta^{-\delta}(\zeta)$$

$$\frac{1}{m_+ a^2} = -2\mu_s \frac{P_{1/2}^2(\zeta)}{\zeta}$$

$$\zeta = -[1 + (\Delta/\mu_s)^2]^{-1/2}$$

$$1 = \zeta^2 + 4(\Delta m_+ a^2)^2 [P_{1/2}(\zeta)]^4$$

$$\begin{aligned} k_F^3 &= 3\pi^2 n_s = 3\pi^2 \int_0^\infty \frac{d^3 k}{(2\pi)^3} \left(1 - \frac{k^2/2m_+ - \mu_s}{\sqrt{(k^2/2m_+ - \mu_s)^2 + \Delta^2}} \right) \\ &= -\frac{3}{2} \sqrt{2} m_+^{3/2} \mu_s^{3/2} (\pi(\zeta^{-2})^{3/4} p_{3/2}(\zeta) + \pi(\zeta^{-2})^{1/4} p_{1/2}(\zeta)) \end{aligned}$$

$$k_F a = (3\pi/4)^{1/3} [(P_{3/2}(\zeta)/P_{1/2}(\zeta) - \zeta)/P_{1/2}^2(\zeta)]^{1/3}$$

$$1 = \zeta^2 + 4 \left(\frac{\Delta}{\mu_s - \left(\frac{3}{2}\right)^{2/3}} \frac{((3\pi/4))[(P_{3/2}(\zeta)/P_{1/2}(\zeta) - \zeta)/P_{1/2}^2(\zeta)]^{2/3}}{2^{1/3}(\pi(\zeta^{-2})^{3/4} p_{3/2}(\zeta) + \pi(\zeta^{-2})^{1/4} p_{1/2}(\zeta))^{2/3}} \right)^2 [P_{1/2}(\zeta)]^4$$

$$\zeta = -[1 + (\Delta/\mu_s)^2]^{-1/2}$$

$$U_s = -\frac{V}{2} \int_0^\infty \frac{d^3 k}{(2\pi)^3} \left(1 - \frac{k^2/2m_+ - \mu_s}{\sqrt{(k^2/2m_+ - \mu_s)^2 + \Delta^2}} \right) = \mu_s (1 - \zeta^{-1} P_{3/2}(\zeta)/P_{1/2}(\zeta))$$

$$V = \frac{4\pi a}{m_+} \mu_\uparrow = \mu_s + U_s + h_s \mu_\downarrow = \mu_s + U_s - h_s$$

$$U_\uparrow = \frac{a}{m_+} \left(-\frac{4\sqrt{2}}{3\pi} \right) (m_r m_\uparrow (\mu_s + U_s - h_s - U_\downarrow))^{3/2}, U_\downarrow = \frac{a}{m_+} \left(-\frac{4\sqrt{2}}{3\pi} \right) (m_\uparrow (\mu_s + U_s + h_s - U_\uparrow))^{3/2}$$

$$\begin{aligned} &\frac{3\sqrt{2}\pi\zeta^2}{64|P_{1/2}(\zeta)|^5} \left((\zeta^{-2} - 5)P_{1/2}(\zeta) + 4\zeta^{-1}P_{3/2}(\zeta) \right) = \\ &m_+ a^5 (m_\uparrow)^{3/2} ((\mu_s + U_s + h_s - U_\uparrow)^{5/2} + (m_r)^{3/2} (\mu_s + U_s - h_s - U_\downarrow)^{5/2}) \end{aligned}$$

$$p_n = \frac{n_\uparrow^n - n_\downarrow^n}{n_\uparrow^n + n_\downarrow^n}$$

$$n_\delta^n = \int d^3 k / (2\pi)^3 = \int N(E_i) dE_i$$

$$E_\uparrow = \left| \frac{k^2}{2m_\uparrow} - \mu_s - h_s - U_s + U_\uparrow \right|, E_\downarrow = \left| \frac{k^2}{2m_\downarrow} - \mu_s + h_s - U_s + U_\downarrow \right|$$

$$p_n = \frac{(\mu_s + h_s + U_s - U_\uparrow)^{3/2} - (m_r)^{3/2} (\mu_s - h_s + U_s - U_\downarrow)^{3/2}}{(\mu_s + h_s + U_s - U_\uparrow)^{3/2} + (m_r)^{3/2} (\mu_s - h_s + U_s - U_\downarrow)^{3/2}}$$

$$p = \frac{n_\uparrow^n - n_\downarrow^n}{n_\uparrow^n + n_\downarrow^n + n_s}$$

$$1 = \frac{-V}{2} \int \frac{d^3 k}{(2\pi)^3} \left(\frac{1 - f(E_\alpha) - f(E_\beta)}{\sqrt{\left(\frac{k^2}{2m_+} - \mu_s\right)^2 + \Delta^2}} - \frac{1}{\frac{k^2}{2m_+}} \right)$$

$$n_{\uparrow}^n = \int d^3 k / (2\pi)^3 f(E_{\uparrow}) = \int d^3 k / (2\pi)^3 f\left(\frac{k^2}{2m_{\uparrow}} - \mu_{\uparrow} + U_{\uparrow}\right)$$

$$\mu_{\uparrow} - U_{\uparrow} \equiv \mu_s + h_s + U_s - U_{\uparrow}$$

$$H_1 = \sum_{\vec{k}, \vec{k}', \sigma, \sigma'} B(\vec{k}\sigma | \vec{k}'\sigma') a_{\vec{k}, \sigma}^{\dagger} a_{\vec{k}', \sigma'}$$

$$B(\vec{k}\sigma | \vec{k}'\sigma')\,B(\vec{k}\sigma | \vec{k}'\sigma')\vec{A}_{\vec{k}-\vec{k}'}\,B(\vec{k}\sigma | \vec{k}'\sigma')\vec{A}_{\vec{k}-\vec{k}'}\cdot(\vec{k}-\vec{k}')$$

$$B(\vec{k}\sigma | \vec{k}'\sigma')B(\vec{k}\sigma | \vec{k}'\sigma')B(\vec{k}\sigma | \vec{k}'\sigma')=B=\text{const}$$

$$a_{k\alpha}^{\dagger}=u_{\vec{k}}\gamma_{k\alpha}^{\dagger}+\sum_{\beta}\rho_{\alpha\beta}v_{\vec{k}}\gamma_{-\vec{k}\beta}$$

$$\rho=\begin{bmatrix}0&-1\\1&0\end{bmatrix}$$

$$H_1 = \sum_{\vec{k}, \vec{k}', \sigma, \sigma'} B \left(u_{\vec{k}} u_{\vec{k}'}^{\dagger} \gamma_{\vec{k}\sigma}^{\dagger} \gamma_{\vec{k}'\sigma'} + v_{\vec{k}} v_{\vec{k}'}^{\dagger} \sum_{\beta, \beta'} \rho_{\sigma\beta} \rho_{\sigma'\beta'} \gamma_{-\vec{k}\beta} \gamma_{-\vec{k}'\beta'}^{\dagger} + \right. \\ \left. u_{\vec{k}} v_{\vec{k}'}^{\dagger} \sum_{\beta'} \rho_{\sigma'\beta'} \gamma_{\vec{k}\sigma}^{\dagger} \gamma_{-\vec{k}'\beta'}^{\dagger} + v_{\vec{k}} u_{\vec{k}'}^{\dagger} \sum_{\beta'} \rho_{\sigma\beta} \gamma_{-\vec{k}\beta} \gamma_{\vec{k}'\sigma'} \right)$$

$$\gamma_{\vec{k}\sigma}^{\dagger}\gamma_{\vec{k}'\sigma'}|\vec{k}'\sigma'\rangle|\vec{k}\sigma\rangle\gamma_{-\vec{k}\beta}\gamma_{-\vec{k}'\beta'}^{\dagger}$$

$$\gamma_{\vec{k}\sigma}^{\dagger}\gamma_{-\vec{k}'\beta'}^{\dagger}\left(\gamma_{-\vec{k}\beta}\gamma_{\vec{k}'\sigma'}\right)$$

$$R_{\vec{k}\rightarrow\vec{k}'}=2\pi|\langle\vec{k}'\sigma'|H_1|\vec{k}\sigma\rangle|^2\Big\{f\left(E_{\vec{k}_\alpha}\right)\Big(1-f\left(E_{\vec{k}'_\alpha}\right)\Big)-f\left(E_{\vec{k}'_\alpha}\right)\Big(1-f\left(E_{\vec{k}_\alpha}\right)\Big)\Big\}\delta\left(E_{\vec{k}'_\alpha}-E_{\vec{k}_\alpha}-\omega\right)$$

$$|\vec{k}\sigma\rangle\equiv a_{\vec{k}\sigma}^{\dagger}\prod_{\vec{k}'\neq k}\left(u_{\vec{k}}+v_{\vec{k}}a_{\vec{k}'\uparrow}^{\dagger}a_{\vec{k}'\downarrow}^{\dagger}\right)|0\rangle$$

$$\gamma_{\vec{k}\sigma}^{\dagger}|\psi_{BCS}\rangle=|\vec{k}\sigma\rangle$$

$$|\psi_{BCS}\rangle\langle\vec{k}'\sigma'|H_1|\vec{k}\sigma\rangle$$

$$\langle\vec{k}'\sigma'|H_1|\vec{k}\sigma\rangle=B(u_{\vec{k}},u_{\vec{k}}-\eta v_{\vec{k}},v_{\vec{k}})$$

$$\frac{dE}{dt} = W = \frac{1}{(2\pi)^6} \sum_{\alpha=1}^2 \sum_{\sigma'=1}^2 \iint d^3k d^3k' R_{\vec{k} \rightarrow \vec{k}'} \omega$$

$$\sum_{\vec{k}} \dots = (1/2\pi^2) \int k^2 dk \dots = \int dE N_s(E) \dots$$

$$W = 2\pi\omega\overline{|B|^2} \int dE dE' N_s(E') N_s(E) \big((u(E')u(E) - \eta v(E')v(E))\big)^2 \big(f(E) - f(E')\big) \delta(E' - E - \omega)$$

$$N(E)=\sum_n\delta(E-E_n)$$

$$N_s(E)=\frac{4\pi k(E)}{\frac{1}{m_-}+\frac{\left(\frac{1}{m_+}\right)\left(\frac{k^2}{2m_+}-\mu_s\right)}{\sqrt{\left(\frac{k^2}{2m_+}-\mu_s\right)^2+\Delta^2}}}$$

$$k^2(E)=\frac{1}{\left(\frac{1}{(2m_-)^2}-\frac{1}{(2m_+)^2}\right)}\Big(-\Big[\frac{\mu_s}{2m_+}-\frac{E_\alpha+h_s}{2m_-}\Big]+ \sqrt{\Big[\frac{\mu_s}{2m_+}-\frac{E_\alpha+h_s}{2m_-}\Big]^2-\Big(\frac{1}{(2m_-)^2}-\frac{1}{(2m_+)^2}\Big)\big((E_\alpha+h_s)^2-\Delta^2-\mu_s^2\big)}\Big)$$

$$\hat{H} = \sum_{i=\uparrow,\downarrow} \int d\mathbf{r} \hat{\Psi}_i^\dagger \left[\frac{-\nabla^2}{2} + V(\mathbf{r}) - \mu + \frac{g_{ii}}{2} \hat{\Psi}_i^\dagger \hat{\Psi}_i \right] \hat{\Psi}_i \\ + g_{\uparrow\downarrow} \int d\mathbf{r} \hat{\Psi}_\uparrow^\dagger \hat{\Psi}_\downarrow^\dagger \hat{\Psi}_\uparrow \hat{\Psi}_\downarrow - \Omega \int d\mathbf{r} (\hat{\Psi}_\uparrow^\dagger \hat{\Psi}_\downarrow + \hat{\Psi}_\downarrow^\dagger \hat{\Psi}_\uparrow)$$

$${}^t\left(\begin{smallmatrix}\hat{\Psi}_{\uparrow}\\\hat{\Psi}_{\downarrow}\end{smallmatrix}\right)=\left(\begin{smallmatrix}\hat{h}_{\uparrow}+g_{\uparrow\uparrow}\hat{\Psi}_{\uparrow}^{\dagger}\hat{\Psi}_{\uparrow}&g_{\uparrow\downarrow}\hat{\Psi}_{\downarrow}^{\dagger}\hat{\Psi}_{\uparrow}\\g_{\uparrow\downarrow}\hat{\Psi}_{\uparrow}^{\dagger}\hat{\Psi}_{\downarrow}&\hat{h}_{\downarrow}+g_{\downarrow\downarrow}\hat{\Psi}_{\downarrow}^{\dagger}\hat{\Psi}_{\downarrow}\end{smallmatrix}\right)\left(\begin{smallmatrix}\hat{\Psi}_{\uparrow}\\\hat{\Psi}_{\downarrow}\end{smallmatrix}\right)\\-\left(\begin{smallmatrix}0&\Omega\\\Omega&0\end{smallmatrix}\right)\left(\begin{smallmatrix}\hat{\Psi}_{\uparrow}\\\hat{\Psi}_{\downarrow}\end{smallmatrix}\right)$$

$$\hat{h}_i=-\nabla^2/2-\mu$$

$$\hat{\Psi}_i(\mathbf{r},t)=\phi_i(\mathbf{r})+\delta\hat{\psi}_i(\mathbf{r},t)$$

$$\langle \delta \hat{\psi}_i \rangle = \langle \delta \hat{\psi}_i^\dagger \rangle = 0$$

$$0=\left(\begin{array}{cc}\hat{h}_{\uparrow}+L_{\uparrow}&g_{\uparrow\downarrow}\langle\delta\hat{\psi}_{\downarrow}^{\dagger}\delta\hat{\psi}_{\uparrow}\rangle-\Omega\\g_{\uparrow\downarrow}\langle\delta\hat{\psi}_{\uparrow}^{\dagger}\delta\hat{\psi}_{\downarrow}\rangle-\Omega&\hat{h}_{\downarrow}+L_{\downarrow}\end{array}\right)\left(\begin{array}{c}\phi_{\uparrow}\\\phi_{\downarrow}\end{array}\right),$$

$$L_i=g_{ii}(n_i+\tilde{n}_i)+g_{i\bar{i}}n_{\bar{i}}$$

$$\bar{i} \!=\! \downarrow \ (\uparrow) \text{ if } i \!=\! \uparrow \ (\downarrow), \, \tilde{n}_i \equiv \langle \delta \hat{\psi}_i^\dagger \delta \hat{\psi}_i \rangle$$

$$n_i = |\phi_i|^2 + \tilde{n}_i$$

$$\tilde{m}_i = \langle \delta \hat{\psi}_i \delta \hat{\psi}_i \rangle, \text{ and } \langle \delta \hat{\psi}_i \delta \hat{\psi}_{\bar{i}} \rangle$$

$$\langle \delta \hat{\psi}_i^\dagger \delta \hat{\psi}_{\bar{i}} \rangle \sum_i n_{ic} + \tilde{n}_i$$

$$\delta \hat{\psi}_i(\mathbf{r},t)=\sum_{j,\mathbf{k}}\left[u_{i,\mathbf{k}}^j\frac{e^{i\mathbf{k}.\mathbf{r}}}{\sqrt{V}}\hat{a}_je^{-i\omega_jt}+v_{i,\mathbf{k}}^{j*}\frac{e^{-i\mathbf{k}.\mathbf{r}}}{\sqrt{V}}\hat{a}_j^\dagger e^{i\omega_jt}\right],$$

$$\omega_j\begin{pmatrix}u_{\uparrow,\mathbf{k}}^j\\v_{\uparrow,\mathbf{k}}^j\\u_{\downarrow,\mathbf{k}}^j\\v_{\downarrow,\mathbf{k}}^j\end{pmatrix}=\mathcal{L}\begin{pmatrix}u_{\uparrow,\mathbf{k}}^j\\v_{\uparrow,\mathbf{k}}^j\\u_{\downarrow,\mathbf{k}}^j\\v_{\downarrow,\mathbf{k}}^j\end{pmatrix},$$

$$\mathcal{L}=\begin{pmatrix}\mathcal{L}_{\uparrow}&g_{\uparrow\uparrow}\phi_{\uparrow}^2&g_{\uparrow\downarrow}(\phi_{\uparrow}\phi_{\downarrow}^*+\langle\delta\hat{\psi}_{\downarrow}^{\dagger}\delta\hat{\psi}_{\uparrow}\rangle)-\Omega&g_{\uparrow\downarrow}\phi_{\uparrow}\phi_{\downarrow}\\-g_{\uparrow\uparrow}\phi_{\uparrow}^{*2}&\hat{\mathcal{L}}_{\uparrow}&-g_{\uparrow\downarrow}\phi_{\uparrow}^*\phi_{\downarrow}^*&-g_{\uparrow\downarrow}\left(\phi_{\uparrow}^*\phi_{\downarrow}+\langle\delta\hat{\psi}_{\downarrow}^{\dagger}\delta\hat{\psi}_{\uparrow}\rangle^*\right)+\Omega\\g_{\uparrow\downarrow}(\phi_{\downarrow}\phi_{\uparrow}^*+\langle\delta\hat{\psi}_{\uparrow}^{\dagger}\delta\hat{\psi}_{\downarrow}\rangle)-\Omega&g_{\uparrow\downarrow}\phi_{\downarrow}\phi_{\uparrow}&\hat{\mathcal{L}}_{\downarrow}&g_{\downarrow\downarrow}\phi_{\downarrow}^2\\-g_{\uparrow\downarrow}\phi_{\downarrow}^*\phi_{\uparrow}^*&-g_{\uparrow\downarrow}\left(\phi_{\downarrow}^*\phi_{\uparrow}+\langle\delta\hat{\psi}_{\uparrow}^{\dagger}\delta\hat{\psi}_{\downarrow}\rangle^*\right)+\Omega&-g_{\downarrow\downarrow}\phi_{\downarrow}^{*2}&\hat{\mathcal{L}}_{\downarrow}\end{pmatrix}.$$

$$\hat{\mathcal{L}}_i=\frac{1}{2}(k_x^2+k_y^2+k_z^2)+2g_{ii}n_i+g_{\uparrow\downarrow}n_{\bar{i}}$$

$$\underline{\mathcal{L}}_i=-\hat{\mathcal{L}}_i$$

$$\tilde{n}_i=(1/V)\sum_{j,\mathbf{k}}'\left\{\left[\left|u_{i,\mathbf{k}}^j\right|^2+\left|v_{i,\mathbf{k}}^j\right|^2\right]N_0(\omega_j)+\left|v_{i,\mathbf{k}}^j\right|^2\right\}$$

$$\langle \delta \hat{\psi}_i^\dagger \delta \hat{\psi}_{\bar{i}} \rangle = (1/V) \sum_{j,\mathbf{k}}' \{ [u_{i,\mathbf{k}}^{j*} u_{\bar{i},\mathbf{k}}^j + v_{i,\mathbf{k}}^j v_{\bar{i},\mathbf{k}}^{j*}] N_0(\omega_j) + v_{i,\mathbf{k}}^j v_{\bar{i},\mathbf{k}}^{j*} \}$$

$$N_0(\omega_j)\equiv (e^{\beta\omega_j}-1)^{-1}$$

$$\tilde{n}_i=(1/V)\sum_{j,\mathbf{k}}'\left|v_{i,\mathbf{k}}^j\right|^2$$

$$\varepsilon=\frac{1}{4}(g+g_{\uparrow\downarrow})n^2+\frac{1}{4}(g-g_{\uparrow\downarrow})s_z^2-\Omega\sqrt{n^2-s_z^2}-\mu n$$

$$\mu=\frac{n}{2}\bigg(g+g_{\uparrow\downarrow}-\frac{\Omega}{\sqrt{n_{\uparrow}n_{\downarrow}}}\bigg).$$

$$s_z\left(g-g_{\uparrow\downarrow}+\frac{2\Omega}{\sqrt{n^2-s_z^2}}\right)=0.$$

$$s_z = \pm n \sqrt{1 - \frac{4\Omega^2}{[(g - g_{\uparrow\downarrow})n]^2}},$$

$$\Omega_{\rm cr}(T=0)=\Omega_{\rm cr}(0)=n(g_{\uparrow\downarrow}-g)/2$$

$$\omega_{\pm}=\sqrt{C_k\pm\sqrt{C_k^2-\frac{k^2}{2}\left(\frac{k^2}{2}+\Omega\frac{n_{\uparrow}+n_{\downarrow}}{\sqrt{n_{\uparrow}n_{\downarrow}}}\right)\left[\prod_i\left(\frac{k^2}{2}+2gn_i+\Omega\sqrt{\frac{n_{\bar{i}}}{n_i}}\right)-\left(2g_{\uparrow\downarrow}\sqrt{n_{\uparrow}n_{\downarrow}}-\Omega\right)^2\right]}},$$

$$C_k=\frac{1}{2}\sum_i\left(\frac{k^2}{2}+\Omega\sqrt{\frac{n_{\bar{i}}}{n_i}}\right)\left(\frac{k^2}{2}+2gn_i+\Omega\sqrt{\frac{n_{\bar{i}}}{n_i}}\right)\\-\Omega(2g_{\uparrow\downarrow}\sqrt{n_{\uparrow}n_{\downarrow}}-\Omega).$$

$$\Delta=\sqrt{2\Omega\sqrt{n^2-s_Z^2}(g-g_{\uparrow\downarrow})+4\Omega^2\frac{n^2}{n^2-s_Z^2}}.$$

$$\delta n_{i,\mathbf{k}}^j(\mathbf{r})=2\mathrm{cos}\left(\mathbf{k}\cdot\mathbf{r}\right)\mathrm{Re}\big[\phi_i(u_{i,\mathbf{k}}^{j*}+v_{i,\mathbf{k}}^j)\big]$$

$$\delta n_{\mathbf{k}}^j=\delta n_{\uparrow,\mathbf{k}}^j+\delta n_{\downarrow,\mathbf{k}}^j \text{ and } \delta s_{\mathbf{k}}^j=\delta n_{\uparrow,\mathbf{k}}^j-\delta n_{\downarrow,\mathbf{k}}^j$$

$$S_{\pm,\mathbf{k}}^j=\left[(\delta n_{\mathbf{k}}^j)^2\pm(\delta s_{\mathbf{k}}^j)^2\right]$$

$$Q_{\mathbf{k}}^j\equiv S_{-,\mathbf{k}}^j/S_{+,\mathbf{k}}^j\cdot Q_{\mathbf{k}}^j=1(-1)$$

$$\Omega_{\rm cr}(T)\approx\Omega_{\rm cr}(0)n_c(T)/n$$

$$gn,1/\sqrt{gn}1/gngn=g_{\uparrow\downarrow}/g$$

$$\Omega_{\rm cr}(T)\approx\Omega_{\rm cr}(0)n_c(T)/n$$

$$k_BT_c=2\pi[(n/2)/\zeta(3/2)]^{2/3}$$

$$n_c(T)/n=1-(T/T_c)^{3/2}$$

$$a_x=(\hbar/m\omega_x)^{1/2}$$

$$\hbar\omega_y=\hbar\omega_z=\hbar\omega_{\perp}\gg kT>\hbar\omega_x$$

$$Na_{ii}a_{\perp}/a_x^2$$

$$Na_{\uparrow\downarrow}a_{\perp}/a_x^2$$

$$a_x,\omega_x^{-1},\hbar\omega_x$$

$$g=2a_{ii}(\omega_{\perp}/\omega_x)/a_x$$

$$g_{\uparrow\downarrow}=2a_{\uparrow\downarrow}(\omega_{\perp}/\omega_x)/a_x$$

$$V(x)=x^2/n_{\uparrow}^{\rm TF},n_{\downarrow}^{\rm TF}$$

$$\delta\hat{\psi}_i(x,t)=\sum_j\left[u_i^j(x)\hat{a}_je^{-i\omega_jt}+v_i^{j*}(x)\hat{a}_j^{\dagger}e^{i\omega_jt}\right]$$

$$\Omega_{\rm cr}(0)=(1/2)n(x=0)(g_{\uparrow\downarrow}-g)$$

$$n(x)=n_{\uparrow}(x)+n_{\downarrow}(x)$$

$$n_{\uparrow,\downarrow}^{\rm TF}(x)=\Big((\mu^{\rm TF}+\Omega)/(g+g_{\uparrow\downarrow})\Big)\Big(1-x^2/R_{\rm TF}^2\Big)\mu^{\rm TF}=[(3/8)N(g+g_{\uparrow\downarrow})]^{2/3}(1/2)^{1/3}-\Omega$$

$$R_{\rm TF}^2=2(\mu+\Omega)$$

$$n(\pm x_c)=2\Omega/(g_{\uparrow\downarrow}-g)$$

$$x_c=\sqrt{2\mu+4\Omega g/(g-g_{\uparrow\downarrow})}$$

$$n_{\uparrow,\downarrow}^{\rm TF}=(\mu-(1/2)x^2+\Omega)/(g+g_{\uparrow\downarrow})$$

$$|x|<x_c, n_{\uparrow,\downarrow}^{\rm TF}=n^{\rm TF}\left(1\pm\left(1-(2\Omega/(g_{\uparrow\downarrow}-g)n^{\rm TF})^2\right)^{1/2}\right)$$

$$n^{\rm TF}=(\mu-x^2/2)/g$$

$$S_{\pm}^j=\int\,dx\left[(\delta n^j(x))^2\pm(\delta s^j(x))^2\right]$$

$$\delta n^j(x)=\delta n_{\uparrow}^j(x)+\delta n_{\downarrow}^j(x), \delta s^j(x)=\delta n_{\uparrow}^j(x)-\delta n_{\downarrow}^j(x)$$

$$\delta n_i^j(x)=2\mathrm{Re}[\phi_i(x)(u_i^{j*}(x)+v_i^j(x))]$$

$$\omega_{\rm SD}^2=\omega_x^2\left(\frac{g-g_{\uparrow\downarrow}}{g+g_{\uparrow\downarrow}}\right)\left[\frac{1+8\Omega n_0(g+g_{\uparrow\downarrow})/5}{1+f(\Omega/(g-g_{\uparrow\downarrow})n_0)}\right]$$

$$f(\alpha)=3\alpha(1-\sqrt{1+\alpha}\mathrm{arccoth}\sqrt{1+\alpha})$$

$$\langle \hat{O} \rangle = \int \, dx \Phi^\dagger(x,t) \hat{O} \Phi(x,t)$$

$$\Phi(x,t)=[\phi_{\uparrow}(x,t),\phi_{\downarrow}(x,t)]^T$$

$$E_{HF} = \int_{\mathbb{R}^3} \left(\frac{1}{2} \sum_{\ell=1}^N |\nabla \phi_\ell|^2 - \sum_{k=1}^M \frac{Z_k}{|x - R_k|} \rho(x) \right) dx + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dx dy \\ - \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|P(x,y)|^2}{|x-y|} dx dy$$

$$P(x,y) = \sum_{\ell=1}^N \phi_\ell(x) \phi_\ell^*(y)$$

$$\rho(x) = P(x,x) = \sum_{\ell=1}^N |\phi_\ell(x)|^2$$

$$-\frac{1}{2}\Delta\phi_\ell+V_{\text{ext}}\phi_\ell+V_{\text{Har}}(\rho)\phi_\ell+V_{\text{x}}(P)\phi_\ell=\lambda_\ell\phi_\ell,\ell=1,\cdots,N,$$

$$V_{\text{ext}}=-\sum_{k=1}^M\frac{Z_k}{|x-R_k|}\\ V_{\text{Har}}(\rho)=\int_{\mathbb{R}^3}\frac{\rho(y)}{|x-y|}dy\\ V_{\text{x}}(P)\phi_\ell=-\int_{\mathbb{R}^3}\frac{P(x,y)}{|x-y|}\phi_\ell(y)dy$$

$$\frac{1}{2}(\nabla\phi_\ell,\nabla\psi)+(V_{\text{ext}}\phi_\ell,\psi)+(V_{\text{Har}}(\rho)\phi_\ell,\psi)+(V_{\text{x}}(P)\phi_\ell,\psi)=(\lambda_\ell\phi_\ell,\psi),\forall\psi\in H_0^1(\Omega)$$

$$(\phi,\psi)=\int_{\Omega}\phi\psi^*d\Omega$$

$$\frac{1}{2}(\nabla\phi_{\ell,h},\nabla\psi_h)+(V_{\text{ext}}\phi_{\ell,h},\psi_h)+(V_{\text{Har}}(\rho_h)\phi_{\ell,h},\psi_h)+(V_{\text{x}}(P_h)\phi_{\ell,h},\psi_h)=(\lambda_{\ell,h}\phi_{\ell,h},\psi_h),\forall\psi_h$$

$$\in V_h$$

$$\frac{1}{2}\Big(\nabla\phi_{\ell,h}^{(p+1)},\nabla\psi_h\Big)+\Big(V_{\text{ext}}\phi_{\ell,h}^{(p+1)},\psi_h\Big)+\Big(V_{\text{Har}}\left(\rho_h^{(p)}\right)\phi_{\ell,h}^{(p+1)},\psi_h\Big)+\Big(V_{\text{x}}\left(P_h^{(p)}\right)\phi_{\ell,h}^{(p+1)},\psi_h\Big)\\ =\Big(\lambda_{\ell,h}^{(p+1)}\phi_{\ell,h}^{(p+1)},\psi_h\Big),\forall\psi_h\in V_h$$

$$|E^{p+1}-E^p|/|E^{p+1}|\leq \text{TOL}$$

$$-\Delta V_{\text{Har}}(\rho_h)=4\pi\rho_h(x)$$

$$\begin{aligned} (V_{\text{x}}(P)\psi_j,\psi_i) &= -\left(\int_{\Omega}\frac{\rho(x,y)}{|x-y|}\psi_j(y)dy,\psi_i(x)\right) \\ &= -\left(\int_{\Omega}\frac{\sum_{\ell=1}^N\phi_{\ell}(x)\phi_{\ell}^*(y)}{|x-y|}\psi_j(y)dy,\psi_i(x)\right) \\ &= -\sum_{\ell=1}^N\int_{\Omega}\left(\int_{\Omega}\frac{\phi_{\ell}^*(y)\psi_j(y)}{|x-y|}dy\right)\phi_{\ell}(x)\psi_i(x)dx \end{aligned}$$

$$\int_{\Omega} \frac{\phi_{\ell}^*(y)\psi_j(y)}{|x-y|} dy$$

$$\begin{aligned} & \frac{1}{2}(\nabla \tilde{\phi}_{\ell,h_{k+1}}, \nabla \psi_{h_{k+1}}) + (V_{\text{ext}} \tilde{\phi}_{\ell,h_{k+1}}, \psi_{h_{k+1}}) + (V_{\text{Har}}(\rho_{h_k}) \tilde{\phi}_{\ell,h_{k+1}}, \psi_{h_{k+1}}) \\ &= (\lambda_{\ell,h_k} \phi_{\ell,h_k}, \psi_{h_{k+1}}) - (V_x(P_{h_k}) \phi_{\ell,h_k}, \psi_{h_{k+1}}), \forall \psi_{h_{k+1}} \in V_{h_{k+1}}. \end{aligned}$$

$$V_{H,h_{k+1}}=V_H+\text{span}\{\tilde{\phi}_{\ell,h_{k+1}}\}$$

$$\begin{aligned} & \frac{1}{2}(\nabla \phi_{\ell,h_{k+1}}, \nabla \psi_{H,h_{k+1}}) + (V_{\text{ext}} \phi_{\ell,h_{k+1}}, \psi_{H,h_{k+1}}) \\ &+ (V_{\text{Har}}(\rho_{h_{k+1}}) \phi_{\ell,h_{k+1}}, \psi_{H,h_{k+1}}) + (V_x(P_{h_{k+1}}) \phi_{\ell,h_{k+1}}, \psi_{H,h_{k+1}}) \\ &= (\lambda_{\ell,h_{k+1}} \phi_{\ell,h_{k+1}}, \psi_{H,h_{k+1}}), \forall \psi_{h_{k+1}} \in V_{H,h_{k+1}}. \end{aligned}$$

$$(\lambda_{\ell,h_{k+1}},\phi_{\ell,h_{k+1}})=\text{HFCorrection}(\lambda_{\ell,h_k},\phi_{\ell,h_k},V_H,V_{h_{k+1}}).$$

$$\mathcal{R}_T\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N\right)$$

$$\mathcal{J}_e\left(\left\{\phi_{\ell,h_k}\right\}_{\ell=1}^N\right)(\lambda_{\ell,h_k},\phi_{\ell,h_k}), \ell=1,\cdots,N$$

$$\mathcal{R}_T\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N\right):=(-\frac{1}{2}\Delta\phi_{\ell,h_k}+V_{\text{ext}}\phi_{\ell,h_k}+V_{\text{Har}}(\rho_{h_k})\phi_{\ell,h_k}+V_x(P_{h_k})\phi_{\ell,h_k}-\lambda_{\ell,h_k}\phi_{\ell,h_k})_{\ell=1}^N,$$

$$\mathcal{J}_e\left(\left\{\phi_{\ell,h_k}\right\}_{\ell=1}^N\right):=\left(\frac{1}{2}\nabla\phi_{\ell,h_k}\Big|_{T^+}\cdot v^++\frac{1}{2}\nabla\phi_{\ell,h_k}\Big|_{T^-}\cdot v^-\right)_{\ell=1}^N,\text{in }T\in\mathcal{T}_{h_k}$$

$$\eta_{h_k}^2\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,T\right)$$

$$\eta_{h_k}^2\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,T\right):=h_T^2\left\|\mathcal{R}_T\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N\right)\right\|_{0,T}^2+\sum_{e\in\mathcal{E}_{h_k},e\subset\partial T}h_e\left\|\mathcal{J}_e\left(\left\{\phi_{\ell,h_k}\right\}_{\ell=1}^N\right)\right\|_{0,e}^2.$$

$$\eta_{h_k}^2\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,\widehat{\Omega}\right)$$

$$\eta_{h_k}^2\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,\widehat{\Omega}\right)=\sum_{T\in\mathcal{T}_{h_k},T\subset\widehat{\Omega}}\eta_{h_k}^2\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,T\right).$$

$$\sum_{T\in\mathcal{M}_{h_k}}\eta_{h_k}^2\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,T\right)\geq\theta\eta_{h_k}^2\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,\Omega\right).$$

$$\begin{aligned} & \frac{1}{2}(\nabla \phi_{\ell,h_1}, \nabla \psi_{h_1}) + (V_{\text{ext}} \phi_{\ell,h_1}, \psi_{h_1}) + (V_{\text{Har}}(\rho_{h_1}) \phi_{\ell,h_1}, \psi_{h_1}) + (V_x(P_{h_1}) \phi_{\ell,h_1}, \psi_{h_1}) \\ &= (\lambda_{\ell,h_1} \phi_{\ell,h_1}, \psi_{h_1}), \ell=1,\cdots,N, \forall \psi_{h_1} \in V_{h_1}. \end{aligned}$$

$$\eta_{h_k}\left(\left\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\right\}_{\ell=1}^N,T\right)T\in\mathcal{T}_{h_k}$$

$$\mathcal{M}_{h_k}\subset\mathcal{T}_{h_k}$$

$$(\lambda_{\ell,h_{k+1}}, \phi_{\ell,h_{k+1}}) = \text{HFCorrection}(\lambda_{\ell,h_k}, \phi_{\ell,h_k}, V_H, V_{h_{k+1}}).$$

$$\begin{pmatrix} A_H & b_{Hh} \\ b_{Hh}^H & \beta \end{pmatrix} \begin{pmatrix} C_H \\ \theta \end{pmatrix} = \lambda_{\ell,h} \begin{pmatrix} M_H & c_{Hh} \\ c_{Hh}^H & \gamma \end{pmatrix} \begin{pmatrix} C_H \\ \theta \end{pmatrix},$$

$$\dim(A_H) = \dim(M_H) = N_H \times N_H, \dim(b_{Hh}) = \dim(c_{Hh}) = N_H \times 1, \dim(C_H) = N_H \times 1$$

$$\dim(\beta) = \dim(\gamma) = \dim(\theta) = 1$$

$$(M_H)_{i,j} = \int_{\Omega} \psi_{j,H} \psi_{i,H} dx, (c_{Hh})_i = \int_{\Omega} \tilde{\phi}_{\ell,h} \psi_{i,H} dx, \gamma = \int_{\Omega} |\tilde{\phi}_{\ell,h}|^2 dx$$

$$\phi_{\ell,Hh} = \tilde{\theta}_{\ell,h} + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H} \phi_{\ell,Hh}$$

$$\begin{aligned} (A_H)_{i,j} &= \frac{1}{2} \int_{\Omega} \nabla \psi_{j,H}(x) \nabla \psi_{i,H}(x) dx + \int_{\Omega} V_{\text{ext}} \psi_{j,H}(x) \psi_{i,H}(x) dx \\ &\quad + \int_{\Omega} V_{\text{Har}}(\rho_{Hh}) \psi_{j,H}(x) \psi_{i,H}(x) dx + \int_{\Omega} (V_x(P_{Hh}) \psi_{j,H}) \psi_{i,H}(x) dx \\ &= \frac{1}{2} \int_{\Omega} \nabla \psi_{j,H}(x) \nabla \psi_{i,H}(x) dx + \int_{\Omega} V_{\text{ext}} \psi_{j,H}(x) \psi_{i,H}(x) dx \\ &\quad + \sum_{s=1}^N \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}(y) \phi_{s,Hh}^*(y)}{|x-y|} dy \psi_{j,H}(x) \psi_{i,H}(x) dx \\ &\quad + \sum_{s=1}^N \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}^*(y) \psi_{j,H}(y)}{|x-y|} dy \phi_{s,Hh}(x) \psi_{i,H}(x) dx \end{aligned}$$

$$\begin{aligned} (A_{\text{Kin}})_{i,j} &= \frac{1}{2} \int_{\Omega} \nabla \psi_{j,H}(x) \nabla \psi_{i,H}(x) dx + \int_{\Omega} V_{\text{ext}} \psi_{j,H}(x) \psi_{i,H}(x) dx \\ (A_{\text{Har},s})_{i,j} &= \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}(y) \phi_{s,Hh}^*(y)}{|x-y|} dy \psi_{j,H}(x) \psi_{i,H}(x) dx \\ (A_{\text{x},s})_{i,j} &= \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}^*(y) \psi_{j,H}(y)}{|x-y|} dy \phi_{s,Hh}(x) \psi_{i,H}(x) dx \end{aligned}$$

$$\begin{aligned} &(A_{\text{Har},s})_{i,j} + (A_{\text{x},s})_{i,j} \\ &= \int_{\Omega} \int_{\Omega} \frac{|\tilde{\phi}_{s,h}(y)|^2}{|x-y|} dy \psi_{j,H}(x) \psi_{i,H}(x) dx \\ &\quad + \int_{\Omega} \int_{\Omega} \frac{\tilde{\phi}_{s,h}^*(y) \psi_{j,H}(y)}{|x-y|} dy \tilde{\phi}_{s,h}(x) \psi_{i,H}(x) dx \end{aligned}$$

$$(A_{\text{Har},\ell})_{i,j} + (A_{\text{x},\ell})_{i,j} = \int_{\Omega} \int_{\Omega} \frac{|\tilde{\theta}_{\ell,h}(y) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(y)|^2}{|x-y|} dy \psi_{j,H}(x) \psi_{i,H}(x) dx$$

$$+ \int_{\Omega} \left\{ \int_{\Omega} \frac{(\tilde{\theta}_{\ell,h}(y) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(y))^* \psi_{j,H}(y)}{|x-y|} dy \right.$$

$$\left. \left(\tilde{\theta}_{\ell,h}(x) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(x) \right) \psi_{i,H}(x) \right\} dx$$

$$\tilde{V}_{s,\ell}(x) = \int_{\Omega} \frac{\tilde{\phi}_{s,h}(y) \tilde{\phi}_{\ell,h}^*(y)}{|x-y|} dy$$

$$\tilde{V}_{s,m}(x) = \int_{\Omega} \frac{\tilde{\phi}_{s,h}(y) \psi_{m,H}(y)}{|x-y|} dy$$

$$V_{m,n}(x) = \int_{\Omega} \frac{\psi_{m,H}(y) \psi_{n,H}(y)}{|x-y|} dy$$

$$(A_{\text{Har},s})_{i,j} + (A_{\text{x},s})_{i,j} = \int_{\Omega} \tilde{V}_{s,s}(x) \psi_{j,H}(x) \psi_{i,H}(x) dx + \int_{\Omega} \tilde{V}_{s,j}^*(x) \tilde{\phi}_{s,h}(x) \psi_{i,H}(x) dx$$

$$(A_{\text{Har},\ell})_{i,j} + (A_{\text{x},\ell})_{i,j} = \int_{\Omega} \left\{ \left(\tilde{\theta}^2 \tilde{V}_{\ell,\ell}(x) + \tilde{\theta} \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,m}(x) + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,m}^*(x) + \sum_{m,n=1}^{N_H} c_{m,H} c_{n,H}^* V_{m,n}(x) \right) \right.$$

$$\left. \psi_{j,H}(x) \psi_{i,H}(x) \right\} dx$$

$$+ \int_{\Omega} \left(\tilde{\theta}^* \tilde{V}_{\ell,j}^*(x) + \sum_{m=1}^{N_H} c_{m,H}^* V_{j,m}(x) \right) \left(\tilde{\theta} \tilde{\phi}_{\ell,h}(x) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(x) \right) \psi_{i,H}(x) dx$$

$$V_{m,n,j,i} = \int_{\Omega} V_{m,n}(x) \psi_{j,H}(x) \psi_{i,H}(x) dx$$

$$\tilde{V}_{\ell,m,j,i} = \int_{\Omega} \tilde{V}_{\ell,m}(x) \psi_{j,H}(x) \psi_{i,H}(x) dx$$

$$\tilde{V}_{\ell,j,i} = \int_{\Omega} \tilde{V}_{\ell,\ell}(x) \psi_{j,H}(x) \psi_{i,H}(x) dx$$

$$\tilde{W}_{\ell,j,i} = \int_{\Omega} \tilde{V}_{\ell,j}(x) \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx$$

$$\tilde{W}_{*,\ell,j,i} = \int_{\Omega} \tilde{V}_{\ell,j}^*(x) \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx$$

$$\tilde{V}_{\ell,i,j,m} = \int_{\Omega} V_{j,m}(x) \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx$$

$$V_{m,n,j,i} V_{m,n,j,i} \tilde{\phi}_{\ell,h} \tilde{V}_{\ell,m,j,i} \tilde{V}_{\ell,j,i} \tilde{W}_{\ell,j,i} \tilde{W}_{*,\ell,j,i}$$

$$(A_{\text{Har},s})_{i,j} + (A_{\text{x},s})_{i,j} = \tilde{V}_{s,j,i} + \tilde{W}_{*,s,j,i}$$

$$\begin{aligned} (A_{\text{Har},\ell})_{i,j} + (A_{\text{x},\ell})_{i,j} = & \tilde{\theta}^2 \tilde{V}_{\ell,j,i} + \tilde{\theta} \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,m,j,i} + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,m,j,i}^* + \sum_{m,n=1}^{N_H} c_{m,H} c_{n,H}^* V_{m,n,j,i} \\ & + \tilde{\theta}^2 \tilde{W}_{*,\ell,j,i} + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,j,m,i}^* + \tilde{\theta} \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,i,j,m} + \sum_{m,n=1}^{N_H} c_{m,H}^* c_{n,H} V_{j,m,n,i}. \end{aligned}$$

$$(b_{Hh})_i = \frac{1}{2} \int_{\Omega} \nabla \tilde{\phi}_{\ell,h}(x) \nabla \psi_{i,H}(x) dx + \int_{\Omega} V_{\text{ext}} \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx$$

$$\begin{aligned} & + \int_{\Omega} V_{\text{Har}}(\rho_{Hh}) \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx + \int_{\Omega} (V_{\text{x}}(P_{Hh}) \tilde{\phi}_{\ell,h}) \psi_{i,H}(x) dx \\ = & \frac{1}{2} \int_{\Omega} \nabla \tilde{\phi}_{\ell,h}(x) \nabla \psi_{i,H}(x) dx + \int_{\Omega} V_{\text{ext}} \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx + \frac{1}{2} \int_{\Omega} \nabla \tilde{\phi}_{\ell,h}(x) \nabla \psi_{i,H}(x) dx + \int_{\Omega} V_{\text{ext}} \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx \\ & + \sum_{s=1}^N \int_{\Omega} \int_{\Omega} \frac{|\phi_{s,Hh}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx \\ & + \sum_{s=1}^N \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}^*(y) \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \phi_{s,Hh}(x) \psi_{i,H}(x) dx \end{aligned}$$

Denote

$$(b_{\text{Kin},\ell})_i = \frac{1}{2} \int_{\Omega} \nabla \tilde{\phi}_{\ell,h}(x) \nabla \psi_{i,H}(x) dx + \int_{\Omega} V_{\text{ext}} \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx$$

$$(b_{\text{Har},s,\ell})_i = \int_{\Omega} \int_{\Omega} \frac{|\phi_{s,Hh}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx$$

$$(b_{\text{x},s,\ell})_i = \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}^*(y) \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \phi_{s,Hh}(x) \psi_{i,H}(x) dx$$

$$\begin{aligned} (b_{\text{Har},\ell})_i + (b_{\text{x},s,\ell})_i & = \int_{\Omega} \int_{\Omega} \frac{|\tilde{\phi}_{s,h}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx + \int_{\Omega} \left\{ \int_{\Omega} \frac{\tilde{\phi}_{s,h}^*(y) \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \tilde{\phi}_{s,h}(x) \psi_{i,H}(x) \right\} dx \\ & = \int_{\Omega} \tilde{V}_{s,s}(x) \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx + \int_{\Omega} \tilde{V}_{\ell,s}(x) \tilde{\phi}_{s,h}(x) \psi_{i,H}(x) dx \end{aligned}$$

$$\begin{aligned}
& (b_{\text{Har},\ell,\ell})_i + (b_{\text{x},\ell,\ell})_i \\
&= \int_{\Omega} \int_{\Omega} \frac{|\tilde{\theta}_{\ell,h}(y) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx \\
&+ \int_{\Omega} \left\{ \int_{\Omega} \frac{(\tilde{\theta}_{\ell,h}(y) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(y))^* \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \right. \\
&\quad \left. \left(\tilde{\theta}_{\ell,h}(x) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(x) \right) \psi_{i,H}(x) \right\} dx \\
&= \int_{\Omega} \left\{ \left(\tilde{\theta}^2 \tilde{V}_{\ell,\ell}(x) + \tilde{\theta} \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,m}(x) + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,m}^*(x) + \sum_{m,n=1}^{N_H} c_{m,H} c_{n,H}^* V_{m,n}(x) \right) \right. \\
&\quad \left. \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) \right\} dx \\
&+ \int_{\Omega} \left(\tilde{\theta}^* \tilde{V}_{\ell,\ell}(x) + \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,m}(x) \right) \left(\tilde{\theta}_{\ell,h}(x) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(x) \right) \psi_{i,H}(x) dx
\end{aligned}$$

$$\tilde{V}_{s,m,\ell,i} = \int_{\Omega} \tilde{V}_{s,m}(x) \tilde{\phi}_{\ell,h}(x) \psi_{i,H}(x) dx$$

$$(b_{\text{Har},s,\ell})_i + (b_{\text{x},s,\ell})_i = \tilde{V}_{s,s,\ell,i} + \tilde{V}_{\ell,s,s,i}$$

$$\begin{aligned}
& (b_{\text{Har},\ell,\ell})_i + (b_{\text{x},\ell,\ell})_i \\
&= | \tilde{\theta}^2 \tilde{V}_{\ell,\ell,\ell,i} + \tilde{\theta} \sum_{m=1}^{N_H} c_{m,H}^* \tilde{W}_{\ell,m,i} + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{W}_{\ell,m,i}^* + \sum_{m,n=1}^{N_H} c_{m,H} c_{n,H}^* \tilde{V}_{\ell,i,m,n} \\
&\quad + | \tilde{\theta}^2 \tilde{V}_{\ell,\ell,\ell,i} + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,m,i} + \tilde{\theta} \sum_{m=1}^{N_H} c_{m,H}^* \tilde{W}_{\ell,m,i} + \sum_{m,n} c_{m,H}^* c_{n,H} \tilde{V}_{\ell,m,n,i}.
\end{aligned}$$

$$\begin{aligned}
\beta &= \frac{1}{2} \int_{\Omega} \nabla \tilde{\phi}_{\ell,h}(x) \nabla \tilde{\phi}_{\ell,h}^*(x) dx + \int_{\Omega} V_{\text{ext}} \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx \\
&+ \int_{\Omega} V_{\text{Har}}(\rho_{Hh}) \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx + \int_{\Omega} (V_{\text{x}}(P_{Hh}) \tilde{\phi}_{\ell,h}) \tilde{\phi}_{\ell,h}^*(x) dx \\
&= \frac{1}{2} \int_{\Omega} \nabla \tilde{\phi}_{\ell,h}(x) \nabla \tilde{\phi}_{\ell,h}^*(x) dx + \int_{\Omega} V_{\text{ext}} \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx \\
&+ \sum_{s=1}^N \int_{\Omega} \int_{\Omega} \frac{|\phi_{s,Hh}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx \\
&+ \sum_{s=1}^N \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}^*(y) \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \phi_{s,Hh}(x) \tilde{\phi}_{\ell,h}^*(x) dx
\end{aligned}$$

$$\beta_{\text{Kin},\ell} = \frac{1}{2} \int_{\Omega} \nabla \tilde{\phi}_{\ell,h}(x) \nabla \tilde{\phi}_{\ell,h}^*(x) dx + \int_{\Omega} V_{\text{ext}} \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx$$

$$\beta_{\text{Har},s,\ell} = \int_{\Omega} \int_{\Omega} \frac{|\phi_{s,Hh}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx$$

$$\beta_{\text{x},s,\ell} = \int_{\Omega} \int_{\Omega} \frac{\phi_{s,Hh}^*(y) \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \phi_{s,Hh}(x) \tilde{\phi}_{\ell,h}^*(x) dx$$

$$\begin{aligned} & \beta_{\text{Har},s,\ell} + \beta_{\text{x},s,\ell} \\ &= \int_{\Omega} \int_{\Omega} \frac{|\tilde{\phi}_{s,h}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx + \int_{\Omega} \int_{\Omega} \frac{\tilde{\phi}_{s,h}^*(y) \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \tilde{\phi}_{s,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx \\ &= \int_{\Omega} \tilde{V}_{s,s}(x) \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx + \int_{\Omega} \tilde{V}_{\ell,s}(x) \tilde{\phi}_{s,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx \end{aligned}$$

$$\begin{aligned} & \beta_{\text{Har},\ell,\ell} + \beta_{\text{x},\ell,\ell} \\ &= \int_{\Omega} \int_{\Omega} \frac{|\tilde{\theta}_{\ell,h}(y) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(y)|^2}{|x-y|} dy \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx \\ & \quad + \int_{\Omega} \left\{ \int_{\Omega} \frac{(\tilde{\theta}_{\ell,h}(y) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(y))^* \tilde{\phi}_{\ell,h}(y)}{|x-y|} dy \right. \\ & \quad \left. \left(\tilde{\theta}_{\ell,h}(x) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(x) \right) \tilde{\phi}_{\ell,h}^*(x) \right\} dx \\ &= \int_{\Omega} \left\{ \left(|\tilde{\theta}|^2 \tilde{V}_{\ell,\ell}(x) + \tilde{\theta} \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,m}(x) + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,m}^*(x) + \sum_{m,n=1}^{N_H} c_{m,H} c_{n,H}^* V_{m,n}(x) \right) \right. \\ & \quad \left. \tilde{\phi}_{\ell,h}(x) \tilde{\phi}_{\ell,h}^*(x) \right\} dx \\ & \quad + \int_{\Omega} \left(\tilde{\theta}^* \tilde{V}_{\ell,\ell}(x) + \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,m}(x) \right) \left(\tilde{\theta}_{\ell,h}(x) + \sum_{m=1}^{N_H} c_{m,H} \psi_{m,H}(x) \right) \tilde{\phi}_{\ell,h}^*(x) dx \end{aligned}$$

$$\tilde{V}_{s,m,j,\ell} = \int_{\Omega} \tilde{V}_{s,m}(x) \tilde{\phi}_{j,h}(x) \tilde{\phi}_{\ell,h}^*(x) dx$$

$$\beta_{\text{Har},s,\ell} + \beta_{\text{x},s,\ell} = \tilde{\tilde{N}}_{s,s,\ell,\ell} + \tilde{\tilde{V}}_{\ell,s,s,\ell}$$

$$\begin{aligned} & \beta_{\text{Har},\ell,\ell} + \beta_{\text{x},\ell,\ell} \\ &= |\tilde{\theta}^2|^2 \tilde{V}_{\ell,\ell,\ell,\ell} + \tilde{\theta}^N \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,\ell,\ell,m} + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,\ell,\ell,m}^* + \sum_{m,n=1}^{N_H} c_{m,H} c_{n,H}^* \tilde{V}_{\ell,m,n} \\ & \quad + |\tilde{\theta}^2|^{\tilde{T}} \tilde{V}_{\ell,\ell,\ell,\ell} + \tilde{\theta}^* \sum_{m=1}^{N_H} c_{m,H} \tilde{V}_{\ell,\ell,\ell,m}^* + \tilde{\theta}^N \sum_{m=1}^{N_H} c_{m,H}^* \tilde{V}_{\ell,\ell,\ell,m} + \sum_{m,n=1}^{N_H} c_{m,H} c_{n,H}^* \tilde{W}_{*,\ell,m,n} \end{aligned}$$

$$(\tilde{\mathbf{V}}_{\ell})_{m,i,j} = \tilde{V}_{\ell,m,i,j}$$

$$(\tilde{\tilde{\mathbf{V}}}_{\ell})_{i,j} = \tilde{\tilde{V}}_{\ell,i,j}, (\tilde{\mathbf{W}}_{\ell})_{i,j} = \tilde{W}_{\ell,i,j}, (\tilde{\mathbf{W}}_{*,\ell})_{i,j} = \tilde{W}_{*,\ell,i,j}$$

$$\left(\widetilde{\mathbf{V}}_{\ell}\right)_i=\widetilde{V}_{\ell,\ell,\ell,i}$$

$$\widetilde{\widetilde{V}}_{\ell}=\widetilde{\widetilde{V}}_{\ell,\ell,\ell,\ell}$$

$$\widetilde{\mathbf{V}}_{\mathbf{1}\ell},\widetilde{\mathbf{V}}_{\mathbf{2}\ell}\left(\widetilde{\mathbf{V}}_{\mathbf{1}\ell}\right)_{s,i}=\widetilde{V}_{s,s,\ell,i},\left(\widetilde{\mathbf{V}}_{\mathbf{2}\ell}\right)_{s,i}=\widetilde{V}_{\ell,s,s,i}$$

$$\frac{\widetilde{V}_{1\ell}}{\widetilde{\widetilde{V}}}\frac{\widetilde{V}_{2\ell}}{\widetilde{V}}\left(\frac{\mathbf{V}_{1\ell}}{\widetilde{V}}\right)_s=\frac{\widetilde{V}_{s,s,\ell,\ell}}{\widetilde{V}}\left(\frac{\mathbf{V}_{2\ell}}{\widetilde{V}}\right)_s=\frac{\widetilde{V}_{\ell,s,s,\ell}}{\widetilde{V}}$$

$$-\Delta \widetilde{V}_{\ell,s}(x)=4\pi \widetilde{\phi}_{\ell,h}\widetilde{\phi}_{s,h}^*,s=1,\cdots,N\\ -\Delta \widetilde{V}_{\ell,m}(x)=4\pi \widetilde{\phi}_{\ell,h}\psi_{m,H},m=1,\cdots,N_H$$

$$-\Delta V_{m,n}(x)=4\pi \psi_{m,H}\psi_{n,H},m,n=1,\cdots,N_H$$

$$\phi_{\ell,Hh}=\tilde{\theta}_{\ell}\tilde{\phi}_{\ell,h}+\sum_{m=1}^{N_H}c_{m,H,\ell}\psi_{m,H}$$

$$\int_{\Omega}\frac{\phi_{\ell,Hh}(y)\phi_{s,Hh}(y)}{|x-y|}dy$$

$$\int_{\Omega}\frac{\phi_{\ell,Hh}(y)\phi_{s,Hh}^*(y)}{|x-y|}dy\\ =\int_{\Omega}\frac{(\tilde{\theta}_{\ell}\tilde{\phi}_{\ell,h}(y)+\sum_{m=1}^{N_H}c_{m,H,\ell}\psi_{m,H}(y))(\tilde{\theta}_s^*\tilde{\phi}_{s,h}^*(y)+\sum_{m=1}^{N_H}c_{m,H,s}^*\psi_{m,H}(y))}{|x-y|}dy\\ =\tilde{\theta}_{\ell}\tilde{\theta}_s^*\tilde{V}_{\ell,s}+\sum_{m=1}^{N_H}c_{m,H,\ell}\tilde{\theta}_s^*\tilde{V}_{s,m}^*+\sum_{m=1}^{N_H}c_{m,H,s}^*\tilde{\theta}_{\ell}\tilde{V}_{\ell,m}+\sum_{m,n=1}^{N_H}c_{m,H,\ell,\ell}^*c_{n,H,s}V_{m,n}$$

$$\eta_{h_k}\left(\{\lambda_{\ell,h_k},\phi_{\ell,h_k}\}_{\ell=1}^N,T\right)$$

$$V_{H,h_{k+1}}=V_H+\mathrm{span}\{\tilde{\phi}_{\ell,h_{k+1}}\}$$

$$A_{\mathrm{Har},s}+A_{\mathrm{x},s}$$

$$A_H=A_{\mathrm{Kin}}+\sum_s\left(A_{\mathrm{Har},s}+A_{\mathrm{x},s}\right)$$

$$b_{\mathrm{Har},s,\ell}+b_{\mathrm{x},s,\ell}$$

$$b_{Hh}=b_{\mathrm{Kin}}+\sum_s\left(b_{\mathrm{Har},s,\ell}+b_{\mathrm{x},s,\ell}\right)$$

$$\beta_{\text{Har},s,\ell} + \beta_{\text{x},s,\ell}$$

$$\beta = \beta_{\text{Kin}} + \sum_s (\beta_{\text{Har},s,\ell} + \beta_{\text{x},s,\ell})$$

$$A_H = A_{\text{Kin}} + \sum_s (A_{\text{Har},s} + A_{\text{x},s}) O(NN_H^2 + N_H^3)$$

$$b_{Hh} = b_{\text{Kin}} + \sum_s (b_{\text{Har},s,\ell} + b_{\text{x},s,\ell}) O(NN_H + N_H^3)$$

$$\beta = \beta_{\text{Kin}} + \sum_s (\beta_{\text{Har},s,\ell} + \beta_{\text{x},s,\ell}) O(N + N_H^2)$$

$$O\left((N+N_H)N_k+\omega(NN_H^2+N_H^3+M_H)\right)$$

$$\tilde{\mathbf{W}}_\ell, \tilde{\mathbf{W}}_{*,\ell}, \tilde{\tilde{\mathbf{V}}}_{\mathbf{1}\ell}, \tilde{\tilde{\mathbf{V}}}_{\mathbf{2}\ell}$$

$$\dim(\tilde{\mathbf{W}}_\ell)=\dim(\tilde{\mathbf{W}}_{*,\ell})=N_H\times N_H, \dim(\tilde{\tilde{\mathbf{V}}}_{\mathbf{1}\ell})=\dim(\tilde{\tilde{\mathbf{V}}}_{\mathbf{2}\ell})=N\times N_H$$

$$O(N_k + NN_H + N_H^2)$$

$$\hat{H}^{\text{full}} = \sum_{\mu=1}^{N_{\text{nuc}}} \frac{-\hbar^2}{2M_{\mu}} \nabla_{\mathbf{R}_{\mu}}^2 + \frac{e^2}{4\pi\epsilon_0} \sum_{\mu=1}^{N_{\text{nuc}}} \sum_{\nu=\mu+1}^{N_{\text{nuc}}} \frac{Z_{\mu}Z_{\nu}}{|\mathbf{R}_{\mu}-\mathbf{R}_{\nu}|} \\ \frac{e^2}{4\pi\epsilon_0} \sum_{\mu=1}^{N_{\text{nuc}}} \sum_{i=1}^N \frac{Z_{\mu}}{|\mathbf{R}_{\mu}-\mathbf{r}_i|} + \frac{-\hbar^2}{2m_e} \sum_{i=1}^N \nabla_{\mathbf{r}_i}^2 + \frac{e^2}{4\pi\epsilon_0} \sum_{i=1}^N \sum_{j=1}^{i-1} \frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}$$

$$\Psi_{\text{full}}\left(\mathbf{X}_1,\ldots,\mathbf{X}_{N_{\text{nuc}}},\mathbf{x}_1,\ldots,\mathbf{x}_N\right)$$

$$\mathbf{X}_{\mu} \coloneqq \mathbf{R}_{\mu} \Sigma_{\mu} \text{ and } \mathbf{x}_i \coloneqq \mathbf{r}_i \sigma_i$$

$$\hat{H} = -\frac{1}{2} \sum_{i=1}^N \nabla_{\mathbf{r}_i}^2 + \sum_{i=1}^N \underbrace{\sum_{\mu=1}^{N_{\text{nuc}}} \frac{-Z_{\mu}}{|\mathbf{R}_{\mu}-\mathbf{r}_i|}}_{=v(\mathbf{r}_i)} + \sum_{1 \leq i < j \leq N} \underbrace{\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}}_{=w(\mathbf{r}_i,\mathbf{r}_j)} + \underbrace{\sum_{1 \leq \mu < \nu \leq N_{\text{nuc}}} \frac{Z_{\mu}Z_{\nu}}{|\mathbf{R}_{\mu}-\mathbf{R}_{\nu}|}}_{=E_{\text{nuc}}}, (1.4)$$

$$a_0=\frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$$



$$\text{Hartree}=\frac{m_e}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2$$

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N),$$

$$L^2(\mathbb{R}^3)\!:=\!\left\{f\!:\!\mathbb{R}^3\rightarrow\mathbb{C}\!:\!\int\,\mathrm{d}\mathbf{r}|f(\mathbf{r})|^2<\infty\right\}$$

$$\langle f \mid g \rangle := \int \mathrm{d}\mathbf{r} f^*(\mathbf{r}) g(\mathbf{r})$$

$$\psi(\mathbf{x})\begin{pmatrix}\psi_{\alpha}(\mathbf{r})\\ \psi_{\beta}(\mathbf{r})\end{pmatrix}$$

$$\mathcal{H}\!:=\!L^2(\mathbb{R}^3)\otimes\mathbb{Z}_2=\left\{f\!:\!\mathbb{R}^3\times\mathbb{Z}_2\rightarrow\mathbb{C}\!:\!\int\,\mathrm{d}\mathbf{x}|f(\mathbf{x})|^2<\infty\right\}.$$

$$\int\,\mathrm{d}\mathbf{x}\!:=\!\int\,\mathrm{d}\mathbf{r}\sum_{\sigma\in\mathbb{Z}_2}=\int\,\mathrm{d}\mathbf{r}\sum_{\sigma\in\{-1,1\}}=\int\,\mathrm{d}\mathbf{r}\sum_{\sigma\in\{\uparrow,\downarrow\}}$$

$$\langle f \mid g \rangle := \int \mathrm{d}\mathbf{x} f^*(\mathbf{x}) g(\mathbf{x}) = \int \mathrm{d}\mathbf{r} \sum_{\sigma \in \mathbb{Z}_2} f^*(\mathbf{r}\sigma) g(\mathbf{r}\sigma).$$

$$\psi(\mathbf{x})=\sum_{i=1}^{\infty}\psi_i\phi_i(\mathbf{x}).$$

$$\psi_i=\langle\phi_i\mid\psi\rangle$$

$$\langle\phi_i\mid\phi_j\rangle=\delta_{ij}$$

$$\mathcal{H}^N\!:=\!\bigotimes_{i=1}^N\mathcal{H}=\underbrace{\mathcal{H}\otimes\cdots\otimes\mathcal{H}}_{N\text{ times}},$$

$$\mathbb{R}^3=\mathbb{R}\times\mathbb{R}\times\mathbb{R}\text{ out }\mathbb{R}$$

$$f(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\sum_{i_1,\ldots,i_N}f_{i_1\ldots i_N}\underbrace{\phi_{i_1}(\mathbf{x}_1)\phi_{i_2}(\mathbf{x}_2)\cdots\phi_{i_N}(\mathbf{x}_N)}_{=:\Phi_{i_1i_2\ldots i_N}(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)}.$$

$$\begin{array}{lll} 1\cdot 1\cdot 1, \\ x_1\cdot 1\cdot 1, & 1\cdot x_2\cdot 1, & 1\cdot 1\cdot x_3 \\ x_1^2\cdot 1\cdot 1, & x_1\cdot x_2\cdot 1, & x_1\cdot 1\cdot x_3 \\ 1\cdot x_2^2\cdot 1, & 1\cdot x_2\cdot x_3, & 1\cdot 1\cdot x_3^2, \text{ etc.} \end{array}$$

$$\Phi_{i_1i_2\ldots i_N}^{\pm}(\mathbf{x}_1,\ldots,\mathbf{x}_N)\!:=\!\frac{1}{\sqrt{N!}}\left|\begin{array}{cccc}\phi_{i_1}(\mathbf{x}_1) & \phi_{i_2}(\mathbf{x}_1) & \cdots & \phi_{i_N}(\mathbf{x}_1) \\ \phi_{i_1}(\mathbf{x}_2) & \phi_{i_2}(\mathbf{x}_2) & \cdots & \phi_{i_N}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{i_1}(\mathbf{x}_N) & \phi_{i_2}(\mathbf{x}_N) & \cdots & \phi_{i_N}(\mathbf{x}_N)\end{array}\right|_{\pm}$$

$$\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_I c_I \Phi_I(\mathbf{x}_1, \ldots, \mathbf{x}_N)$$

$$\sum_J (H_{IJ} - ES_{IJ})c_J = 0$$

$$\langle \Phi_I | \hat{O} | \Phi_J \rangle.$$

$$\begin{aligned}\hat{O}_0 &= o_0 = \text{constant}, \\ \hat{O}_1 &= \sum_i \hat{o}_i = \sum_i \hat{o}(\mathbf{x}_i), \\ \hat{O}_2 &= \sum_{i < j} \hat{o}_{ij} = \frac{1}{2} \sum_{i \neq j} \hat{o}(\mathbf{x}_i, \mathbf{x}_j), \\ &\vdots \\ \hat{O}_n &= \sum_{i_1 < \dots < i_n} \hat{o}_{i_1 \dots i_n} = \frac{1}{n!} \sum_{i_1 \neq \dots \neq i_n} \hat{o}(\mathbf{x}_{i_1}, \dots, \mathbf{x}_{i_n}).\end{aligned}$$

$$\hat{T}=-\frac{1}{2}\sum_i\nabla_i^2$$

$$\hat{V}_{\rm nuc}=\sum_i v_{\rm nuc}\left(\mathbf{r}_i\right)$$

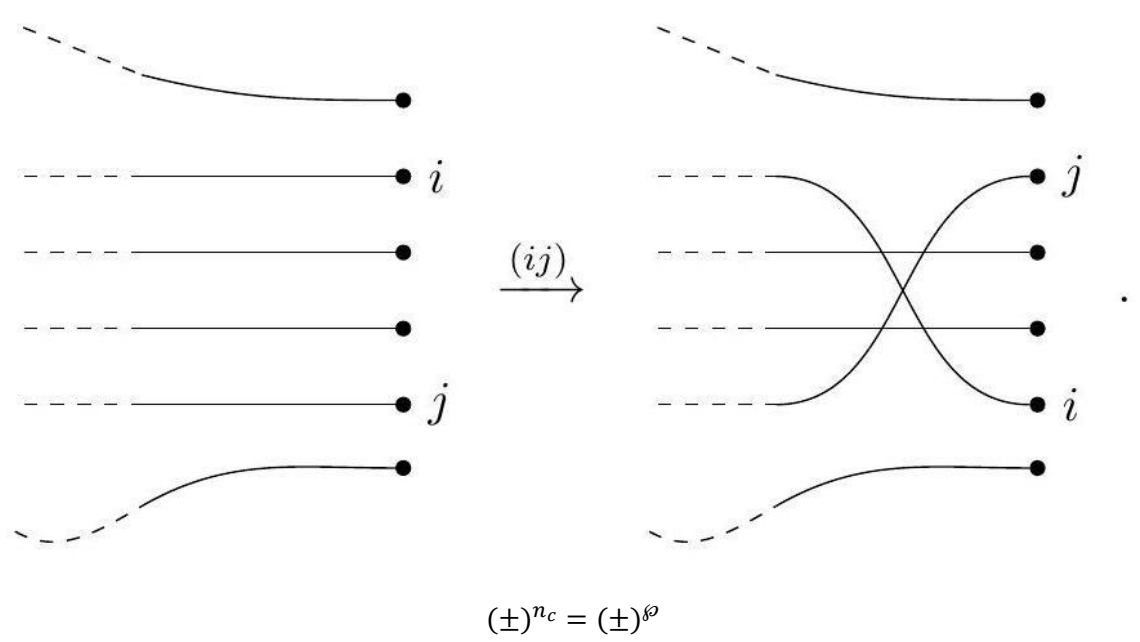
$$\hat{W} = \frac{1}{2} \sum_{i \neq j} w(\mathbf{r}_i, \mathbf{r}_j)$$

$$\hat{S}^2\!:=\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{S}}=\sum_{i\neq j}\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j+\sum_i\hat{S}_i^2$$

$$\begin{aligned}\langle \Phi | \hat{O}_0 | \Psi \rangle &= \langle \Phi | o_0 | \Psi \rangle = o_0 \langle \Phi | \Psi \rangle, \\ \langle \Phi | \hat{O}_1 | \Psi \rangle &= N \langle \Phi | \hat{o}_1 | \Psi \rangle, \\ \langle \Phi | \hat{O}_2 | \Psi \rangle &= \frac{N(N-1)}{2} \langle \Phi | \hat{o}_{12} | \Psi \rangle, \\ &\vdots \\ \langle \Phi | \hat{O}_n | \Psi \rangle &= \binom{N}{n} \langle \Phi | \hat{o}_{1\dots n} | \Psi \rangle.\end{aligned}$$

$$|A|_{\pm}:=\sum_{\wp}(\pm)^{\wp}\prod_{i=1}^nA_{i_{\wp(i)}}$$

$$\wp(1,2,\ldots,n)=(\wp(1),\wp(2),\ldots,\wp(n)=(1',2',\ldots,n')$$



$$\begin{aligned}
|A|_{\pm} &= \begin{array}{ccc} & A_{11} & \\ 1 \bullet & \text{---} & \bullet 1 \\ & A_{22} & \\ 2 \bullet & \text{---} & \bullet 2 \end{array} + \begin{array}{ccc} & A_{11} & \\ 1 \bullet & \text{---} & \bullet 1 \\ & A_{22} & \\ 2 \bullet & \text{---} & \bullet 2 \end{array} \\
&= A_{11}A_{22} \pm A_{12}A_{21}.
\end{aligned}$$

$$\int d\mathbf{x}_1 \int d\mathbf{x}_2 \cdots \int d\mathbf{x}_N \phi_{i_1}^*(\mathbf{x}_1) \phi_{i_2}^*(\mathbf{x}_2) \cdots \phi_{i_N}^*(\mathbf{x}_N) \phi_{j_1}(\mathbf{x}_1) \phi_{j_2}(\mathbf{x}_2) \cdots \phi_{j_N}(\mathbf{x}_N)$$

$$\begin{aligned}
& \begin{array}{ccc} & \delta_{i_1 j_1} & \\ i_1 \bullet & \text{---} & \bullet j_1 \\ & \delta_{i_2 j_2} & \\ i_2 \bullet & \text{---} & \bullet j_2 \\ & \delta_{i_3 j_3} & \\ i_3 \bullet & \text{---} & \bullet j_3 \\ & \delta_{i_4 j_4} & \\ i_4 \bullet & \text{---} & \bullet j_4 \\ \vdots & & \vdots \\ & \delta_{i_N j_N} & \\ i_N \bullet & \text{---} & \bullet j_N \end{array} = \delta_{i_1 j_1} \delta_{i_2 j_2} \cdots \delta_{i_N j_N} =: \delta_{IJ},
\end{aligned}$$

$$\int d\mathbf{x}_1 \int d\mathbf{x}_2 \cdots \int d\mathbf{x}_N \phi_{i_1}^*(\mathbf{x}_1) \phi_{i_2}^*(\mathbf{x}_2) \cdots \phi_{i_N}^*(\mathbf{x}_N) \phi_{j_1}(\mathbf{x}_1) \phi_{j_2}(\mathbf{x}_2) \cdots \phi_{j_N}(\mathbf{x}_N)$$

$$\begin{aligned}
& \begin{array}{ccc} & \int d\mathbf{x} \phi_{i_k}^*(\mathbf{x}_k) \phi_{j_k}(\mathbf{x}_k) & \\ i_1 \bullet & \text{---} & \bullet j_1 \\ & \downarrow \mathbf{x}_1 & \\ i_2 \bullet & \text{---} & \bullet j_2 \\ & \downarrow \mathbf{x}_2 & \\ i_3 \bullet & \text{---} & \bullet j_3 \\ & \downarrow \mathbf{x}_3 & \\ i_4 \bullet & \text{---} & \bullet j_4 \\ \vdots & & \vdots \\ & \downarrow \mathbf{x}_N & \\ i_N \bullet & \text{---} & \bullet j_N \end{array} = \begin{array}{ccc} & \langle \phi_{i_1} | \phi_{j_1} \rangle & \\ i_1 \bullet & \text{---} & \bullet j_1 \\ & \langle \phi_{i_2} | \phi_{j_2} \rangle & \\ i_2 \bullet & \text{---} & \bullet j_2 \\ & \langle \phi_{i_3} | \phi_{j_3} \rangle & \\ i_3 \bullet & \text{---} & \bullet j_3 \\ & \langle \phi_{i_4} | \phi_{j_4} \rangle & \\ i_4 \bullet & \text{---} & \bullet j_4 \\ \vdots & & \vdots \\ & \langle \phi_{i_N} | \phi_{j_N} \rangle & \\ i_N \bullet & \text{---} & \bullet j_N \end{array}
\end{aligned}$$

$$\begin{array}{c}
\begin{array}{ccccc}
& & \delta_{i_1 j_1} & & \\
i_1 & \bullet & \text{---} & \bullet & j_1 \\
& & \delta_{i_2 j_2} & & \\
i_2 & \bullet & \text{---} & \bullet & j_2 \\
& & \delta_{i_3 j_3} & & \\
= & i_3 & \bullet & \text{---} & \bullet & j_3 \\
& & \delta_{i_4 j_4} & & \\
i_4 & \bullet & \text{---} & \bullet & j_4 \\
& \vdots & & & \vdots \\
& & \delta_{i_N j_N} & & \\
i_N & \bullet & \text{---} & \bullet & j_N
\end{array}
& = \delta_{i_1 j_1} \delta_{i_2 j_2} \cdots \delta_{i_N j_N} =: \delta_{IJ},
\end{array}$$

$$\begin{array}{ccccc}
& & \delta_{i_2 j_4} & & \\
i_1 & \bullet & \text{---} & \bullet & j_1 \\
& & \delta_{i_1 j_1} & & \\
i_2 & \bullet & \text{---} & \bullet & j_2 \\
& & \delta_{i_3 j_2} & & \\
i_3 & \bullet & \text{---} & \bullet & j_3 \\
& & \delta_{i_4 j_3} & & \\
i_4 & \bullet & \text{---} & \bullet & j_4 \\
& \vdots & & & \vdots \\
& & \delta_{i_N j_N} & & \\
i_N & \bullet & \text{---} & \bullet & j_N
\end{array} = 0$$

$$\begin{array}{ccccc}
& & \delta_{i_4 j_4} & & \\
i_1 & \bullet & \text{---} & \bullet & j_1 \\
& & \delta_{i_1 j_1} & & \\
i_2 & \bullet & \text{---} & \bullet & j_2 \\
& & \delta_{i_3 j_3} & & \\
i_3 & \bullet & \text{---} & \bullet & j_3 \\
& & \delta_{i_2 j_2} & & \\
i_4 & \bullet & \text{---} & \bullet & j_4 \\
& \vdots & & & \vdots \\
& & \delta_{i_N j_N} & & \\
i_N & \bullet & \text{---} & \bullet & j_N
\end{array} = \begin{array}{ccccc}
& & \delta_{i_2 j_2} & & \\
i_1 & \bullet & \text{---} & \bullet & j_1 \\
& & \delta_{i_N j_N} & & \\
i_2 & \bullet & \text{---} & \bullet & j_2 \\
& & \delta_{i_1 j_1} & & \\
i_3 & \bullet & \text{---} & \bullet & j_3 \\
& & \delta_{i_3 j_3} & & \\
i_4 & \bullet & \text{---} & \bullet & j_4 \\
& \vdots & & & \vdots \\
& & \delta_{i_4 j_4} & & \\
i_N & \bullet & \text{---} & \bullet & j_N
\end{array} = \delta_{IJ}.$$

$$\langle \Phi_I | \Phi_J \rangle = \delta_{IJ}.$$

$$\begin{array}{ccc}
 \langle \phi_{i_1} | \hat{o}_1 | \phi_{i_1} \rangle & & \langle \phi_{i_1} | \hat{o}_1 | \phi_{i_1} \rangle \\
 i_1 \bullet \text{---} \bullet i_1 & & i_1 \bullet \text{---} \bullet i_1 \\
 \delta_{i_2 i_2} & & \delta_{i_4 i_4} \\
 i_2 \bullet \text{---} \bullet i_2 & & i_2 \bullet \text{---} \bullet i_2 \\
 \delta_{i_3 i_3} & = & \delta_{i_2 i_2} \\
 i_3 \bullet \text{---} \bullet i_3 & & i_3 \bullet \text{---} \bullet i_3 \\
 \delta_{i_4 i_4} & & \delta_{i_3 i_3} \\
 i_4 \bullet \text{---} \bullet i_4 & & i_4 \bullet \text{---} \bullet i_4 \\
 \vdots & & \vdots \\
 \delta_{i_N i_N} & & \delta_{i_N i_N} \\
 i_N \bullet \text{---} \bullet i_N & & i_N \bullet \text{---} \bullet i_N \\
 & & = \langle \phi_{i_1} | \hat{o}_1 | \phi_{i_1} \rangle.
 \end{array}$$

$$\begin{array}{ccc}
 \langle \phi_{i_k} | \hat{o}_1 | \phi_{i_k} \rangle & & \langle \phi_{i_k} | \hat{o}_1 | \phi_{i_k} \rangle \\
 i_1 \bullet \text{---} \bullet i_1 & & i_k \bullet \text{---} \bullet i_k \\
 \delta_{i_2 i_2} & & \delta_{i_2 i_2} \\
 i_2 \bullet \text{---} \bullet i_2 & & i_1 \bullet \text{---} \bullet i_1 \\
 \delta_{i_1 i_1} & = & \delta_{i_1 i_1} \\
 i_3 \bullet \text{---} \bullet i_3 & & i_2 \bullet \text{---} \bullet i_2 \\
 \vdots & & \vdots \\
 i_k \bullet \text{---} \bullet i_k & & i_{k-1} \bullet \text{---} \bullet i_{k-1} \\
 \vdots & & \vdots \\
 i_N \bullet \text{---} \bullet i_N & & i_N \bullet \text{---} \bullet i_N \\
 & & = \langle \phi_{i_k} | \hat{o}_1 | \phi_{i_k} \rangle.
 \end{array}$$

$$\begin{array}{ccc}
\begin{array}{c}
\langle \phi_{i_1} | \hat{O}_1 | \phi_{i_1} \rangle \\
i_1 \bullet \text{---} \bullet i_1 \\
\delta_{i_2 i_2} \\
i_2 \bullet \text{---} \bullet i_2 \\
\delta_{i_3 i_3} \\
i_3 \bullet \text{---} \bullet i_3 \\
\delta_{i_4 i_4} \\
i_4 \bullet \text{---} \bullet i_4 \\
\vdots \\
\delta_{i_N i_N} \\
i_N \bullet \text{---} \bullet i_N
\end{array}
& = &
\begin{array}{c}
\langle \phi_{i_1} | \hat{O}_1 | \phi_{i_1} \rangle \\
i_1 \bullet \text{---} \bullet i_1 \\
\delta_{i_4 i_4} \\
i_2 \bullet \text{---} \bullet i_2 \\
\delta_{i_2 i_2} \\
i_3 \bullet \text{---} \bullet i_3 \\
\delta_{i_3 i_3} \\
i_4 \bullet \text{---} \bullet i_4 \\
\vdots \\
\delta_{i_N i_N} \\
i_N \bullet \text{---} \bullet i_N
\end{array} \\
& & = \langle \phi_{i_1} | \hat{O}_1 | \phi_{i_1} \rangle.
\end{array}$$

$$\begin{array}{ccc}
\begin{array}{c}
\langle \phi_{i_k} | \hat{O}_1 | \phi_{i_k} \rangle \\
i_1 \bullet \text{---} \bullet i_1 \\
\delta_{i_2 i_2} \\
i_2 \bullet \text{---} \bullet i_2 \\
\delta_{i_1 i_1} \\
i_3 \bullet \text{---} \bullet i_3 \\
\vdots \\
i_k \bullet \text{---} \bullet i_k \\
\vdots \\
i_N \bullet \text{---} \bullet i_N
\end{array}
& = &
\begin{array}{c}
\langle \phi_{i_k} | \hat{O}_1 | \phi_{i_k} \rangle \\
i_k \bullet \text{---} \bullet i_k \\
\delta_{i_2 i_2} \\
i_1 \bullet \text{---} \bullet i_1 \\
\delta_{i_1 i_1} \\
i_2 \bullet \text{---} \bullet i_2 \\
\vdots \\
i_{k-1} \bullet \text{---} \bullet i_{k-1} \\
\vdots \\
i_N \bullet \text{---} \bullet i_N
\end{array} \\
& & = \langle \phi_{i_k} | \hat{O}_1 | \phi_{i_k} \rangle.
\end{array}$$

$$\langle \Phi_I | \hat{O}_1 | \Phi_I \rangle = \frac{N(N-1)!}{N!} \sum_{k=1}^N \langle \phi_{i_k} | \hat{O}_1 | \phi_{i_k} \rangle = \sum_{k=1}^N \langle \phi_{i_k} | \hat{O}_1 | \phi_{i_k} \rangle,$$

$$= (-1)^{k-l} \langle \phi_{i_k} | \hat{o}_1 | \phi_{j_l} \rangle$$

$$= (-1)^{k-l} \langle \phi_{i_k} | \hat{o}_1 | \phi_{j_l} \rangle$$

$$\langle \Phi_I | \hat{O}_1 | \Phi_J \rangle = (-1)^{k-l} \langle \phi_{i_k} | \hat{o}_1 | \phi_{j_l} \rangle,$$

$$\langle \Phi_I | \hat{O}_1 | \Phi_J \rangle = \begin{cases} \sum_{k=1}^N \langle \phi_{i_k} | \hat{o}_1 | \phi_{i_k} \rangle & \text{if } I = J, \\ (-1)^{k-l} \langle \phi_{i_k} | \hat{o}_1 | \phi_{j_l} \rangle & \text{if only } i_k \neq j_l, \\ 0 & \text{otherwise.} \end{cases}$$

$$\begin{aligned} \langle i_k i_l | \hat{o}_{12} | j_m j_n \rangle &:= \langle \phi_{i_k} \phi_{i_l} | \hat{o}_{12} | \phi_{j_m} \phi_{j_n} \rangle \\ &:= \int d\mathbf{x}_1 \int d\mathbf{x}_2 \phi_{i_k}^*(\mathbf{x}_1) \phi_{i_l}^*(\mathbf{x}_1) \hat{o}(\mathbf{x}_1, \mathbf{x}_2) \phi_{j_m}(\mathbf{x}_1) \phi_{j_n}(\mathbf{x}_2) \end{aligned}$$

$$\langle kl | \hat{o}_{12} | mn \rangle := \langle kl | \hat{o}_{12} | mn \rangle - \langle kl | \hat{o}_{12} | nm \rangle.$$

$$=$$

$$= \langle i_1 i_2 | \hat{O}_{12} | i_1 i_2 \rangle$$

$$\begin{array}{ccc}
 \langle i_2 i_1 | \hat{O}_{12} | i_1 i_2 \rangle & & \langle i_2 i_1 | \hat{O}_{12} | i_1 i_2 \rangle \\
 \begin{array}{c} i_1 \bullet \quad \quad \bullet i_1 \\ i_2 \bullet \quad \quad \bullet i_2 \\ \vdots \\ i_N \bullet \quad \quad \bullet i_N \end{array} & = & \begin{array}{c} i_1 \bullet \quad \quad \bullet i_1 \\ i_2 \bullet \quad \quad \bullet i_2 \\ \vdots \\ i_N \bullet \quad \quad \bullet i_N \end{array} \\
 \delta_{i_3 i_3} & & \delta_{i_3 i_3} \\
 \delta_{i_4 i_4} & & \delta_{i_4 i_4} \\
 \delta_{i_N i_N} & & \delta_{i_N i_N} \\
 \end{array}$$

$$= \langle i_1 i_2 | \hat{O}_{12} | i_2 i_1 \rangle.$$

$$2(N-2)! (\langle i_1 i_2 | \hat{O}_{12} | i_1 i_2 \rangle - \langle i_1 i_2 | \hat{O}_{12} | i_2 i_1 \rangle).$$

$$\begin{aligned}
 \langle \Phi_I | \hat{O}_2 | \Phi_I \rangle &= \sum_{r < s} (\langle i_r i_s | \hat{O}_{12} | i_r i_s \rangle - \langle i_r i_s | \hat{O}_{12} | i_s i_r \rangle) \\
 &= \sum_{r < s} \langle i_r i_s | \hat{O}_{12} | i_r i_s \rangle
 \end{aligned}$$

$$\begin{array}{ccc}
 \langle i_k i_r | \hat{O}_{12} | j_m i_r \rangle & & \langle i_k i_r | \hat{O}_{12} | j_m i_r \rangle \\
 \begin{array}{c} i_1 \bullet \quad \quad \bullet j_1 \\ i_2 \bullet \quad \quad \bullet j_2 \\ \vdots \\ i_k \bullet \quad \quad \bullet j_k \\ \vdots \\ i_{r-1} \bullet \quad \bullet j_{r-1} \\ i_r \bullet \quad \quad \bullet j_r \\ \vdots \\ i_m \bullet \quad \quad \bullet j_m \\ \vdots \end{array} & = (-1)^{k-m} & \begin{array}{c} i_k \bullet \quad \quad \bullet j_m \\ i_1 \bullet \quad \quad \bullet j_1 \\ i_2 \bullet \quad \quad \bullet j_2 \\ \vdots \\ i_{r-1} \bullet \quad \bullet j_{r-2} \\ i_r \bullet \quad \quad \bullet j_{r-1} \\ \vdots \end{array}
 \end{array}$$

$$\begin{array}{c}
\langle i_k i_r | \hat{O}_{12} | j_m i_r \rangle \\
\begin{array}{ccc}
i_k & \cdots & j_m \\
i_r & \cdots & j_{r-1} \\
i_1 & \cdots & j_1 \\
i_2 & \cdots & j_2 \\
\vdots & & \vdots
\end{array}
\end{array}
= (-1)^{k-m} \langle i_k i_r | \hat{O}_{12} | j_m i_r \rangle$$

$$(-1)^{k-m} 2(N-2)! (\langle i_k i_r | \hat{O}_{12} | j_m i_r \rangle - \langle i_k i_r | \hat{O}_{12} | i_r j_m \rangle)$$

$$\begin{aligned}
\langle \Phi_I | \hat{O}_2 | \Phi_J \rangle &= (-1)^{k-m} \sum_{r \neq k} (\langle i_k i_r | \hat{O}_{12} | j_m i_r \rangle - \langle i_k i_r | \hat{O}_{12} | i_r j_m \rangle) \\
&= (-1)^{k-m} \sum_{r \neq k} \langle i_k i_r | \hat{O}_{12} | j_m i_r \rangle
\end{aligned}$$

$$\begin{array}{c}
\langle i_k i_l | \hat{O}_{12} | j_m j_n \rangle \\
\begin{array}{ccc}
i_1 & \cdots & j_1 \\
i_2 & \cdots & j_2 \\
\vdots & & \vdots \\
i_k & \cdots & j_m \\
\vdots & & \vdots \\
i_l & \cdots & j_n \\
\vdots & & \vdots
\end{array}
\end{array}
= (-1)^{k-m} \begin{array}{c}
\langle i_k i_l | \hat{O}_{12} | j_m j_n \rangle \\
\begin{array}{ccc}
i_k & \cdots & j_m \\
i_1 & \cdots & j_1 \\
i_2 & \cdots & j_2 \\
\vdots & & \vdots \\
i_l & \cdots & j_n \\
\vdots & & \vdots
\end{array}
\end{array}$$

$$\begin{array}{c}
\langle i_k i_l | \hat{O}_{12} | j_m j_n \rangle \\
\begin{array}{ccc}
i_k & \cdots & j_m \\
i_l & \cdots & j_n \\
i_1 & \cdots & j_1 \\
i_2 & \cdots & j_2 \\
\vdots & & \vdots
\end{array}
\end{array}
= (-1)^{k+l-m-n} \begin{array}{c}
\langle i_k i_l | \hat{O}_{12} | j_m j_n \rangle \\
\begin{array}{ccc}
i_k & \cdots & j_m \\
i_l & \cdots & j_n \\
i_1 & \cdots & j_1 \\
i_2 & \cdots & j_2 \\
\vdots & & \vdots
\end{array}
\end{array}$$

$$= (-1)^{k+l-m-n} \langle i_k i_l | \hat{O}_{12} | j_m j_n \rangle$$

$$\begin{aligned}\langle \Phi_I | \hat{O}_2 | \Phi_J \rangle &= (-1)^{k+l-m-n} (\langle i_k i_l | \hat{o}_{12} | j_m j_n \rangle - \langle i_k i_l | \hat{o}_{12} | j_n j_m \rangle) \\ &= (-1)^{k+l-m-n} \langle i_k i_l || \hat{o}_{12} || j_m j_n \rangle \\ \langle \Phi_I | \hat{O}_2 | \Phi_J \rangle &= \begin{cases} \sum_{r < s} \langle i_r i_s || \hat{o}_{12} || i_r i_s \rangle & \text{if } I = J, \\ (-1)^{k-m} \sum_{r \neq k} \langle i_k i_r || \hat{o}_{12} || j_m i_r \rangle & \text{if only } i_k \neq j_m, \\ (-1)^{k+l-m-n} \langle i_k i_l || \hat{o}_{12} || j_m j_n \rangle & \text{if } i_k \neq j_m \text{ and } i_l \neq j_n, \\ 0 & \text{otherwise.} \end{cases}\end{aligned}$$

$$\begin{aligned}\langle ij \mid kl \rangle &:= \langle ij | \hat{w}_{12} | kl \rangle = \langle \phi_i \phi_j | \hat{w}_{12} | \phi_k \phi_l \rangle \\ &= \int d\mathbf{x}_1 \int d\mathbf{x}_2 \phi_i^*(\mathbf{x}_1) \phi_j^*(\mathbf{x}_2) w(\mathbf{r}_1, \mathbf{r}_2) \phi_k(\mathbf{x}_1) \phi_l(\mathbf{x}_2)\end{aligned}$$

$$(ij \mid kl) := \int d\mathbf{x}_1 \int d\mathbf{x}_2 \phi_i^*(\mathbf{x}_1) \phi_j(\mathbf{x}_1) w(\mathbf{r}_1, \mathbf{r}_2) \phi_k^*(\mathbf{x}_2) \phi_l(\mathbf{x}_2)$$

$$\begin{aligned}\langle ij || kl \rangle &:= \langle ij \mid kl \rangle - \langle ij \mid lk \rangle, \\ (ij || kl) &:= (ij \mid kl) - (il \mid kj).\end{aligned}$$

$$E^{\mathrm{HF}}[\{\phi_i\}] = \sum_{i=1}^N \langle \phi_i | \hat{h} | \phi_i \rangle + \frac{1}{2} \sum_{i,j=1}^N \langle \phi_i \phi_j || \phi_i \phi_j \rangle + E_{\mathrm{nuc}}$$

$$\hat{h} \colon = -\frac{1}{2} \nabla^2 + v(\mathbf{r})$$

$$\langle ij || kl \rangle = (ik || jl)$$

$$\chi_A(\mathbf{r}) = N_\zeta \mathrm{e}^{-\zeta|\mathbf{r}-\mathbf{R}_A|} \; \chi_B(\mathbf{r}) = N_\zeta \mathrm{e}^{-\zeta|\mathbf{r}-\mathbf{R}_B|}$$

$$N_\zeta = \sqrt{\frac{\zeta^3}{\pi}}$$

$$s\colon=\langle\chi_A\mid\chi_B\rangle=\left(1+\rho+\frac{\rho^2}{3}\right)\mathrm{e}^{-\rho}$$

$$\rho\colon=\zeta R \text{ and } R\colon=|\mathbf{R}_A-\mathbf{R}_B|$$

$$\chi_{A/B} = N_\zeta \mathrm{e}^{-\frac{\rho}{2}(\xi \mp \eta)}$$

$$\sigma_g = \frac{\chi_A + \chi_B}{\sqrt{2(1+s)}} \text{ and } \sigma_u = \frac{\chi_A - \chi_B}{\sqrt{2(1-s)}}.$$

$$\langle \chi_A | \hat{h} | \chi_A \rangle = \langle \chi_B | \hat{h} | \chi_B \rangle = \frac{\zeta^2}{2} - \zeta + \frac{\zeta}{\rho} (e^{-2\rho}(1+\rho) - 1)$$

$$\langle \chi_A | \hat{h} | \chi_B \rangle = \left[\frac{\zeta^2}{2} \left(1 + \rho - \frac{\rho^2}{3} \right) - 2\zeta(1+\rho) \right] e^{-\rho}$$

$$\left(-\frac{1}{2} \nabla^2 - \frac{\zeta}{r_{A/B}} \right) \chi_{A/B} = -\frac{\zeta^2}{2} \chi_{A/B}.$$

$$\langle \sigma_g | \hat{h} | \sigma_g \rangle = \frac{\langle \chi_A | \hat{h} | \chi_A \rangle + \langle \chi_A | \hat{h} | \chi_B \rangle}{1+s}.$$

$$(\sigma_g \sigma_g | \sigma_g \sigma_g) = \frac{1}{2(1+s)^2} [(AA | AA) + 4(AA | AB) + (AA | BB) + 2(AB | AB)]$$

$$(AA | BB) = \zeta \left[\frac{1}{\rho} - e^{-2\rho} \left(\frac{1}{\rho} + \frac{11}{8} + \frac{3\rho}{4} + \frac{\rho^2}{6} \right) \right]$$

$$(AA | AB) = \frac{\zeta e^{-\rho}}{16\rho} (5 + 2\rho + 16\rho^2 - (5 + 2\rho)e^{-2\rho})$$

$$v_A(\mathbf{r}') = \int \mathrm{d}\mathbf{r} \frac{|\chi_A(\mathbf{r})|^2}{|\mathbf{r}' - \mathbf{r}|}$$

$$\int \mathrm{d}\mathbf{r} |\chi_B(\mathbf{r})|^2 v_A(\mathbf{r})$$

$$(AA | AA) = \lim_{R \rightarrow 0} (AA | BB) = \frac{5\zeta}{8}$$

$$(AB | AB) = \frac{\zeta e^{-2\rho}}{120\rho} [75\rho - 138\rho^2 - 72\rho^3 - 8\rho^4 + 16(\gamma + \ln(\rho))(9 + 18\rho + 15\rho^2 + 6\rho^3 + \rho^4) - 32(9 - 3\rho^2 + \rho^4)e^{2\rho}\mathrm{Ei}(-2\rho) + 16(3 - 3\rho + \rho^2)^2 e^{4\rho}\mathrm{Ei}(-4\rho)]$$

$$\gamma := -\int_0^\infty \mathrm{d}z e^{-z} \ln(z) = 0.5772156649 \dots$$

$$\mathrm{Ei}(-x) := -\int_x^\infty \mathrm{d}z \frac{e^{-z}}{z}$$

$$E_{\mathrm{RHF}}\left[(\sigma_g)^2\right] = 2\langle\sigma_g|\hat{h}|\sigma_g\rangle + (\sigma_g\sigma_g | \sigma_g\sigma_g) + \frac{1}{R}$$

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}=\frac{2}{R}\sum_{l=0}^{\infty}\sum_{m=-l}^l\alpha_{ml}\mathrm{P}_l^{|m|}(\xi_{<})\mathrm{Q}_l^{|m|}(\xi_{>})\times\\ \mathrm{P}_l^{|m|}(\eta_1)\mathrm{P}_l^{|m|}(\eta_2)\mathrm{e}^{im(\phi_1-\phi_2)}$$

$$\mathrm{P}_l^{|m|}(x)\mathrm{Q}_l^{|m|}(x)$$



$$\alpha_{lm}=(-1)^m(2l+1)\left(\frac{(l-|m|)!}{(l+|m|)!}\right)^2$$

$$\xi_{>}=\max(\xi_1,\xi_2)$$

$$\xi_{<}=\min(\xi_1,\xi_2)$$

$$\begin{array}{ll} \min_{x,y\in\mathbb{R}} & f(x,y)=(x-1)^2+(y-2)^2 \\ \text{subject to} & (x-1)^2=5y \end{array}$$

$$\begin{aligned} L[\{\phi_i,\psi_i^*\},\epsilon]&=E_{\text{HF}}[\{\phi_i,\psi_i^*\}]-E_{\text{nuc}}-\sum_{r,s=1}^N\epsilon_{rs}(\langle\psi_i\mid\phi_r\rangle-\delta_{sr})\\ &=\sum_{r=1}^N\langle\psi_r|\hat{h}|\phi_r\rangle+\frac{1}{2}\sum_{r,s=1}^N\langle\psi_r\psi_s\|\phi_r\phi_s\rangle-\sum_{r,s=1}^N\epsilon_{rs}(\langle\psi_s\mid\phi_r\rangle-\delta_{sr}) \end{aligned}$$

$$\psi_i=\phi_i \text{ and } \langle\phi_i\mid\phi_j\rangle=\delta_{ij}$$

$$\begin{aligned} \delta L = & \sum_{i=1}^N \langle \delta \psi_i | \hat{h} | \phi_i \rangle + \frac{1}{2} \sum_{i,j=1}^N \left(\langle \delta \psi_i \psi_j | \phi_i \phi_j \rangle + \langle \psi_i \delta \psi_j | \phi_i \phi_j \rangle \right) + \\ & \sum_{i=1}^N \langle \psi_i | \hat{h} | \delta \phi_i \rangle + \frac{1}{2} \sum_{i,j=1}^N \left(\langle \psi_i \psi_j | \delta \phi_i \phi_j \rangle + \langle \psi_i \psi_j | \phi_i \delta \phi_j \rangle \right) - \\ & \sum_{i,j=1}^N \epsilon_{ji} \left(\langle \delta \psi_j | \phi_i \rangle + \langle \psi_j | \delta \phi_i \rangle \right) \end{aligned}$$

$$\delta L = \sum_{i=1}^N \int \mathrm{d}\mathbf{x} \left(\delta \phi_i^*(\mathbf{x}) \frac{\delta L}{\delta \phi_i^*(\mathbf{x})} + \frac{\delta L}{\delta \phi_i(\mathbf{x})} \delta \phi_i(\mathbf{x}) \right),$$

$$\begin{aligned} \frac{\delta L}{\delta \phi_i^*(\mathbf{x})} = & \hat{h} \phi_i(\mathbf{x}) - \sum_{j=1}^N \phi_j(\mathbf{x}) \epsilon_{ji} + \\ & \sum_{j=1}^N \int \mathrm{d}\mathbf{x}' \phi_j^*(\mathbf{x}') \frac{\phi_j(\mathbf{x}') \phi_i(\mathbf{x}) - \phi_j(\mathbf{x}) \phi_i(\mathbf{x}')}{|\mathbf{r} - \mathbf{r}'|} \\ \frac{\delta L}{\delta \phi_i(\mathbf{x})} = & \hat{h} \phi_i^*(\mathbf{x}) - \sum_{j=1}^N \epsilon_{ij} \phi_j^*(\mathbf{x}) + \\ & \sum_{j=1}^N \int \mathrm{d}\mathbf{x}' \frac{\phi_i^*(\mathbf{x}) \phi_j^*(\mathbf{x}') - \phi_i^*(\mathbf{x}') \phi_j^*(\mathbf{x})}{|\mathbf{r} - \mathbf{r}'|} \phi_j(\mathbf{x}') \end{aligned}$$

$$\delta L/\delta \phi_i(\mathbf{x}) \text{ and } \delta L/\delta \phi_i^*(\mathbf{x})$$

$$L[\{\phi_i,\psi_i^*\},\epsilon]=\Re E_{\text{HF}}[\{\phi_i,\psi_i^*\}]-\sum_{r\geq s=1}^N(\epsilon_{rs}\langle\psi_s\mid\phi_r\rangle+\epsilon_{sr}\langle\phi_r\mid\psi_s\rangle-2\delta_{sr})$$

$$\Re c_i = 1/\|\phi_i\|$$

$$\rho(\mathbf{x}) = \sum_{i=1}^N |\phi(\mathbf{x})|^2 \rightarrow v_{\mathrm{H}}[\rho](\mathbf{x}) := \int \mathrm{d}\mathbf{x}' \frac{\rho(\mathbf{x}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$v_{\mathbf{x}}[\{\phi_i\}](\mathbf{x},\mathbf{x}') := -\sum_{j=1}^N \frac{\phi_j(\mathbf{x})\phi_j^*(\mathbf{x}')}{|\mathbf{r}-\mathbf{r}'|}.$$

$$-\sum_{j=1}^N \int \mathrm{d}\mathbf{x}' \phi_j^*(\mathbf{x}') \frac{\phi_j(\mathbf{x})\phi_i(\mathbf{x}')}{|\mathbf{r}-\mathbf{r}'|} = \int \mathrm{d}\mathbf{x}' v_{\mathbf{x}}(\mathbf{x},\mathbf{x}') \phi_i(\mathbf{x}') =: (\hat{v}_{\mathbf{x}}\phi_i)(\mathbf{x})$$

$$t(\mathbf{x},\mathbf{x}')=\frac{1}{2}\sum_r \nabla \chi_r(\mathbf{x})\cdot \nabla \chi_r^*(\mathbf{x}'),$$

$$\int \mathrm{d}\mathbf{x}' t(\mathbf{x},\mathbf{x}') \psi(\mathbf{x}') = -\frac{1}{2} \nabla^2 \psi(\mathbf{x})$$

$$v_{\mathrm{H}}(\mathbf{x},\mathbf{x}')=v_{\mathrm{H}}(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}')$$

$$\hat{f}[\{\phi_i\}]\!:=\hat{h}+\hat{v}_{\mathrm{H}}[\{\phi_i\}]+\hat{v}_{\mathbf{x}}[\{\phi_i\}]$$

$$\frac{\delta L}{\delta \phi_i^*(\mathbf{x})} = \hat{f} \phi_i(\mathbf{x}) - \sum_{j=1}^N \phi_j(\mathbf{x}) \epsilon_{ji}$$

$$\frac{\delta L}{\delta \phi_i(\mathbf{x})} = \hat{f}^* \phi_i^*(\mathbf{x}) - \sum_{j=1}^N \epsilon_{ij} \phi_j^*(\mathbf{x})$$

$$\hat{f}\phi_i(\mathbf{x})=\sum_{j=1}^N\phi_j(\mathbf{x})\epsilon_{ji},\qquad \hat{f}^*\phi_i^*(\mathbf{x})=\sum_{j=1}^N\epsilon_{ij}\phi_j^*(\mathbf{x})$$

$$\langle \phi_j | \hat{f} | \phi_i \rangle = \epsilon_{ji}, \langle \phi_j | \hat{f} | \phi_i \rangle^* = \epsilon_{ij}$$

$$\langle \phi_i \mid \phi_j \rangle = \delta_{ij}$$

$$\epsilon_{ij} = \langle \phi_j | \hat{f} | \phi_i \rangle^* = \epsilon_{ji}^*$$

$$\hat{f}[\{\phi\}]\phi_i(\mathbf{x})=\varepsilon_i\phi_i(\mathbf{x}),$$

$$\phi_i'(\mathbf{x})=\sum_{j=1}^N\phi_j(\mathbf{x})U_{ji}$$

$$\phi_i(\mathbf{x})=\sum_j\chi_j(\mathbf{x})S_{ji}^{-1/2}$$

$$\boldsymbol{s}=\left(\begin{smallmatrix}1&s\\s&1\end{smallmatrix}\right)$$

$$\mathbf{S}^{-1/2} = \frac{1}{\sqrt{1-s^2}} \begin{pmatrix} \cos \theta & -\sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix},$$

$$\phi_{a/b}(\mathbf{r}) = \frac{1}{\sqrt{1-s^2}} (\cos(\theta)\chi_{A/B}(\mathbf{r}) - \sin(\theta)\chi_{B/A}(\mathbf{r})).$$

$$\langle \phi_a | \hat{h} | \phi_a \rangle = \langle \phi_b | \hat{h} | \phi_b \rangle = \frac{\langle \chi_A | \hat{h} | \chi_A \rangle - s \langle \chi_A | \hat{h} | \chi_B \rangle}{1-s^2}$$

$$\langle \phi_a | \hat{h} | \phi_b \rangle = \langle \phi_a | \hat{h} | \phi_b \rangle = \frac{\langle \chi_A | \hat{h} | \chi_B \rangle - s \langle \chi_A | \hat{h} | \chi_A \rangle}{1-s^2}$$

$$(aa | aa) = \frac{1}{(1-s^2)^2} \left[\left(1 - \frac{s^2}{2} \right) (AA | AA) + \frac{s^2}{2} (AA | BB) - \right. \\ \left. 2s(AA | AB) + s^2(AB | AB) \right]$$

$$(aa | bb) = \frac{1}{(1-s^2)^2} \left[\left(1 - \frac{s^2}{2} \right) (AA | BB) + \frac{s^2}{2} (AA | AA) - \right. \\ \left. 2s(AA | AB) + s^2(AB | AB) \right]$$

$$(aa | ab) = \frac{1}{(1-s^2)^2} \left[(1+s^2)(AA | AB) - s(AB | AB) - \right. \\ \left. \frac{s}{2} ((AA | AA) + (AA | BB)) \right]$$

$$(ab | ab) = \frac{1}{(1-s^2)^2} \left[(AB | AB) - 2s(AA | AB) - \right. \\ \left. \frac{s^2}{2} ((AA | AA) + (AA | BB)) \right]$$

$$E_{\text{HF}}^{\text{loc}} = 2\langle \phi_a | \hat{h} | \phi_a \rangle + (\phi_a \phi_a | \phi_b \phi_b) + \frac{1}{R}.$$

$$\psi(\mathbf{r})_{a/b} = \cos(\alpha)\phi_{a/b}(\mathbf{r}) + \sin(\alpha)\phi_{b/a}(\mathbf{r})$$

$$E_{\text{UHF}} = 2(\langle a | \hat{h} | a \rangle + \sin(2\alpha)\langle a | \hat{h} | b \rangle) + \\ (aa | bb) + \frac{\sin^2(2\alpha)}{2} ((aa | aa) - (aa | bb)) + \frac{1}{R}$$

$$\rho(\mathbf{x},\mathbf{x}')=\sum_{i=1}^N\delta(\mathbf{x}-\mathbf{x}').$$

$$\rho(\mathbf{x})=\sum_{i=1}^N|\phi_i(\mathbf{x})|^2$$

$$\phi_i(\mathbf{x})=\sum_{v=1}^m\chi_v(\mathbf{x})C_{vi}$$

$$\sum_{v=1}^m \underbrace{\langle \chi_\mu | \hat{f} | \chi_\nu \rangle}_{=: f_{\mu\nu}} C_{vi} = \sum_v \underbrace{\langle \chi_\mu | \chi_\nu \rangle}_{=: S_{\mu\nu}} C_{vi} \varepsilon_i$$

$$\mathbf{f}\mathbf{C} = \mathbf{S}\mathbf{C}\text{diag}(\boldsymbol{\varepsilon}),$$

$$\mathbf{f}\mathbf{C} = \mathbf{C}\text{diag}(\boldsymbol{\varepsilon})$$

$$f_{\mu\nu}[\mathbf{C}]:=\langle\chi_{\mu}|\hat{f}[\mathbf{C}]\chi_{\nu}\rangle=\langle\chi_{\mu}|\hat{h}+\hat{v}_{\text{H}}[\mathbf{C}]+\hat{v}_{\text{x}}[\mathbf{C}]\chi_{\nu}\rangle.$$

$$\rho(\mathbf{x})=\sum_{i=1}^N|\phi_i(\mathbf{x})|^2=\sum_{\mu,\nu}\chi_{\mu}(\mathbf{x})\underbrace{\sum_{i=1}^N c_{\mu i}c_{i\nu}^{\dagger}}_{=:\gamma_{\mu\nu}^{\text{HF}}}\chi_{\nu}^*(\mathbf{x})$$

$$\begin{aligned} N &= \sum_{i=1}^N \langle \phi_i | \phi_i \rangle = \sum_{\mu,\nu} \sum_{i=1}^N c_{i\nu}^{\dagger} \langle \chi_{\mu} | \chi_{\nu} \rangle c_{\mu i} \\ &= \sum_{\mu,\nu} \gamma_{\mu\nu}^{\text{HF}} S_{\nu\mu} = \text{Tr}\{\boldsymbol{\gamma}^{\text{HF}} \mathbf{S}\} \end{aligned}$$

$$\text{Tr}\{\boldsymbol{\gamma}^{\text{HF}} \mathbf{S}\} = \sum_A \sum_{\mu \in A} (\boldsymbol{\gamma}^{\text{HF}} \mathbf{S})_{\mu\mu}.$$

$$\rho_A^{\text{Mulliken}} = \sum_{\mu \in A} (\boldsymbol{\gamma}^{\text{HF}} \mathbf{S})_{\mu\mu}$$

$$Q_A^{\text{Mulliken}} = Z_A - \rho_A^{\text{Mulliken}}$$

$$v_{\text{H}}(\mathbf{x}) = \int \text{d}\mathbf{x}' \frac{\rho(\mathbf{x}')}{|\mathbf{r}-\mathbf{r}'|} = \sum_{\mu,\nu} \gamma_{\mu\nu}^{\text{HF}} \int \text{d}\mathbf{x}' \frac{\chi_{\mu}(\mathbf{x}') \chi_{\nu}^*(\mathbf{x}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$\langle\chi_{\mu}|\hat{v}_{\text{H}}|\chi_{\nu}\rangle=\sum_{i=1}^N\langle\chi_{\mu}\phi_i\mid\chi_{\nu}\phi_i\rangle=\sum_{\rho\sigma}\gamma_{\sigma\rho}^{\text{HF}}\langle\chi_{\mu}\chi_{\rho}\mid\chi_{\nu}\chi_{\sigma}\rangle$$

$$\gamma^{\text{HF}}(\mathbf{x},\mathbf{x}')=\sum_{i=1}^N\phi_i(\mathbf{x})\phi_i^*(\mathbf{x}')=\sum_{\mu,\nu}\chi_{\mu}(\mathbf{x})\gamma_{\mu\nu}^{\text{HF}}\chi_{\nu}^*(\mathbf{x}')$$

$$v_{\text{x}}(\mathbf{x},\mathbf{x}')=-\frac{\gamma^{\text{HF}}(\mathbf{x},\mathbf{x}')}{|\mathbf{r}-\mathbf{r}'|}=-\sum_{\mu,\nu}\chi_{\mu}(\mathbf{x})\frac{\gamma_{\mu\nu}^{\text{HF}}}{|\mathbf{r}-\mathbf{r}'|}\chi_{\nu}^*(\mathbf{x}')$$

$$\langle\chi_{\mu}|\hat{v}_{\text{x}}|\chi_{\nu}\rangle=-\sum_{\rho,\sigma}\gamma_{\sigma\rho}^{\text{HF}}\langle\mu\rho\mid\sigma\nu\rangle$$

$$\gamma_{rs}^{\text{HF}}=\langle\phi_r|\hat{\gamma}^{\text{HF}}|\phi_s\rangle=\begin{cases}1&\text{if }r=s\leq N\\0&\text{otherwise}\end{cases}$$

$$\boldsymbol{\gamma}^{\text{HF}}\mathbf{S}\boldsymbol{\gamma}^{\text{HF}}=\boldsymbol{\gamma}^{\text{HF}}.$$

$$\langle \Phi_0 | \hat{H} | \Phi_i^a \rangle = 0,$$

$$\hat{H}^{(0)} = \sum_{i=1}^N \hat{f}(\mathbf{x}_i).$$

$$E_{\text{HF}} \neq \langle \Phi_{\text{HF}} | \hat{H}^{(0)} | \Phi_{\text{HF}} \rangle$$

$$\begin{aligned} E_{\text{HF}} &= \langle \Phi_{\text{HF}} | \hat{H} | \Phi_{\text{HF}} \rangle \\ &= \langle \Phi_{\text{HF}} | \hat{H}^{(0)} | \Phi_{\text{HF}} \rangle + \langle \Phi_{\text{HF}} | \hat{H} - \hat{H}^{(0)} | \Phi_{\text{HF}} \rangle = E^{(1)} \end{aligned}$$

$$\hat{H}^{(0)} | \Phi_{\text{HF}} \rangle = E^{(0)} | \Phi_{\text{HF}} \rangle \text{ where } E^{(0)} = \sum_{i=1}^N \epsilon_i.$$

$$E_{\text{HF}} = \sum_{i=1}^N \epsilon_i - \frac{1}{2} \sum_{i,j=1}^N \langle ij || ij \rangle = \frac{1}{2} \sum_{i=1}^N (\langle i | \hat{h} | i \rangle + \epsilon_i).$$

$$\begin{aligned} \text{IP}_i^{\text{HF}} &= E_{\text{HF}}^{N-1} - E_{\text{HF}}^N \approx -\epsilon_i, \\ \text{EA}_a^{\text{HF}} &= E_{\text{HF}}^N - E_{\text{HF}}^{N+1} \approx -\epsilon_a. \end{aligned}$$

$$\phi_i(\mathbf{x}) = \begin{cases} \psi_{(i+1)/2}(\mathbf{r})\alpha(\sigma) & \text{for } i \text{ odd} \\ \psi_{i/2}(\mathbf{r})\beta(\sigma) & \text{for } i \text{ even} \end{cases}$$

$$E^{\text{RHF}} = 2 \sum_{i=1}^{N/2} \langle \psi_i | \hat{h} | \psi_i \rangle + \sum_{i,j=1}^{N/2} (2 \langle \psi_i \psi_j | \psi_i \psi_j \rangle - \langle \psi_i \psi_j | \psi_j \psi_i \rangle)$$

$$\epsilon_i \psi_i(\mathbf{r}) = \hat{f} \psi_i(\mathbf{r}) = (\hat{h} + \hat{v}_{\text{H}} + \hat{v}_{\text{x}}) \psi_i(\mathbf{r})$$

$$\begin{aligned} v_{\text{H}}(\mathbf{r}) &= \int \mathrm{d}\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ v_{\text{x}}(\mathbf{r}, \mathbf{r}') &= -\frac{1}{2} \frac{\gamma^{\text{HF}}(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \end{aligned}$$

$$\gamma^{\text{HF}}(\mathbf{r}, \mathbf{r}') = \sum_{\sigma} \gamma^{\text{HF}}(\mathbf{r}\sigma, \mathbf{r}'\sigma) = 2 \sum_{i=1}^{N/2} \psi_i(\mathbf{r}) \psi_i^*(\mathbf{r}')$$

$$\rho(\mathbf{r}) = \sum_{\sigma} \rho(\mathbf{r}\sigma) = 2 \sum_{i=1}^{N/2} |\psi_i(\mathbf{r})|^2 = \gamma^{\text{HF}}(\mathbf{r}, \mathbf{r})$$

$$\begin{aligned} \hat{S}^2 &= \hat{\mathbf{S}} \cdot \hat{\mathbf{S}} = \sum_{i,j} \mathbf{S}(\sigma_i) \cdot \mathbf{S}(\sigma_j) \\ &= \sum_{i,j} [\hat{S}_x(\sigma_i) \hat{S}_x(\sigma_j) + \hat{S}_y(\sigma_i) \hat{S}_y(\sigma_j) + \hat{S}_z(\sigma_i) \hat{S}_z(\sigma_j)] \\ &= \sum_{i,j} \left[\frac{1}{2} (\hat{S}_+(\sigma_i) \hat{S}_-(\sigma_j) + \hat{S}_-(\sigma_i) \hat{S}_+(\sigma_j)) + \hat{S}_z(\sigma_i) \hat{S}_z(\sigma_j) \right] \end{aligned}$$

$$|\Phi\rangle = |\psi_1\alpha, \ldots, \psi_{N/2}\alpha, \psi_{N/2+1}\beta, \ldots, \psi_N\beta\rangle.$$

$$\hat{S}^2 = \frac{1}{2}(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+) + \hat{S}_z^2$$

$$\begin{aligned}\Psi_{\text{HL}}^1 &= \frac{1}{2}(\chi_A(\mathbf{r}_1)\chi_B(\mathbf{r}_2) + \chi_A(\mathbf{r}_2)\chi_B(\mathbf{r}_1)) \\ &\quad (\alpha(\sigma_1)\beta(\sigma_2) - \alpha(\sigma_2)\beta(\sigma_1)) \\ \Psi_{\text{HL}}^3 &= \frac{1}{2}(\chi_A(\mathbf{r}_1)\chi_B(\mathbf{r}_2) - \chi_A(\mathbf{r}_2)\chi_B(\mathbf{r}_1)) \\ &\quad (\alpha(\sigma_1)\beta(\sigma_2) + \alpha(\sigma_2)\beta(\sigma_1))\end{aligned}$$

$$\begin{aligned}E_u &= \langle (\sigma_u)^2 | \hat{H} | (\sigma_u)^2 \rangle = 2 \langle \sigma_u | \hat{h} | \sigma_u \rangle + (\sigma_u \sigma_u | \sigma_u \sigma_u) \\ V &= \langle (\sigma_u)^2 | \hat{H} | (\sigma_g)^2 \rangle = (\sigma_g \sigma_u | \sigma_g \sigma_u) \\ E_g &= E_{\text{RHF}} = 2 \langle \sigma_g | \hat{h} | \sigma_g \rangle + (\sigma_g \sigma_g | \sigma_g \sigma_g)\end{aligned}$$

$$\begin{aligned}\langle \sigma_u | \hat{h} | \sigma_u \rangle &= \frac{\langle A | \hat{h} | A \rangle - \langle A | \hat{h} | B \rangle}{1-s}, \\ (\sigma_u \sigma_u | \sigma_u \sigma_u) &= \frac{1}{2(1-s)^2} [(AA | AA) + (AA | BB) - \\ &\quad 4(AA | AB) - 2(AB | AB)], \\ (\sigma_g \sigma_u | \sigma_g \sigma_u) &= \frac{1}{2(1-s^2)} [(AA | AA) + (AA | BB)].\end{aligned}$$

$$|\Psi_1^{\text{CI}}\rangle = \cos{(\alpha)}\left|(\sigma_g)^2\right\rangle + \sin{(\alpha)}|(\sigma_u)^2\rangle$$

$$\int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{x}' w(\mathbf{x},\mathbf{x}') |\psi(\mathbf{x},\mathbf{x}')|^2 > 0$$

$$\begin{aligned}h_k &= \langle \phi_k | \hat{h} | \phi_k \rangle \\ W_{k,l} &= \frac{1}{2} \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{x}' |\phi_k(\mathbf{x}) \phi_l(\mathbf{x}') - \phi_l(\mathbf{x}) \phi_k(\mathbf{x}')|^2 w(\mathbf{x},\mathbf{x}')\end{aligned}$$

$$\begin{aligned}\langle \Phi_{\text{HF}} | \hat{H} | \Phi_{\text{HF}} \rangle &= \sum_{k=1}^N h_k + \frac{1}{2} \sum_{k,l=1}^N W_{k,l} \\ \langle \tilde{\Phi} | \hat{H} | \tilde{\Phi} \rangle &= \sum_{k=1}^{N-1} h_k + \frac{1}{2} \sum_{k,l=1}^{N-1} W_{k,l} + h_{N+1} + \sum_{l=1}^{N-1} W_{l,N+1}\end{aligned}$$

$$\epsilon_k = \langle \phi_k | \hat{f} | \phi_k \rangle = h_k + \sum_{l=1}^N W_{l,k}.$$

$$\begin{aligned}\langle \tilde{\Phi} | \hat{H} | \tilde{\Phi} \rangle &= \langle \Phi_{\text{HF}} | \hat{H} | \Phi_{\text{HF}} \rangle + h_{N+1} - h_N + \sum_{l=1}^{N-1} (W_{l,N+1} - W_{l,N}) \\ &= \langle \Phi_{\text{HF}} | \hat{H} | \Phi_{\text{HF}} \rangle + \epsilon_{N+1} - \epsilon_N - W_{N,N+1} \\ &\leq \langle \Phi_{\text{HF}} | \hat{H} | \Phi_{\text{HF}} \rangle - W_{N,N+1}\end{aligned}$$

$$\langle v | w \rangle = \sum_{i=1}^N v_i^* w_i = \mathbf{v}^\dagger \mathbf{w}$$

$$\langle f | g \rangle = \int d\mathbf{r} f^*(\mathbf{r}) g(\mathbf{r})$$

$$\hat{1} = \sum_{i,j} |\phi_i\rangle (\mathbf{S}^{-1})_{ij} \langle \phi_j|,$$

$$S_{ij} := \langle \phi_i | \phi_j \rangle$$

$$|f\rangle = \hat{1}|f\rangle = \sum_{i,j} |\phi_i\rangle (\mathbf{S}^{-1})_{ij} \langle \phi_j | f \rangle,$$

$$\sum_j (\mathbf{S}^{-1})_{ij} \langle \phi_j | f \rangle$$

$$|f\rangle = \sum_k |\phi_k\rangle f_k$$

$$f_i = \sum_j (\mathbf{S}^{-1})_{ij} \langle \phi_j | f \rangle$$

$$\langle \phi_i | \phi_j \rangle = S_{ij} = \delta_{ij}.$$

$$|u_1\rangle = |v_1\rangle,$$

$$|u_2\rangle = |v_2\rangle - \frac{\langle u_1 | v_2 \rangle}{\langle u_1 | u_1 \rangle} |u_1\rangle,$$

$$|u_3\rangle = |v_3\rangle - \frac{\langle u_1 | v_3 \rangle}{\langle u_1 | u_1 \rangle} |u_1\rangle - \frac{\langle u_2 | v_3 \rangle}{\langle u_2 | u_2 \rangle} |u_2\rangle$$

$$\vdots$$

$$|u_n\rangle = |v_n\rangle - \sum_{i=1}^{n-1} \frac{\langle u_i | v_n \rangle}{\langle u_i | u_i \rangle} |u_i\rangle = \left(\hat{1} - \sum_{i=1}^{n-1} \frac{|u_i\rangle \langle u_i|}{\langle u_i | u_i \rangle} \right) |v_n\rangle$$

$$u_i = \sum_j |v_j\rangle (\mathbf{S}^{-1/2})_{ji}$$

$$|u_i\rangle = \sum_j |v_j\rangle (L^{-\dagger})_{ji}$$

$$L^{-\dagger} := (L^{-1})^\dagger = (L^\dagger)^{-1}$$

$$\begin{array}{ll} \text{completeness} & \sum_i^{\text{discrete, } |\phi_i\rangle} |\phi_i\rangle\langle\phi_i| = \hat{1} \quad \int^{\text{continuous, } |\mathbf{r}\rangle} d\mathbf{r} |\mathbf{r}\rangle\langle\mathbf{r}| = \hat{1} \\ \text{orthonormality} & \langle\phi_i|\phi_j\rangle = \delta_{ij} \quad \langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') \end{array}$$

$$\begin{aligned} |\phi_i\rangle &= \hat{1}|\phi_i\rangle = \int d\mathbf{x} |\mathbf{r}\rangle\langle\mathbf{r}|\phi_i\rangle = \int d\mathbf{r} |\mathbf{r}\rangle\phi_i(\mathbf{r}), \\ |\mathbf{r}\rangle &= \hat{1}|\mathbf{r}\rangle = \sum_i |\phi_i\rangle\langle\phi_i|\mathbf{r}\rangle = \sum_i |\phi_i\rangle\phi_i^*(\mathbf{r}). \end{aligned}$$

$$\begin{aligned} \langle\phi_i|\hat{O}|\phi_j\rangle &= \int d\mathbf{r} \int d\mathbf{r}' \langle\phi_i|\mathbf{r}\rangle\langle\mathbf{r}|\hat{O}|\mathbf{r}'\rangle\langle\mathbf{r}'|\phi_j\rangle \\ &= \int d\mathbf{r} \int d\mathbf{r}' \phi_i^*(\mathbf{r})\langle\mathbf{r}|\hat{O}|\mathbf{r}'\rangle\phi_j(\mathbf{r}') \end{aligned}$$

$$\langle\mathbf{r}|\hat{v}_{\text{loc}}|\mathbf{r}'\rangle = v_{\text{loc}}(\mathbf{r},\mathbf{r}') = v_{\text{loc}}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$$

$$\langle\mathbf{k}|\hat{p}|\mathbf{k}'\rangle = \mathbf{k}\delta(\mathbf{k}-\mathbf{k}') \text{ and } \langle\mathbf{k}|\hat{T}|\mathbf{k}'\rangle = \frac{|\mathbf{k}|^2}{2}\delta(\mathbf{k}-\mathbf{k}')$$

$$\begin{aligned} \langle\mathbf{r}|\hat{p}|\mathbf{r}'\rangle &= i\nabla_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}') = -i\nabla_{\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}') \\ \langle\mathbf{r}|\hat{T}|\mathbf{r}'\rangle &= -\frac{1}{2}\nabla_{\mathbf{r}'}^2\delta(\mathbf{r}-\mathbf{r}') = \frac{1}{2}\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{r}'}\delta(\mathbf{r}-\mathbf{r}') \end{aligned}$$

$$\delta(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^d} \int d\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

$$\psi_{nlm}(r,\theta,\phi) = N_{nl} e^{-\rho/2} \rho^l L_{n-l-1}^{2l+1}(\rho) Y_l^m(\theta,\phi),$$

$$\left(-\frac{1}{2}\nabla^2+\frac{Z}{r}\right)\phi_{\mathbf{k}}(\mathbf{r})=\frac{k^2}{2}\phi_{\mathbf{k}}(\mathbf{r}),$$

$$F_{\eta l}(\rho) = \tilde{N}_{\eta l} \rho^{l+1} e^{\mp i \rho} M(l+1 \mp i \eta, 2l+2, \pm 2 i \rho),$$

$$\tilde{\psi}_{\eta lm}(r,\theta,\phi) = F_{\eta l}(\rho) Y_l^m(\theta,\rho).$$

$$\hat{1} = \underbrace{\sum_{n,l,m} |\psi_{nlm}\rangle\langle\psi_{nlm}|}_{\text{discrete part}} + \underbrace{\int_0^\infty d\eta \sum_{l,m} |\tilde{\psi}_{\eta lm}\rangle\langle\tilde{\psi}_{\eta lm}|}_{\text{continuous part}}.$$

$$\mathrm{e}^{-\alpha r_A^2}\mathrm{e}^{-\beta r_B^2}=\mathrm{e}^{-\mu R_{AB}^2}\mathrm{e}^{-pr_P^2},$$

$$p = \alpha + \beta, \quad \mathbf{P} = \frac{\alpha \mathbf{A} + \beta \mathbf{B}}{p}$$

$$\mu = \frac{\alpha\beta}{p}, \quad R_{AB} = |\mathbf{A} - \mathbf{B}|$$

$$\frac{1}{r_c} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dt e^{-r_c^2 t^2}$$

$$F_n(x)=\int_0^1 dt t^{2n} \mathrm{e}^{-xt^2}$$

$$E=T[\gamma]+V[\rho]+W[P].$$

$$\int \, \mathrm{d}\mathbf{x}\!:=\sum_{\sigma}\int \, \mathrm{d}\mathbf{r}$$

$$\begin{aligned} T &= \int \, \mathrm{d}\mathbf{x}_1 \cdots \, \mathrm{d}\mathbf{x}_N \Psi^*(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \sum_{i=1}^N -\frac{1}{2} \nabla_i^2 \Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\ &= -\frac{1}{2} \int \, \mathrm{d}\mathbf{x}_1 \cdots \, \mathrm{d}\mathbf{x}_N \Psi^*(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \nabla_{\mathbf{r}_1}^2 \Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) + \cdots + \\ &\quad -\frac{1}{2} \int \, \mathrm{d}\mathbf{x}_1 \cdots \, \mathrm{d}\mathbf{x}_N \Psi^*(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \nabla_{\mathbf{r}_N}^2 \Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\ &= -\frac{N}{2} \int \, \mathrm{d}\mathbf{x}_1 \cdots \, \mathrm{d}\mathbf{x}_N \Psi^*(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \nabla_{\mathbf{r}_1}^2 \Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\ &= -\frac{1}{2} \int \, \mathrm{d}\mathbf{x}_1 \big[\nabla_{\mathbf{r}_1}^2 \gamma(\mathbf{x}_1, \mathbf{x}'_1) \big]_{\mathbf{x}'_1 = \mathbf{x}_1} \end{aligned}$$

$$\gamma(\mathbf{x}_1,\mathbf{x}'_1)\!:=\!N\int \, \mathrm{d}\mathbf{x}_2\cdots \mathrm{d}\mathbf{x}_N \Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)\times \\ \Psi^*(\mathbf{x}'_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)$$

$$\gamma(\mathbf{r},\mathbf{r}')\!:=\!\sum_{\sigma}\gamma(\mathbf{r}\sigma,\mathbf{r}'\sigma)$$

$$T[\gamma] = -\frac{1}{2} \int \, \mathrm{d}\mathbf{r} [\nabla_{\mathbf{r}}^2 \gamma(\mathbf{r},\mathbf{r}')]_{\mathbf{r}'=\mathbf{r}} = \frac{1}{2} \int \, \mathrm{d}\mathbf{r} [\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{r}'} \gamma(\mathbf{r},\mathbf{r}')]_{\mathbf{r}'=\mathbf{r}}$$

$$\rho(\mathbf{x}_1):=N\int \, \mathrm{d}\mathbf{x}_2\cdots \mathbf{x}_N |\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)|^2$$

$$P(\mathbf{x}_1,\mathbf{x}_2):=N(N-1)\int \, \mathrm{d}\mathbf{x}_3\cdots \mathbf{x}_N |\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)|^2$$

$$V[\rho] \, = \int \, \mathrm{d}\mathbf{r} v(\mathbf{r}) \rho(\mathbf{r})$$

$$W[P] \, = \frac{1}{2} \int \, \mathrm{d}\mathbf{r}_1 \int \, \mathrm{d}\mathbf{r}_2 w(|\mathbf{r}_1 - \mathbf{r}_2|) P(\mathbf{r}_1, \mathbf{r}_2)$$

$$\Gamma(\mathbf{x}_1\mathbf{x}_2,\mathbf{x}'_2\mathbf{x}'_1)\!:=\!N(N-1)\int \, \mathrm{d}\mathbf{x}_3\cdots \mathrm{d}\mathbf{x}_N \Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\ldots,\mathbf{x}_N)\times \\ \Psi^*(\mathbf{x}'_1,\mathbf{x}'_2,\mathbf{x}_3,\ldots,\mathbf{x}_N)$$

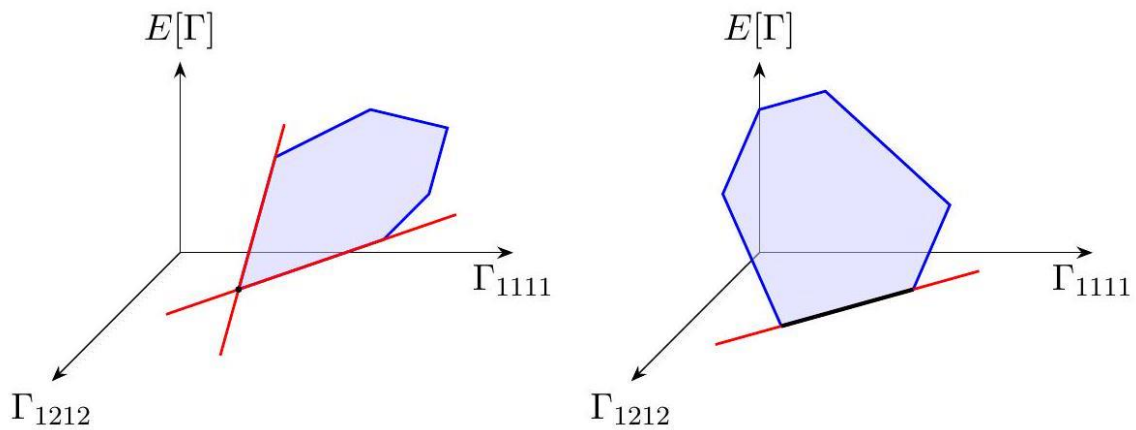
$$\begin{aligned}
P(\mathbf{x}_1, \mathbf{x}_2) &= \Gamma(\mathbf{x}_1 \mathbf{x}_2, \mathbf{x}_2 \mathbf{x}_1) \\
\gamma(\mathbf{x}_1, \mathbf{x}'_1) &= \frac{1}{N-1} \int d\mathbf{x}_2 \Gamma(\mathbf{x}_1 \mathbf{x}_2, \mathbf{x}_2 \mathbf{x}'_1) \\
\rho(\mathbf{x}) &= \gamma(\mathbf{x}, \mathbf{x}) = \frac{1}{N-1} \int d\mathbf{x}' \Gamma(\mathbf{x} \mathbf{x}', \mathbf{x}' \mathbf{x})
\end{aligned}$$

$$\inf_{\Xi} E[\Xi] = -\infty$$

$$E_{\text{gs}} = \min_{N\text{-representable } \Gamma} E[\Gamma].$$

$$E[\gamma] = \text{Tr}\{\hat{L}\hat{\Gamma}\} = \int d\mathbf{x}_1 \int d\mathbf{x}_2 \hat{L}\Gamma(\mathbf{x}_1 \mathbf{x}_2, \mathbf{x}'_2 \mathbf{x}'_1) \Big|_{\mathbf{x}'_1=\mathbf{x}_1, \mathbf{x}'_2=\mathbf{x}_2}$$

$$\hat{L} = \frac{1}{2(N-1)} \left(-\frac{1}{2} (\nabla_{\mathbf{r}_1}^2 + \nabla_{\mathbf{r}_2}^2) + v(\mathbf{r}_1) + v(\mathbf{r}_2) \right) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$



$$v(\mathbf{r}) \stackrel{\hat{H}\Psi=E\Psi}{\mapsto} \Psi \stackrel{\int d\mathbf{r}}{\mapsto} \rho(\mathbf{r}).$$

$$\begin{aligned}
(\hat{T} + \hat{V}_1 + \hat{W})\Psi &= E_1\Psi \\
(\hat{T} + \hat{V}_2 + \hat{W})\Psi &= E_2\Psi
\end{aligned}$$

$$(E_1 - E_2)\Psi = (\hat{V}_1 - \hat{V}_2)\Psi = \sum_{i=1}^N (v_1(\mathbf{r}_i) - v_2(\mathbf{r}_i))\Psi$$

$$\sum_{i=1}^N (v_1(\mathbf{r}_i) - v_2(\mathbf{r}_i)) = E_1 - E_2 = \text{constant}$$

$$\begin{aligned}
E_1 &= \langle \Psi_1 | \hat{T} + \hat{V}_1 + \hat{W} | \Psi_1 \rangle \\
\langle \Psi_2 | \hat{T} + \hat{V}_1 + \hat{W} | \Psi_2 \rangle &= \langle \Psi_2 | \hat{T} + \hat{V}_2 + \hat{W} | \Psi_2 \rangle + \langle \Psi_2 | \hat{V}_1 - \hat{V}_2 | \Psi_2 \rangle \\
&= E_2 + \int d\mathbf{r} \rho(\mathbf{r}) (v_1(\mathbf{r}) - v_2(\mathbf{r}))
\end{aligned}$$

$$E_2 < E_1 + \int d\mathbf{r} \rho(\mathbf{r}) (v_2(\mathbf{r}) - v_1(\mathbf{r}))$$

$$E_1 + E_2 < E_1 + E_2$$

$$v(\mathbf{r}) \overset{\text{HK-I}}{\longleftrightarrow} \Psi \overset{\text{HK-II}}{\longleftrightarrow} \rho(\mathbf{r}),$$

$$O[\rho] = \langle \Psi[\rho] | \hat{O} | \Psi[\rho] \rangle$$

$$E[\rho] = \langle \Psi[\rho] | \hat{H} | \Psi[\rho] \rangle = F_{\text{HK}}[\rho] + \int d\mathbf{r} \rho(\mathbf{r}) v(\mathbf{r})$$

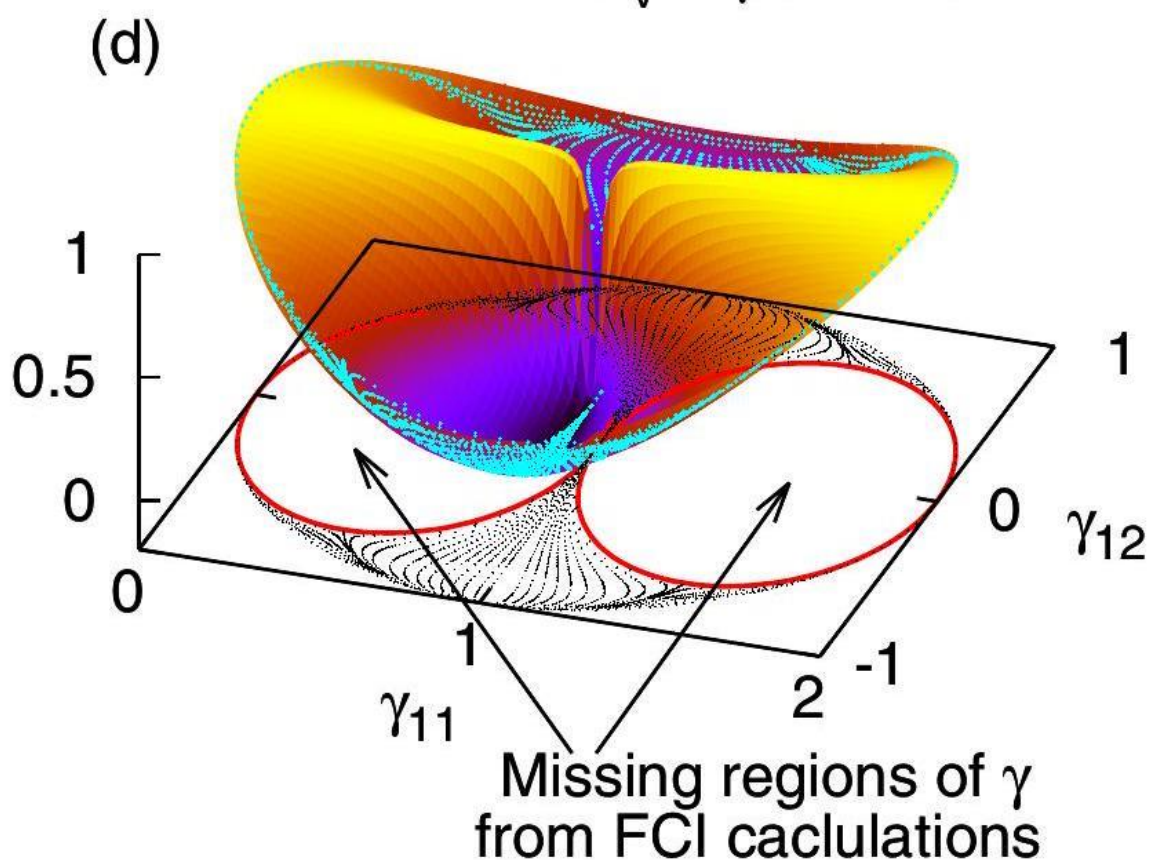
$$F_{\text{HK}}[\rho] := \langle \Psi[\rho] | \hat{T} + \hat{W} | \Psi[\rho] \rangle$$

$$\hat{v}\psi(\mathbf{x}) = (\hat{v}\psi)(\mathbf{x}) = \int d\mathbf{x}' v(\mathbf{x}, \mathbf{x}') \psi(\mathbf{x}')$$

$$\hat{V} = \sum_{i=1}^N \hat{v}(\mathbf{x}_i, \mathbf{x}'_i)$$

$$\langle \Psi | \hat{V} | \Psi \rangle = \int d\mathbf{x} \int d\mathbf{x}' v(\mathbf{x}', \mathbf{x}) \gamma(\mathbf{x}, \mathbf{x}')$$

$$E_v^{\text{FCI}} - \gamma.v \quad \bullet, \bullet$$



$$\begin{aligned} E_{\text{gs}} &= \min_{\Psi} \langle \Psi | \hat{T} + \hat{V} + \hat{W} | \Psi \rangle \\ &= \min_{\rho} \left(\min_{\Psi \rightarrow \rho} \langle \Psi | \hat{T} + \hat{W} | \Psi \rangle + \int d\mathbf{r} \rho(\mathbf{r}) v(\mathbf{r}) \right) \end{aligned}$$

$$F_{\text{LL}}[\rho] := \min_{\Psi \rightarrow \rho} \langle \Psi | \hat{T} + \hat{W} | \Psi \rangle$$

$$W_{\text{H}}[\rho] := \frac{1}{2} \int \mathrm{d}\mathbf{r}_1 \int \mathrm{d}\mathbf{r}_2 \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$T_{\text{TF}}[\rho] := C_{\text{TF}} \int \mathrm{d}\mathbf{r} \rho(\mathbf{r})^{5/3}, C_{\text{TF}} := \frac{3}{10} (3\pi^2)^{2/3}$$

$$E[\rho] \approx E_{\text{TF}}[\rho] := T_{\text{TF}}[\rho] + V[\rho] + W_{\text{H}}[\rho].$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = \Omega^{-1/2} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$$

$$k_i = \frac{2\pi n_i}{L} \quad i = x,y,z \quad n_i = 0, \pm 1, \pm 2, \dots$$

$$\epsilon(\mathbf{k}) = \frac{1}{2} |\mathbf{k}|^2$$

$$\sum_{n_x,n_y,n_z} = \frac{\Omega}{(2\pi)^3} \sum_{k_x,k_y,k_z} \stackrel{L\rightarrow\infty}{\rightarrow} \frac{\Omega}{(2\pi)^3} \int \mathrm{d}\mathbf{k}.$$

$$T_s[\rho] := \min_{\Psi_s \rightarrow \rho} \langle \Psi_s | \hat{T} | \Psi_s \rangle.$$

$$\Psi_s(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(\mathbf{x}_1)&\phi_2(\mathbf{x}_1)&\ldots&\phi_N(\mathbf{x}_1)\\ \phi_1(\mathbf{x}_2)&\phi_2(\mathbf{x}_2)&\ldots&\phi_N(\mathbf{x}_2)\\ \vdots&\vdots&\ddots&\vdots\\ \phi_1(\mathbf{x}_N)&\phi_2(\mathbf{x}_N)&\ldots&\phi_N(\mathbf{x}_N)\end{vmatrix}.$$

$$\gamma_s(\mathbf{x},\mathbf{x}')=\sum_{i=1}^N\phi_i(\mathbf{x})\phi_i^*(\mathbf{x}').$$

$$\tilde{T}_s[\{\phi,\phi^*\}]=-\frac{1}{2}\int\mathrm{d}\mathbf{x}[\nabla_{\mathbf{r}}^2\gamma_s(\mathbf{x},\mathbf{x}')]\big|_{\mathbf{x}'=\mathbf{x}}=-\frac{1}{2}\sum_{i=1}^N\langle\phi_i|\nabla^2|\phi_i\rangle,$$

$$L_{\rho}[\{\phi,\phi^*\},v_s,\epsilon] := \tilde{T}_s[\{\phi,\phi^*\}] - \sum_{ij} \epsilon_{ji} (\langle \phi_i | \phi_j \rangle - \delta_{ij}) + \\ \int \mathrm{d}\mathbf{r} v_s(\mathbf{r}) \left(\sum_{i,\sigma} |\phi_i(\mathbf{r}\sigma)|^2 - \rho(\mathbf{r}) \right)$$

$$0=\delta L_{\rho}=\int\mathrm{d}\mathbf{x}\sum_{i=1}^N\left(\delta\phi_i^*(\mathbf{x})\frac{\delta L_{\rho}}{\delta\phi_i^*(\mathbf{x})}+\frac{\delta L_{\rho}}{\delta\phi_i(\mathbf{x})}\delta\phi_i(\mathbf{x})\right)$$

$$0=\frac{\delta L_{\rho}}{\delta\phi_i^*(\mathbf{x})}=-\frac{1}{2}\nabla^2\phi_i(\mathbf{x})-\sum_{j=1}^N\phi_j(\mathbf{x})\epsilon_{ji}+v_s(\mathbf{r})\phi_i(\mathbf{x}).$$

$$\left(-\frac{1}{2}\nabla^2 + v_s(\mathbf{r})\right)\phi_i(\mathbf{x}) = \sum_{j=1}^N \phi_j(\mathbf{x})\epsilon_{ji}.$$

$$\tilde{T}_s = \frac{1}{2}\sum_{i=1}^N \langle \nabla\phi_i | \nabla\phi_i \rangle = -\frac{1}{2}\sum_{i=1}^N \langle \nabla^2\phi_i | \phi_i \rangle.$$

$$\left(-\frac{1}{2}\nabla^2 + v_s(\mathbf{r})\right)\phi_i^*(\mathbf{x}) = \sum_{j=1}^N \epsilon_{ij}\phi_j^*(\mathbf{x})$$

$$\left(-\frac{1}{2}\nabla^2 + v_s(\mathbf{r})\right)\phi_k(\mathbf{x}) = \epsilon_k\phi_k(\mathbf{x})$$

$$\phi_k(\mathbf{x}) = \phi_k(\mathbf{r}\sigma) = \begin{cases} \psi_{(k+1)/2}(\mathbf{r})\alpha(\sigma) & \text{for } k \text{ odd} \\ \psi_{k/2}(\mathbf{r})\beta(\sigma) & \text{for } k \text{ even.} \end{cases}$$

$$\gamma_s(\mathbf{r},\mathbf{r}')=2\sum_{i=1}^{N/2}\psi_i(\mathbf{r})\psi_i^*(\mathbf{r}')$$

$$\int \mathrm{d}\mathbf{r} \frac{\delta W_{\mathrm{H}}}{\delta \rho(\mathbf{r})} \delta \rho(\mathbf{r})$$

$$T_s[\rho] = L_\rho[\{\phi_i[\rho], \phi_i^*[\rho]\}, v_s[\rho], \epsilon[\rho]]$$

$$\begin{aligned} \frac{\delta T_s}{\delta \rho(\mathbf{r})} = & \sum_i \int \mathrm{d}\mathbf{x}' \left(\frac{\partial L_\rho}{\partial \phi_i(\mathbf{x}')}\bigg|_\rho \frac{\delta \phi_i(\mathbf{x}')}{\delta \rho(\mathbf{r})} + \frac{\partial L_\rho}{\partial \phi_i^*(\mathbf{x}')}\bigg|_\rho \frac{\delta \phi_i^*(\mathbf{x}')}{\delta \rho(\mathbf{r})} \right) + \\ & \int \mathrm{d}\mathbf{r}' \frac{\partial L_\rho}{\partial v_s(\mathbf{r}')}\bigg|_\rho \frac{\delta v_s(\mathbf{r}')}{\delta \rho(\mathbf{r})} + \sum_i \frac{\partial L_\rho}{\partial \epsilon_{ij}}\bigg|_\rho \frac{\delta \epsilon_{ij}}{\delta \rho(\mathbf{r})} + \frac{\partial L_\rho}{\partial \rho(\mathbf{r})}\bigg|_\rho = -v_s[\rho](\mathbf{r}) \end{aligned}$$

$$E[\rho] = F[\rho] + V[\rho] = T_s[\rho] + V[\rho] + \underbrace{F[\rho] - T_s[\rho]}_{=:E_{\mathrm{Hxc}}[\rho]},$$

$$E_{\mathrm{xc}}[\rho] := E_{\mathrm{Hxc}}[\rho] - W_{\mathrm{H}}[\rho] = \underbrace{T[\rho] - T_s[\rho]}_{=:T_{\mathrm{c}}[\rho]} + W_{\mathrm{xc}}[\rho]$$

$$\int \mathrm{d}\mathbf{r} \delta \rho(\mathbf{r}) = 0$$

$$0 = \delta E = \int \mathrm{d}\mathbf{r} \frac{\delta E}{\delta \rho(\mathbf{r})} \delta \rho(\mathbf{r}) \Rightarrow c = \frac{\delta E}{\delta \rho(\mathbf{r})} = \frac{\delta F}{\delta \rho(\mathbf{r})} + v(\mathbf{r})$$

$$c = \frac{\delta E}{\delta \rho(\mathbf{r})} = \frac{\delta T_s}{\delta \rho(\mathbf{r})} + v(\mathbf{r}) + \frac{\delta E_{\mathrm{Hxc}}}{\delta \rho(\mathbf{r})}$$

$$v_s[\rho](\mathbf{r}) = v(\mathbf{r}) + v_{\mathrm{H}}[\rho](\mathbf{r}) + v_{\mathrm{xc}}[\rho](\mathbf{r}),$$

$$v_{\mathrm{H}}[\rho](\mathbf{r}) := \frac{\delta W_{\mathrm{H}}}{\delta \rho(\mathbf{r})} = \int \mathrm{d}\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, v_{\mathrm{xc}}[\rho](\mathbf{r}) := \frac{\delta E_{\mathrm{xc}}}{\delta \rho(\mathbf{r})}.$$

$$W = \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{P(\mathbf{r}_1, \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

$$\rho(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) := \frac{P(\mathbf{r}, \mathbf{r}_{\text{ref}})}{\rho(\mathbf{r}_{\text{ref}})}$$

$$W = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}_{\text{ref}} \frac{\rho(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) \rho(\mathbf{r}_{\text{ref}})}{|\mathbf{r} - \mathbf{r}_{\text{ref}}|}$$

$$\begin{aligned} W_{\text{xc}} &:= W - W_{\text{H}} = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}_{\text{ref}} \frac{\rho(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) \rho(\mathbf{r}_{\text{ref}}) - \rho(\mathbf{r}) \rho(\mathbf{r}_{\text{ref}})}{|\mathbf{r} - \mathbf{r}_{\text{ref}}|} \\ &= \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}_{\text{ref}} \rho(\mathbf{r}_{\text{ref}}) \frac{\rho_{\text{xc}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}})}{|\mathbf{r} - \mathbf{r}_{\text{ref}}|} \end{aligned}$$

$$\rho_{\text{xc}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) := \rho(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) - \rho(\mathbf{r}) = \frac{P(\mathbf{r}, \mathbf{r}_{\text{ref}})}{\rho(\mathbf{r}_{\text{ref}})} - \rho(\mathbf{r})$$

$$\int d\mathbf{r} \rho_{\text{xc}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) = -1$$

$$P_s(\mathbf{r}_1, \mathbf{r}_2) = \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) - \frac{1}{2} |\gamma_s(\mathbf{r}_1, \mathbf{r}_2)|^2.$$

$$\rho_{\text{x}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) := -\frac{1}{2} \frac{|\gamma_s(\mathbf{r}, \mathbf{r}_{\text{ref}})|^2}{\rho(\mathbf{r}_{\text{ref}})}.$$

$$\rho_{\text{xc}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) =: \rho_{\text{x}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) + \rho_{\text{c}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}}).$$

$$\int d\mathbf{r}_1 \int d\mathbf{r}_2 P(\mathbf{r}_1, \mathbf{r}_2) = N(N-1).$$

$$P_s(\mathbf{x}_1, \mathbf{x}_2) = \rho(\mathbf{x}_1) \rho(\mathbf{x}_2) - |\gamma_s(\mathbf{x}_1, \mathbf{x}_2)|^2$$

$$P_s(\mathbf{r}_1, \mathbf{r}_2) = \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) - \frac{1}{2} |\gamma_s(\mathbf{r}_1, \mathbf{r}_2)|^2$$

$$\rho_{\text{x}}(\mathbf{r} \mid \mathbf{r}_{\text{ref}}) = -\rho(\mathbf{r})/2$$

$$E_{\lambda} = \langle \Psi_{\lambda} | \hat{H}_{\lambda} | \Psi_{\lambda} \rangle = \langle \Psi_{\lambda} | \hat{T} + \hat{V}_{\lambda} + \lambda \hat{W} | \Psi_{\lambda} \rangle.$$

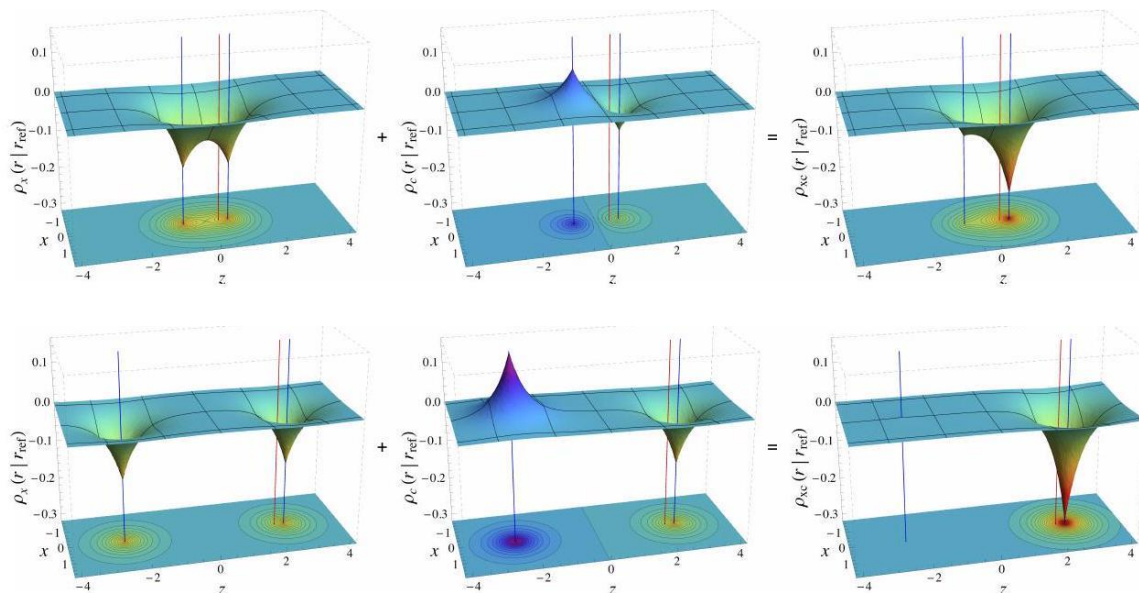
$$\begin{aligned} \frac{\partial E_{\lambda}}{\partial \lambda} &= \langle \Psi_{\lambda} | \frac{\partial \hat{H}_{\lambda}}{\partial \lambda} | \Psi_{\lambda} \rangle \text{ (Hellman-Feynman)} \\ &= \langle \Psi_{\lambda} | \frac{\partial \hat{V}_{\lambda}}{\partial \lambda} | \Psi_{\lambda} \rangle + \langle \Psi_{\lambda} | \hat{W} | \Psi_{\lambda} \rangle \\ &= \int d\mathbf{r} \rho(\mathbf{r}) \frac{\partial v_{\lambda}(\mathbf{r})}{\partial \lambda} + \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{P_{\lambda}(\mathbf{r}_1, \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} \end{aligned}$$

$$\begin{aligned} E_1 - E_0 &= \int_0^1 d\lambda \frac{\partial E}{\partial \lambda} \\ &= \int d\mathbf{r} \rho(\mathbf{r}) (v_1(\mathbf{r}) - v_0(\mathbf{r})) + \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{\bar{P}(\mathbf{r}_1, \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} \end{aligned}$$



$$\bar{P}(\mathbf{r}_1, \mathbf{r}_2) := \int_0^1 d\lambda P_\lambda(\mathbf{r}_1, \mathbf{r}_2)$$

$$E_{\text{Hxc}} = T - T_s + W_{\text{Hxc}} = \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{\bar{P}(\mathbf{r}_1, \mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$



$$E_{\text{xc}} = \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{\bar{P}(\mathbf{r}_1, \mathbf{r}_2) - \rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

$$\bar{\rho}_{\text{xc}}(\mathbf{r} | \mathbf{r}_{\text{ref}}) := \frac{\bar{P}(\mathbf{r}, \mathbf{r}_{\text{ref}})}{\rho(\mathbf{r}_{\text{ref}})} - \rho(\mathbf{r}).$$

$$\rho_{\text{x}}(\mathbf{r} | \mathbf{r}_{\text{ref}}) = -\frac{1}{2} \rho(\mathbf{r}),$$

$$E_{\text{HF}}(R_{\text{H-H}} \rightarrow \infty) = C - \frac{1}{2R_{\text{H-H}}}$$

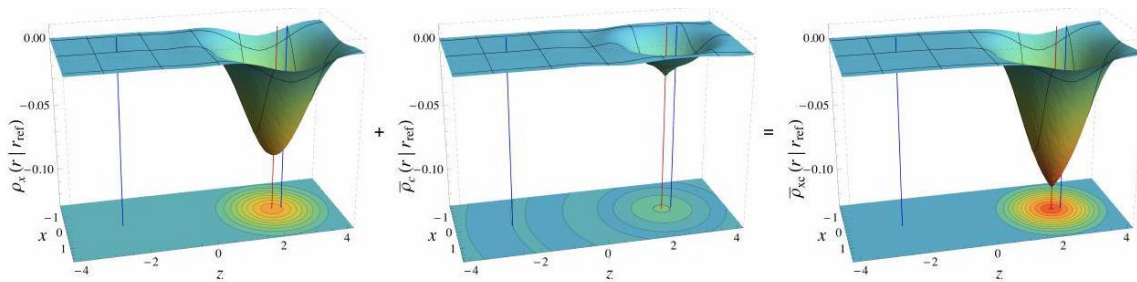
$$C = \lim_{R \rightarrow \infty} E_{\text{RHF}}(R) \approx 2\langle A | \hat{h} | A \rangle + \frac{1}{2} (AA | AA) = \zeta^2 - 2\zeta + \frac{5\zeta}{16},$$

$$\bar{\rho}_{\text{xc}}^{\text{LDA}}(\mathbf{r} | \mathbf{r}_{\text{ref}}) := \bar{\rho}_{\text{xc}}^{\text{HEG}}(\rho(\mathbf{r}_{\text{ref}}), |\mathbf{r} - \mathbf{r}_{\text{ref}}|).$$

$$\gamma_s^{\text{HEG}}(k_F, r_{12}) = \frac{k_F^3}{\pi^2} J(k_F r_{12}), J(y) = \frac{j_1(y)}{y} = \frac{\sin(y) - y \cos(y)}{y^3},$$

$$W_{\text{x}}^{\text{LDA}}[\rho] = -C_{\text{x}} \int d\mathbf{r} \rho(\mathbf{r})^{4/3}, C_{\text{x}} := \frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3}$$

$$W_{\text{x}}^{\text{X}\alpha}[\rho] = \frac{3}{2} \alpha W_{\text{x}}^{\text{LDA}}[\rho]$$



$$\int \mathrm{d}\mathbf{r} \rho_{\mathbf{x}}^{\mathrm{LDA}}(\mathbf{r} \mid \mathbf{r}_{\mathrm{ref}}) = -\frac{2}{\pi} \int_0^\infty \mathrm{d}x (q(x))^2.$$

$$\gamma_s^{\mathrm{HEG}}(k_F,r_{12})=\frac{1}{4\pi^3}\int_{\Omega_F}\mathrm{d}\mathbf{k}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{12}}$$

$$\int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{\mathrm{i}kx} = 2\pi \delta(k),$$

$$s:=|\nabla\rho|/(2k_F\rho)$$

$$\bar{\rho}_{\mathrm{xc}}^{\mathrm{GEA}}(\mathbf{r} \mid \mathbf{r}_{\mathrm{ref}}) \mathop{:}= \bar{\rho}_{\mathrm{xc}}^{\mathrm{HEG}}(\rho(\mathbf{r}_{\mathrm{ref}}), |\nabla \rho(\mathbf{r}_{\mathrm{ref}})|, |\mathbf{r} - \mathbf{r}_{\mathrm{ref}}|),$$

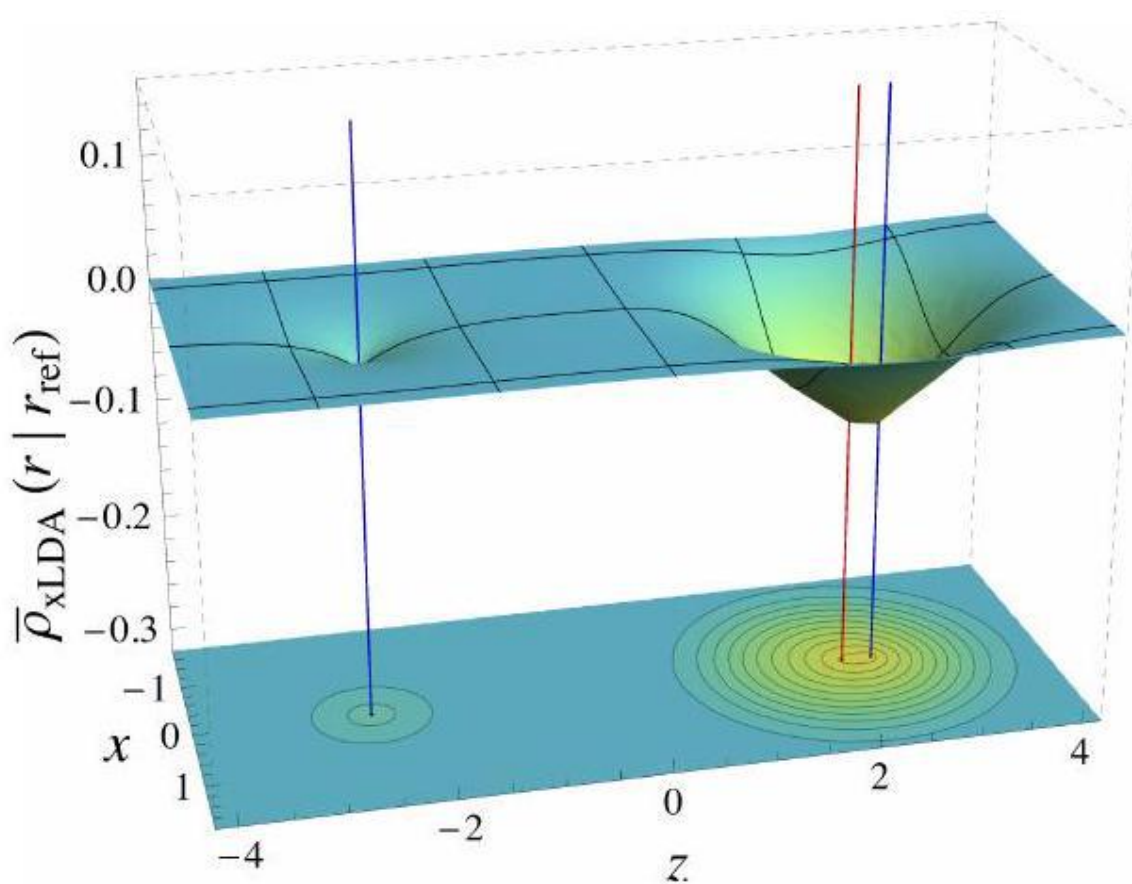
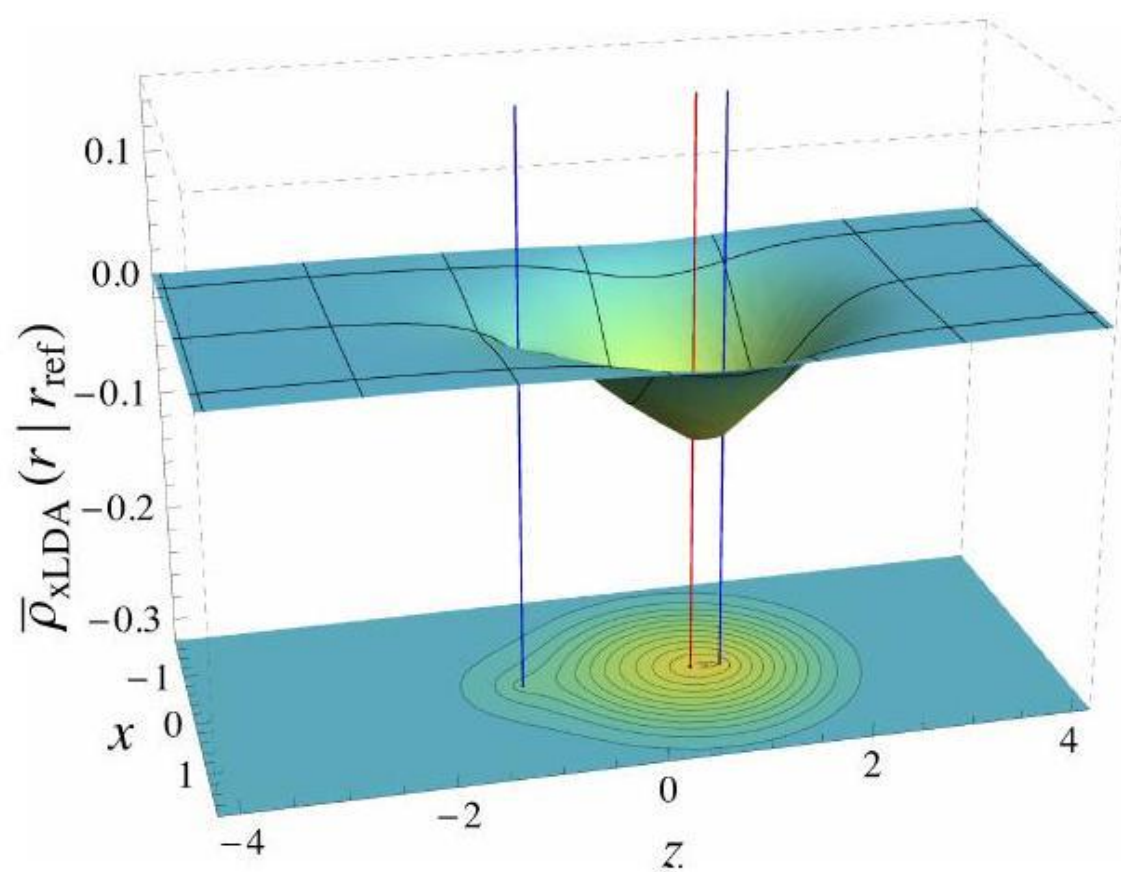
$$\tau_s(\mathbf{x})\mathop{:}=\frac{1}{2}\sum_{i=1}^N|\nabla\phi_i(\mathbf{x})|^2.$$

$$\alpha(\mathbf{r})=\frac{\tau_s(\mathbf{r})-\tau_{\mathrm{W}}(\mathbf{r})}{\tau^{\mathrm{HEG}}(\mathbf{r})},$$

$$\tau_{\mathrm{W}}(\mathbf{r})=\frac{1}{8}\frac{|\nabla\rho(\mathbf{r})|^2}{\rho(\mathbf{r})}$$

$$\tau^{\mathrm{HEG}}(\mathbf{r})=C_{\mathrm{TF}}\rho(\mathbf{r})^{5/3};\;C_{\mathrm{TF}}=\frac{3}{10}(3\pi^2)^{2/3}$$

$$\tau_s(\mathbf{x})=\sum_{i=1}^N\varepsilon_i|\phi_i(\mathbf{x})|^2-v_s(\mathbf{r})\rho(\mathbf{x})+\frac{1}{4}\nabla^2\rho(\mathbf{x}).$$



$$E_{\rm xc}^{\rm B3PW91} = E_{\rm xc}^{\rm VW5} + a_0 (E_{\rm x}^{\rm exact} - E_{\rm x}^{\rm VWN5}) + \\ a_x (E_{\rm x}^{\rm B88} - E_{\rm x}^{\rm VWN5}) + a_c (E_{\rm c}^{\rm PW91} - E_{\rm c}^{\rm VWN5}),$$

$$\varepsilon_{\rm HOMO} = -I_0 = E_0(N) - E_0(N-1).$$

$$\rho(r\rightarrow\infty)\sim\mathrm{e}^{-2\sqrt{2I_0}r}$$

$$\psi_k(r\rightarrow\infty)\sim\mathrm{e}^{-\sqrt{-2\epsilon_k}r}$$

$$F_{\rm L}[\rho] = \min_{\hat{\Gamma} \rightarrow \rho} {\rm Tr}\{\hat{\Gamma}(\hat{T} + \hat{W})\}$$

$$\hat{\Gamma} = \sum_K w_K |\Psi_K\rangle \langle \Psi_K|$$

$$\sum_K w_K = 1$$

$$\phi(\mathbf{r}) = \sqrt{\cos^2\left(\theta\right) \left|\sigma_g(\mathbf{r})\right|^2 + \sin^2\left(\theta\right) \left|\sigma_u(\mathbf{r})\right|^2}$$

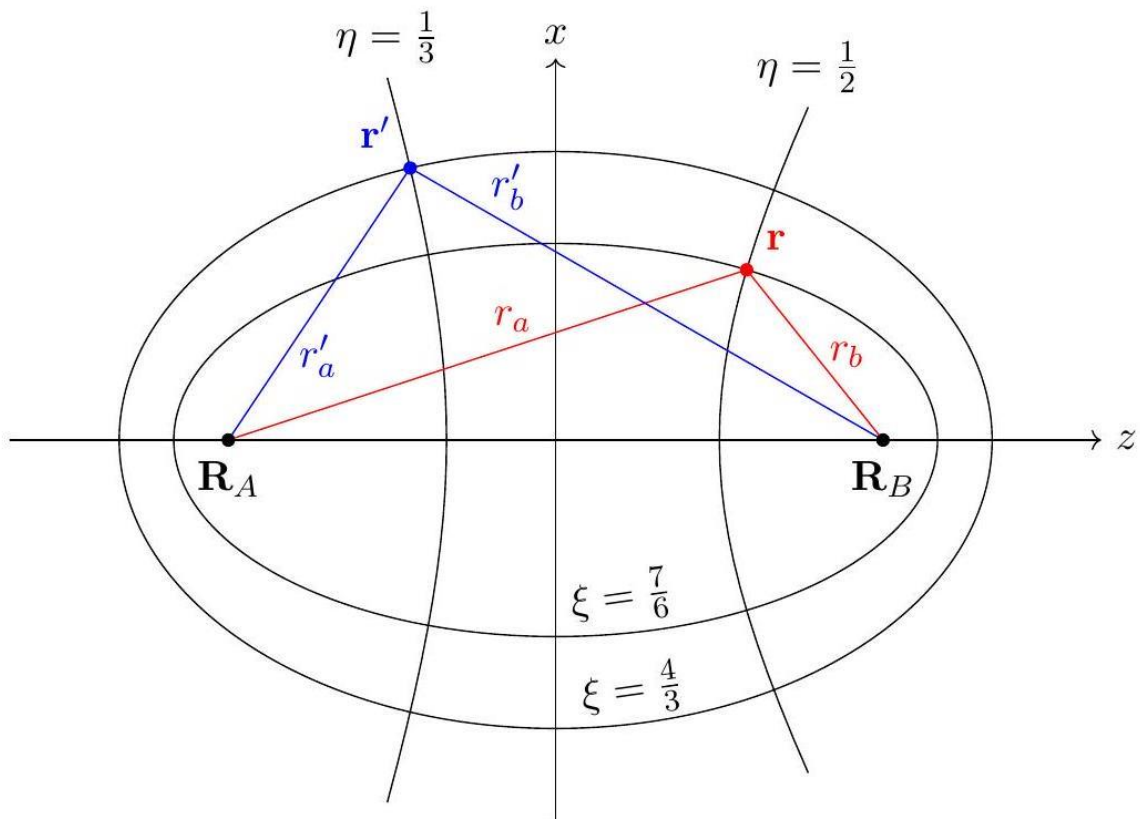
$$W_{\rm SCE}[\rho] = \min_{\hat{\Gamma} \rightarrow \rho} {\rm Tr}\{\hat{\Gamma} \hat{W}\}$$

$$F[\rho] \geq T_s[\rho] + W_{\rm SCE}[\rho]$$

$$N_e(x)=\int_{-\infty}^x\mathrm{d}y\rho(y)$$

$$\xi\!:=\!\frac{r_A+r_B}{R}\;\;\text{and}\;\;\eta\!:=\!\frac{r_B-r_A}{R}\,,$$

$$x=\frac{R}{2}\sqrt{(\xi^2-1)(1-\eta^2)}\;\;\text{and}\;\;z=\frac{R}{2}\xi\eta$$



$$\mathbf{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{R}{2} \begin{pmatrix} \sqrt{(\xi^2 - 1)(1 - \eta^2)} \cos(\phi) \\ \sqrt{(\xi^2 - 1)(1 - \eta^2)} \sin(\phi) \\ \xi\eta \end{pmatrix}.$$

$$\begin{aligned} (\mathbf{e}_\xi \quad \mathbf{e}_\eta \quad \mathbf{e}_\phi) &= \mathbf{J} = \begin{pmatrix} \frac{\partial \mathbf{r}}{\partial \xi} & \frac{\partial \mathbf{r}}{\partial \eta} & \frac{\partial \mathbf{r}}{\partial \phi} \end{pmatrix} \\ &= \frac{R}{2} \begin{pmatrix} \xi \sqrt{\frac{1 - \eta^2}{\xi^2 - 1}} \cos(\phi) & -\eta \sqrt{\frac{\xi^2 - 1}{1 - \eta^2}} \cos(\phi) & -\sqrt{(\xi^2 - 1)(1 - \eta^2)} \sin(\phi) \\ \xi \sqrt{\frac{1 - \eta^2}{\xi^2 - 1}} \sin(\phi) & -\eta \sqrt{\frac{\xi^2 - 1}{1 - \eta^2}} \sin(\phi) & \sqrt{(\xi^2 - 1)(1 - \eta^2)} \cos(\phi) \\ \eta & \xi & 0 \end{pmatrix} \end{aligned}$$

$$\lambda_\xi = |\mathbf{e}_\xi| = \frac{R}{2} \sqrt{\frac{\xi^2 - \eta^2}{\xi^2 - 1}}$$

$$\lambda_\eta = |\mathbf{e}_\eta| = \frac{R}{2} \sqrt{\frac{\xi^2 - \eta^2}{1 - \eta^2}}$$

$$\lambda_\phi = |\mathbf{e}_\phi| = \frac{R}{2} \sqrt{(\xi^2 - 1)(1 - \eta^2)}$$

$$d\mathbf{r} = \lambda_\xi \lambda_\eta \lambda_\phi d\xi d\eta d\phi = \frac{R^3}{8} (\xi^2 - \eta^2) d\xi d\eta d\phi$$

$$\begin{aligned}\nabla^2 &= \frac{1}{\lambda_\xi \lambda_\eta \lambda_\phi} \left(\frac{\partial}{\partial \xi} \frac{\lambda_\eta \lambda_\phi}{\lambda_\xi} \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} \frac{\lambda_\xi \lambda_\phi}{\lambda_\eta} \frac{\partial}{\partial \eta} + \frac{\partial}{\partial \phi} \frac{\lambda_\xi \lambda_\eta}{\lambda_\phi} \frac{\partial}{\partial \phi} \right) \\ &= \frac{4}{R^2(\xi^2 - \eta^2)} \left[\frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} + \right. \\ &\quad \left. \left(\frac{1}{\xi^2 - 1} + \frac{1}{1 - \eta^2} \right) \frac{\partial^2}{\partial \phi^2} \right]\end{aligned}$$

$$F\colon X\rightarrow K,$$

$$F_i[\boldsymbol{v}]=v_i.$$

$$\frac{\partial F_i[\boldsymbol{v}]}{\partial v_k}=\delta_{ik}.$$

$$F_{\alpha}[\boldsymbol{v}]=\sum_{i=1}^n v_i^{\alpha}$$

$$\frac{\partial F_{\alpha}[\boldsymbol{v}]}{\partial v_k}=\alpha v_k^{\alpha-1}.$$

$$\begin{aligned}\frac{\partial F_{\alpha}[\boldsymbol{v}]}{\partial v_k} &= \frac{\partial}{\partial v_k} \sum_{i=1}^n (F_i[\boldsymbol{v}])^{\alpha} = \sum_{i=1}^n \frac{\partial}{\partial v_k} (F_i[\boldsymbol{v}])^{\alpha} \\ &= \sum_{i=1}^n \alpha (F_i[\boldsymbol{v}])^{\alpha-1} \frac{\partial F_i[\boldsymbol{v}]}{\partial v_k} = \sum_{i=1}^n \alpha v_i^{\alpha-1} \delta_{ik} = \alpha v_k^{\alpha-1}\end{aligned}$$

$$F_{\mathbf{x}}[f]=f(\mathbf{x})$$

$$\frac{\delta F_{\mathbf{x}}[f]}{\delta f(\mathbf{x}')}=\delta(\mathbf{x}-\mathbf{x}')=\delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}$$

$$F_{\alpha}[f]=\int\,\mathrm{d}\mathbf{x}(f(\mathbf{x}))^{\alpha}$$

$$\frac{\delta F_{\alpha}[f]}{\delta f(\mathbf{y})}=\alpha (f(\mathbf{y}))^{\alpha-1}$$

$$\begin{aligned}\frac{\delta F_{\alpha}[f]}{\delta f(\mathbf{y})} &= \frac{\delta}{\delta f(\mathbf{y})} \int\,\mathrm{d}\mathbf{x}(F_{\mathbf{x}}[f])^{\alpha} = \int\,\mathrm{d}\mathbf{x} \frac{\delta}{\delta f(\mathbf{y})} (F_{\mathbf{x}}[f])^{\alpha} \\ &= \int\,\mathrm{d}\mathbf{x} \alpha (F_{\mathbf{x}}[f])^{\alpha-1} \frac{\delta F_{\mathbf{x}}[f]}{\delta f(\mathbf{y})} \\ &= \int\,\mathrm{d}\mathbf{x} \alpha (f(x))^{\alpha-1} \delta(\mathbf{x}-\mathbf{y}) = \alpha (f(\mathbf{y}))^{\alpha-1}\end{aligned}$$

$$D_hF[f]=\lim_{\epsilon\rightarrow 0}\frac{F[f+\epsilon h]-F[f]}{\epsilon}=\frac{\mathrm{d}F[f+\epsilon h]}{\mathrm{d}\epsilon}\Big|_{\epsilon=0}$$

$$\begin{aligned}
D_h F_\alpha[f] &= \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \int d\mathbf{x} [(f(\mathbf{x}) + \epsilon h(\mathbf{x}))^\alpha - (f(\mathbf{x}))^\alpha] \\
&= \lim_{\epsilon \rightarrow 0} \int d\mathbf{x} \alpha (f(\mathbf{x}))^{\alpha-1} h(\mathbf{x}) + \mathcal{O}(\epsilon) \\
&= \int d\mathbf{x} \underbrace{\alpha (f(\mathbf{x}))^{\alpha-1}}_{=\frac{\delta F_\alpha}{\delta f}} h(\mathbf{x})
\end{aligned}$$

$$L[f] = \int d\mathbf{x} \mathcal{L}(f(\mathbf{x}), \nabla f(\mathbf{x}))$$

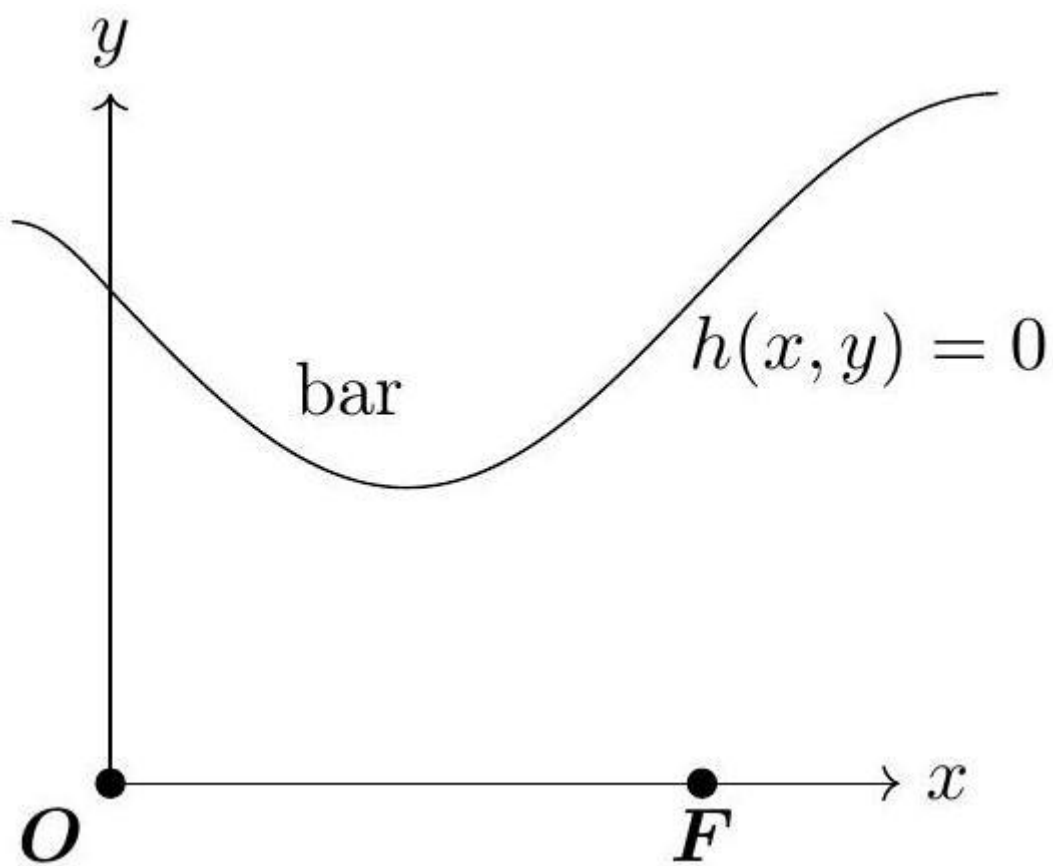
$$\begin{aligned}
D_h L[f] &= \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \int d\mathbf{x} [\mathcal{L}(f(\mathbf{x}) + \epsilon h(\mathbf{x}), \nabla(f(\mathbf{x}) + \epsilon h(\mathbf{x}))) - \mathcal{L}(f(\mathbf{x}), \nabla f(\mathbf{x}))] \\
&= \lim_{\epsilon \rightarrow 0} \int d\mathbf{x} \left[\frac{\partial \mathcal{L}}{\partial f}(\mathbf{x}) h(\mathbf{x}) + \frac{\partial \mathcal{L}}{\partial \nabla f}(\mathbf{x}) \cdot \nabla h(\mathbf{x}) + \mathcal{O}(\epsilon) \right] \\
&= \int d\mathbf{x} \left[\frac{\partial \mathcal{L}}{\partial f}(\mathbf{x}) - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla f}(\mathbf{x}) \right] h(\mathbf{x})
\end{aligned}$$

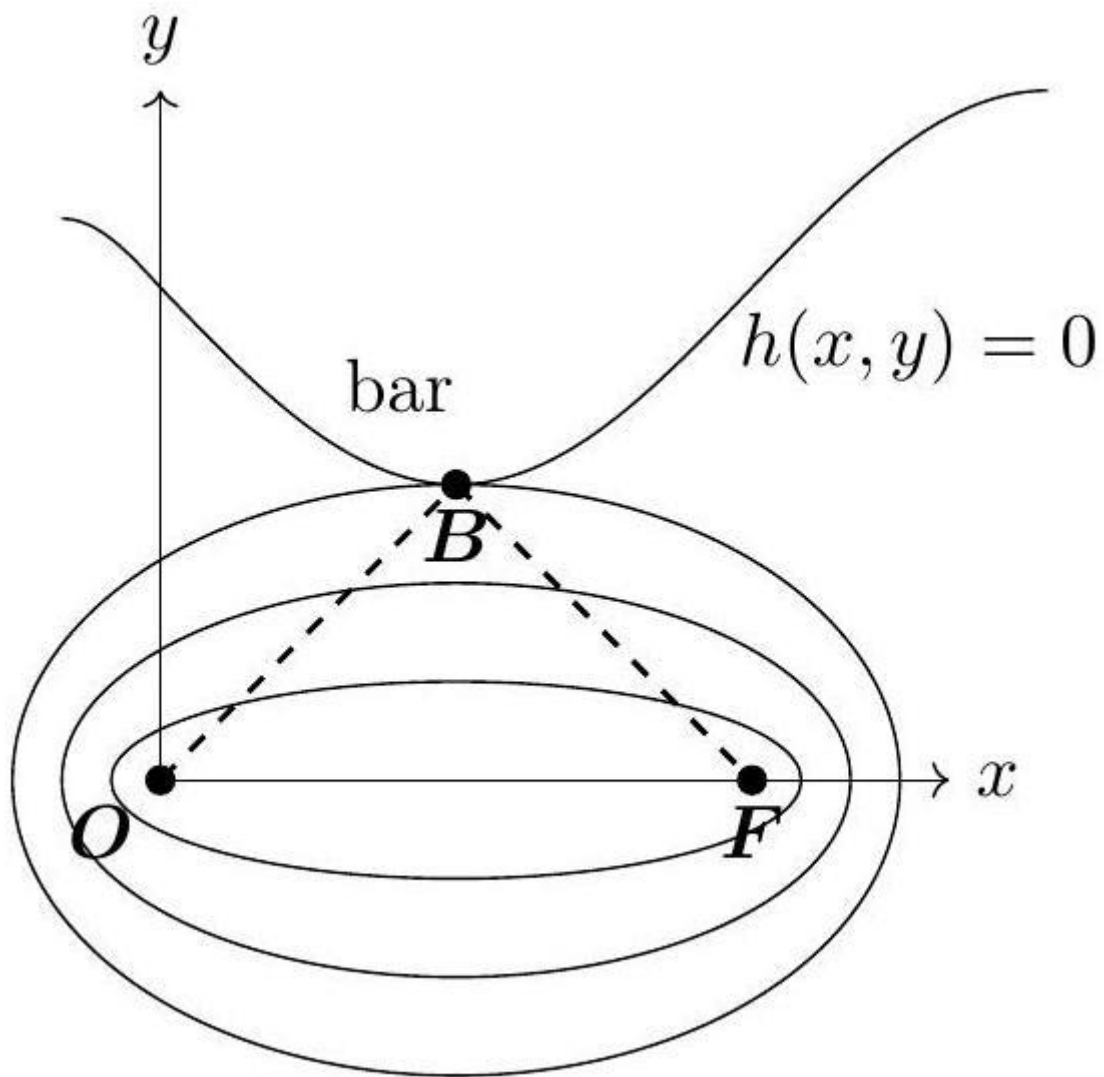
$$\frac{\partial \mathcal{L}}{\partial f}(\mathbf{x}) - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla f}(\mathbf{x})$$

$$\frac{\delta L}{\delta f(\mathbf{x})} = \frac{\partial \mathcal{L}}{\partial f}(\mathbf{x}) - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla f}(\mathbf{x}) = \frac{\partial L}{\partial f(\mathbf{x})} - \nabla \cdot \frac{\partial L}{\partial \nabla f(\mathbf{x})}$$

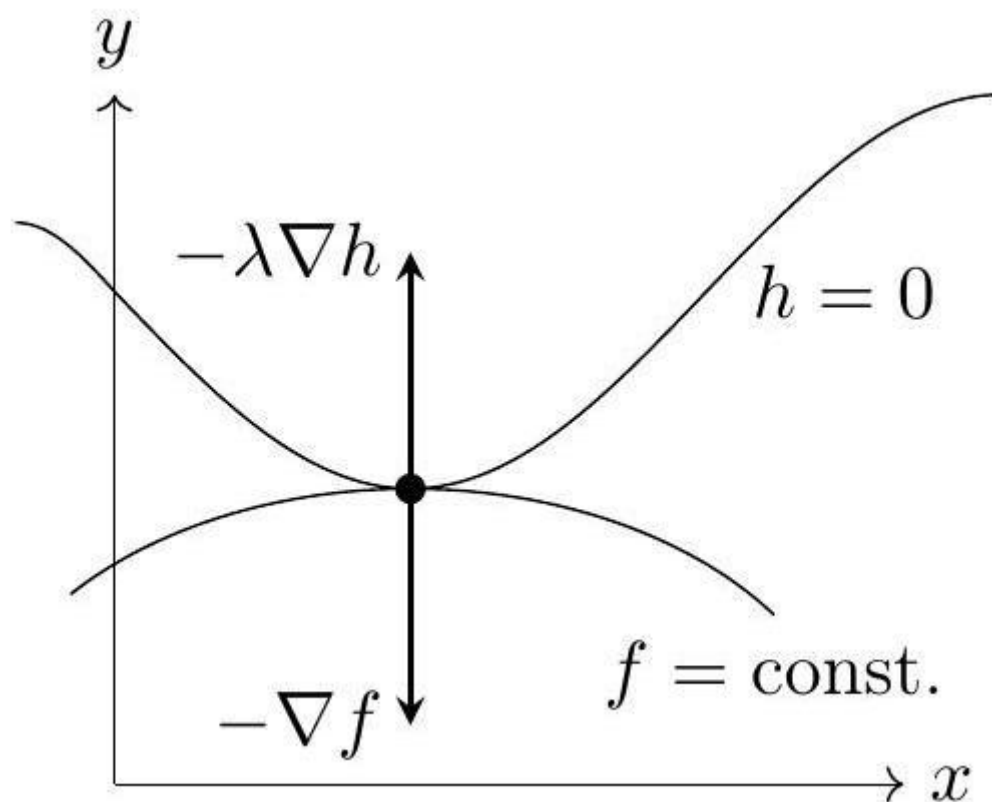
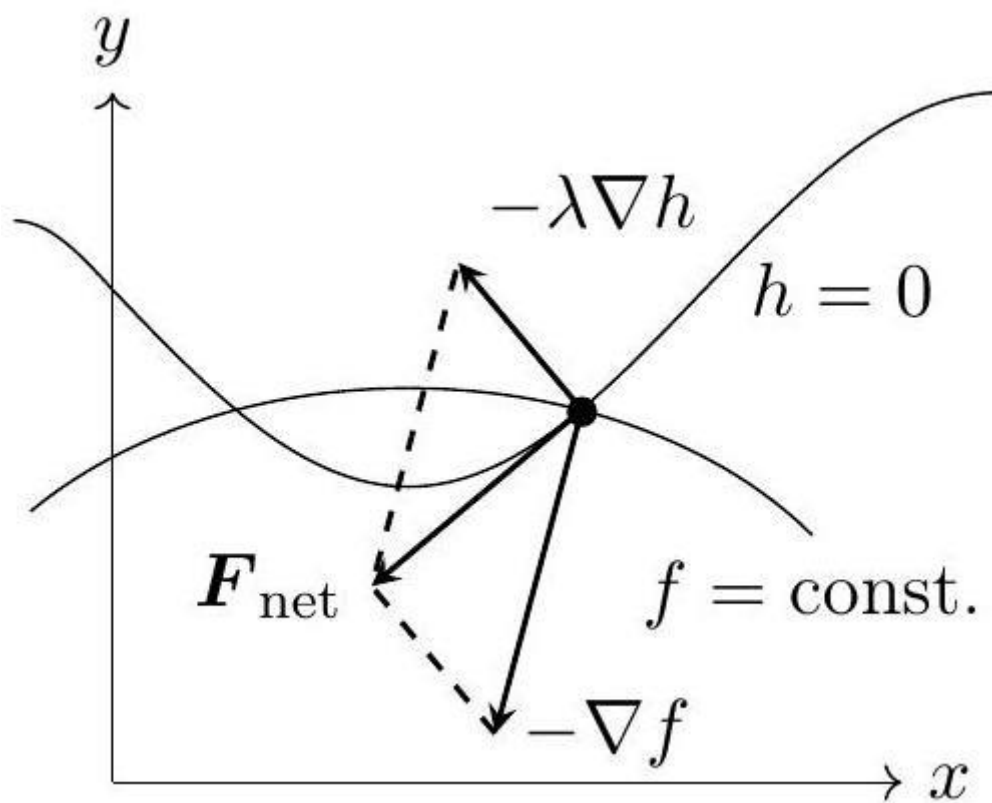
$$\begin{aligned}
&\min_{\mathbf{r} \in \mathbb{R}^N} f(\mathbf{r}) \\
&\text{subject to } h_j(\mathbf{r}) = 0 \text{ for } j = 1, \dots, l,
\end{aligned}$$

$$f = d_{OB} + d_{BF}.$$





$$\nabla f(\mathbf{P}) + \lambda \nabla h(\mathbf{P}) = 0.$$



$$L(\mathbf{r}, \boldsymbol{\lambda}) = f(\mathbf{r}) + \sum_{j=1}^l \lambda_j h_j(\mathbf{r})$$

$$\begin{aligned}\nabla f(\mathbf{r}) + \sum_{j=1}^l \lambda_j \nabla h_j(\mathbf{r}) &= \mathbf{0} \\ h_j(\mathbf{r}) &= 0 \text{ for } j = 1, \dots, l\end{aligned}$$

$$\begin{aligned}\min_{x,y \in \mathbb{R}} f(x,y) &= x^2 y \\ \text{subject to } x^2 + y^2 &= 3\end{aligned}$$

$$L(x, y, \lambda) = f(x, y) + \lambda h(x, y) = x^2 y + \lambda(x^2 + y^2 - 3).$$

$$\frac{\partial L}{\partial x} = 2xy + 2\lambda x = 0,$$

$$\frac{\partial L}{\partial y} = x^2 + 2\lambda y = 0,$$

$$\frac{\partial L}{\partial \lambda} = x^2 + y^2 - 3 = 0.$$

$$x^2 - 2y^2 = 0 \Rightarrow x^2 = 2y^2.$$

$$3y^2 = 3 \Rightarrow y = \pm 1.$$

$$h(x, y) = y - (\alpha x + h),$$

$$\nabla h(x, y) = (-\alpha, 1)^T$$

$$f(x, y) = d_{OB} + d_{BF} = \sqrt{x^2 + y^2} + \sqrt{(x - c)^2 + y^2}$$

$$\frac{\partial f}{\partial x} = \frac{2x}{2\sqrt{x^2 + y^2}} + \frac{2(x - c)}{2\sqrt{(x - c)^2 + y^2}} = \frac{x}{d_{OB}} + \frac{x - c}{d_{BF}},$$

$$\frac{\partial f}{\partial y} = \frac{2y}{2\sqrt{x^2 + y^2}} + \frac{2y}{2\sqrt{(x - c)^2 + y^2}} = \frac{y}{d_{OB}} + \frac{y}{d_{BF}}.$$

$$\frac{\partial L}{\partial x} = \frac{\partial f}{\partial x} + \lambda \frac{\partial g}{\partial x} = \frac{x}{d_{OP}} + \frac{x - c}{d_{PC}} - \alpha\lambda = 0,$$

$$\begin{aligned}\frac{\partial L}{\partial y} &= \frac{\partial f}{\partial y} + \lambda \frac{\partial g}{\partial y} = \frac{y}{d_{OP}} + \frac{y}{d_{PC}} + \lambda = 0, \\ \alpha x + h &= y.\end{aligned}$$

$$\begin{aligned}&\left(\frac{1}{d_{OP}} + \frac{1}{d_{PC}}\right)x - \frac{c}{d_{PC}} + \alpha\left(\frac{1}{d_{OP}} + \frac{1}{d_{PC}}\right)y = 0 \\ \Leftrightarrow &\left(\frac{1}{d_{OP}} + \frac{1}{d_{PC}}\right)(x + \alpha y) = \frac{c}{d_{PC}}\end{aligned}$$

$$\Leftrightarrow \left(\frac{d_{PC}}{d_{OP}} + 1\right)(x + \alpha y) = c$$

$$\Leftrightarrow \frac{d_{PC}}{d_{OP}} = \frac{c}{x + \alpha y} - 1$$

$$\Leftrightarrow \sqrt{\frac{(x - c)^2 + y^2}{x^2 + y^2}} = \frac{c - x - \alpha y}{x + \alpha y}.$$



$$\begin{aligned}\frac{(x-c)^2+y^2}{x^2+y^2} &= \frac{(x+\alpha y-c)^2}{(x+\alpha y)^2} \\ \Leftrightarrow & ((x-c)^2+y^2)(x+\alpha y)^2 = (x^2+y^2)(x+\alpha y-c)^2 \\ \Leftrightarrow & (x^2+y^2)(x+\alpha y)^2 + (c^2-2cx)(x+\alpha y)^2 \\ \Leftrightarrow & = (x^2+y^2)(x+\alpha y)^2 + (x^2+y^2)(c^2-2c(x+\alpha y)) \\ \Leftrightarrow & (c-2x)(x+\alpha y)^2 = (x^2+y^2)(c-2(x+\alpha y)).\end{aligned}$$

$$\begin{aligned}\text{l.h.} &= (c-2x)(x+\alpha(\alpha x+h))^2 \\ &= (c-2x)((1+\alpha^2)x+\alpha h)^2 \\ &= (c-2x)((1+\alpha^2)^2x^2+2\alpha h(1+\alpha^2)x+\alpha^2h^2) \\ &= -2(1+\alpha^2)^2x^3-4\alpha h(1+\alpha^2)x^2+c(1+\alpha^2)^2x^2- \\ &\quad 2\alpha^2h^2x+2\alpha ch(1+\alpha^2)x+\alpha^2ch^2, \\ \text{r.h.} &= (x^2+(\alpha x+h)^2)(c-2(x+\alpha(\alpha x+h))) \\ &= ((1+\alpha^2)x^2+2\alpha hx+h^2)(c-2\alpha h-2(1+\alpha^2)x) \\ &= -2(1+\alpha^2)^2x^3-4\alpha h(1+\alpha^2)x^2+(c-2\alpha h)(1+\alpha^2)x^2- \\ &\quad 2h^2(1+\alpha^2)x+2\alpha h(c-2\alpha)x+h^2(c-2\alpha h).\end{aligned}$$

$$\begin{aligned}0 &= \text{l.h.} - \text{r.h.} \\ &= [(1+\alpha^2)(c(1+\alpha^2)-(c-2\alpha h))]x^2 + [\alpha^2ch^2-h^2(c-2\alpha h)] + \\ &\quad 2[\alpha ch(1+\alpha^2)-\alpha^2h^2+h^2(1+\alpha^2)-\alpha h(c-2\alpha)]x \\ &= (1+\alpha^2)(c+\alpha^2c-c+2\alpha h)x^2 + [\alpha^2ch^2-ch^2+2\alpha h^3] \\ &\quad 2(\alpha ch+\alpha^3ch-\alpha^2h^2+h^2+\alpha^2h^2-\alpha ch+2\alpha^2h)x \\ &= \alpha(1+\alpha^2)(\alpha c+2h)x^2 + 2h(\alpha^3c+2\alpha^2h+h)x + h^2(\alpha^2c+2\alpha h-c).\end{aligned}$$

$$\begin{aligned}D &= h^2(\alpha^3c+2\alpha^2h+h)^2 + h^2(c-\alpha^2c-2\alpha h)\alpha(1+\alpha^2)(\alpha c+2h) \\ &= h^2[(\alpha^3c+2\alpha^2h+h)\{\alpha^3c+2\alpha^2h+h\} + \\ &\quad (\alpha c - (\alpha^3c+2\alpha^2h))(\{\alpha^3c+2\alpha^2h+h\} + h + \alpha c)] \\ &= h^2[h(\alpha^3c+2\alpha^2h+h) + \alpha c(\alpha^3c+2\alpha^2h+2h+\alpha c) - \\ &\quad (\alpha^3c+2\alpha^2h)(h+\alpha c)] \\ &= h^2(h^2+2\alpha ch+\alpha^2c^2) \\ &= h^2(\alpha c+h)^2\end{aligned}$$

$$x = \frac{-h(\alpha^3c+2\alpha h+h) + h(\alpha c+h)}{\alpha(1+\alpha^2)(\alpha c+2h)} = h \frac{c-2\alpha h-\alpha^2c}{(1+\alpha^2)(\alpha c+2h)}.$$

$$\begin{aligned}y &= h \left(\alpha \frac{c-2\alpha h-\alpha^2c}{(1+\alpha^2)(\alpha c+2h)} + 1 \right) \\ &= h \frac{\alpha c - 2\alpha^2h - \alpha^3c + \alpha c + 2h + \alpha^3c + 2\alpha^2h}{(1+\alpha^2)(\alpha c+2h)} \\ &= \frac{2h(\alpha c+h)}{(1+\alpha^2)(\alpha c+2h)}\end{aligned}$$

$$H^1(\mathbb{R}^3) := \left\{ f: \mathbb{R}^3 \rightarrow \mathbb{C}: \int \mathrm{d}\mathbf{r} (|f(\mathbf{r})|^2 + |\nabla f(\mathbf{r})|^2) < \infty \right\}$$

$$\int \mathrm{d}\mathbf{s} L[f(\mathbf{s}), \nabla f(\mathbf{s}), \nabla^2 f(\mathbf{s}), \dots]$$



$$\frac{\delta L_\rho}{\delta f(\mathbf{s})} = \frac{\partial L}{\partial f(\mathbf{s})} - \nabla \cdot \frac{\partial L}{\partial \nabla f(\mathbf{s})} + \nabla^2 \frac{\partial L}{\partial \nabla^2 f(\mathbf{s})} + \dots$$

$$\begin{aligned} H = & \sum_{pq} h_{pq} E_{pq} + \frac{1}{2} \sum_{pqrs} g_{pqrs} e_{pqrs} + h_{nuc} \\ & + \frac{1}{2} \sum_{pqrs} (\boldsymbol{\lambda} \cdot \mathbf{d})_{pq} (\boldsymbol{\lambda} \cdot \mathbf{d})_{rs} E_{pq} E_{rs} \\ & - \sqrt{\frac{\omega}{2}} \sum_{pq} (\boldsymbol{\lambda} \cdot \mathbf{d})_{pq} E_{pq} (b^\dagger + b) \\ & + \omega b^\dagger b \end{aligned}$$

$$|\text{GS}\rangle = U_X |S\rangle \otimes |0\rangle.$$

$$U_{\text{QED-HF}} = \exp \left(-\gamma (b - b^\dagger) \right)$$

$$U_{\text{SC}} = \exp \left(- \left(\sum_p \frac{\eta_p}{\omega} \tilde{E}_{pp} \right) (b - b^\dagger) \right)$$

$$(\mathbf{d} \cdot \boldsymbol{\lambda}) = \sum_p (\widetilde{\mathbf{d} \cdot \boldsymbol{\lambda}})_{pp} \tilde{E}_{pp}$$

$$\gamma = -\frac{\boldsymbol{\lambda} \cdot \langle \mathbf{d} \rangle_{\text{QED-HF}}}{\sqrt{2\omega}}$$

$$\begin{aligned} U_{\text{QED-HF}}^\dagger H U_{\text{QED-HF}} = & \sum_{pq} h_{pq} E_{pq} + \frac{1}{2} \sum_{pqrs} g_{pqrs} e_{pqrs} + h_{nuc} \\ & + \frac{1}{2} \sum_{pqrs} \left(\boldsymbol{\lambda} \cdot (\mathbf{d} - \langle \mathbf{d} \rangle_{\text{QED-HF}}) \right)_{pq} \left(\boldsymbol{\lambda} \cdot (\mathbf{d} - \langle \mathbf{d} \rangle_{\text{QED-HF}}) \right)_{rs} E_{pq} E_{rs} \\ & - \sqrt{\frac{\omega}{2}} \sum_{pq} \left(\boldsymbol{\lambda} \cdot (\mathbf{d} - \langle \mathbf{d} \rangle_{\text{QED-HF}}) \right)_{pq} E_{pq} (b + b^\dagger) + \omega b^\dagger b, \end{aligned}$$

$$F_{pq} = F_{pq}^e + \frac{1}{2} \left(\sum_a (\boldsymbol{\lambda} \cdot \mathbf{d}_{pa}) (\boldsymbol{\lambda} \cdot \mathbf{d}_{aq}) - \sum_i (\boldsymbol{\lambda} \cdot \mathbf{d}_{pi}) (\boldsymbol{\lambda} \cdot \mathbf{d}_{iq}) \right),$$

$$U_{\text{SC}}^\dagger \tilde{a}_p^\dagger U_{\text{SC}} = \tilde{a}_p^\dagger \exp \left(\frac{\eta_p}{\omega} (b - b^\dagger) \right)$$

$$\begin{aligned} H_{\text{SC}} = U_{\text{SC}}^\dagger H U_{\text{SC}} = & \sum_{pq} \tilde{h}_{pq} \tilde{E}_{pq} \exp \left(\frac{1}{\omega} (\eta_p - \eta_q) (b - b^\dagger) \right) \\ & + \frac{1}{2} \sum_{pqrs} \tilde{g}_{pqrs} \tilde{e}_{pqrs} \exp \left(\frac{1}{\omega} (\eta_p + \eta_r - \eta_q - \eta_s) (b - b^\dagger) \right) + h_{nuc} \\ & + \omega \left(b^\dagger - \sum_p \left(\frac{\lambda}{\sqrt{2\omega}} (\widetilde{\mathbf{d} \cdot \boldsymbol{\epsilon}})_{pp} - \frac{\eta_p}{\omega} \right) \tilde{E}_{pp} \right) \left(b - \sum_p \left(\frac{\lambda}{\sqrt{2\omega}} (\widetilde{\mathbf{d} \cdot \boldsymbol{\epsilon}})_{pp} - \frac{\eta_p}{\omega} \right) \tilde{E}_{pp} \right). \end{aligned}$$

$$H_{\infty} = \omega b^{\dagger} b - \lambda \sqrt{\frac{\omega}{2}} (\mathbf{d} \cdot \boldsymbol{\epsilon}) (b^{\dagger} + b) + \frac{\lambda^2}{2} (\mathbf{d} \cdot \boldsymbol{\epsilon})^2.$$

$$\eta_p = \sqrt{\frac{\omega}{2}} (\widetilde{\mathbf{d} \cdot \boldsymbol{\lambda}})_{pp}$$

$$\begin{aligned} |R(t)\rangle &= \exp(-i\Lambda(t))|S,0\rangle \\ &= \exp(-i\boldsymbol{\kappa}(t))\exp\left(-i(\gamma(t)b^{\dagger} + \gamma^*(t)b)\right)|R\rangle \end{aligned}$$

$$|R\rangle = |S\rangle \otimes |0\rangle$$

$$\boldsymbol{\kappa}(t) = \frac{1}{\sqrt{2}} \sum_{ai} (\kappa_{ai} E_{ai} + \kappa_{ai}^* E_{ia})$$

$$H_X = U_X^\dagger H U_X,$$

$$\begin{aligned} \Lambda(t) &= \Lambda^{(1)}(t) + \Lambda^{(2)}(t) + \cdots \\ &= \int \mathrm{d}\omega_1 e^{-i\omega_1 t} \Lambda^{\omega_1} + \frac{1}{2} \int \mathrm{d}\omega_1 \mathrm{d}\omega_2 e^{-i\omega_1 t} e^{-i\omega_2 t} \Lambda^{\omega_1, \omega_2} + \cdots \end{aligned}$$

$$\begin{aligned} \Lambda^{\omega_1} &= \frac{1}{\sqrt{2}} \sum_{ai} (\kappa_{ai}^{\omega_1} E_{ai} + [\kappa_{ai}^{-\omega_1}]^* E_{ia}) + (\gamma^{\omega_1} b^{\dagger} + [\gamma^{-\omega_1}]^* b) \\ \Lambda^{\omega_1, \omega_2} &= \frac{1}{\sqrt{2}} \sum_{ai} (\kappa_{ai}^{\omega_1, \omega_2} E_{ai} + [\kappa_{ai}^{-\omega_1, -\omega_2}]^* E_{ia}) + (\gamma^{\omega_1, \omega_2} b^{\dagger} + [\gamma^{-\omega_1, -\omega_2}]^* b). \end{aligned}$$

$$\begin{aligned} \langle A \rangle(t) &= \langle A \rangle_{\rm R} + \int \mathrm{d}\omega_1 e^{-i\omega_1 t} \langle \langle A; V^{\omega_1} \rangle \rangle_{\omega_1} \\ &\quad + \frac{1}{2} \int \mathrm{d}\omega_1 \mathrm{d}\omega_2 e^{-i\omega_1 t} e^{-i\omega_2 t} \langle \langle A; V^{\omega_1}, V^{\omega_2} \rangle \rangle_{\omega_1, \omega_2} + \cdots \end{aligned}$$

$$\left[\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{B}^* & \boldsymbol{A}^* \end{pmatrix} - \omega_1 \begin{pmatrix} \boldsymbol{1} & \boldsymbol{0} \\ \boldsymbol{0} & -\boldsymbol{1} \end{pmatrix} \right] \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} = i \begin{pmatrix} \boldsymbol{g}_1 \\ \boldsymbol{g}_2 \end{pmatrix} \equiv i \boldsymbol{g}$$

$$\boldsymbol{X} = \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \end{pmatrix} \boldsymbol{Y} = \begin{pmatrix} [\gamma^{-\omega_1}]^* \\ [\kappa_{ai}^{-\omega_1}]^* \end{pmatrix}$$

$$\boldsymbol{g}_1 = \begin{pmatrix} \langle [b, V_X^{\omega_1}] \rangle_{\rm R} \\ \frac{1}{\sqrt{2}} \langle [E_{ia}, V_X^{\omega_1}] \rangle_{\rm R} \end{pmatrix} \boldsymbol{g}_2 = \begin{pmatrix} \langle [b^{\dagger}, V_X^{\omega_1}] \rangle_{\rm R} \\ \frac{1}{\sqrt{2}} \langle [E_{ai}, V_X^{\omega_1}] \rangle_{\rm R} \end{pmatrix},$$

$$\begin{aligned} \boldsymbol{A} &= \begin{pmatrix} \left\langle [b, [H_X, b^{\dagger}]] \right\rangle_{\rm R} & \frac{1}{\sqrt{2}} \left\langle [b, [H_X, E_{ai}]] \right\rangle_{\rm R} \\ \frac{1}{\sqrt{2}} \left\langle [b^{\dagger}, [H_X, E_{ia}]] \right\rangle_{\rm R} & \frac{1}{2} \left\langle [E_{jb}, [H_X, E_{ai}]] \right\rangle_{\rm R} \end{pmatrix} \\ \boldsymbol{B} &= \begin{pmatrix} \left\langle [b, [H_X, b]] \right\rangle_{\rm R} & \frac{1}{\sqrt{2}} \left\langle [b, [H_X, E_{ia}]] \right\rangle_{\rm R} \\ \frac{1}{\sqrt{2}} \left\langle [b^{\dagger}, [H_X, E_{ai}]] \right\rangle_{\rm R} & \frac{1}{2} \left\langle [E_{bj}, [H_X, E_{ai}]] \right\rangle_{\rm R} \end{pmatrix}. \end{aligned}$$

$$\omega_1 \langle \langle A; V^{\omega_1} \rangle \rangle_{\omega_1} = \langle \langle [A, H]; V^{\omega_1} \rangle \rangle_{\omega_1} + \langle 0 | [A, V^{\omega_1}] | 0 \rangle.$$

$$i\boldsymbol{p}_i = [\boldsymbol{r}_i, H]$$

$$\omega_n \langle 0 | \boldsymbol{r}_i | n \rangle = i \langle 0 | \boldsymbol{p}_i | n \rangle,$$

$$q=\frac{1}{\sqrt{2\omega}}(b+b^\dagger)$$

$$p=i\sqrt{\frac{\omega}{2}}(b^\dagger-b)$$

$$ip=[q,H]$$

$$\omega_n \langle 0 | q | n \rangle = i \langle 0 | p | n \rangle$$

$$\omega_1 \langle \langle b; V^{\omega_1} \rangle \rangle_{\omega_1} = \left\langle \left\langle -\sqrt{\frac{\omega}{2}} \boldsymbol{d} \cdot \boldsymbol{\lambda} - \omega b; V^{\omega_1} \right\rangle \right\rangle_{\omega_1} + \langle 0 | [b, V^{\omega_1}] | 0 \rangle$$

$$\omega_1 \langle \langle b^\dagger; V^{\omega_1} \rangle \rangle_{\omega_1} = \left\langle \left\langle \sqrt{\frac{\omega}{2}} \boldsymbol{d} \cdot \boldsymbol{\lambda} + \omega b^\dagger; V^{\omega_1} \right\rangle \right\rangle_{\omega_1} + \langle 0 | [b^\dagger, V^{\omega_1}] | 0 \rangle$$

$$\omega_n \langle 0 | q | n \rangle = i \langle 0 | p | n \rangle = \langle 0 | \boldsymbol{d} \cdot \boldsymbol{\lambda} | n \rangle \frac{\omega_n \omega}{\omega_n^2 - \omega^2}$$

$$U_{\rm SC}^\dagger \tilde{E}_{pq} U_{\rm SC} = \tilde{E}_{pq} \exp\left(\frac{\omega_p - \omega_q}{\omega} (b - b^\dagger)\right)$$

$$U_{\rm SC}^\dagger b U_{\rm SC} = b + \sum_p \frac{\eta_p}{\omega} \tilde{E}_{pp}$$

$$\vartheta_n=\gamma_n^2$$

$$q=\frac{1}{\sqrt{2\omega}}(b+b^\dagger)$$

$$\langle n | b^\dagger b | n \rangle = \sqrt{\frac{\omega}{2}} (b - b^\dagger)$$

$$\langle n | p | n \rangle = |\langle R | p | n \rangle|^2,$$

$$f_l=\frac{2}{3}\omega_{LP}|\langle\text{GS}|\boldsymbol{d}|\text{LP}\rangle|^2\quad f_v=\frac{2}{3}\frac{1}{\omega_{LP}}|\langle\text{GS}|\boldsymbol{p}|\text{LP}\rangle|^2$$

$$f_l=\frac{2}{3}\omega_{LP}|\langle\text{GS}|\boldsymbol{d}|\text{LP}\rangle|^2$$

$$f_v = \frac{2}{3} \frac{1}{\omega_{LP}} |\langle \text{GS} | \mathbf{p} | \text{LP} \rangle|^2$$

$$q = \frac{1}{\sqrt{2}\omega}(b+b^\dagger)$$

$$ip = \sqrt{\frac{\omega}{2}}(b-b^\dagger)$$

$$\langle 0 | \mathbf{d} \cdot \boldsymbol{\lambda} | n \rangle = \frac{\omega_n^2 - \omega^2}{\omega} \langle 0 | q | n \rangle = i \frac{\omega_n^2 - \omega^2}{\omega_n \omega} \langle 0 | p | n \rangle,$$

$$\omega_n \langle 0 | q | n \rangle = i \langle 0 | p | n \rangle$$

$$\omega_n \langle 0 | \mathbf{r}_i | n \rangle = i \langle 0 | \mathbf{p}_i | n \rangle$$

$$\omega_1 \langle \langle A; V^{\omega_1} \rangle \rangle_{\omega_1} = \langle \langle [A, H]; V^{\omega_1} \rangle \rangle_{\omega_1} + \langle 0 | [A, V^{\omega_1}] | 0 \rangle$$

$$iP=[Q,H]$$

$$\langle \langle P; V^{\omega_1} \rangle \rangle_{\omega_1} = -i\omega_1 \langle \langle Q; V^{\omega_1} \rangle \rangle_{\omega_1} + i \langle 0 | [A, V^{\omega_1}] | 0 \rangle.$$

$$\begin{aligned} \langle \langle P, V \rangle \rangle_{\omega_1 + i\epsilon} = & \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [[Q_X, H_X], E_{ai}] \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [[Q_X, H_X], E_{ia}] \rangle_R \\ & + \gamma^{\omega_1} \left\langle [[Q_X, H_X], b^\dagger] \right\rangle_R + \gamma^{-\omega_1} \langle [[Q_X, H_X], b] \rangle_R \end{aligned}$$

$$Q_X=U_X^\dagger Q U_X$$

$$|R\rangle = |\text{HF}\rangle \otimes |0\rangle.$$

$$\boldsymbol{d}_X=U_X^\dagger \boldsymbol{d} U_X=\boldsymbol{d} \, p_X=U_X^\dagger p U_X=p$$

$$q_X=U_X^\dagger q U_X=\frac{b+b^\dagger}{\sqrt{2}\omega}+\frac{2}{\omega}\frac{1}{\sqrt{2}\omega}\sum_p\eta_p\tilde{E}_{pp}$$

$$Q=\frac{1}{\sqrt{2}}\sum_{ai}\left(Q_{ai}E_{ai}+Q_{ai}^*E_{ia}\right)+\delta Q$$

$$\delta Q = \frac{1}{\sqrt{2}} \sum_{ab} Q_{ab} E_{ab} + \frac{1}{\sqrt{2}} \sum_{ij} Q_{ij} E_{ij}$$

$$\begin{aligned}
\langle\langle P, V \rangle\rangle_{\omega_1+i\epsilon} &= \frac{1}{2} \sum_{aibj} \kappa_{ai}^{\omega_1} \left\langle \left[[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], E_{ai} \right] \right\rangle_R + \frac{1}{2} \sum_{aibj} \kappa_{ia}^{-\omega_1} \left\langle \left[[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], E_{ia} \right] \right\rangle_R \\
&+ \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [\delta Q, H_X], E_{ai} \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [\delta Q, H_X], E_{ia} \rangle_R \\
&+ \frac{1}{\sqrt{2}} \sum_{abj} \gamma_\alpha^{\omega_1} \left\langle \left[[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], b_\alpha^\dagger \right] \right\rangle_R + \frac{1}{\sqrt{2}} \sum_{abj} \gamma_\alpha^{-\omega_1} \left\langle \left[[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], b_\alpha \right] \right\rangle_R \\
&+ \sum_\alpha \gamma_\alpha^{\omega_1} \langle [\delta Q, H_X], b_\alpha^\dagger \rangle_R + \sum_\alpha \gamma_\alpha^{-\omega_1} \langle [\delta Q, H_X], b_\alpha \rangle_R \\
&= \begin{pmatrix} 0 & Q_{ai}^* & 0 \\ & Q_{ai} \end{pmatrix} \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \\
&+ \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [\delta Q, H_X], E_{ai} \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [\delta Q, H_X], E_{ia} \rangle_R \\
&+ \sum_\alpha \gamma_\alpha^{\omega_1} \langle [\delta Q, H_X], b_\alpha^\dagger \rangle_R + \sum_\alpha \gamma_\alpha^{-\omega_1} \langle [\delta Q, H_X], b_\alpha \rangle_R \\
&= \begin{pmatrix} 0 & Q_{ai}^* & 0 & Q_{ai} \end{pmatrix} \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \\
&- \sum_{ai} \kappa_{ai}^{\omega_1} \langle [E_{ai}, \delta Q], H_X \rangle_R - \sum_{ai} \kappa_{ai}^{-\omega_1} \langle [H_X, E_{ai}], \delta Q \rangle_R \\
&- \sum_{ai} \kappa_{ia}^{\omega_1} \langle [E_{ia}, \delta Q], H_X \rangle_R - \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [H_X, E_{ia}], \delta Q \rangle_R \\
&- \sum_\alpha \gamma_\alpha^{\omega_1} \langle [b_\alpha^\dagger, \delta Q], H_X \rangle_R - \sum_\alpha \gamma_\alpha^{-\omega_1} \langle [H_X, b_\alpha], \delta Q \rangle_R \\
&- \sum_\alpha \gamma_\alpha^{\omega_1} \langle [b_\alpha^\dagger, \delta Q], H_X \rangle_R - \sum_\alpha \gamma_\alpha^{-\omega_1} \langle [H_X, b_\alpha], \delta Q \rangle_R
\end{aligned}$$

$$\begin{aligned}
\langle\langle P, V \rangle\rangle_{\omega_1+i\epsilon} &= \frac{1}{2} \sum_{aibj} \kappa_{ai}^{\omega_1} \langle [[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], E_{ai}] \rangle_R + \frac{1}{2} \sum_{aibj} \kappa_{ia}^{-\omega_1} \langle [[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], E_{ia}] \rangle_R \\
&+ \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [[\delta Q, H_X], E_{ai}] \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [[\delta Q, H_X], E_{ia}] \rangle_R \\
&+ \frac{1}{\sqrt{2}} \sum_{\alpha bj} \gamma_{\alpha}^{\omega_1} \langle [[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], b_{\alpha}^{\dagger}] \rangle_R + \frac{1}{\sqrt{2}} \sum_{\alpha bj} \gamma_{\alpha}^{-\omega_1} \langle [[Q_{bj}E_{bj} + Q_{bj}^*E_{jb}, H_X], b_{\alpha}] \rangle_R \\
&+ \sum_{\alpha} \gamma_{\alpha}^{\omega_1} \langle [[\delta Q, H_X], b_{\alpha}^{\dagger}] \rangle_R + \sum_{\alpha} \gamma_{\alpha}^{-\omega_1} \langle [[\delta Q, H_X], b_{\alpha}] \rangle_R \\
&= \begin{pmatrix} 0 & Q_{ai}^* & 0 & Q_{ai} \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \\
&+ \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [[\delta Q, H_X], E_{ai}] \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [[\delta Q, H_X], E_{ia}] \rangle_R \\
&+ \sum_{\alpha} \gamma_{\alpha}^{\omega_1} \langle [[\delta Q, H_X], b_{\alpha}^{\dagger}] \rangle_R + \sum_{\alpha} \gamma_{\alpha}^{-\omega_1} \langle [[\delta Q, H_X], b_{\alpha}] \rangle_R \\
&= \begin{pmatrix} 0 & Q_{ai}^* & 0 & Q_{ai} \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \\
&- \sum_{ai} \kappa_{ai}^{\omega_1} \langle [[E_{ai}, \delta Q], H_X] \rangle_R - \sum_{ai} \kappa_{ai}^{-\omega_1} \langle [[H_X, E_{ai}], \delta Q] \rangle_R \\
&- \sum_{ai} \kappa_{ia}^{\omega_1} \langle [[E_{ia}, \delta Q], H_X] \rangle_R - \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [[H_X, E_{ia}], \delta Q] \rangle_R \\
&- \sum_{\alpha} \gamma_{\alpha}^{\omega_1} \langle [[b_{\alpha}^{\dagger}, \delta Q], H_X] \rangle_R - \sum_{\alpha} \gamma_{\alpha}^{-\omega_1} \langle [[H_X, b_{\alpha}], \delta Q] \rangle_R \\
&- \sum_{\alpha} \gamma_{\alpha}^{\omega_1} \langle [[b_{\alpha}^{\dagger}, \delta Q], H_X] \rangle_R - \sum_{\alpha} \gamma_{\alpha}^{-\omega_1} \langle [[H_X, b_{\alpha}], \delta Q] \rangle_R.
\end{aligned}$$

$$\begin{aligned}
[E_{lm}, E_{ai}] &= E_{li}\delta_{am} - E_{am}\delta_{il} \\
[E_{cd}, E_{ia}] &= E_{ca}\delta_{di} - E_{id}\delta_{ac}
\end{aligned}$$

$$\begin{aligned}
&= (0 \quad O_{ai}^* \quad 0 \quad O_{ai}) \left[i \begin{pmatrix} \langle [b, V^{\omega_1}] \rangle_R \\ \frac{1}{\sqrt{2}} \langle [E_{ja}, V^{\omega_1}] \rangle_R \\ \langle [b^\dagger, V^{\omega_1}] \rangle_R \\ \frac{1}{\sqrt{2}} \langle [E_{aj}, V^{\omega_1}] \rangle_R \end{pmatrix} + \omega_1 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \right] \\
&= i \langle [O, V^{\omega_1}] \rangle_R + \omega_1 (O_{ia} \kappa_{ai}^{\omega_1} - O_{ai} \kappa_{ia}^{-\omega_1}) \\
&= i \langle [O, V^{\omega_1}] \rangle_R + \omega_1 \frac{1}{\sqrt{2}} (\langle [O, E_{ai}] \rangle_R \kappa_{ai}^{\omega_1} + \langle [O, E_{ia}] \rangle_R \kappa_{ia}^{-\omega_1})
\end{aligned}$$

$$\begin{aligned}
&= \begin{pmatrix} 0 & O_{ai}^* & 0 & O_{ai} \end{pmatrix} \left[i \begin{pmatrix} \langle [b, V^{\omega_1}] \rangle_R \\ \frac{1}{\sqrt{2}} \langle [E_{ja}, V^{\omega_1}] \rangle_R \\ \langle [b^\dagger, V^{\omega_1}] \rangle_R \\ \frac{1}{\sqrt{2}} \langle [E_{aj}, V^{\omega_1}] \rangle_R \end{pmatrix} + \omega_1 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \right] \\
&= i \langle [O, V^{\omega_1}] \rangle_R + \omega_1 (O_{ia} \kappa_{ai}^{\omega_1} - O_{ai} \kappa_{ia}^{-\omega_1}) \\
&= i \langle [O, V^{\omega_1}] \rangle_R + \omega_1 \frac{1}{\sqrt{2}} \left(\langle [O, E_{ai}] \rangle_R \kappa_{ai}^{\omega_1} + \langle [O, E_{ia}] \rangle_R \kappa_{ia}^{-\omega_1} \right),
\end{aligned}$$

$$\omega_n \langle 0 | \mathbf{r}_i | n \rangle = i \langle 0 | \mathbf{p}_i | n \rangle.$$

$$\omega_n \langle 0 | q | n \rangle = i \langle 0 | p | n \rangle.$$

$$Q_X = \frac{1}{\sqrt{2}} \sum_{ai} (Q_{ai} E_{ai} + Q_{ai}^* E_{ia}) + \delta Q + \frac{b + b^\dagger}{\sqrt{2\omega}}$$



$$\begin{aligned}
\langle\langle P, V \rangle\rangle_{\omega_1+i\epsilon} &= \frac{1}{2} \sum_{aibj} \kappa_{ai}^{\omega_1} \left\langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], E_{ai} \right] \right\rangle_R \\
&\quad + \frac{1}{2} \sum_{aibj} \kappa_{ia}^{-\omega_1} \left\langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], E_{ia} \right] \right\rangle_R \\
&\quad + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [\delta Q, H_X], E_{ai} \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [\delta Q, H_X], E_{ia} \rangle_R \\
&\quad + \frac{1}{\sqrt{2}} \sum_{\alpha bj} \gamma_\alpha^{\omega_1} \left\langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], b_\alpha^\dagger \right] \right\rangle_R \\
&\quad + \frac{1}{\sqrt{2}} \sum_{\alpha bj} \gamma_\alpha^{-\omega_1} \left\langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], b_\alpha \right] \right\rangle_R \\
&\quad + \sum_\alpha \gamma_\alpha^{\omega_1} \langle [\delta Q, H_X], b_\alpha^\dagger \rangle_R + \sum_\alpha \gamma_\alpha^{-\omega_1} \langle [\delta Q, H_X], b_\alpha \rangle_R \\
&= \left(\frac{1}{\sqrt{2\omega}} Q_{ai}^* \frac{1}{\sqrt{2\omega}} Q_{ai} \right) \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \\
&\quad + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [\delta Q, H_X], E_{ai} \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [\delta Q, H_X], E_{ia} \rangle_R \\
&\quad + \sum_\alpha \gamma_\alpha^{\omega_1} \langle [\delta Q, H_X], b_\alpha^\dagger \rangle_R + \sum_\alpha \gamma_\alpha^{-\omega_1} \langle [\delta Q, H_X], b_\alpha \rangle_R.
\end{aligned}$$

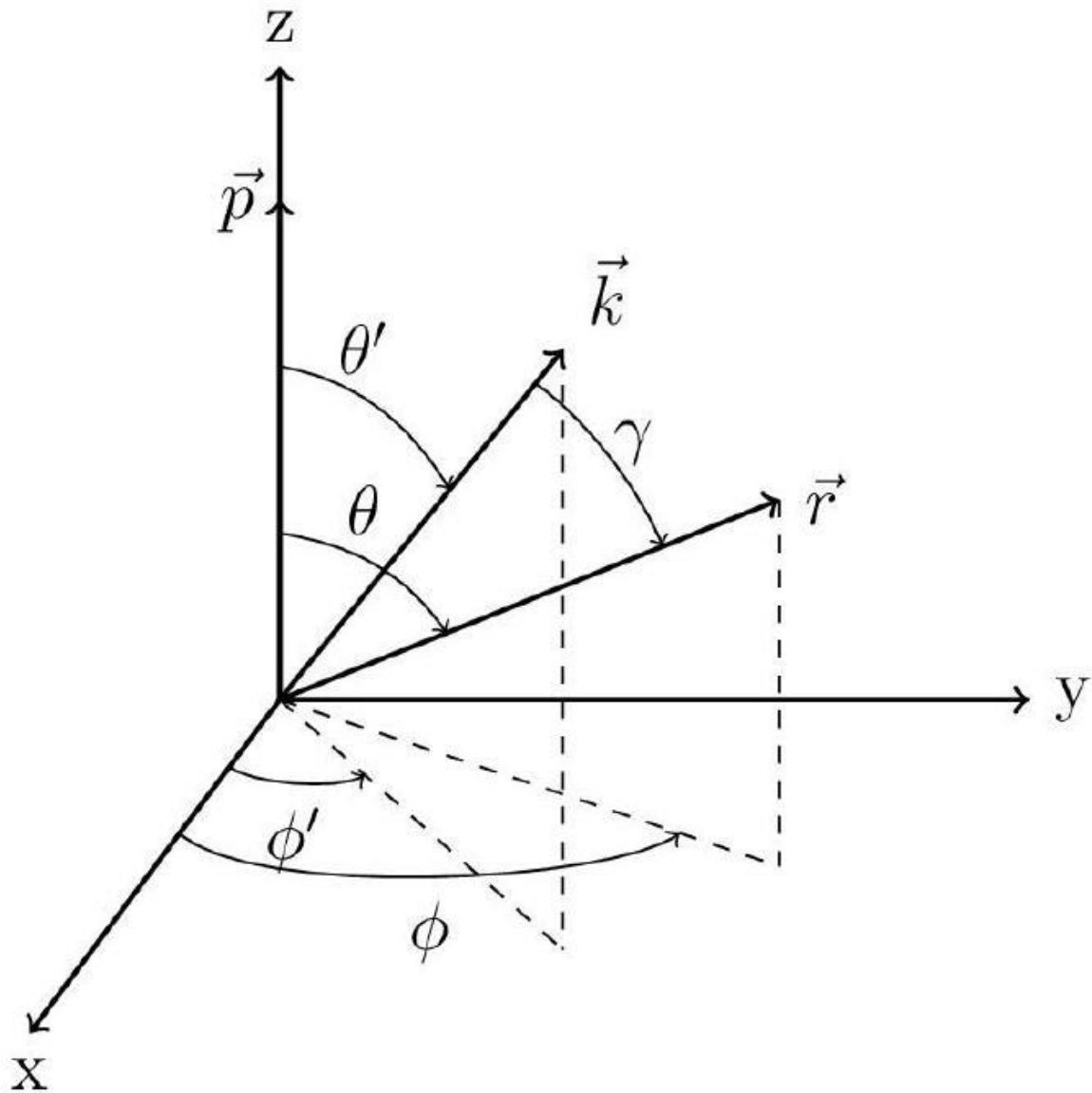
$$\begin{aligned}
\langle\langle P, V \rangle\rangle_{\omega_1+i\epsilon} &= \frac{1}{2} \sum_{aibj} \kappa_{ai}^{\omega_1} \langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], E_{ai} \right] \rangle_R \\
&\quad + \frac{1}{2} \sum_{aibj} \kappa_{ia}^{-\omega_1} \langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], E_{ia} \right] \rangle_R \\
&\quad + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [\delta Q, H_X], E_{ai} \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [\delta Q, H_X], E_{ia} \rangle_R \\
&\quad + \frac{1}{\sqrt{2}} \sum_{\alpha bj} \gamma_\alpha^{\omega_1} \langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], b_\alpha^\dagger \right] \rangle_R \\
&\quad + \frac{1}{\sqrt{2}} \sum_{\alpha bj} \gamma_\alpha^{-\omega_1} \langle \left[\left[Q_{bj} E_{bj} + Q_{bj}^* E_{jb} + \frac{b+b^\dagger}{\sqrt{\omega}}, H_X \right], b_\alpha \right] \rangle_R \\
&\quad + \sum_\alpha \gamma_\alpha^{\omega_1} \langle [\delta Q, H_X], b_\alpha^\dagger \rangle_R + \sum_\alpha \gamma_\alpha^{-\omega_1} \langle [\delta Q, H_X], b_\alpha \rangle_R
\end{aligned}$$

$$\begin{aligned}
&= \begin{pmatrix} \frac{1}{\sqrt{2\omega}} & Q_{ai}^* & \frac{1}{\sqrt{2\omega}} & Q_{ai} \end{pmatrix} \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* \end{pmatrix} \begin{pmatrix} \gamma^{\omega_1} \\ \kappa_{ai}^{\omega_1} \\ \gamma^{-\omega_1} \\ \kappa_{ia}^{-\omega_1} \end{pmatrix} \\
&+ \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ai}^{\omega_1} \langle [[\delta Q, H_X], E_{ai}] \rangle_R + \frac{1}{\sqrt{2}} \sum_{ai} \kappa_{ia}^{-\omega_1} \langle [[\delta Q, H_X], E_{ia}] \rangle_R \\
&+ \sum_{\alpha} \gamma_{\alpha}^{\omega_1} \langle [[\delta Q, H_X], b_{\alpha}^{\dagger}] \rangle_R + \sum_{\alpha} \gamma_{\alpha}^{-\omega_1} \langle [[\delta Q, H_X], b_{\alpha}] \rangle_R.
\end{aligned}$$

$$\omega_n \langle 0|q|n\rangle = i \langle 0|p|n\rangle$$

$$[b,b^{\dagger}]=1$$

$$V_{\vec{p}-\vec{k}}=\int d^3rV(r)e^{-i(\vec{p}-\vec{k})\vec{r}}$$



$$V_{\vec{p}-\vec{k}} = \int d^3r V(r) e^{-ipr \cos \theta} e^{ikr \cos \gamma}$$

$$e^{ikr \cos \alpha} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos \alpha) j_l(kr)$$

$$P_{l'}(\cos \gamma) = P_{l'}(\cos \theta) P_{l'}(\cos \theta') + 2 \sum_{m=1}^{l'} \frac{(l'-m)!}{(l'+m)!} P_{l'}^m(\cos \theta) P_{l'}^m(\cos \theta') \cos [m(\varphi - \varphi')]$$

$$\int_0^{\pi} d\theta \sin \theta P_l(\cos \theta) P_{l'}(\cos \theta) = \frac{2}{2l+1} \delta_{l,l'}$$

$$V_{\vec{p}-\vec{k}} = \sum_{l=0}^{\infty} V_l(p, k) P_l(\cos \theta')$$

$$V_l(p,k) = 4\pi(2l+1) \int_0^\infty dr r^2 V(r) j_l(pr) j_l(kr)$$

$$\varepsilon_p = \frac{p^2}{2m} - \int \frac{d^3k}{(2\pi)^3} V_{\vec{p}-\vec{k}}$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{1}{(2\pi)^2} \int_0^{p_F} \int_0^\pi dk k^2 \sin \theta' d\theta' \sum_{l=0}^\infty V_l(p,k) P_l(\cos \theta')$$

$$\int_{-1}^1 dx x^m P_n(x) = 0$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{1}{2\pi^2} \int_0^{p_F} dk k^2 V_0(p,k)$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{2}{\pi} \int_0^{p_F} dk k^2 \int_0^\infty dr r^2 V(r) j_0(pr) j_0(kr)$$

$$j_\nu(z) = \sqrt{\frac{\pi}{2z}} J_{\nu+\frac{1}{2}}(z)$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{1}{\sqrt{p}} \int_0^\infty dr r V(r) J_{\frac{1}{2}}(pr) \int_0^{p_F} dk k^{3/2} J_{\frac{1}{2}}(kr)$$

$$\varepsilon_p = \frac{p^2}{2m} - p_F \sqrt{\frac{p_F}{p}} \int_0^\infty dr V(r) J_{\frac{1}{2}}(pr) J_{\frac{3}{2}}(p_F r)$$

$$V(r) = \frac{A}{r^\eta}$$

$$\varepsilon_p = \frac{p^2}{2m} - A p_F^\eta \sqrt{\frac{1}{y}} \int_0^\infty dz z^{-\eta} J_{\frac{1}{2}}(yz) J_{\frac{3}{2}}(z)$$

$$\varepsilon_p = \frac{p^2}{2m} - A p_F^\eta \begin{cases} \frac{\Gamma\left(\frac{3-\eta}{2}\right)}{2^\eta \Gamma\left(\frac{1}{2}\right) \Gamma\left(1+\frac{\eta}{2}\right)} F\left(\frac{3-\eta}{2}, -\frac{\eta}{2}; \frac{3}{2}; y^2\right) & ; y < 1 \\ \frac{\Gamma(\eta) \Gamma\left(\frac{3-\eta}{2}\right)}{2^\eta \Gamma\left(\frac{\eta}{2}\right) \Gamma\left(1+\frac{\eta}{2}\right) \Gamma\left(\frac{3+\eta}{2}\right)} & ; y = 1 \\ \frac{\Gamma\left(\frac{3-\eta}{2}\right)}{2^\eta y^{3-\eta} \Gamma\left(\frac{5}{2}\right) \Gamma\left(\frac{\eta}{2}\right)} F\left(\frac{3-\eta}{2}, 1-\frac{\eta}{2}; \frac{5}{2}; \frac{1}{y^2}\right) & ; y > 1 \end{cases}$$

$$F(\alpha,\beta;\gamma;z) = \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)} F(\alpha,\beta;\alpha+\beta-\gamma+1;1-z) + \\ + (1-z)^{\gamma-\alpha-\beta} \frac{\Gamma(\gamma)\Gamma(\alpha+\beta-\gamma)}{\Gamma(\alpha)\Gamma(\beta)} F(\gamma-\alpha,\gamma-\beta;\gamma-\alpha-\beta+1;1-z)$$

$$\begin{aligned}\varepsilon_p &\simeq \frac{p_F^2}{2m} - Ap_F^\eta \frac{\Gamma\left(\frac{3-\eta}{2}\right)}{2^\eta \Gamma\left(1+\frac{\eta}{2}\right)} \times \\ &\times \left\{ \frac{\Gamma(\eta)}{\Gamma\left(\frac{\eta}{2}\right) \Gamma\left(\frac{3+\eta}{2}\right)} \mathcal{F}_1 + (1-y^2)^\eta \frac{\Gamma(-\eta)}{\Gamma\left(\frac{3-\eta}{2}\right) \Gamma\left(-\frac{\eta}{2}\right)} \mathcal{F}_2 \right\} \\ \mathcal{F}_{1,2} &\simeq 1 \mp \frac{\eta(3 \mp \eta)}{4(1 \mp \eta)} (1-y^2) \\ \varepsilon_p &\simeq \frac{p_F^2}{2m} - Ap_F^\eta \frac{\Gamma\left(\frac{3-\eta}{2}\right)}{2^\eta y^{3-\eta} \Gamma\left(\frac{\eta}{2}\right)} \times \\ &\times \left\{ \frac{\Gamma(\eta)}{\Gamma\left(1+\frac{\eta}{2}\right) \Gamma\left(\frac{3+\eta}{2}\right)} \mathcal{F}_3 + \left(1-\frac{1}{y^2}\right)^\eta \frac{\Gamma(-\eta)}{\Gamma\left(\frac{3-\eta}{2}\right) \Gamma\left(1-\frac{\eta}{2}\right)} \mathcal{F}_4 \right\} \\ \mathcal{F}_{3,4} &\simeq 1 + \frac{(2 \mp \eta)(3 \mp \eta)}{4(1 \mp \eta)} \left(1 - \frac{1}{y^2}\right)\end{aligned}$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{2e^2 p_F}{\pi} \begin{cases} F\left(1, -\frac{1}{2}; \frac{3}{2}; y^2\right) & ; y < 1 \\ \frac{1}{2} & ; y = 1 \\ \frac{1}{3y^2} F\left(1, \frac{1}{2}; \frac{5}{2}; \frac{1}{y^2}\right) & ; y > 1 \end{cases}$$

$$F\left(1, -\frac{1}{2}; \frac{3}{2}; y^2\right) = \frac{1}{2} + \frac{1-y^2}{4y} \ln\left(\frac{1+y}{1-y}\right)$$

$$F\left(1, \frac{1}{2}; \frac{5}{2}; x^2\right) = \frac{3}{2x^2} \left[1 - \frac{1-x^2}{2x} \ln\left(\frac{1+x}{1-x}\right)\right]$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{2e^2 p_F}{\pi} \left[\frac{1}{2} + \frac{1-y^2}{4y} \ln\left|\frac{1+y}{1-y}\right| \right]$$

$$E_{HF} = E_{HF}^{(1)} + E_{HF}^{(2)}$$

$$E_{HF}^{(1)} = \frac{3}{5} \frac{p_F^2}{2m} N$$

$$E_{HF}^{(2)} = - \frac{Ap_F^{\eta+3} \Gamma\left(\frac{3-\eta}{2}\right) I_\eta}{2^{\eta+1} \pi^2 \Gamma\left(\frac{3}{2}\right) \Gamma\left(1+\frac{\eta}{2}\right)}$$

$$I_\eta = \int_0^1 dy y^2 F\left(\frac{3-\eta}{2}, -\frac{\eta}{2}; \frac{3}{2}; y^2\right)$$

$$E_{HF}^{(2)} = -\frac{e^2 p_F^4}{4\pi^3}$$

$$\int_0^1 dx x^{\gamma-1} (1-x)^{\rho-1} F(\alpha, \beta; \gamma; x) = \frac{\Gamma(\gamma)\Gamma(\rho)\Gamma(\gamma+\rho-\alpha-\beta)}{\Gamma(\gamma+\rho-\alpha)\Gamma(\gamma+\rho-\beta)}$$

$$\frac{E_{HF}}{N} = \frac{3}{5} \frac{p_F^2}{2m} - A \left(\frac{p_F}{2} \right)^\eta \frac{12\Gamma\left(\frac{3-\eta}{2}\right)\Gamma(\eta)}{\eta(\eta+1)(\eta+3)\Gamma\left(\frac{1+\eta}{2}\right)\left[\Gamma\left(\frac{\eta}{2}\right)\right]^2}$$

$$v_p = \frac{p}{m} + \frac{2}{3} A p_F^{\eta-2} \frac{\eta \Gamma\left(\frac{5-\eta}{2}\right)}{2^\eta \Gamma\left(\frac{3}{2}\right) \Gamma\left(1+\frac{\eta}{2}\right)} p F\left(\frac{5-\eta}{2}, 1-\frac{\eta}{2}; \frac{5}{2}; \frac{p^2}{p_F^2}\right)$$

$$v_p = \frac{p}{m} + 2A p_F^{\eta-1} \frac{\Gamma\left(\frac{5-\eta}{2}\right)}{2^\eta \Gamma\left(\frac{5}{2}\right) \Gamma\left(\frac{\eta}{2}\right)} \left(\frac{p_F}{p}\right)^{4-\eta} \times \left\{ F\left(\frac{3-\eta}{2}, 1-\frac{\eta}{2}; \frac{5}{2}; \frac{p_F^2}{p^2}\right) + \frac{2}{5} \left(1-\frac{\eta}{2}\right) \left(\frac{p_F}{p}\right)^2 F\left(\frac{5-\eta}{2}, 2-\frac{\eta}{2}; \frac{7}{2}; \frac{p_F^2}{p^2}\right) \right\}$$

$$F(a,b;c;x) = \frac{c-1}{a-1} x^{-1} [F(a-1,b;c-1;x) - F(a-1,b-1;c-1;x)]$$

$$F(1,b;c;x) = \frac{c-1}{b-1} (1-x)^{-1} - \frac{c-b}{b-1} (1-x)^{-1} F(1,b-1;c;x)$$

$$v_p = \frac{p}{m} + \frac{e^2}{\pi} \frac{1}{y} \left[\frac{1+y^2}{2y} \ln \left| \frac{1+y}{1-y} \right| - 1 \right]$$

$$N(p) = \frac{p^2}{\pi^2 |v_p|}$$

$$v_{p \rightarrow p_F} \simeq \frac{p_F}{m} + \frac{2}{3} A p_F^{\eta-1} \frac{\eta \Gamma\left(\frac{5-\eta}{2}\right)}{2^\eta \Gamma\left(\frac{3}{2}\right) \Gamma\left(1+\frac{\eta}{2}\right)} \times \left\{ \frac{\Gamma\left(\frac{5}{2}\right) \Gamma(-1+\eta)}{\Gamma\left(\frac{\eta}{2}\right) \Gamma\left(\frac{3+\eta}{2}\right)} Q_1 + (1-y^2)^{-1+\eta} \frac{\Gamma\left(\frac{5}{2}\right) \Gamma(1-\eta)}{\Gamma\left(\frac{5-\eta}{2}\right) \Gamma\left(1-\frac{\eta}{2}\right)} Q_2 \right\}$$

$$Q_1 = F\left(\frac{5-\eta}{2}, 1-\frac{\eta}{2}; 2-\eta; 1-y^2\right) \simeq 1 + \frac{5-\eta}{4} (1-y^2)$$

$$Q_2 = F\left(\frac{\eta}{2}, \frac{3+\eta}{2}; \eta; 1-y^2\right) \simeq 1 + \frac{3+\eta}{4} (1-y^2)$$

$$v_{p=p_F} = \frac{p_F}{2} \left[\frac{2}{m} + A \left(\frac{p_F}{2} \right)^{\eta-2} \mathcal{M}(\eta) \right]$$

$$\mathcal{M}(\eta) = \frac{\Gamma\left(\frac{5-\eta}{2}\right)\Gamma(-1+\eta)}{\left[\Gamma\left(\frac{\eta}{2}\right)\right]^2\Gamma\left(\frac{3+\eta}{2}\right)}$$

$$N(p_F) = \frac{2p_F}{\pi^2 \left[\frac{2}{m} + A \left(\frac{p_F}{2} \right)^{\eta-2} \mathcal{M}(\eta) \right]}$$

$$v_{p \rightarrow p_F} \simeq \frac{A\Gamma(1-\eta)}{\pi} \left(\frac{p_F}{2} \right)^{\eta-1} \left(1 - \frac{p^2}{p_F^2} \right)^{-1+\eta} \sin \left(\frac{\pi\eta}{2} \right)$$

$$N(p \rightarrow p_F) \simeq \frac{2^{\eta-1}}{\pi A \Gamma(1-\eta) \left| \sin \left(\frac{\pi\eta}{2} \right) \right|} p_F^{3-\eta} \left(1 - \frac{p^2}{p_F^2} \right)^{1-\eta}$$

$$v_{p \rightarrow p_F} \simeq \frac{p_F}{m} + 2Ap_F^{\eta-1} \frac{\Gamma\left(\frac{5-\eta}{2}\right)}{2^{\eta}\Gamma\left(\frac{5}{2}\right)\Gamma\left(\frac{\eta}{2}\right)} \\ \times \left\{ \frac{\Gamma\left(\frac{5}{2}\right)\Gamma(\eta)}{\Gamma\left(1+\frac{\eta}{2}\right)\Gamma\left(\frac{3+\eta}{2}\right)} \mathcal{F}_3 + \left(1 - \frac{1}{y^2}\right)^{\eta} \frac{\Gamma\left(\frac{5}{2}\right)\Gamma(-\eta)}{\Gamma\left(\frac{3-\eta}{2}\right)\Gamma\left(1-\frac{\eta}{2}\right)} \mathcal{F}_4 + \right. \\ \left. + \frac{2}{5} \left(1 - \frac{\eta}{2}\right) \left[\frac{\Gamma\left(\frac{7}{2}\right)\Gamma(-1+\eta)}{\Gamma\left(1+\frac{\eta}{2}\right)\Gamma\left(\frac{3+\eta}{2}\right)} \mathcal{S}_1 + \left(1 - \frac{1}{y^2}\right)^{-1+\eta} \frac{\Gamma\left(\frac{7}{2}\right)\Gamma(1-\eta)}{\Gamma\left(\frac{5-\eta}{2}\right)\Gamma\left(2-\frac{\eta}{2}\right)} \mathcal{S}_2 \right] \right\}$$

$$\mathcal{S}_1 \simeq 1 + \frac{(4-\eta)(5-\eta)}{4(2-\eta)} \left(1 - \frac{1}{y^2}\right)$$

$$\mathcal{S}_2 \simeq 1 + \frac{(2+\eta)(3+\eta)}{4\eta} \left(1 - \frac{1}{y^2}\right)$$

$$N(p \rightarrow p_F) \simeq \frac{2^{\eta-1}}{\pi A \Gamma(1-\eta) \left| \sin \left(\frac{\pi\eta}{2} \right) \right|} p_F^{3-\eta} \left(1 - \frac{p_F^2}{p^2} \right)^{1-\eta}$$

$$V_{\vec{p}-\vec{k}} = \int d^2r V(r) e^{-i(\vec{p}-\vec{k})\vec{r}}$$

$$V_{\vec{p}-\vec{k}} = \int_0^\infty dr r V(r) \int_0^{2\pi} d\theta e^{-i p r \cos \theta} e^{i k r \cos \alpha}$$

$$e^{iz\cos\varphi}=J_0(z)+2\sum_{n=1}^\infty i^nJ_n(z)\cos\left(n\varphi\right)$$

$$I=2\pi\sum_{l=0}^\infty \varepsilon_l J_l(pr)J_l(kr)\cos\left(l\theta'\right)$$

$$V_{\vec{p}-\vec{k}} = \sum_{l=0}^{\infty} V_l(p, k) \cos(l\theta')$$

$$V_l(p, k) = 2\pi\epsilon_l \int_0^\infty dr r V(r) J_l(pr) J_l(kr)$$

$$\epsilon_p = \frac{p^2}{2m} - \int_0^{p_F} \int_0^{2\pi} \frac{k dk d\theta'}{(2\pi)^2} \sum_{l=0}^{\infty} V_l(p, k) \cos(l\theta')$$

$$\epsilon_p = \frac{p^2}{2m} - \int_0^{p_F} k dk \int_0^\infty dr r V(r) J_0(pr) J_0(kr)$$

$$\epsilon_p = \frac{p^2}{2m} - A p_F^\eta \int_0^\infty dz z^{-\eta} J_0(yz) J_1(z)$$

$$\epsilon_p = \frac{p^2}{2m} - A p_F^\eta \begin{cases} \frac{\Gamma(1-\frac{\eta}{2})}{2^\eta \Gamma(1+\frac{\eta}{2})} F(1-\frac{\eta}{2}, -\frac{\eta}{2}; 1; y^2) & ; y < 1 \\ \frac{\Gamma(\eta) \Gamma(1-\frac{\eta}{2})}{2^\eta \Gamma(\frac{\eta}{2}) [\Gamma(1+\frac{\eta}{2})]^2} & ; y = 1 \\ \frac{\Gamma(1-\frac{\eta}{2})}{2^\eta y^{2-\eta} \Gamma(\frac{\eta}{2})} F(1-\frac{\eta}{2}, 1-\frac{\eta}{2}; 2; \frac{1}{y^2}) & ; y > 1 \end{cases}$$

$$\epsilon_p \simeq \frac{p_F^2}{2m} - A p_F^\eta \frac{\Gamma(1-\frac{\eta}{2})}{2^\eta \Gamma(1+\frac{\eta}{2})} \times \left\{ \frac{\Gamma(\eta)}{\Gamma(\frac{\eta}{2}) \Gamma(1+\frac{\eta}{2})} \mathcal{G}_1 + (1-y^2)^\eta \frac{\Gamma(-\eta)}{\Gamma(1-\frac{\eta}{2}) \Gamma(-\frac{\eta}{2})} \mathcal{G}_2 \right\}$$

$$\mathcal{G}_{1,2} \simeq 1 \mp \frac{\eta(2 \mp \eta)}{4(1 \mp \eta)} (1-y^2)$$

$$\epsilon_p \simeq \frac{p_F^2}{2m} - A p_F^\eta \frac{\Gamma(1-\frac{\eta}{2})}{2^\eta y^{2-\eta} \Gamma(\frac{\eta}{2})} \times \left\{ \frac{\Gamma(\eta)}{[\Gamma(1+\frac{\eta}{2})]^2} \mathcal{G}_3 + \left(1-\frac{1}{y^2}\right)^\eta \frac{\Gamma(-\eta)}{[\Gamma(1-\frac{\eta}{2})]^2} \mathcal{G}_4 \right\}$$

$$\mathcal{G}_{3,4} \simeq 1 + \frac{(2 \mp \eta)^2}{4(1 \mp \eta)} \left(1 - \frac{1}{y^2}\right)$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{2e^2 p_F}{\pi} \begin{cases} \frac{\pi}{2} F\left(\frac{1}{2}, -\frac{1}{2}; 1; y^2\right) & ; y < 1 \\ 1 & ; y = 1 \\ \frac{\pi}{4y} F\left(\frac{1}{2}, \frac{1}{2}; 2; \frac{1}{y^2}\right) & ; y > 1 \end{cases}$$

$$\frac{\pi}{2} F\left(\frac{1}{2}, -\frac{1}{2}; 1; y^2\right) = E(y)$$

$$F\left(\frac{1}{2}, \frac{1}{2}; 2; \frac{1}{y^2}\right) = \frac{4y^2}{\pi} \left[E\left(\frac{1}{y}\right) - \left(1 - \frac{1}{y^2}\right) K\left(\frac{1}{y}\right) \right]$$

$$\varepsilon_p = \frac{p^2}{2m} - \frac{2e^2 p_F}{\pi} \begin{cases} E(y) & ; y < 1 \\ 1 & ; y = 1 \\ y \left[E\left(\frac{1}{y}\right) - \left(1 - \frac{1}{y^2}\right) K\left(\frac{1}{y}\right) \right] & ; y > 1 \end{cases}$$

$$E_{HF} = E_{HF}^{(1)} + E_{HF}^{(2)}$$

$$E_{HF}^{(1)} = \frac{1}{2} \frac{p_F^2}{2m} N$$

$$E_{HF}^{(2)} = - \frac{A p_F^{\eta+2} \Gamma\left(1 - \frac{\eta}{2}\right) Y_\eta}{2^{\eta+1} \pi \Gamma\left(1 + \frac{\eta}{2}\right)}$$

$$Y_\eta = \int_0^1 dy y F\left(1 - \frac{\eta}{2}, -\frac{\eta}{2}; 1; y^2\right)$$

$$E_{HF}^{(2)} = - \frac{2e^2 p_F^3}{3\pi^2}$$

$$\frac{E_{HF}}{N} = \frac{1}{2} \frac{p_F^2}{2m} - A \left(\frac{p_F}{2}\right)^\eta \frac{\Gamma\left(1 - \frac{\eta}{2}\right) \Gamma(\eta)}{\left(1 + \frac{\eta}{2}\right) \left(\frac{\eta}{2}\right)^2 \left[\Gamma\left(\frac{\eta}{2}\right)\right]^3}$$

$$v_p = \frac{p}{m} + A p_F^{\eta-2} \frac{\eta \Gamma\left(2 - \frac{\eta}{2}\right)}{2\eta \Gamma\left(1 + \frac{\eta}{2}\right)} p F\left(2 - \frac{\eta}{2}, 1 - \frac{\eta}{2}; 2; \frac{p^2}{p_F^2}\right)$$

$$v_p = \frac{p}{m} + \frac{e^2}{2} y F\left(\frac{3}{2}, \frac{1}{2}; 2; y^2\right)$$

$$\frac{\pi}{2} F\left(\frac{1}{2}, \frac{1}{2}; 1; y^2\right) = K(y)$$

$$v_p = \frac{p}{m} + \frac{2e^2}{\pi y} [K(y) - E(y)]$$

$$v_p = \frac{p}{m} + 2Ap_F^{\eta-1} \frac{\Gamma\left(2 - \frac{\eta}{2}\right)}{2^\eta \Gamma\left(\frac{\eta}{2}\right)} \left(\frac{p_F}{p}\right)^{3-\eta} \times$$

$$\times \left\{ F\left(1 - \frac{\eta}{2}, 1 - \frac{\eta}{2}; 2; \frac{p_F^2}{p^2}\right) + \frac{1}{2}\left(1 - \frac{\eta}{2}\right) \left(\frac{p_F}{p}\right)^2 F\left(2 - \frac{\eta}{2}, 2 - \frac{\eta}{2}; 3; \frac{p_F^2}{p^2}\right) \right\}$$

$$v_p = \frac{p}{m} + \frac{2e^2}{\pi} \left[K\left(\frac{1}{y}\right) - E\left(\frac{1}{y}\right) \right]$$

$$v_{p \rightarrow p_F} \simeq \frac{p_F}{m} + Ap_F^{\eta-1} \frac{\eta \Gamma\left(2 - \frac{\eta}{2}\right)}{2^\eta \Gamma\left(1 + \frac{\eta}{2}\right)}$$

$$\times \left\{ \frac{\Gamma(-1 + \eta)}{\Gamma\left(\frac{\eta}{2}\right) \Gamma\left(1 + \frac{\eta}{2}\right)} \mathcal{J}_1 + (1 - y^2)^{-1+\eta} \frac{\Gamma(1 - \eta)}{\Gamma\left(2 - \frac{\eta}{2}\right) \Gamma\left(1 - \frac{\eta}{2}\right)} \mathcal{J}_2 \right\}$$

$$\mathcal{J}_1 \simeq 1 + \frac{4 - \eta}{4} (1 - y^2)$$

$$\mathcal{J}_2 \simeq 1 + \frac{2 + \eta}{4} (1 - y^2)$$

$$v_{p=p_F} = \frac{p_F}{2} \left\{ \frac{2}{m} + A \left(\frac{p_F}{2}\right)^{\eta-2} \frac{2}{\eta} \frac{\Gamma\left(2 - \frac{\eta}{2}\right) \Gamma(-1 + \eta)}{\left[\Gamma\left(\frac{\eta}{2}\right)\right]^3} \right\}$$

$$v_{p \rightarrow p_F} \simeq \frac{A \Gamma(1 - \eta)}{\pi} \left(\frac{p_F}{2}\right)^{\eta-1} \left(1 - \frac{p^2}{p_F^2}\right)^{-1+\eta} \sin\left(\frac{\pi \eta}{2}\right)$$

$$v_{p \rightarrow p_F} \simeq \frac{p_F}{m} + 2Ap_F^{\eta-1} \frac{\Gamma\left(2 - \frac{\eta}{2}\right)}{2^\eta \Gamma\left(\frac{\eta}{2}\right)} \times \left\{ \frac{\Gamma(\eta)}{\left[\Gamma\left(1 + \frac{\eta}{2}\right)\right]^2} \mathcal{Z}_1 + \left(1 - \frac{1}{y^2}\right)^\eta \frac{\Gamma(-\eta)}{\left[\Gamma\left(1 - \frac{\eta}{2}\right)\right]^2} \mathcal{Z}_2 \right. \\ \left. + \frac{1}{2} \left(1 - \frac{\eta}{2}\right) \left[\frac{2\Gamma(-1 + \eta)}{\left[\Gamma\left(1 + \frac{\eta}{2}\right)\right]^2} \mathcal{H}_1 + \left(1 - \frac{1}{y^2}\right)^{-1+\eta} \frac{2\Gamma(1 - \eta)}{\left[\Gamma\left(2 - \frac{\eta}{2}\right)\right]^2} \mathcal{H}_2 \right] \right\}$$

$$\mathcal{Z}_{1,2} \simeq 1 + \frac{(2 \mp \eta)^2}{4(1 \mp \eta)} \left(1 - \frac{1}{y^2}\right)$$

$$\mathcal{H}_1 \simeq 1 + \frac{(4 - \eta)^2}{4(2 - \eta)} \left(1 - \frac{1}{y^2}\right)$$

$$\mathcal{H}_2 \simeq 1 + \frac{(2 + \eta)^2}{4\eta} \left(1 - \frac{1}{y^2}\right)$$

$$v_{p \rightarrow p_F} \simeq \frac{A \Gamma(1 - \eta)}{\pi} \left(\frac{p_F}{2}\right)^{\eta-1} \left(1 - \frac{p_F^2}{p^2}\right)^{-1+\eta} \sin\left(\frac{\pi \eta}{2}\right)$$

$$N(p) = \frac{p}{\pi|v_p|}$$

$$N(p_F) = \frac{1}{\pi \left\{ \frac{1}{m} + A \left(\frac{p_F}{2} \right)^{\eta-2} \frac{\Gamma \left(2 - \frac{\eta}{2} \right) \Gamma(-1 + \eta)}{\eta \left[\Gamma \left(\frac{\eta}{2} \right) \right]^3} \right\}}$$

$$N(p \rightarrow p_F) \simeq \frac{2^{\eta-1}}{A\Gamma(1-\eta) \left| \sin \left(\frac{\pi\eta}{2} \right) \right|} p_F^{2-\eta} \times \begin{cases} \left(1 - \frac{p^2}{p_F^2} \right)^{1-\eta} & ; p < p_F \\ \left(1 - \frac{p_F^2}{p^2} \right)^{1-\eta} & ; p > p_F \end{cases}$$

$$\begin{aligned} H^{\text{ferm}} &= \sum_{p,q}^M h_{pq}(C) \alpha_p^\dagger \alpha_q + \frac{1}{2} \sum_{p,q,r,s}^M g_{pqrs}(C) \alpha_p^\dagger \alpha_r^\dagger \alpha_s \alpha_q \\ &= \sum_{p,q}^M h_{pq} \alpha_p^\dagger \alpha_q + \frac{1}{2} \sum_{p,q,r,s}^M g_{pqrs} \alpha_p^\dagger \alpha_r^\dagger \alpha_s \alpha_q \end{aligned}$$

$$U(\vec{\kappa}) = e^{-\hat{k}(\vec{\kappa})}, \text{ where } \hat{k} = \sum_{p>q}^M \kappa_{pq} (\alpha_p^\dagger \alpha_q - \alpha_q^\dagger \alpha_p)$$

$$\hat{k}^\dagger = -\hat{k}$$

$$\kappa_{pq}=-\kappa_{qp}^*\frac{M(M-1)}{2}$$

$$\begin{aligned} H^{\text{ferm}} &\mapsto H^{\text{ferm}}(\vec{\kappa}) = e^{-\hat{k}(\vec{\kappa})} H^{\text{ferm}} e^{\hat{k}(\vec{\kappa})} \\ &= \sum_{mn}^M \bar{h}_{mn}(\vec{\kappa}) \alpha_m^\dagger \alpha_n + \sum_{mn\mu\nu}^M \frac{\bar{g}_{mn\mu\nu}(\vec{\kappa})}{2} \alpha_m^\dagger \alpha_n^\dagger \alpha_\mu \alpha_\nu \end{aligned}$$

$$\begin{aligned} H_D^{\text{ferm}}(\vec{\kappa}) &= \sum_n^M \bar{h}_{nn}(\vec{\kappa}) \alpha_n^\dagger \alpha_n + \\ &\frac{1}{2} \sum_{\substack{\bar{m},\bar{n} \\ m \neq n}}^M (\bar{g}_{mmnn}(\vec{\kappa}) - \bar{g}_{mnnm}(\vec{\kappa})) \alpha_m^\dagger \alpha_m \alpha_n^\dagger \alpha_n \end{aligned}$$

$$\begin{aligned} E_{HF}^{\text{ferm}} &= \min_{\vec{\kappa}} [\langle HF^{\text{ferm}} | e^{-\hat{k}(\vec{\kappa})} H^{\text{ferm}} e^{\hat{k}(\vec{\kappa})} | HF^{\text{ferm}} \rangle] \\ &= \min_{\vec{\kappa}} [\langle HF^{\text{ferm}} | H_D^{\text{ferm}}(\vec{\kappa}) | HF^{\text{ferm}} \rangle] \end{aligned}$$

$$|HF^{\text{ferm}}\rangle = \prod_{i\in\mathcal{O}_\alpha\cup\mathcal{O}_\beta} \alpha_i^\dagger|vac\rangle$$

$$\begin{aligned}
H_D(R) &= \sum_n^M \frac{\bar{h}_{nn}(R)}{2} (I - Z_n) + \\
&\sum_{\substack{m,n \\ m \neq n}}^M \frac{\bar{g}_{mmnn}(R) - \bar{g}_{nnmm}(R)}{8} (I - Z_n - Z_m + Z_m Z_n) \\
&= \sum_{j=1}^{1+\frac{M(M+1)}{2}} c_j(R) P_j
\end{aligned}$$

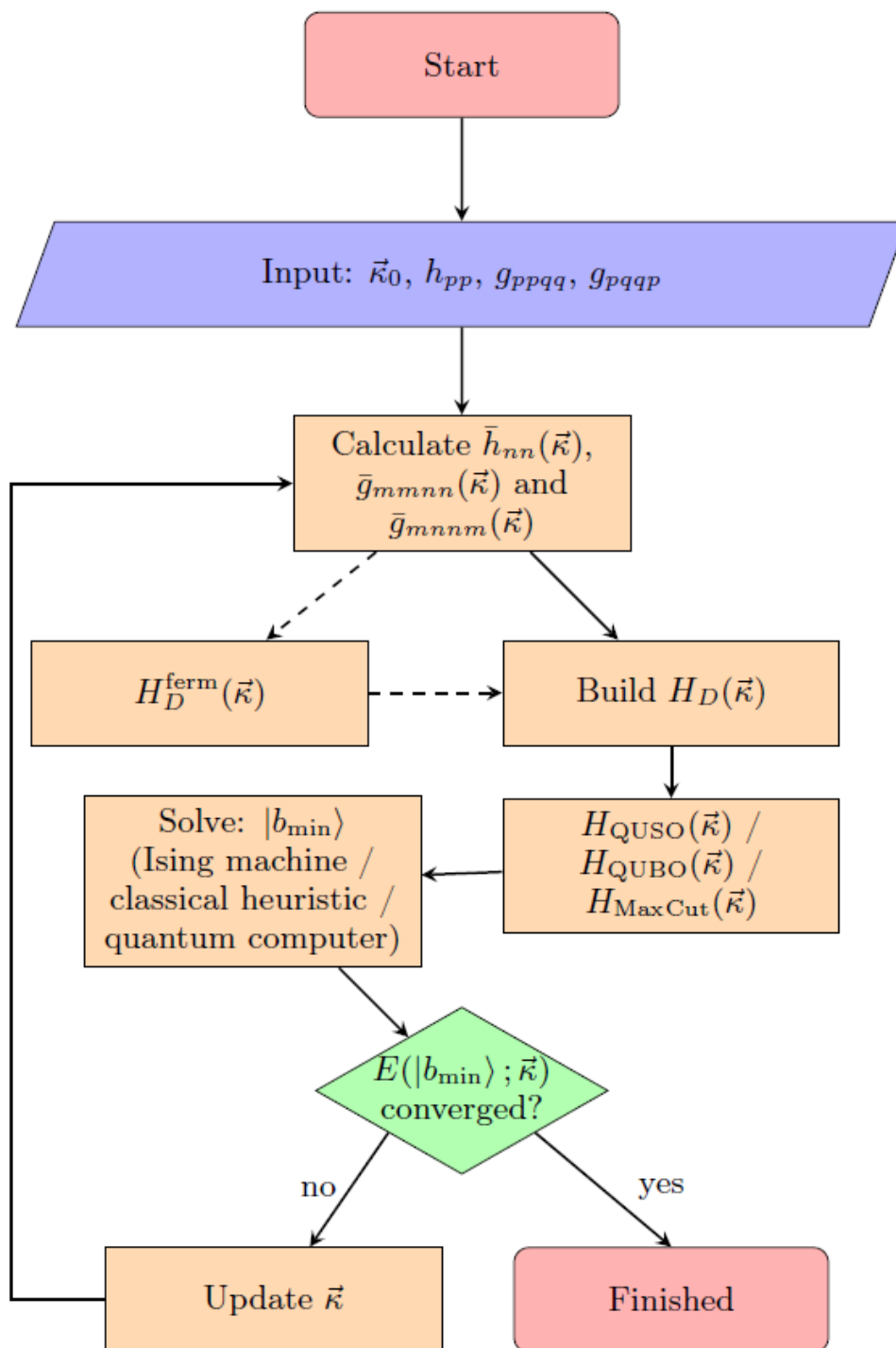
$$\min\{f(\vec{x}): \vec{x} \in \{0,1\}^n\}.$$

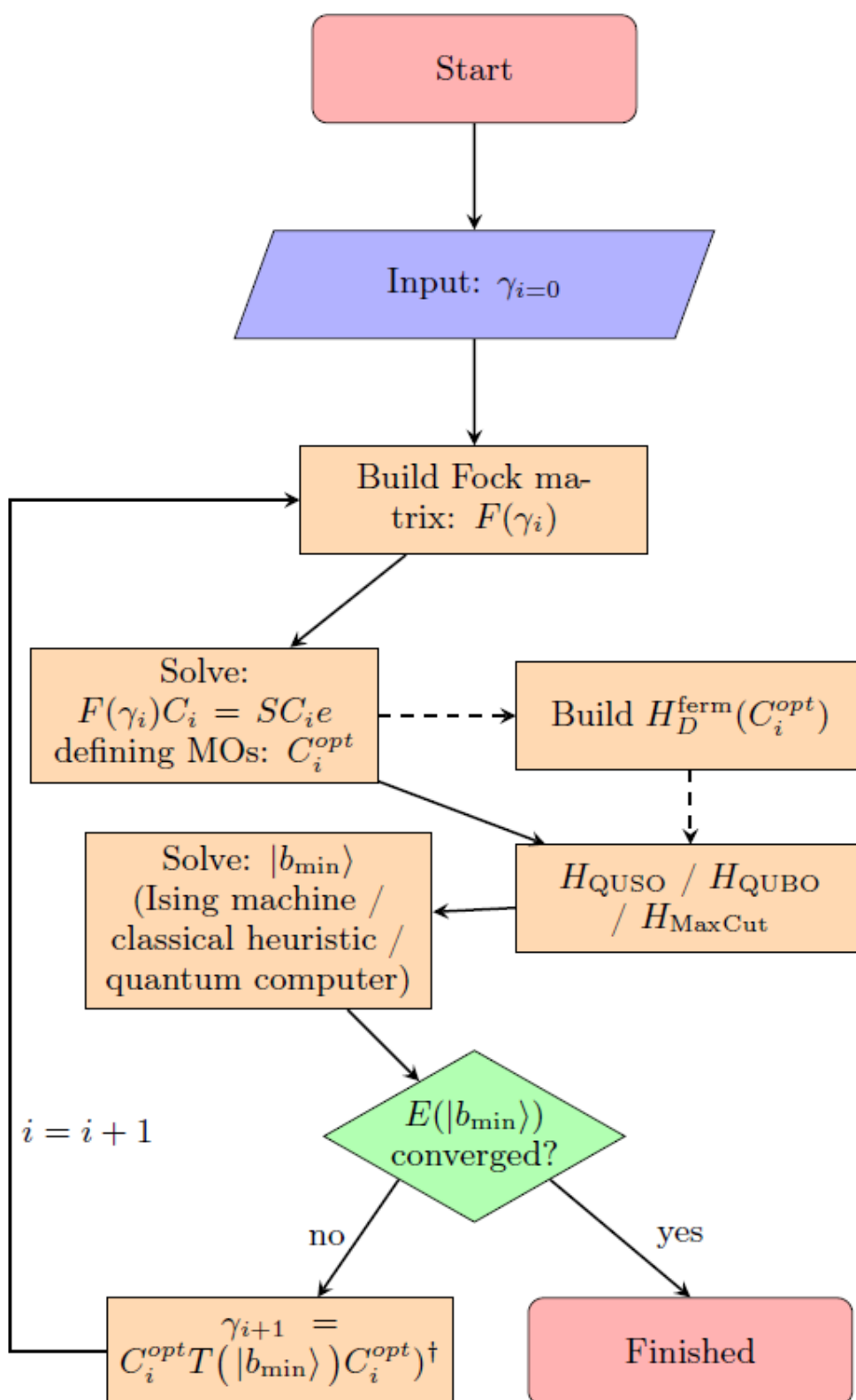
$$\begin{aligned}
g(\vec{x}) &= \vec{x}^T Q \vec{x} + \vec{b}^T \vec{x} + c, \\
&= \sum_{ij} Q_{ij} x_i x_j + \sum_i b_i x_i + c. (9)
\end{aligned}$$

$$x_i \leftrightarrow \frac{1-z_i}{2},$$

$$E_{\text{Alg-1}}^{\text{min-eig}} = \min_{\vec{\kappa}} \left[\min_{[|b\rangle \in \mathcal{S} \subset \mathcal{D}} [\langle b | H_D(\vec{\kappa}) | b \rangle] \right]$$







$$E_{\text{Alg-2}}^{\text{min-eig}} = \min_C \left[\min_{|b\rangle \in \mathcal{S} \subset \mathcal{D}} [\langle b | H_D(C) | b \rangle] \right],$$

$$H_D^{\text{ferm}}(C) = \sum_n^M \bar{h}_{nn}(C) \alpha_n^\dagger \alpha_n + \\ \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M (\bar{g}_{mmnn}(C) - \bar{g}_{mnnm}(C)) \alpha_m^\dagger \alpha_m \alpha_n^\dagger \alpha_n$$

$$E_{QUSO}^{V_P} = \min_R \left[\min_{|b\rangle \in \mathcal{D}} [\langle b|H_D(R) + \lambda V_P|b\rangle] \right].$$

$$E_{QUSO}^{V_P} = \underbrace{\min_R}_{\text{classical algorithm}} \left[\underbrace{\min_{|b\rangle \in \mathcal{D}} [\langle b|H_D(R) + \lambda V_P|b\rangle]}_{\text{quantum algorithm}} \right],$$

$$E_{QAOA-SCF} = \min_R \left[\min_{\vec{g}, \vec{b}} [\langle \vec{g}, \vec{b} | H_c(R) | \vec{g}, \vec{b} \rangle] \right]$$

$$|\vec{g}, \vec{b}\rangle = \prod_{k=l}^1 e^{-ib_k H_m} e^{-ig_k H_c(R)} |s\rangle \\ = e^{-ib_l H_m} e^{-ig_l H_c(R)} \dots e^{-ib_1 H_m} e^{-ig_1 H_c(R)} |s\rangle.$$

$$|s\rangle = H^{\otimes n} |0\rangle = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} |k\rangle$$

$$\max_{\vec{z}} \left[\sum_{ij} A_{ij} \frac{I - z_i z_j}{2} \right] \mapsto \max_{\vec{x}} \left[\sum_{ij} A_{ij} (x_i \oplus x_j) \right]$$

$$x_i \oplus x_j = \begin{cases} 1, & \text{if } A_{ij} > 0 \\ 0, & \text{if } A_{ij} < 0 \end{cases}$$

$$[\hat{k},a_r^\dagger]=\sum_{pq}k_{pq}[a_p^\dagger a_q,a_r^\dagger] \\ =\sum_{pq}k_{pq}(a_p^\dagger \underbrace{[a_q,a_r^\dagger]}_{=\delta_{qr}}+\underbrace{[a_p^\dagger,a_r^\dagger]}_{=0}a_q) \\ =\sum_{pq}k_{pq}a_p^\dagger \delta_{qr} \\ =\sum_pk_{pr}a_p^\dagger\equiv k_{pr}a_p^\dagger$$

$$\begin{aligned}
[\hat{k}, a_r] &= \sum_{pq} k_{pq} [a_p^\dagger a_q, a_r] \\
&= \sum_{pq} k_{pq} (a_p^\dagger \underbrace{[a_q, a_r]}_{=0} + \underbrace{[a_p^\dagger, a_r]}_{=-[a_r, a_p^\dagger] = -\delta_{pr}} a_q) \\
&= \sum_{pq} -k_{pq} a_q \delta_{pr} \\
&= \sum_q -k_{rq} a_q \\
&= \sum_q k_{qr}^* a_q \equiv k_{qr}^* a_q
\end{aligned}$$

$$[(A)^n, B] = \underbrace{[A, \dots [A, [A, B]] \dots]}_{n \text{ times}}, [(A)^0, B] = B.$$

$$\begin{aligned}
e^{\hat{k}} a_p^\dagger e^{-\hat{k}} &= \sum_{n=0}^{\infty} \frac{[(\hat{k})^n, a_p^\dagger]}{n!} \\
&= a_p^\dagger + [\hat{k}, a_p^\dagger] + \frac{1}{2} [\hat{k}, [\hat{k}, a_p^\dagger]] + \frac{1}{6} [\hat{k}, [\hat{k}, [\hat{k}, a_p^\dagger]]] + \dots \\
&= a_p^\dagger + a_r^\dagger k_{pr} + \frac{1}{2} [\hat{k}, a_r^\dagger k_{pr}] + \frac{1}{6} [\hat{k}, [\hat{k}, a_r^\dagger k_{pr}]] + \dots \\
&= a_p^\dagger + a_r^\dagger k_{pr} + \frac{(k_{pr} k_{rm})}{2} a_m^\dagger + \frac{[\hat{k}, (k_{pr} k_{rm}) a_m^\dagger]}{6} + \dots \\
&= a_p^\dagger + a_r^\dagger k_{pr} + \frac{(k_{pr} k_{rm})}{2} a_m^\dagger + \frac{(k_{pr} k_{rm} k_{mn})}{6} a_n^\dagger + \dots \\
&= a_p^\dagger + a_r^\dagger k_{pr} + \frac{(K^2)_{pm}}{2} a_m^\dagger + \frac{(K^3)_{pn}}{6} a_n^\dagger + \dots \\
&= a_p^\dagger (I)_{pr} + a_r^\dagger (K)_{pr} + \frac{(K^2)_{pr}}{2} a_r^\dagger + \frac{(K^3)_{pr}}{6} a_r^\dagger + \dots = \sum_s a_s^\dagger [e^K]_{ps} \\
&= a_p^\dagger (I)_{rp} - a_r^\dagger (K)_{rp} + \frac{(K^2)_{rp}}{2} a_r^\dagger - \frac{(K^3)_{rp}}{6} a_r^\dagger + \dots = \sum_s a_s^\dagger [e^{-K}]_{sp}.
\end{aligned}$$

$$e^{\hat{k}} a_p e^{-\hat{k}} = a_p (I)_{rp} - a_r (K)_{rp}^* + \frac{(K^2)_{rp}^*}{2} a_r - \frac{(K^3)_{rp}^*}{6} a_r + \dots = \sum_s a_s [e^{-K}]_{sp}^*.$$



$$\begin{aligned}
e^{-\hat{k}} H e^{\hat{k}} &= \sum_{pq}^M h_{pq} e^{-\hat{k}} \alpha_p^\dagger \alpha_q e^{\hat{k}} + \frac{1}{2} \sum_{pqrs}^M g_{pqrs} e^{-\hat{k}} \alpha_p^\dagger \alpha_r^\dagger \alpha_s \alpha_q e^{\hat{k}} \\
&= \sum_{pq}^M h_{pq} e^{-\hat{k}} \alpha_p^\dagger (e^{\hat{k}} e^{-\hat{k}}) \alpha_q e^{\hat{k}} + \frac{1}{2} \sum_{pqrs}^M g_{pqrs} e^{-\hat{k}} \alpha_p^\dagger (e^{\hat{k}} e^{-\hat{k}}) \alpha_r^\dagger (e^{\hat{k}} e^{-\hat{k}}) \alpha_s (e^{\hat{k}} e^{-\hat{k}}) \alpha_q e^{\hat{k}} \\
&= \sum_{pq}^M h_{pq} \left(\sum_m^M a_m^\dagger [e^{-K}]_{mp} \right) \left(\sum_n^M a_n [e^{-K}]_{nq}^* \right) + \\
&\quad \frac{1}{2} \sum_{pqrs}^M g_{pqrs} \left(\sum_m^M a_m^\dagger [e^{-K}]_{mp} \right) \left(\sum_n^M a_n^\dagger [e^{-K}]_{nr} \right) \left(\sum_\mu^M a_\mu [e^{-K}]_{\mu s}^* \right) \left(\sum_\nu^M a_\nu [e^{-K}]_{\nu q}^* \right) \\
&= \sum_{mn}^M a_m^\dagger a_n \sum_{pq}^M h_{pq} ([e^{-K}]_{mp}) ([e^{-K}]_{nq}^*) + \\
&\quad \frac{1}{2} \sum_{mn\mu\nu}^M a_m^\dagger a_n^\dagger a_\mu a_\nu \sum_{pqrs}^M g_{pqrs} ([e^{-K}]_{mp}) ([e^{-K}]_{nr}) ([e^{-K}]_{\mu s}^*) ([e^{-K}]_{\nu q}^*) \\
&= \sum_{mn}^M \bar{h}_{mn} \alpha_m^\dagger \alpha_n + \frac{1}{2} \sum_{mn\mu\nu}^M \bar{g}_{mn\mu\nu} \alpha_m^\dagger \alpha_n^\dagger \alpha_\mu \alpha_\nu.
\end{aligned}$$

$$\begin{aligned}
\bar{h}_{mn} &= \sum_{pq}^M V(\vec{k})_{mp} V(\vec{k})_{nq}^* \cdot h_{pq} \\
\bar{g}_{mn\mu\nu} &= \sum_{pqrs}^M V(\vec{k})_{mp} V(\vec{k})_{nr} V(\vec{k})_{\mu s}^* V(\vec{k})_{\nu q}^* \cdot g_{pqrs} \\
&= \sum_{pqrs}^M V(\vec{k})_{mp} V(\vec{k})_{nr} \cdot g_{pqrs} \cdot [V(\vec{k})^\dagger]_{s\mu} [V(\vec{k})^\dagger]_{q\nu}
\end{aligned}$$

$$V(\vec{k}) = e^{-K}, \text{ with } K = \text{skew}(\vec{k}) = \begin{pmatrix} 0 & k_{12} & k_{13} & \dots & k_{1M} \\ -k_{21}^* & 0 & k_{23} & \dots & k_{2M} \\ -k_{31}^* & -k_{32}^* & \ddots & \dots & k_{3M} \\ \vdots & \vdots & \vdots & 0 & \vdots \\ -k_{M1}^* & -k_{M2}^* & -k_{M3}^* & \dots & 0 \end{pmatrix}.$$

$$\int \phi_p^*(\vec{r}) \phi_q(\vec{r}) d\vec{r} = \langle \phi_p | \phi_q \rangle = \delta_{pq} \forall p, q$$

$$\begin{aligned}
h_{pq} &= \langle p | h | q \rangle = \int \phi_p^*(\vec{r}_1) \hat{h}(\vec{r}_1) \phi_q(\vec{r}_1) d\vec{r}_1 \\
g_{pqrs} &= \langle pq | rs \rangle \\
&= \int \phi_p^*(\vec{r}_1) \phi_r^*(\vec{r}_2) \frac{1}{|\vec{r}_1 - \vec{r}_2|} \phi_q(\vec{r}_1) \phi_s(\vec{r}_2) d\vec{r}_1 d\vec{r}_2
\end{aligned}$$

$$\hat{h}(\vec{r}_1) = -\frac{\nabla_{\vec{r}_1}^2}{2} - \sum_I^{N_{\text{atoms}}} \frac{Z_I}{|\vec{r}_1 - \vec{R}_I|}$$



$$\phi_p(\vec{r}) = \sum_{\mu}^M C_{\mu p} \chi_{\mu p}(\vec{r}).$$

$$\delta_{pq} = \sum_{\mu\nu} C_{\mu p}^* S_{\mu\nu} C_{\nu q},$$

$$S_{\mu\nu} = \int d\vec{r} \chi_{\mu}^*(\vec{r}) \chi_{\nu}(\vec{r})$$

$$E_{QCSO} = \min_R \left[\min_{|b\rangle \in \mathcal{S} \subset \mathcal{D}} [\langle b | H_D(R) | b \rangle] \right]$$

$$E_{QUSO}^{V_P} = \min_R \left[\min_{|b\rangle \in \mathcal{D}} [\langle b | H_D(R) + \lambda V_P | b \rangle] \right].$$

$$\sum_{\mathcal{K} \in \mathcal{X}} \prod_{i \in \mathcal{K}} \left(\frac{I - Z_i}{2}\right) = \sum_{\mathcal{K} \in \mathcal{S}} \bar{z}_{\mathcal{K}} = \Omega$$

$$\begin{aligned} V_P(\lambda) &= \lambda \left[\sum_{\mathcal{K} \in \mathcal{X}} \prod_{i \in \mathcal{K}} \left(\frac{I - Z_i}{2}\right) - \Omega \right]^2 \\ &= \lambda \left[\sum_{\mathcal{K} \in \mathcal{X}} \bar{z}_{\mathcal{K}} - \Omega \right]^2 \end{aligned}$$

$$V_P^{\alpha}(\lambda) \, = \, \lambda \left(\sum_{i \in \mathcal{X}_{\alpha}} \left(\frac{I - Z_i}{2} \right) - N_{\alpha} \right)^2$$

$$V_P^{\beta}(\lambda) \, = \, \lambda \left(\sum_{i \in \mathcal{X}_{\beta}} \left(\frac{I - Z_i}{2} \right) - N_{\beta} \right)^2$$

$$S^2=S_z+S_z^2+S_-S_+$$

$$V_P^{S^2}(\lambda) = \lambda [N_{\beta} - \sum_{k=0}^{M/2-1} \left(\frac{I + Z_{2k}Z_{2k+1}}{2}\right) - \underbrace{S^2}_{\text{desired value}}]^2.$$

$$V_P^{S^2}(\lambda) = \lambda \left[N_{\beta} - \sum_{k=0}^{M/2-1} \left(\frac{I + Z_{2k}Z_{2k+1}}{2}\right) \right].$$

$$\langle S^2 \rangle = \left(\frac{N_{\alpha} - N_{\beta}}{2}\right)^2 + \left(\frac{N_{\alpha} - N_{\beta}}{2}\right) + N_{\beta} - \sum_{j \in O_{\alpha}} \sum_{k \in O_{\beta}} \left| \left\langle \psi_j^{\alpha} \mid \psi_k^{\beta} \right\rangle \right|^2$$

$$\left\langle \psi_j^{\alpha} \mid \psi_k^{\beta} \right\rangle = \delta_{jk}$$

$$\langle \psi_p | \psi_q \rangle = \sum_{\mu\nu} C_{\mu p}^* S_{\mu\nu} C_{\nu q} = \delta_{pq}.$$

$$S_{\mu\nu} = \int d\vec{r} \chi_{\mu}^*(\vec{r}) \chi_{\nu}(\vec{r})$$

$$\begin{aligned} \langle S_{ROHF}^2 \rangle &= \left(\frac{N_{\alpha} - N_{\beta}}{2} \right)^2 + \left(\frac{N_{\alpha} - N_{\beta}}{2} \right) + N_{\beta} - \sum_{j \in O_{\alpha}} \sum_{k \in O_{\beta}} \delta_{jk} \\ &= \left(\frac{N_{\alpha} - N_{\beta}}{2} \right)^2 + \left(\frac{N_{\alpha} - N_{\beta}}{2} \right) + N_{\beta} - N_{\text{paired}} \\ &= \left(\frac{N_{\alpha} - N_{\beta}}{2} \right)^2 + \left(\frac{N_{\alpha} - N_{\beta}}{2} \right) + N_{\text{unpaired } \beta} \end{aligned}$$

$$f(\vec{x}) = \min_{\vec{y} \in \{0,1\}^m} \{g(\vec{x}, \vec{y})\} \quad \forall \vec{x} \in \{0,1\}^n$$

$$H_D(R) = \sum_n^M \bar{h}_{nn} \left(\frac{I - Z_n}{2} \right) + \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} (I - Z_n - Z_m + Z_m Z_n)$$

$$\mapsto \\ H_{QUSO}(R) = \sum_n^M \bar{h}_{nn} \left(\frac{1 - z_n}{2} \right) + \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} (1 - z_n - z_m + z_m z_n)$$

$$\begin{aligned} H_{QUBO}(R) &= \sum_n^M \bar{h}_{nn} \left(\frac{1 - (1 - 2x_n)}{2} \right) + \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} (1 - (1 - 2x_n) - (1 - 2x_m) + (1 - 2x_n)(1 - 2x_m)) \\ &= \sum_n^M \bar{h}_{nn}(x_n) + \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} (4x_n x_m) \\ &= \sum_n^M \bar{h}_{nn}(x_n) + \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M ([\bar{g}_{mmnn} - \bar{g}_{mnnm}] x_n x_m). \end{aligned}$$

$$\begin{aligned} C_{\text{MaxCut}} &= \sum_{ij}^M A_{ij} \left(\frac{I - Z_i Z_j}{2} \right) \\ &= \sum_{ij}^M \left(\frac{A_{ij} I}{2} + \frac{-A_{ij} Z_i Z_j}{2} \right) \end{aligned}$$

$$H_D^{\text{ferm}}(R) = \sum_n^M \bar{h}_{nn} \alpha_n^\dagger \alpha_n + \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M ([\bar{g}_{mmnn} - \bar{g}_{mnnm}] \alpha_m^\dagger \alpha_m \alpha_n^\dagger \alpha_n)$$

$$\mapsto \\ H_D^{JW}(R) = \sum_n^M \bar{h}_{nn} \left(\frac{I - Z_n}{2} \right) + \frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} (I - Z_n - Z_m + Z_m Z_n).$$

$$\begin{aligned}
H_{\omega}^{\text{ferm}}(R) &= \sum_{n=1}^M \bar{h}_{nn}(\alpha_n^{\dagger}\alpha_n + \alpha_{\omega}^{\dagger}\alpha_{\omega} - 2\alpha_n^{\dagger}\alpha_n\alpha_{\omega}^{\dagger}\alpha_{\omega}) + \\
&\frac{1}{2} \sum_{\substack{m,n=1 \\ m \neq n}}^M \left([\bar{g}_{mmnn} - \bar{g}_{mnnm}](\alpha_{\omega}^{\dagger}\alpha_{\omega} + \alpha_m^{\dagger}\alpha_m\alpha_n^{\dagger}\alpha_n - \alpha_n^{\dagger}\alpha_n\alpha_{\omega}^{\dagger}\alpha_{\omega} - \alpha_m^{\dagger}\alpha_m\alpha_{\omega}^{\dagger}\alpha_{\omega}) \right) \\
&\mapsto \\
H_{\omega}^{\text{JW}}(R) &= \sum_{n=1}^M \bar{h}_{nn} \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \frac{1}{2} \sum_{\substack{m,n=1 \\ m \neq n}}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} (I - Z_n Z_{\omega} - Z_m Z_{\omega} + Z_m Z_n). \\
\\
H_{|1\rangle_{\omega}}^{\text{ferm}}(R) &= \sum_n^M \bar{h}_{nn}(1 - \alpha_n^{\dagger}\alpha_n) + \\
&\frac{1}{2} \sum_{\substack{m,n \\ m \neq n}}^M \left([\bar{g}_{mmnn} - \bar{g}_{mnnm}](1 + \alpha_m^{\dagger}\alpha_m\alpha_n^{\dagger}\alpha_n - \alpha_n^{\dagger}\alpha_n - \alpha_m^{\dagger}\alpha_m) \right) \\
\\
H_{\text{MaxCut}}^{\text{JW}}(R) &= \sum_{n=1}^M -\bar{h}_{nn} \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \sum_{\substack{m,n=1 \\ m \neq n}}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \left(\frac{I - Z_n Z_{\omega} - Z_m Z_{\omega} + Z_m Z_n}{2} \right). \\
\\
H_{\text{MaxCut}}^{\text{JW}}(R) &= \sum_{n=1}^M \left(-\bar{h}_{nn} + \left[\sum_{m=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \right] \right) \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \sum_{m,n=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \left(\frac{-Z_m Z_{\omega} + Z_m Z_n}{2} \right) \\
&= \sum_{n=1}^M \left(-\bar{h}_{nn} + \left[\sum_{m=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \right] \right) \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \sum_{m=1}^M \left(\left[\sum_{n=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \right] \right) \left(\frac{-Z_m Z_{\omega}}{2} \right) \\
&\quad + \sum_{m,n=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \left(\frac{Z_m Z_n}{2} \right) \\
&= \sum_{n=1}^M \left(-\bar{h}_{nn} + \left[\sum_{m=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \right] \right) \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \underbrace{\sum_{m=1}^M \left(\left[\sum_{n=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \right] \right)}_{\text{relabelled } m \leftrightarrow n \text{ (as dummy index)}} \left(\frac{I - Z_n Z_{\omega} - I}{2} \right) \\
&\quad + \sum_{m,n=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \left(\frac{Z_m Z_n}{2} \right) \\
&= \sum_{n=1}^M \left(-\bar{h}_{nn} + \left[\sum_{m=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} + \frac{\bar{g}_{nnmm} - \bar{g}_{nnmm}}{4} \right] \right) \left(\frac{I - Z_n Z_{\omega}}{2} \right) \\
&\quad + \sum_{m,n=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \left(\frac{Z_m Z_n}{2} \right) - \sum_{n=1}^M \left(\left[\sum_{m=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \right] \right) \left(\frac{I}{2} \right) \\
\\
H_{\text{MaxCut}}^{\text{JW}}(R) &= \sum_{n=1}^M [-\bar{h}_{nn} + G_n] \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \sum_{m,n=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} \left(\frac{Z_m Z_n}{2} \right) - c \frac{I}{2} \\
&= \sum_{n=1}^M [-\bar{h}_{nn} + G_n] \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \sum_{m,n=1}^M \underbrace{\frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4}}_{\times -1} \underbrace{\left(\frac{-Z_m Z_n}{2} \right)}_{\times -1} - c \frac{I}{2} \\
&= \sum_{n=1}^M [-\bar{h}_{nn} + G_n] \left(\frac{I - Z_n Z_{\omega}}{2} \right) + \sum_{m,n=1}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} \left(\frac{I - Z_m Z_n}{2} - \frac{I}{2} \right) - c \frac{I}{2},
\end{aligned}$$

$$G_n = \left[\sum_{m=1}^M \frac{\bar{g}_{mnnm} - \bar{g}_{mmnn}}{4} + \frac{\bar{g}_{nmmn} - \bar{g}_{nnmm}}{4} \right]$$

$$c = \sum_{n=1}^M \left(\left[\sum_{m=1}^M \frac{\bar{g}_{nmmn} - \bar{g}_{nnmm}}{4} \right] \right)$$

$$H_{\text{MaxCut}}^{\text{JW}}(R) = \sum_{n=1}^M [-\bar{h}_{nn} + G_n] \left(\frac{I - Z_n Z_\omega}{2} \right) + \sum_{m,n=1}^M \frac{\bar{g}_{mmnn} - \bar{g}_{mnnm}}{4} \left(\frac{I - Z_m Z_n}{2} \right),$$

$$P = \left(\sum_{j=1}^M \alpha_j^\dagger \alpha_j - N \right)^2$$

$$\mapsto$$

$$P_\omega = \left(\sum_{j=1}^M [\alpha_j^\dagger \alpha_j + \alpha_\omega^\dagger \alpha_\omega - 2\alpha_j^\dagger \alpha_j \alpha_\omega^\dagger \alpha_\omega] - N \right)^2.$$

$$H_\omega^{\text{ferm}}(R) = \left(\begin{array}{cccc|cccc} a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & c & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a \end{array} \right) = |0\rangle_\omega \langle 0|_\omega \otimes \left(\begin{array}{cccc} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & c \end{array} \right) + |1\rangle_\omega \langle 1|_\omega \otimes \left(\begin{array}{cccc} c & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & a \end{array} \right)$$

$$S_{\text{D}}^2 = \sum_{p=1}^{M/2} \frac{3}{4} (a_{2p}^\dagger a_{2p} + a_{2p+1}^\dagger a_{2p+1} - a_{2p}^\dagger a_{2p} a_{2p+1}^\dagger a_{2p+1} - a_{2p+1}^\dagger a_{2p+1} a_{2p}^\dagger a_{2p}) +$$

$$\sum_{p=1}^{M/2} \sum_{m=1}^{M/2} \frac{1}{4} (a_{2p}^\dagger a_{2p} a_{2m}^\dagger a_{2m} - a_{2p}^\dagger a_{2p} a_{2m+1}^\dagger a_{2m+1} - a_{2p+1}^\dagger a_{2p+1} a_{2m}^\dagger a_{2m} + a_{2p+1}^\dagger a_{2p+1} a_{2m+1}^\dagger a_{2m+1})$$

$$\text{Maximize} \left[\frac{1}{2} \sum_{i < j}^M w_{ij} (1 - z_i \cdot z_j) \right]$$

$$\text{s.t. } z_k \in \{-1, 1\}.$$

$$\text{Maximize} \left[\frac{1}{2} \sum_{i < j}^M w_{ij} (1 - v_i \cdot v_j) \right]$$

$$\text{s.t. } v_k \in \mathbb{R}^M, \|v_k\| = 1$$

$$\begin{aligned} & \text{Maximize} \left[\frac{1}{2} \sum_{i < j}^M w_{ij} (1 - X_{ij}) \right] \\ & \text{s.t. } X \succeq 0 \\ & [X]_{ii} = 1, \forall i = 1, \dots, M. \end{aligned}$$

$$\vec{z}_{cut} = \text{sign}[\tilde{V} \cdot \vec{r}],$$

$$\begin{aligned} \max_{z_i \in \{-1,1\}} \left[\sum_{i < j}^M w_{ij} \left(\frac{1 - z_i z_j}{2} \right) \right] &\geq \mathbb{E}[\text{cut}(H)] = \sum_{i < j}^M w_{ij} (\text{Pr}[(i,j) \text{ in cut }]) \geq \alpha_{G.W} \left[\sum_{i < j}^M w_{ij} \left(\frac{1 - v_i \cdot v_j}{2} \right) \right] \\ &\geq \alpha_{G.W} \left[\sum_{i < j}^M w_{ij} \left(\frac{1 - \tilde{z}_i \cdot \tilde{z}_j}{2} \right) \right] \end{aligned}$$

$$\max_{z_i \in \{-1,1\}} \left[\sum_{i < j}^M w_{ij} \left(\frac{1 - z_i \cdot z_j}{2} \right) \right] - W^- \geq \alpha_{G.W} \left(\left[\sum_{i < j}^M w_{ij} \left(\frac{1 - \tilde{z}_i \tilde{z}_j}{2} \right) \right] - W^- \right),$$

$$W^- = \sum_{\substack{i,j \\ \forall w_{ij} < 0}}^M w_{ij}.$$

$$\max_{z_i \in \{-1,1\}} \left[\sum_{i < j}^M w_{ij} \left(\frac{1 - z_i z_j}{2} \right) \right] \geq \alpha_{G.W} \left[\sum_{i < j}^M w_{ij} \left(\frac{1 - \tilde{z}_i \tilde{z}_j}{2} \right) \right] + (1 - \alpha_{G.W}) W^-,$$

$$(pq \mid rs) = g_{pqrs} = \sum_{\mu\nu\lambda\sigma}^{N_s} C_{\mu p} C_{\nu q} (\mu\nu \mid \lambda\sigma) C_{\lambda r} C_{\sigma s}.$$

$$(pq \mid qp) = W_{pq}^{(pq \mid pq)} = \sum_{\mu\nu\lambda\sigma}^{N_s} C_{\mu p} C_{\nu q} (\mu\nu \mid \lambda\sigma) C_{\lambda q} C_{\sigma p},$$

$$(pp \mid qq) = W_{pq}^{(pp \mid qq)} = \sum_{\mu\nu\lambda\sigma}^{N_s} C_{\mu p} C_{\nu p} (\mu\nu \mid \lambda\sigma) C_{\lambda q} C_{\sigma q}.$$

Scaling	Current	Remaining
$(N_s)^5$	$\mu\nu\lambda\sigma, \mu p \mapsto \nu\lambda\sigma p$	$\nu q, \lambda r, \sigma s, \nu\lambda\sigma p \mapsto p q r s$
$(N_s)^5$	$\nu\lambda\sigma p, \nu q \mapsto \lambda\sigma p q$	$\lambda r, \sigma s, \lambda\sigma p q \mapsto p q r s$

$$(N_s)^5 \quad \lambda\sigma pq, \lambda r \mapsto \sigma pqr \quad \sigma s, \sigma pqr \mapsto pqrs$$

$$(N_s)^5 \quad \sigma pqr, \sigma s \mapsto pqrs \quad pqrs \mapsto pqrs$$

Scaling	Current	Remaining
$(N_s)^3$	$\sigma s, \mu p \mapsto \sigma p\mu$	$\nu q, \mu\nu\lambda\sigma, \lambda q, \sigma p\mu \mapsto pq$
$(N_s)^3$	$\lambda q, \nu q \mapsto \lambda q\nu$	$\mu\nu\lambda\sigma, \sigma p\mu, \lambda q\nu \mapsto pq$
$(N_s)^5$	$\sigma p\mu, \mu\nu\lambda\sigma \mapsto p\nu\lambda$	$\lambda q\nu, p\nu\lambda \mapsto pq$
$(N_s)^4$	$p\nu\lambda, \lambda q\nu \mapsto pq$	$pq \mapsto pq$

Scaling	Current	Remaining
$(N_s)^3$	$\nu p, \mu p \mapsto \nu p\mu$	$\mu\nu\lambda\sigma, \lambda q, \sigma q, \nu p\mu \mapsto pq$
$(N_s)^5$	$\nu p\mu, \mu\nu\lambda\sigma \mapsto p\lambda\sigma$	$\lambda q, \sigma q, p\lambda\sigma \mapsto pq$
$(N_s)^3$	$\sigma q, \lambda q \mapsto \sigma ql$	$p\lambda\sigma, \sigma ql \mapsto pq$
$(N_s)^4$	$\sigma ql, p\lambda\sigma \mapsto pq$	$pq \mapsto pq$

$H_D(\vec{\kappa}) \leftarrow$ Build Hamiltonian

$$|b_{min}\rangle \leftarrow \operatorname{argmin}_{|b\rangle \in \mathcal{D}} \left[\langle b | H_D(\vec{\kappa}) | b \rangle \right]$$

$$E_{prev} \leftarrow \langle b_{min} | H_D(\vec{\kappa}) | b_{min} \rangle$$

$$\text{converged} \leftarrow 0$$



$$\vec{\kappa} \leftarrow \operatorname{argmin}_{\vec{\kappa}} \left[\langle b_{min} | H_D(\vec{\kappa}) | b_{min} \rangle \right]$$

$$H_D(\vec{\kappa}) \leftarrow \text{Build Hamiltonian}$$

$$|b_{min}\rangle \leftarrow \operatorname{argmin}_{|b\rangle \in \mathcal{D}} \left[\langle b | H_D(\vec{\kappa}) | b \rangle \right]$$

$$E_{new} \leftarrow \langle b_{min} | H_D(\vec{\kappa}) | b_{min} \rangle$$

if $(E_{prev} - E_{new}) < \epsilon$ **then**
 converged $\leftarrow 1$

Require: $H_{core}, (\mu\nu|\lambda\sigma), \gamma^{initial}, S, \epsilon$
 $U, \Sigma, V^\dagger \leftarrow \text{SVD}(S)$
 $A \leftarrow U\Sigma^{-1/2}V^\dagger$

$J \leftarrow \sum_{\lambda,\sigma} (\mu\nu|\lambda\sigma) \gamma_{\lambda\sigma}$
 $K \leftarrow \sum_{\lambda,\sigma} (\mu\nu|\lambda\sigma) \gamma_{\lambda\sigma}$
 $F \leftarrow H_{core} + 2J - K$

$F' \leftarrow A^\dagger F A$
 $O, C' \leftarrow \text{eigh}(F')$
 $C_{opt} \leftarrow U C'$

$H_D(C^{opt}) \leftarrow \text{Build Hamiltonian}$

$|b_{min}\rangle \leftarrow \text{argmin}_{|b\rangle \in \mathcal{D}} \left[\langle b | H_D(C^{opt}) | b \rangle \right]$

$T_{pq} \leftarrow \langle b_{min} | (a_{2p}^\dagger a_{2q} + a_{2p+1}^\dagger a_{2q+1}) | b_{min} \rangle$
 $\gamma \leftarrow C^{opt} T (C^{opt})^\dagger$

$J \leftarrow \sum_{\lambda,\sigma} (\mu\nu|\lambda\sigma) \gamma_{\lambda\sigma}$
 $K \leftarrow \sum_{\lambda,\sigma} (\mu\nu|\lambda\sigma) \gamma_{\lambda\sigma}$
 $F \leftarrow H_{core} + 2J - K$
 $E_{prev} \leftarrow 0.5 \sum_{\mu,\nu} \gamma_{\mu\nu} (H_{core} + F_{\mu\nu})$
 $\text{converged} \leftarrow 0$

while converged $\neq 1$ **do**

$F' \leftarrow A^\dagger F A$
 $O, C' \leftarrow \text{eigh}(F')$
 $C_{opt} \leftarrow U C'$

```

 $H_D(C^{opt}) \leftarrow \text{Build Hamiltonian}$ 
 $|b_{min}\rangle \leftarrow \operatorname{argmin}_{|b\rangle \in \mathcal{D}} \left[ \langle b| H_D(C^{opt}) |b\rangle \right]$ 
 $T_{pq} \leftarrow \langle b_{min}| (a_{2p}^\dagger a_{2q} + a_{2p+1}^\dagger a_{2q+1}) |b_{min}\rangle$ 
 $\gamma \leftarrow C^{opt} T (C^{opt})^\dagger$ 

 $J \leftarrow \sum_{\lambda, \sigma} (\mu\nu | \lambda\sigma) \gamma_{\lambda\sigma}$ 
 $K \leftarrow \sum_{\lambda, \sigma} (\mu\nu | \lambda\sigma) \gamma_{\lambda\sigma}$ 
 $F \leftarrow H_{core} + 2J - K$ 
 $E_{new} \leftarrow 0.5 \sum_{\mu, \nu} \gamma_{\mu\nu} (H_{core} + F_{\mu\nu})$ 
if  $(E_{prev} - E_{new}) < \epsilon$  then
    converged  $\leftarrow 1$ 
else
     $E_{prev} \leftarrow E_{new}$ 
end if
end while

Return:  $E_{new}$ ,  $C^{opt}$  and  $|b_{min}\rangle$ 

```

$$\hat{\mathcal{H}} = \hat{H} + \lambda[\hat{S}^2 - S(S+1)].$$

$$\frac{\partial}{\partial \lambda} \langle \text{c-UHF}(S) | \hat{\mathcal{H}} | \text{c-UHF}(S) \rangle = \langle \text{c-UHF}(S) | \hat{S}^2 | \text{c-UHF}(S) \rangle - S(S+1) \equiv 0$$

$$\mathcal{E}(S) = \langle \text{c-UHF}(S) | \hat{H} | \text{c-UHF}(S) \rangle$$

$$E_{\text{UHF}} = \min_S \mathcal{E}(S)$$

$$|\text{c-UHF}\rangle = \prod_{i=0}^{\frac{N}{2}-1} a_{2i\uparrow}^\dagger \prod_{j=0}^{\frac{N}{2}-1} a_{2j+1\downarrow}^\dagger |\theta\rangle$$

$$\begin{aligned}\{a_{2i\uparrow}^\dagger, a_{2j\uparrow}\} &= \{a_{2i+1\downarrow}^\dagger, a_{2j+1\downarrow}\} = \delta_{ij}, \\ \{a_{2i\uparrow}^\dagger, a_{2j+1\downarrow}\} &= \{a_{2i\downarrow}^\dagger, a_{2j+1\uparrow}\} = 0, \\ \{a_{2i\uparrow}^\dagger, a_{2j+1\uparrow}\} &= \{a_{2i\downarrow}^\dagger, a_{2j+1\downarrow}\} = G_{2i,2j+1}, \forall i, j = 0 \dots L-1 \\ \{a_{i\sigma}^\dagger, a_{j\tau}^\dagger\} &= \{a_{i\sigma}, a_{j\tau}\} = 0, \forall i, j = 0 \dots 2L-1 \forall \sigma, \tau = \uparrow, \downarrow.\end{aligned}$$

$$\{b_{i\sigma}^\dagger, b_{j\tau}^\dagger\} = \{b_{i\sigma}, b_{j\tau}\} = 0, \{b_{i\sigma}^\dagger, b_{j\tau}\} = \delta_{ij}\delta_{\sigma\tau}. \forall ij = 1 \dots L, \sigma, \tau = \uparrow, \downarrow.$$

$$a_{2i\uparrow}^\dagger = \sum_{j=1}^L U_{ij}^\uparrow b_{j\uparrow}^\dagger, a_{2i+1\downarrow}^\dagger = \sum_{j=1}^L U_{ij}^\downarrow b_{j\downarrow}^\dagger,$$

$$\boldsymbol{U}^\uparrow (\boldsymbol{U}^\downarrow)^\dagger = \boldsymbol{G}.$$

$$\hat{S}^+ = \sum_{i=1}^L b_{i\uparrow}^\dagger b_{i\downarrow}, \hat{S}^- = (\hat{S}^+)^\dagger = \sum_{i=1}^L b_{i\downarrow}^\dagger b_{i\uparrow}, \hat{S}_0 = \frac{1}{2} \sum_{i=1}^L [b_{i\uparrow}^\dagger b_{i\uparrow} - b_{i\downarrow}^\dagger b_{i\downarrow}],$$

$$[\hat{S}_0, \hat{S}^\pm] = \pm \hat{S}^\pm, [\hat{S}^+, \hat{S}^-] = 2\hat{S}_0$$

$$\hat{S}^2 = \hat{S}_0^2 + \frac{1}{2} [\hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+]$$

$$\begin{aligned}[\hat{S}^\pm, a_{im}^\dagger] &= \sqrt{\left(\frac{1}{2} \mp m\right) \left(\frac{1}{2} \pm m + 1\right)} a_{im\pm 1}^\dagger \\ [\hat{S}_0, a_{im}^\dagger] &= m a_{im}^\dagger\end{aligned}$$

$$\hat{R}(\Omega) a_{im}^\dagger \hat{R}(\Omega)^{-1} = \sum_{m'=\pm\frac{1}{2}} a_{im'}^\dagger \mathcal{D}_{m'm}^{\frac{1}{2}}(\Omega)$$

$$\hat{P}^S = \prod_{S' \neq S} \frac{\hat{S}^2 - S'(S' + 1)}{S(S + 1) - S'(S' + 1)}$$

$$\hat{P}_{MK}^S = \int \mathcal{D}_{MK}^S(\Omega)^* \hat{R}(\Omega) d\Omega$$

$$\hat{P}_{MK}^S a_{0,\frac{1}{2}}^\dagger a_{1,-\frac{1}{2}}^\dagger |\theta\rangle = \int d\Omega \mathcal{D}_{MK}^S(\Omega)^* \hat{R}(\Omega) a_{0,\frac{1}{2}}^\dagger \hat{R}(\Omega)^{-1} \hat{R}(\Omega) a_{1,-\frac{1}{2}}^\dagger \hat{R}(\Omega)^{-1} \hat{R}(\Omega) |\theta\rangle$$

$$\hat{P}_{MK}^S a_{0,\frac{1}{2}}^\dagger a_{1,-\frac{1}{2}}^\dagger |\theta\rangle = \sum_{m_0=\pm\frac{1}{2}} \sum_{m_1=\pm\frac{1}{2}} a_{0,m_0}^\dagger a_{1,m_1}^\dagger |\theta\rangle \int d\Omega \mathcal{D}_{MK}^S(\Omega)^* \mathcal{D}_{m_0,\frac{1}{2}}^{\frac{1}{2}}(\Omega) \mathcal{D}_{m_1,-\frac{1}{2}}^{\frac{1}{2}}(\Omega)$$

$$\mathcal{D}_{m_1k_1}^{j_1}(\Omega)\mathcal{D}_{m_2k_2}^{j_2}(\Omega)=\sum_{j,mk}\langle j_1m_1,j_2m_2\mid jm\rangle\langle j_1k_1,j_2k_2\mid jk\rangle\mathcal{D}_{mk}^j(\Omega)$$

$$\int d\Omega \mathcal{D}_{m_1k_1}^{j_1}(\Omega)^*\mathcal{D}_{m_2k_2}^{j_2}(\Omega)=\frac{(4\pi)^2}{2(2j_1+1)}\delta_{j_1j_2}\delta_{m_1m_2}\delta_{k_1k_2}$$

$$\hat{P}_{MK}^S a_{0,\frac{1}{2}}^\dagger a_{1,-\frac{1}{2}}^\dagger |\theta\rangle = \frac{(4\pi)^2}{2(2S+1)} \left\langle \frac{1}{2} \frac{1}{2}, \frac{1}{2} - \frac{1}{2} \right| SK \rangle [a_0^\dagger a_1^\dagger]_M^S |\theta\rangle$$

$$[a_0^\dagger a_1^\dagger]_M^S |\theta\rangle = \sum_{m_0, m_1 = \pm \frac{1}{2}} \left\langle \frac{1}{2} m_0, \frac{1}{2} m_1 \right| SM \rangle a_{0m_0}^\dagger a_{1m_1}^\dagger |\theta\rangle,$$

$$a_{0,+\frac{1}{2}}^\dagger a_{1,-\frac{1}{2}}^\dagger |\theta\rangle = a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger |\theta\rangle$$

$$a_{0,-\frac{1}{2}}^\dagger a_{1,+\frac{1}{2}}^\dagger |\theta\rangle = a_{0\downarrow}^\dagger a_{1\uparrow}^\dagger |\theta\rangle$$

$$a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle$$

$$\hat{P}_{MK}^S a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle = \frac{(4\pi)^2}{4(2S+1)} \delta_{K0} \sum_{S_{01}, S_{23}} (-)^{S_{01}+S_{23}} \langle S_{01} 0, S_{23}, 0 | S0 \rangle \left[[a_0^\dagger a_1^\dagger]^{S_{01}} [a_2^\dagger a_3^\dagger]^{S_{23}} \right]_M^S |\theta\rangle.$$

$$\hat{P}_{00}^1 a_{0\uparrow}^\dagger a_{1,\downarrow}^\dagger |\theta\rangle = \frac{(4\pi)^2}{6\sqrt{2}} [a_0^\dagger a_1^\dagger]_0^1 |\theta\rangle,$$

$$a_{1\downarrow}^\dagger = \sum_{i=0}^{L-1} G_{2i,1} a_{2i\downarrow}^\dagger,$$

$$\hat{P}_{00}^1 a_{0\uparrow}^\dagger a_{1,\downarrow}^\dagger |\theta\rangle = \frac{(4\pi)^2}{6\sqrt{2}} \sum_{i=0}^{L-1} G_{2i,1} [a_0^\dagger a_{2i}^\dagger]_0^1 |\theta\rangle = \frac{(4\pi)^2}{6\sqrt{2}} \sum_{i=1}^{L-1} G_{2i,1} [a_0^\dagger a_{2i}^\dagger]_0^1 |\theta\rangle,$$

$$\hat{P}_{00}^1 a_{0\uparrow}^\dagger a_{0,\downarrow}^\dagger |\theta\rangle = 0.$$

$$\{a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle, a_{0\uparrow}^\dagger a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle, a_{0\downarrow}^\dagger a_{1\uparrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle, a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\downarrow}^\dagger a_{3\uparrow}^\dagger |\theta\rangle, a_{0\downarrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\uparrow}^\dagger |\theta\rangle, a_{0\downarrow}^\dagger a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger a_{3\uparrow}^\dagger |\theta\rangle\}.$$

$$a_{0\uparrow}^\dagger a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle = a_{0\uparrow}^\dagger a_{0\uparrow}^\dagger a_{2\downarrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle = 0$$

$$a_{0\downarrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\uparrow}^\dagger |\theta\rangle = a_{0\downarrow}^\dagger a_{0\downarrow}^\dagger a_{2\downarrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle = 0$$

$$a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle = a_{0\uparrow}^\dagger a_{0\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle$$

$$a_{0\downarrow}^\dagger a_{1\uparrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle = a_{0\downarrow}^\dagger a_{0\uparrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle$$

$$a_{0\downarrow}^\dagger a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger a_{3\uparrow}^\dagger |\theta\rangle$$

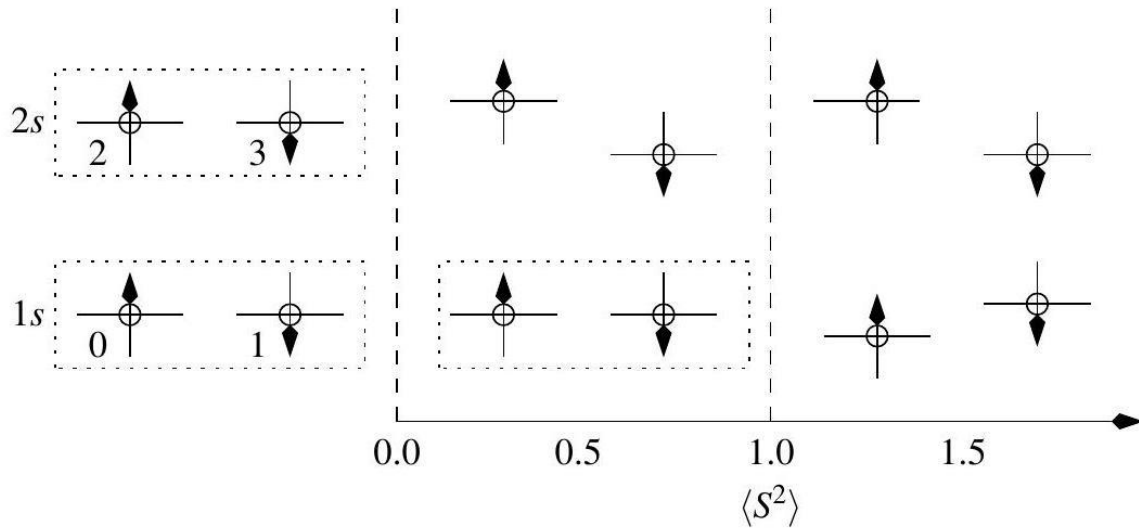
$$a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\downarrow}^\dagger a_{3\uparrow}^\dagger |\theta\rangle$$

$$a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger a_{3\downarrow}^\dagger |\theta\rangle \text{ and } a_{0\uparrow}^\dagger a_{1\downarrow}^\dagger a_{2\downarrow}^\dagger a_{3\uparrow}^\dagger |\theta\rangle$$

$$k_{\text{eff}} = \binom{M}{M/2}$$



$$0 \leq \langle c - \text{UHF} | S^2 | c - \text{UHF} \rangle \leq \frac{N}{2}.$$



$$|(S_{01}S_{23})S\rangle = \left[[a_0^\dagger a_1^\dagger]^{S_{01}} [a_2^\dagger a_3^\dagger]^{S_{23}} \right]_0^S |\theta\rangle$$

$$\begin{pmatrix} |(00)0\rangle \\ |(11)0\rangle \\ |(01)1\rangle \\ |(10)1\rangle \\ |(11)1\rangle \\ |(11)2\rangle \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & 0 \\ \frac{\sqrt{3}}{3} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{3} \\ 0 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix} \begin{pmatrix} |01\bar{2}\bar{3}\rangle \\ |0\bar{1}2\bar{3}\rangle \\ |\bar{0}12\bar{3}\rangle \\ |0\bar{1}\bar{2}3\rangle \\ |\bar{0}\bar{1}\bar{2}3\rangle \\ |\bar{0}\bar{1}23\rangle \end{pmatrix}$$

$$\mathbf{G} = \begin{pmatrix} 1 & G_{01} & 0 & G_{03} \\ G_{10} & 1 & G_{12} & 0 \\ 0 & G_{21} & 1 & G_{23} \\ G_{30} & 0 & G_{32} & 1 \end{pmatrix}$$

$$\mathbf{M} = \begin{pmatrix} f_1 & -G_{21}^2 & -f_3f_4 & -f_3f_4 & -G_{03}^2 & f_4^2 \\ -G_{21}^2 & 1 & -G_{01}^2 & -G_{23}^2 & (f_3-f_4)^2 & -G_{03}^2 \\ -f_3f_4 & -G_{01}^2 & f_2 & f_3^2 & -G_{23}^2 & -f_3f_4 \\ -f_3f_4 & -G_{23}^2 & f_3^2 & f_2 & -G_{01}^2 & -f_3f_4 \\ -G_{03}^2 & (f_3-f_4)^2 & -G_{23}^2 & -G_{01}^2 & 1 & -G_{21}^2 \\ f_4^2 & -G_{03}^2 & -f_3f_4 & -f_3f_4 & -G_{21}^2 & f_1 \end{pmatrix}$$

$$f_1 = (1 - G_{01}^2)(1 - G_{23}^2)$$

$$f_2 = (1 - G_{03}^2)(1 - G_{21}^2)$$

$$f_3 = G_{01}G_{23}$$

$$f_4 = G_{03}G_{21}$$



$$U_R M U_R^T = \begin{pmatrix} M_{11}^{(0)} & M_{12}^{(0)} & \cdot & \cdot & \cdot & \cdot \\ M_{21}^{(0)} & M_{22}^{(0)} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & M_{11}^{(1)} & M_{12}^{(1)} & M_{13}^{(1)} & \cdot \\ \cdot & \cdot & M_{21}^{(1)} & M_{22}^{(1)} & M_{23}^{(1)} & \cdot \\ \cdot & \cdot & M_{31}^{(1)} & M_{32}^{(1)} & M_{33}^{(1)} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & M_{11}^{(2)} \end{pmatrix}$$

$$M_{11}^{(0)} = 1 + G_{01}^2 + G_{23}^2 - \frac{1}{2}G_{03}^2 - \frac{1}{2}G_{21}^2 + f_3^2 - f_3f_4 + f_4^2$$

$$M_{12}^{(0)} = M_{21}^{(0)} = -\frac{\sqrt{3}}{2}[G_{03}^2 + G_{21}^2 - 2f_3f_4]$$

$$M_{22}^{(0)} = 1 - G_{01}^2 - G_{23}^2 + \frac{1}{2}G_{03}^2 + \frac{1}{2}G_{21}^2 + f_3^2 + f_3f_4 + f_4^2$$

$$M_{11}^{(1)} = 1 + G_{01}^2 - G_{23}^2 - \frac{1}{2}G_{03}^2 - \frac{1}{2}G_{21}^2 - f_3^2 + f_3f_4$$

$$M_{12}^{(1)} = M_{21}^{(1)} = \frac{1}{2}G_{03}^2 + \frac{1}{2}G_{21}^2 + f_3f_4 - f_4^2$$

$$M_{22}^{(1)} = 1 - G_{01}^2 + G_{23}^2 - \frac{1}{2}G_{03}^2 - \frac{1}{2}G_{21}^2 - f_3^2 + f_3f_4$$

$$M_{13}^{(1)} = M_{23}^{(1)} = M_{31}^{(1)} = M_{32}^{(1)} = \frac{\sqrt{2}}{2}[G_{03}^2 - G_{21}^2]$$

$$M_{33}^{(1)} = 1 - G_{01}^2 - G_{23}^2 + f_3^2 - f_4^2$$

$$M_{11}^{(2)} = 1 - G_{01}^2 - G_{23}^2 - G_{03}^2 - G_{12}^2 + (f_3 - f_4)^2$$

$$G_{01} = 1, G_{03} = G_{21} = 0$$

$$M_{11}^{(0)} = 2 + 2G_{23}^2$$

$$M_{11}^{(1)} = 2 - 2G_{23}^2,$$

$$G_{23} = 1,$$

$$M_{11}^{(0)} = 4$$

$$\bar{x}_i \cdot b = b \cdot M_{x_i}$$

$$\bar{\xi}_i^{(j)} v_j = v_j \cdot M_{x_i}$$

$$f_1(x_1,x_2,\ldots,x_n)=f_2(x_1,x_2,\ldots,x_n)=\cdots=f_t(x_1,x_2,\ldots,x_n)=0$$

$$(x_1,x_2,\ldots,x_n)=\left(\bar{\xi}_1^{(j)},\bar{\xi}_2^{(j)},\ldots,\bar{\xi}_n^{(j)}\right)$$

$$\bar{\xi}_i^{(j)}=\frac{(v_j\cdot M_{x_i},v_j)}{(v_j,v_j)}$$

$$\left|v_j\right\rangle\left|\text{Ancilla}_1\right\rangle\left|\text{Ancilla}_2\right\rangle\cdots\left|\text{Ancilla}_n\right\rangle\rightarrow\left|v_j\right\rangle\left|\bar{\xi}_1^{(j)}\right\rangle\left|\bar{\xi}_2^{(j)}\right\rangle\cdots\left|\bar{\xi}_n^{(j)}\right\rangle$$

$$\begin{pmatrix} V(x,y) & -1 \\ -1 & V(x,y) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = e \begin{pmatrix} x \\ y \end{pmatrix}$$

$$I=(xV(x,y)-y-ex,yV(x,y)-x-ey,x^2+y^2-1)$$

$$I_{std}=(e^2-1,2y^2-1,x+ye)$$

$$(x,y,e)=\left(\pm\frac{1}{\sqrt{2}},\pm\frac{1}{\sqrt{2}},-1\right),\left(\pm\frac{1}{\sqrt{2}},\mp\frac{1}{\sqrt{2}},1\right)$$

$$b[0]=ye$$

$$b[1]=y$$

$$b[2]=e$$

$$b[3]=1$$

$$m_x=\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -0.5 & 0 & 0 \\ -0.5 & 0 & 0 & 0 \end{pmatrix}$$

$$m_y=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \end{pmatrix}$$

$$m_e=\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} v & (vm_x,v) & (vm_y,v) & (vm_e,v) \\ \left(-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},-1,1\right) & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -1 \\ \left(\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},-1,1\right) & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -1 \\ \left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},1,1\right) & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1 \\ \left(-\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},1,1\right) & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 1 \end{pmatrix}$$

$$E_{HF}=\sum_i\langle i|h|i\rangle+\frac{1}{2}\sum_{ij}([\textit{ii}|\textit{jj}]-[\textit{ij}|\textit{ji}])$$

$$\langle i|h|i\rangle=\int d\mathbf{x}_1\chi_i^*(\mathbf{x}_1)h(\mathbf{r}_1)\chi_j(\mathbf{x}_1)$$

$$[ij\mid kl]=\int d\mathbf{x}_1d\mathbf{x}_2\chi_i^*(\mathbf{x}_1)\chi_j(\mathbf{x}_1)\frac{1}{r_{12}}\chi_i^*(\mathbf{x}_2)\chi_j(\mathbf{x}_2)$$

$$\chi_i(\mathbf{x})=\left(x\phi_{1s,He}(r-R_{He})+y\phi_{1s,H}(r-R_H)\right)\sigma_i$$

$$\sigma_i\colon \text{spin function}$$

$$\phi_{1s}^{STO-3G}(\mathbf{r})=\sum_{i=1}^3c(i)\exp{(-z(i)r^2)}$$

$$i=\alpha,\beta$$



$$h(\mathbf{r})=-\frac{1}{2}\nabla^2-\frac{Z_{He}}{|\mathbf{r}-\mathbf{R}_{He}|}-\frac{Z_H}{|\mathbf{r}-\mathbf{R}_H|}$$

$$R=|\mathbf{R}_{He}-\mathbf{R}_H|, Z_{He}=2, Z_H=1$$

$$E_{tot}(x,y,e,R)=E_{HF}(x,y,R)-e\sum_i\left(\langle\chi_i|\chi_j\rangle-1\right)+\frac{Z_{He}Z_H}{R}$$

$$I=\left(\frac{\partial f_{obj}}{\partial x},\frac{\partial f_{obj}}{\partial y},\frac{\partial f_{obj}}{\partial e},\frac{\partial f_{obj}}{\partial R}\right)$$

$$I=\left(\frac{\partial f_{obj}}{\partial x},\frac{\partial f_{obj}}{\partial y},\frac{\partial f_{obj}}{\partial e},100R-146\right)$$

$$\tilde{A}=(\langle 0|^{\otimes a}\otimes I_n)U(|0\rangle^{\otimes a}\otimes I_n)$$

$$U(|0\rangle^{\otimes a}\otimes|\phi\rangle)=|0\rangle^{\otimes a}\otimes\tilde{A}|\phi\rangle+\sqrt{1-\|\tilde{A}|\phi\rangle\|^2}|\sigma^\perp\rangle$$

$$(\langle 0|^{\otimes a}\otimes I_n)|\sigma^\perp\rangle=0$$

$$\| |\sigma^\perp\rangle \| = 1$$

$$|0\rangle^{\otimes a}\|\tilde{A}|\phi\rangle\}^2\frac{\|\tilde{A}|\phi\rangle}{\|\tilde{A}|\phi\rangle\|}$$

$$O_A|0\rangle|i\rangle|j\rangle=\left(a_{ij}+\sqrt{1-|a_{ij}|^2}\right)|i\rangle|j\rangle$$

$$O_A=\left(\begin{array}{cccccccc} c_{00} & & & & & & & -s_{00} \\ & c_{01} & & & & & & -s_{01} \\ & & \ddots & & & & & \ddots \\ & & & c_{N-1,N-1} & & & & -s_{N-1,N-1} \\ s_{00} & & & & c_{00} & & & \\ & s_{01} & & & & c_{01} & & \\ & & \ddots & & & & \ddots & \\ & & & s_{N-1,N-1} & & & & c_{N-1,N-1} \end{array}\right)$$

$$c_{ij}=\cos\left(\theta_{ij}\right),s_{ij}=\sin\left(\theta_{ij}\right)$$

$$\theta_{ij}=\arccos\left(a_{ij}\right)$$

$$U_A=(I_1\otimes H^{\otimes n}\otimes I_n)(I_1\otimes \text{SWAP})O_A(I_1\otimes H^{\otimes n}\otimes I_n)$$

$$\langle 0|\langle 0|^{\otimes n}\langle i|U_A|0\rangle|0\rangle^{\otimes n}|j\rangle=\frac{1}{2^n}a_{ij}$$

$$\frac{1}{\sqrt{2}}\Big(|0\rangle+\alpha e^{i2^k\lambda}|1\rangle\Big)\otimes|\psi\rangle$$

$$|0\rangle+e^{i2^k\lambda}|1\rangle$$

$$\frac{\alpha}{\sqrt{2}}\Big(|0\rangle+e^{i2^k\lambda}|1\rangle\Big)$$

$$(\phi|A|\phi)(\phi|\exp{(-iA)}|\phi)A=m_x^T,m_y^T(\phi|O_{\rm exp}|\phi)O_{\rm exp}=O_{\rm exp}(-iM)$$

$$\frac{\lambda}{2\pi}=\frac{j_1}{2^1}+\frac{j_2}{2^2}+\cdots+\frac{j_n}{2^n}$$

$$|0\rangle|\phi\rangle\overset{H}{\rightarrow}\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|\phi\rangle$$

$$\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|\phi\rangle\overset{\Lambda(U^{2^{n-1}})}{\rightarrow}\frac{1}{\sqrt{2}}(|0\rangle+e^{i(2\pi)j_n}|1\rangle)|\phi\rangle$$

$$\frac{1}{\sqrt{2}}(|0\rangle+e^{i(2\pi)j_n}|1\rangle)|\phi\rangle\overset{H}{\rightarrow}|j_n\rangle|\phi\rangle$$

$$\frac{1}{\sqrt{2}}(|0\rangle+\exp{(-2^k\cdot 2\pi v)}e^{i(2\pi)j_n}|1\rangle)|\phi\rangle,$$

$$|\exp{(-2^k(2\pi)v)}|$$

$$|\psi_{init}\rangle=\sum\beta_j|E_j\rangle|\bar{E}_j\rangle$$

$$e^{2\pi i\lambda_j\Delta T}|E_j\rangle|\bar{E}_j\rangle$$

$$e^{2\pi i\mu_j\Delta T}|E_j\rangle|\bar{E}_j\rangle$$

$$|\lambda_j\rangle|\mu_j\rangle|E_j\rangle|\bar{E}_j\rangle$$

$$\begin{pmatrix} 0 & (A-\lambda I) \\ (A^T-\lambda I) & 0 \end{pmatrix} \begin{pmatrix} 0 \\ x_k \end{pmatrix} = \begin{pmatrix} x_{k-1} \\ 0 \end{pmatrix}$$

$$\sum_s|\beta\rangle\rightarrow\sum_s|\beta\rangle|e_s\rangle$$

$$\sum_s\sum_jc_j|v_j\rangle|e_s\rangle$$

$$\sum_s\sum_jc_j(A-e_s)^{-N}|v_j\rangle|e_s\rangle$$



$$\sum_s \sum_l D_l |v_{e_s}(l)\rangle |e_s\rangle$$

$$|\beta\rangle|\beta'\rangle(A(\lambda+i\mu)I)^{-1}\otimes(A-(\lambda-i\mu)I)^{-1}\sum C_j|E_j\rangle|\hat{E}_j\rangle$$

$$|\hat{\lambda}(e_s)\rangle|e_s\rangle$$

$$|\psi\rangle=(p|\lambda+i\mu)+q|\lambda-i\mu\rangle|e_s\rangle.$$

$$\sum_s \sum_k C_k |k\rangle |e_s\rangle$$

$$C_1\sum_i x_i+C_2\sum_{i_1,i_2} x_{i_1}x_{i_2}+\cdots+C_n\sum_{i_1,\ldots,i_n} x_{i_1}\cdots x_{i_n}-e=0$$

$$x_i^2-x_i=0 \text{ for } i=1,\ldots,n.$$

$$v_1=\left(-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},-1,1\right)\\v_2=\left(\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},-1,1\right)$$

$$w_1=\frac{1}{2}(v_1+v_2)=(0,0,-1,1)\\w_2=\frac{1}{\sqrt{2}}(v_1-v_2)=(-1,1,0,0)$$

$$\begin{aligned}w_1m_x &= (-1/2,1/2,0,0)\\w_2m_x &= (0,0,1,-1)\\w_1m_y &= (-1/2,1/2,0,0)\\w_2m_y &= (0,0,-1,1)\end{aligned}$$

$$m_1^Tv_1=E_vv_1,m_1^Tv_2=E_vv_2.$$

$$\left[\begin{pmatrix} (v_1|m_2^T|v_1) & (v_1|m_2^T|v_2) \\ (v_2|m_2^T|v_1) & (v_2|m_2^T|v_2) \end{pmatrix}-E_j\begin{pmatrix} (v_1|v_1) & (v_1|v_2) \\ (v_2|v_1) & (v_2|v_2) \end{pmatrix}\right]\begin{pmatrix} c_1^j \\ c_2^j \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$w_j=c_1^jv_1+c_2^jv_2 \text{ for } j=1,2$$

$$\begin{aligned}|\psi\rangle&=(p|v_1\rangle+q|v_2\rangle)\,|\text{Ancilla}_1\rangle\,|\text{Ancilla}_2\rangle\cdots|\text{Ancilla}_N\rangle\\&=(s|w_1\rangle+t|w_2\rangle)\,|\text{Ancilla}_1\rangle\,|\text{Ancilla}_2\rangle\cdots|\text{Ancilla}_N\rangle.\end{aligned}$$

$$|\psi\rangle=(s|w_1\rangle+t|w_2\rangle)|E_v\rangle\,|\text{Ancilla}_2\rangle\cdots|\text{Ancilla}_N\rangle$$

$$\begin{aligned}|\psi\rangle&=s|w_1\rangle|E_v\rangle|E_{w_1}\rangle\cdots|\text{Ancilla}_N\rangle\\&\quad+t|w_2\rangle|E_v\rangle|E_{w_2}\rangle\cdots|\text{Ancilla}_N\rangle\end{aligned}$$

$$O\left(mD\binom{n+D-1}{D}^\omega\right)\text{ as }D\rightarrow\infty$$



$$S(f_i,f_j)=\frac{a_{ij}}{g_j}f_i-\frac{a_{ij}}{g_i}f_j$$

$$S(f_i,f_j)=\sum_l c_l f_l+r$$

$$\begin{cases} i\partial_t X=-\Delta X+(w*\mathbb{E}[|X|^2])X-\int_{\mathbb{R}^d}w(x-y)\mathbb{E}[\overline{X(y)}X(x)]X(y)dy,\\ X(t=0)=X_0 \end{cases}$$

$$i\partial_t\gamma=[-\Delta+w*\rho+\mathcal{X},\gamma]$$

$$k(x,y)=\mathbb{E}(X(x)\overline{X(y)})$$

$$\gamma=\sum_{i=1}^N|\varphi_i\rangle\langle\varphi_i|$$

$$X=\sum_{i=1}^N g_i \varphi_i$$

$$i\partial_tX=-\Delta X+(w*\mathbb{E}[|X|^2])X,$$

$$i\partial_t\gamma=[-\Delta+w*\rho,\gamma]$$

$$Y_f=\int_{\mathbb{R}^d}f(\xi)e^{i(\xi x-\theta(\xi)t)}dW(\xi)$$

$$\theta(\xi)=|\xi|^2+\int_{\mathbb{R}^d}w dx\int_{\mathbb{R}^d}f^2dx-(2\pi)^{d/2}(\hat{w}*f^2)(\xi)$$

$$(\xi)=(2\pi)^{-d/2}\int e^{-i\xi x}w(x)dx$$

$$\mathbb{E}[\overline{dW(\xi)}dW(\xi')]=\delta(\xi-\xi')d\xi d\xi'$$

$$X_{|t=0}=Y_f+Z_0$$

$$S(t)Z(x)=\frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}e^{i(\eta x-\theta(\eta)t)}\hat{Z}(\eta)d\eta$$

$$\tilde{\theta}=-(2\pi)^{d/2}\hat{w}*f^2$$

$$\tilde{\theta}\in C^{d+2}\cap W^{d+2,\infty}\cap W^{4,1}$$

$$\eta^\top \nabla^{\otimes 2} \theta(\xi) \eta > \lambda_* |\eta|^2$$

$$\nabla^{\otimes 2}a^\top b=\sum_{k=1}^da_kb_k$$

$$C\left(\|\nabla^{\otimes 3}\tilde{\theta}\|_{L^\infty},\lambda_*\right)>0$$

$$\| \langle y \rangle w \|_M \| \nabla g \|_{W^{2,1}} \leq C \left(\| \nabla^{\otimes 3} \tilde{\theta} \|_{L^\infty}, \lambda_* \right)$$

$$\|Z_0\|_{L^2\big(\Omega,H^{sc}(\mathbb{R}^d)\big)\cap L^{2d/(d+2)}(\mathbb{R}^d,L^2(\Omega))}\leq \delta$$

$$Z\in C\left(\mathbb{R},L^2\left(\Omega,H^{sc}(\mathbb{R}^d)\right)\right)$$

$$Z_{\pm}\in L^2\left(\Omega,H^{sc}(\mathbb{R}^d)\right)$$

$$X(t)=Y_f(t)+S(t)Z_{\pm}+o_{L^2\big(\Omega,H^{sc}(\mathbb{R}^d)\big)}(1)$$

$$C(\mathbb{R},H^s)\cap L^{2\frac{d+2}{d}}\left(\mathbb{R},W^{s_c,2\frac{d+2}{d}}(\mathbb{R}^d)\right)$$

$$g[\rho,T,\mu](\xi)=\rho C_{\frac{\mu}{T}}T^{-\frac{d}{2}}\frac{1}{e^{(|\xi|^2-\mu)/T}+1}$$

$$C_{\tilde{\mu}}=\left(\int\frac{d\xi}{e|\xi|^2-\tilde{\mu}+1}\right)^{-1}$$

$$\|\nabla^s g\|_{L^1}=\rho T^{-\frac{s}{2}}\frac{\left\|\nabla^s\frac{1}{e^{|\xi|^2-\mu/T}+1}\right\|_{L^1}}{\left\|\frac{1}{e^{|\xi|^2-\mu/T}+1}\right\|_{L^1}}\approx\rho T^{-\frac{s}{2}}\left(\frac{\mu}{T}\right)_+^{\frac{s}{2}-1}$$

$$\|\nabla^s\tilde{\theta}\|_{L^\infty}\leq \|w\|_M\|\nabla^s g\|_{L^1}\lesssim \rho T^{-\frac{s}{2}}\left(\frac{\mu}{T}\right)_+^{\frac{s}{2}-1}$$

$$\begin{aligned}\mathcal{E}_N(\psi) &= -\int_{\mathbb{R}^{dN}} \bar{\psi} \sum_{i=1}^N \Delta_i \psi d\underline{x} + \int_{\mathbb{R}^{dN}} \sum_{i<j} w(x_i-x_j) |\psi|^2 d\underline{x} \\ &= \mathcal{E}_{kin} + \mathcal{E}_{pot}\end{aligned}$$

$$\underline{x}=(x_1,\ldots,x_N)\in\mathbb{R}^{dN}$$

$$\psi(\underline{x})=\frac{1}{\sqrt{N!}}\sum_{\sigma\in\mathfrak{S}_N}\varepsilon(\sigma)^t\prod_{j=1}^Nu_{\sigma(j)}(x_j)$$

$$\begin{aligned}\mathcal{E}_{pot}(\psi) &= \int_{\mathbb{R}^{dN}} \frac{1}{N!} \sum_{i<j} w(x_i-x_j) \sum_{\sigma_1,\sigma_2\in\mathfrak{S}_N} \varepsilon(\sigma_1\sigma_2) \prod_{k=1}^N \overline{u_{\sigma_1(k)}(x_k)} u_{\sigma_2(k)}(x_k) d\underline{x} \\ &= \frac{1}{N!} \sum_{\sigma_1,\sigma_2\in\mathfrak{S}_N} \varepsilon(\sigma_1\sigma_2) \sum_{i<j} \langle u_{\sigma_1(i)} \bar{u}_{\sigma_2(i)}, w * (\bar{u}_{\sigma_1(j)} u_{\sigma_2(j)}) \rangle \prod_{k\neq i,j} \langle u_{\sigma_1(k)}, u_{\sigma_2(k)} \rangle\end{aligned}$$

$$\prod_{k\neq i,j}\langle u_{\sigma_1(k)},u_{\sigma_2(k)}\rangle=\begin{cases}1&\text{if }\sigma_1=\sigma_2\text{ or }\sigma_2=\sigma_1\circ(ij),\\0&\text{otherwise.}\end{cases}$$

$$\mathcal{E}_{pot}(\psi) = \sum_{i < j} \left(\langle |u_{\sigma_1(i)}|^2, w * |u_{\sigma_1(j)}|^2 \rangle - \langle u_{\sigma_1(i)} \bar{u}_{\sigma_1(j)}, w * (\bar{u}_{\sigma_1(j)} u_{\sigma_1(i)}) \rangle \right).$$

$$\mathcal{E}_{pot}(\psi) = \frac{1}{2} \sum_{i' \neq j'} \left(\langle |u_{i'}|^2, w * |u_{j'}|^2 \rangle - \langle u_{i'} \bar{u}_{j'}, w * (\bar{u}_{j'} u_{i'}) \rangle \right)$$

$$\mathcal{E}_{kin}(\psi) = - \sum_{j'=1}^N \langle u_{j'}, \Delta u_{j'} \rangle.$$

$$\mathcal{E}_N(\psi) = - \sum_{j'=1}^N \langle u_{j'}, \Delta u_{j'} \rangle + \frac{1}{2} \sum_{i' \neq j'} \left(\langle |u_{i'}|^2, w * |u_{j'}|^2 \rangle - \langle u_{i'} \bar{u}_{j'}, w * (\bar{u}_{j'} u_{i'}) \rangle \right)$$

$$\sum_{i' \neq j'} \sum_{i', j'}$$

$$i\partial_t u_j(x) = -\Delta u_j(x) + \sum_k \int_{\mathbb{R}^d} w(x-y) (|u_k(y)|^2 u_j(x) - \overline{u_k(y)} u_j(y) u_k(x)) dy$$

$$X(x,\omega)\colon=\sum_k u_k(x)g_k(\omega)$$

$$i\partial_t X = -\Delta X + (w * \mathbb{E}[|X|^2])X - \int_{\mathbb{R}^d} w(\cdot - y) \mathbb{E}[\overline{X(y)} X(\cdot)] X(y) dy$$

$$Y_f = \int_{\mathbb{R}^d} f(\xi) e^{i(\xi x - \theta(\xi) t)} dW(\xi)$$

$$g=f^2$$

$$\theta(\xi)=|\xi|^2+\tilde{\theta}(\xi)+\theta_0$$

$$\tilde{\theta} = -(2\pi)^{\frac{d}{2}} \hat{w} * g \text{ and } \theta_0 = (2\pi)^d \hat{w}(0) \hat{g}(0)$$

$$\mathbb{E}[\overline{Y_f(t,x)}Y_f(t,y)]=\int_{\mathbb{R}^d}f^2(\xi)e^{i\xi(y-x)}d\xi=(2\pi)^{d/2}\hat{g}(x-y)$$

$$\left(w * \mathbb{E}\left[|Y_f|^2\right]\right)(x) = (2\pi)^d \hat{w}(0) \hat{g}(0)$$

$$\begin{aligned} \int_{\mathbb{R}^d} w(x-y) \mathbb{E}[\overline{Y_f(y)} Y_f(x)] Y(y) dy &= \int_{\mathbb{R}^{3d}} w(x-y) g(\xi') e^{i\xi'(x-y)} f(\xi) e^{i(\xi y - \theta(\xi) t)} d\xi' dW(\xi) dy \\ &= (2\pi)^{\frac{d}{2}} \int \hat{w}(\xi - \xi') g(\xi') f(\xi) e^{i(\xi x - \theta(\xi) t)} d\xi' dW(\xi) \\ &= (2\pi)^{\frac{d}{2}} (\hat{w} * g)(D) Y_f \end{aligned}$$

$$\xi x = \sum_1^d \xi_i x_i$$

$$\hat{f}(\xi)=\mathcal{F}f(\xi)=(2\pi)^{-\frac{d}{2}}\int_{\mathbb{R}^d}e^{-ix\xi}f(x)dx$$

$$\mathcal{F}(s(D)f)(\xi)=s(\xi)\hat{f}(\xi)$$

$$(1-\Delta_x)^{-\frac{s}{2}}L^p\left(\mathbb{R},L^q\left(\mathbb{R}^d,L^2(\Omega)\right)\right)$$

$$\|u\|_{L^p_tW^{s,q}_xL^2_\omega}=\|\langle \nabla \rangle^su\|_{L^p_tL^q_xL^2_\omega}$$

$$L^p_tH^{s,x}_\omega,L^2_\omega=L^p_tW^{s,2}_x,L^2_\omega$$

$$L^p_tB^{s,t}_qL^2_\omega=L^pB^{s,t}_qL^2_\omega$$

$$\|u\|_{L^pB^{s,t}_qL^2_\omega}=\left\|\left(\sum_{j<0}2^{2js}\|u_j\|^2_{L^q_xL^2_\omega}+\sum_{j\geq 0}2^{2jt}\|u_j\|^2_{L^q_xL^2_\omega}\right)^{\frac{1}{2}}\right\|_{L^p(\mathbb{R})}$$

$$\begin{aligned}\mathbb{E}[w*|X|^2]X-\mathbb{E}[w*|Y|^2]Y&=\mathbb{E}[w*|Y|^2]Z+\mathbb{E}[w*(|X|^2-|Y|^2-1)]X\\&=\theta_0Z+\mathbb{E}[w*(|X|^2-|Y|^2-1)]X\end{aligned}$$

$$\begin{aligned}&\int_{\mathbb{R}^d}w(x-y)\mathbb{E}[\overline{X(y)}X(x)]X(y)dy-\int_{\mathbb{R}^d}w(x-y)\mathbb{E}[\overline{Y(y)}Y(x)]Y(y)dy\\&=\int_{\mathbb{R}^d}w(x-y)\mathbb{E}[\overline{Y(y)}Y(x)]Z(y)dy+\int_{\mathbb{R}^d}w(x-y)\mathbb{E}[\overline{X(y)}X(x)-\overline{Y(y)}Y(x)]X(y)dy\\&=\tilde{\theta}(D)Z+\int_{\mathbb{R}^d}w(x-y)\mathbb{E}[\overline{X(y)}X(x)-\overline{Y(y)}Y(x)]X(y)dy\end{aligned}$$

$$i\partial_tZ=\theta(D)Z+\mathbb{E}[w*(|X|^2-|Y|^2-1)]X-\int_{\mathbb{R}^d}w(\cdot-y)\mathbb{E}[\overline{X(y)}X(\cdot)-\overline{Y(y)}Y(\cdot)]X(y)dy$$

$$\begin{aligned}V(x,z)&=\mathbb{E}[\bar{X}(x+z)X(x)-\bar{Y}(x+z)Y(x)]\\&=\mathbb{E}[\overline{Y(x+z)}Z(x)+\overline{Z(x+z)}Y(x)+\overline{Z(x+z)}Z(x)].\end{aligned}$$

$$i\partial_tZ=\theta(D)Z+(w*V(\cdot,0))(Y+Z)-\int_{\mathbb{R}^d}w(z)V(x,z)(Y+Z)(x+z)dz$$

$$\begin{aligned}Z&=S(t)Z_0-i\int_0^tS(t-\tau)\left[(w*V(\cdot,0))Y-\int w(z)V(x,z)Y(x+z)dz\right]d\tau\\&\quad -i\int_0^tS(t-\tau)\left[(w*V(\cdot,0))Z-\int w(z)V(x,z)Z(x+z)dz\right]d\tau\end{aligned}$$

$$Z=S(t)Z_0+L_1(V)+L_2(V)+Q_1(Z,V)+Q_2(Z,V)$$

$$L_1(V) = -i \int_0^t S(t-\tau) [(w * V(\cdot, 0))Y] d\tau$$

$$L_2(V) = i \int_0^t S(t-\tau) \left[\int dz w(z) V(x, z) Y(x+z) \right] d\tau$$

$$Q_1(Z, V) = -i \int_0^t S(t-\tau) [(w * V(\cdot, 0))Z] d\tau$$

$$Q_2(Z, V) = i \int_0^t S(t-\tau) \left[\int dz w(z) V(x, z) Z(x+z) \right] d\tau$$

$$V = \mathbb{E}(\overline{Y(x+y)} S(t) Z_0(x) + \overline{S(t) Z_0(x+y)} Y(x)) \\ + L_3(V) + L_4(V) \\ + Q_3(Z, V) + Q_4(Z, V) + \mathbb{E}(\overline{Z(x+y)} Z(x))$$

$$L_k(V) = \mathbb{E}[\overline{Y(x+y)} L_{k-2}(V)(x)] + \mathbb{E}[\overline{L_{k-2}(V)(x+y)} Y(x)] \\ Q_k(Z, V) = \mathbb{E}[\overline{Y(x+y)} Q_{k-2}(Z, V)(x)] + \mathbb{E}[\overline{Q_{k-2}(Z, V)(x+y)} Y(x)].$$

$$\binom{Z}{V} = \mathcal{A}_{Z_0} \binom{Z}{V} = \begin{pmatrix} \mathcal{A}_{Z_0}^{(1)}(Z, V) \\ \mathcal{A}_{Z_0}^{(2)}(Z, V) \end{pmatrix}$$

$$\mathcal{A}_{Z_0}^{(1)}(Z, V) = S(t)Z_0 + L_1(V) + L_2(V) + Q_1(Z, V) + Q_2(Z, V)$$

$$\mathcal{A}_{Z_0}^{(2)}(Z, V) = \mathbb{E}[\overline{Y(x+y)} S(t) Z_0(x) + \overline{S(t) Z_0(x+y)} Y(x)] \\ + L_3(V) + L_4(V) + Q_3(Z, V) + Q_4(Z, V) + \mathbb{E}[\overline{Z(x+y)} Z(x)]$$

$$E_Z = C\left(\mathbb{R}, L^2\left(\Omega, H^{s_c}(\mathbb{R}^d)\right)\right) \cap L^p\left(\mathbb{R}, W^{s_c, p}(\mathbb{R}^d, L^2(\Omega))\right) \\ \cap L^{d+2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega)) \cap L^4\left(\mathbb{R}, L^q(\mathbb{R}^d, L^2(\Omega))\right)$$

$$E_V = C\left(\mathbb{R}^d, L^{\frac{d+2}{2}}(\mathbb{R} \times \mathbb{R}^d)\right) \cap C\left(\mathbb{R}^d, L^2\left(\mathbb{R}, B_2^{-\frac{1}{2}, s_c}(\mathbb{R}^d)\right)\right)\Bigg)$$

$$p=2\frac{d+2}{d}, s_c=\frac{d}{2}-1, q=\frac{4d}{d+1}$$

$$\|\cdot\|_Z = \|\cdot\|_{L^\infty\left(\mathbb{R}, L^2\left(\Omega, H^s(\mathbb{R}^d)\right)\right)} + \|\cdot\|_{L^p\left(\mathbb{R}, W^{s_c, p}(\mathbb{R}^d, L^2(\Omega))\right)} \\ + \|\cdot\|_{L^{d+2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} + \|\cdot\|_{L^4\left(\mathbb{R}, B_q^{0, \frac{1}{4}}(\mathbb{R}^d, L^2(\Omega))\right)}$$

$$\|\cdot\|_V = \|\cdot\|_{C\left(\mathbb{R}^d, L^{\frac{d+2}{2}}(\mathbb{R} \times \mathbb{R}^d)\right)} + \|\cdot\|_{C\left(\mathbb{R}^d, L^2\left(\mathbb{R}, B_2^{-\frac{1}{2}, s_c}(\mathbb{R}^d)\right)\right)}$$

$$C\left(\mathbb{R}, L^2\left(\Omega, H^{s_c}(\mathbb{R}^d)\right)\right)$$

$$\tilde{\theta} \in C^{d+2}(\mathbb{R}^d) \cap W^{d+2,\infty}(\mathbb{R}^d)$$

$$\frac{2}{p}+\frac{d}{q}=\frac{d}{2}, (p,q)\neq (2,\infty) \text{ if } d=2$$

$$\|e^{-it\theta(D)}u_0\|_{L^p_tL^q_x}\leq C\|u_0\|_{L^2_x}$$

$$\| \langle y \rangle^2 w \|_M \| g \|_{L^1} < C(d)$$

$$\|w\|_M\|\nabla^2g\|_{L^1}<C(d)$$

$$\theta=\theta_0+|\xi|^2-(2\pi)^{d/2}\rho\hat{w}\ast g^*$$

$$\chi_0(\xi)+\sum_{\lambda\in 2^{\mathbb{N}}}\chi(\lambda^{-1}\xi)=1$$

$$c\leq \chi_0^2(\xi)+\sum_{\lambda\in 2^{\mathbb{N}}}\chi^2(\lambda^{-1}\xi)\leq 1$$

$$\chi_\lambda(\xi)\!:=\!\chi(\lambda^{-1}\xi), \lambda\in 2^{\mathbb{N}}$$

$$u_\lambda(t,x)\!:=\!e^{-it\theta(D)}\chi_\lambda(D)u_0(x), \lambda\in 2^{\mathbb{N}}\cup\{0\}$$

$$\begin{aligned} u_\lambda(t,x) &= (2\pi)^{-d}\int_{\mathbb{R}^d}\left[\int_{\mathbb{R}^d}e^{-it\theta(\xi)+i(x-y)\cdot\xi}\chi_\lambda(\xi)d\xi\right]u_0(y)dy\\ &= \int_{\mathbb{R}^d}I_\lambda(t,x-y)u_0(y)dy=[I_\lambda(t,\cdot)\ast u_0(\cdot)](x) \end{aligned}$$

$$I_\lambda(t,x)\!:=\!(2\pi)^{-d}\int_{\mathbb{R}^d}e^{-it\theta(\xi)+ix\xi}\chi_\lambda(\xi)d\xi$$

$$I(\mu)=\int_{\mathbb{R}^d}e^{i\mu\phi(\xi)}\psi(\xi)d\xi$$

$$\phi\in C^{d+2}(\mathbb{R}^d), \psi\in C_0^{d+1}(\mathbb{R}^d)$$

$$\mathcal{M}_{d+2}(\phi)=\sum_{2\leq|\alpha|\leq d+2}\sup_{\xi\in K_{\epsilon_0}}|\nabla^{\otimes\alpha}\phi(\xi)|<+\infty$$

$$\mathcal{N}_{d+1}(\psi)=\sum_{|\alpha|\leq d+1}\sup_{\xi\in K}|\nabla^{\otimes\alpha}\psi(\xi)|<+\infty$$

$$a_0=\inf_{\xi\in K_{\epsilon_0}}|\det\nabla^{\otimes 2}\phi(\xi)|>0$$

$$\xi\mapsto \nabla\psi(\xi)$$

$$|I(\mu)|\leq \mu^{-\frac{d}{2}}Ca_0^{-1}\left(1+\mathcal{M}_{d+2}^{\frac{d}{2}}\right)\mathcal{N}_{d+1}.$$

$$\phi(t,x,\xi):=-\theta(\xi)+\frac{x}{t}\cdot\xi$$

$$I_\lambda(t,x)=(2\pi)^{-d}\int_{\mathbb{R}^d}e^{it\phi(t,x,\xi)}\chi_\lambda(\xi)d\xi$$

$$\inf_{\xi\in\mathbb{R}^d}|\det\nabla^{\otimes 2}(-\tilde{\theta}(\xi))|>0$$

$$\inf_{\xi\in\mathbb{R}^d}|\det\nabla^{\otimes 2}\phi(\xi)|\geq c_1$$

$$\begin{aligned}\nabla\tilde{\phi}(\xi_1)-\tilde{\nabla}\tilde{\phi}(\xi_2)&=\int_0^1\frac{d}{ds}\big[\nabla\tilde{\phi}(s\xi_1+(1-s)\xi_2)\big]ds\\&=\int_0^1\nabla^{\otimes 2}\tilde{\phi}(s\xi_1+(1-s)\xi_2)\cdot(\xi_1-\xi_2)ds\end{aligned}$$

$$|\nabla\tilde{\phi}(\xi_1)-\nabla\tilde{\phi}(\xi_2)| |\xi_1-\xi_2|\geq \langle \nabla\tilde{\phi}(\xi_1)-\nabla\tilde{\phi}(\xi_2),\xi_1-\xi_2\rangle\geq c_1|\xi_1-\xi_2|^2$$

$$\begin{aligned}\|e^{it\theta(D)}\chi_\lambda(D)u_0\|_{L^\infty_x}&\leq \|I_\lambda(t,\cdot)\|_{L^\infty_x}\|u_0\|_{L^1_x}\\&\leq Ct^{-\frac{d}{2}}\|u_0\|_{L^1_x}\end{aligned}$$

$$\|U(t)f\|_{L^2_x}\lesssim \|f\|_H$$

$$\|U(s)U^*(t)g\|_{L^\infty}\lesssim |t-s|^{-\sigma}\|g\|_{L^1}$$

$$\|U(t)f\|_{L^q_tL^r_x}\lesssim \|f\|_H$$

$$\frac{1}{q}+\frac{\sigma}{r}=\frac{\sigma}{2},(q,r,\sigma)\neq(2,\infty,1)$$

$$P=\left(2,\frac{2\sigma}{\sigma-1}\right)$$

$$U(t)=e^{-it\theta(D)}\chi_\lambda(D)\colon L^2_x\rightarrow L^2_x,\,\sigma=\frac{d}{2}$$

$$\|e^{-it\theta(D)}\chi_\lambda(D)u_0\|_{L^p_tL^q_x}\leq C\|u_0\|_{L^2_x}$$

$$(p,q)\in [2,+\infty]^2$$

$$\frac{2}{p}+\frac{d}{q}=\frac{d}{2},(p,q)\neq(2,\infty)\text{ if }d=2$$

$$\|\chi_\lambda(D)u_0\|_{L^2_x}\tilde{\chi}_\lambda\in C_c^\infty\tilde{\chi}_\lambda\chi_\lambda=\chi_\lambda$$

$$\|e^{-it\theta(D)}\chi_\lambda(D)u_0\|_{L^p_tL^q_x}=\|e^{-it\theta(D)}\tilde{\chi}_\lambda\chi_\lambda(D)u_0\|_{L^p_tL^q_x}\leq C\|\chi_\lambda(D)u_0\|_{L^2_x}$$

$$\big[e^{-it\theta(D)},\chi_\lambda(D)\big]=0$$

$$\begin{aligned}
\|e^{-it\theta(D)}u_0\|_{L_t^p L_x^q} &\simeq \left\| \|e^{-it\theta(D)}\chi_0(D)u_0\|_{L_x^q} + \left\| \left(\sum_{\lambda \in 2^{\mathbb{N}}} |e^{-it\theta(D)}\chi_\lambda(D)u_0|^2 \right)^{\frac{1}{2}} \right\|_{L_x^q} \right\|_{L_t^p} \\
&\leq \|e^{-it\theta(D)}\chi_0(D)u_0\|_{L_t^p L_x^q} + \left(\sum_{\lambda \in 2^{\mathbb{N}}} \|e^{-it\theta(D)}\chi_\lambda(D)u_0\|_{L_t^p L_x^q}^2 \right)^{\frac{1}{2}} \\
&\leq \|\chi_0(D)u_0\|_{L_x^2} + \left(\sum_{\lambda \in 2^{\mathbb{N}}} \|\chi_\lambda(D)u_0\|_{L_x^2}^2 \right)^{\frac{1}{2}} \\
&\simeq \|u_0\|_{L_x^2}.
\end{aligned}$$

$$\theta \in C^{n_0}(\mathbb{R}^d), n_0 > \frac{d+2}{2} \text{ and } \langle \xi \rangle^{n-2} \nabla^{\otimes n} \tilde{\theta} \in L^\infty \text{ for any } n = 2, \dots, n_0$$

$$\frac{1}{r}=\frac{1}{r_2}+\frac{s_2}{d} \text{ and } \frac{2}{q_2}+\frac{d}{r_2}+s_2=\frac{d}{2}$$

$$F\in L^{q_1'}_tH^{s_2,r_1'}_x$$

$$\left\| S(t)u_0-i\int_0^tS(t-\tau)F(\tau)d\tau\right\|_{L^{q_2}_{t}L^{r_2}_{x}}\leq C\left[\|u_0\|_{H^{s_2}_x}+\|F\|_{L^{q_1'}_tH^{s_2,r_1'}_x}\right]$$

$$\mathcal{T}_{\xi}(t)U(x)=\frac{1}{(2\pi)^{\frac{d}{2}}}\int e^{-i(\theta(\eta+\xi)-\theta(\eta)-\theta(\xi))t}e^{i\eta x}\hat{U}(\eta)d\eta$$

$$L_1(V) \, = \, -i \int\!\!\int_0^t f(\xi) e^{i\xi x - i\theta(\xi)t} \mathcal{T}_{\xi}(t-\tau) S(t-\tau) [w * V(\cdot, 0, \tau)] d\tau dW(\xi)$$

$$L_2(V) \, = \, i \int\!\!\int\!\!\int_0^t f(\xi) e^{i\xi x - i\theta(\xi)t} e^{i\xi z} w(z) \mathcal{T}_{\xi}(t-\tau) S(t-\tau) V(\cdot, z, \tau) d\tau dz dW(\xi)$$

$$L_3(V) \, = \, i \int\!\!\int\!\!\int_0^t (g(\xi+\zeta)-g(\xi)) e^{-i(\theta(\xi+\zeta)-\theta(\xi))(t-\tau)} e^{i\zeta x - i\xi y} \hat{W}(\zeta) \hat{V}(\zeta, 0, \tau) d\tau d\xi d\zeta$$

$$L_4(V)$$

$$= -i(2\pi)^{-\frac{d}{2}}\iiint\int_0^t (g(\xi+\zeta)-g(\xi))e^{-i(t-\tau)(\theta(\xi+\zeta)-\theta(\xi))}e^{i\zeta x+i\xi(z-y)}w(z)\hat{V}(\zeta,z,\tau)d\tau dzd\xi d\zeta$$

$$|\nabla_\eta(\theta(\xi+\eta)-\theta(\eta)-\theta(\xi))|\approx|\xi| \text{ and } \frac{\xi}{|\xi|}\cdot\nabla_\eta(\theta(\xi+\eta)-\theta(\eta)-\theta(\xi))\approx|\xi|$$

$$i\partial_t u=\theta(D)u+V$$

$$\overline{V(x,y)}=V(x+y,-y)$$

$$\overline{\hat{V}(\eta,y)}=\hat{V}(-\eta,-y)e^{-i\eta y}.$$

$$\begin{aligned} L_1(V) &= -i \int_0^t S(t-\tau) [(w * V(\cdot, 0))Y] d\tau \\ &= -i \iint_0^t f(\xi) e^{-i\theta(\xi)\tau} S(t-\tau) [(w * V(\cdot, 0))e^{i\xi x}] d\tau dW(\xi) \end{aligned}$$

$$e^{i\theta(\xi)t} S(t) (e^{i\xi x} U) = e^{i\xi x} \mathcal{T}_\xi(t) S(t) U$$

$$\begin{aligned} L_2(V) &= -i \int_0^t S(t-\tau) \left[\int dz w(z) V(x, z) Y(x+z) \right] d\tau \\ &= -i \iiint_0^t f(\xi) e^{-i\theta(\xi)\tau} e^{i\xi z} w(z) S(t-\tau) [V(x, z) e^{i\xi x}] d\tau dz dW(\xi) \end{aligned}$$

$$\begin{aligned} L_3(V) &= \mathbb{E}[\overline{Y(x+y)} L_1(V)(x)] + \mathbb{E}[\overline{L_1(V)(x+y)} Y(x)] \\ &= L_3^{(1)}(V) + L_3^{(2)}(V). \end{aligned}$$

$$\overline{L_3^{(1)}(V)(x, y)} = L_3^{(2)}(V)(x+y, -y)$$

$$\begin{aligned} \widehat{L_3^{(1)}(V)}(\eta, y) &= \frac{1}{(2\pi)^{\frac{d}{2}}} \int \overline{L_3^{(2)}(V)(x+y, -y)} e^{-i\eta x} dx \\ &= \frac{1}{(2\pi)^{\frac{d}{2}}} \widehat{L_3^{(2)}(V)}(z, -y) e^{i\eta(z-y)} dx \\ &= e^{i\eta y} \overline{L_3^{(2)}(V)}(-\eta, -y) \end{aligned}$$

$$\widehat{L_3(V)}(\zeta, y) = \widehat{L_3^{(1)}(V)}(\zeta, y) + e^{i\zeta y} \widehat{L_3^{(1)}(V)}(-\zeta, -y).$$

$$L_1(V) = -i \iiint_0^t f(\xi) e^{i\xi x - i\theta(\xi)t} e^{i\zeta x} e^{-i(t-\tau)(\theta(\zeta+\xi) - \theta(\xi))} \hat{w}(\zeta) \hat{V}(\zeta, 0, \tau) d\tau d\zeta dW(\xi)$$

$$L_3^{(1)}(x, y) = -i \iint_0^t f^2(\xi) e^{-i\xi y} e^{i\zeta x} e^{-i(t-\tau)(\theta(\zeta+\xi) - \theta(\xi))} \hat{w}(\zeta) \hat{V}(\zeta, 0, \tau) d\tau d\zeta d\xi$$

$$\widehat{L_3^{(1)}(V)}(\zeta, y) = -i(2\pi)^{\frac{d}{2}} \hat{w}(\zeta) \iint_0^t f^2(\xi) e^{-i(\theta(\xi+\zeta) - \theta(\xi))(t-\tau)} e^{-i\xi y} \hat{V}(\zeta, 0, \tau) d\tau d\xi$$

$$\widehat{L_3(V)}(\zeta, y) = -i(2\pi)^{\frac{d}{2}} \hat{w}(\zeta) \int_0^t \hat{V}(\zeta, 0) \int (f(\xi)^2 - f(\xi+\zeta)^2) e^{-i(\theta(\xi+\zeta) - \theta(\xi))(t-\tau)} e^{-i\xi y} d\tau d\xi$$

$$\begin{aligned} L_4(V) &= \mathbb{E}[\overline{Y(x+y)} L_2(V)(x)] + \mathbb{E}[\overline{L_2(V)(x+y)} Y(x)] \\ &= L_4^{(1)}(V) + L_4^{(2)}(V). \end{aligned}$$

$$\widehat{L_4^{(1)}(V)}(\eta, y) = e^{i\eta y} \widehat{L_4^{(2)}(V)}(-\eta, -y)$$

$$L_2(V)(x) = \frac{i}{(2\pi)^{\frac{d}{2}}} \int_0^t \iiint f(\xi) w(z) \hat{V}(\eta - \xi, z, \tau) e^{i\eta x + i\xi z} e^{-i(t-\tau)\theta(\eta) - i\tau\theta(\xi)} dz d\eta d\tau dW(\xi)$$

$$L_4^{(1)}(x,y)=\frac{i}{(2\pi)^{\frac{d}{2}}}\int_0^t\iiint f^2(\xi)w(z)\hat{V}(\eta-\xi,z,\tau)e^{i(\eta-\xi)x+i\xi(z-y)}e^{i(t-\tau)(\theta(\xi)-\theta(\eta))}dzd\eta d\tau d\xi$$

$$\widehat{L_4^{(1)}}(\zeta,y)=i\int_0^t\iint f^2(\xi)w(z)\hat{V}(\zeta,z,\tau)e^{i\xi(z-y)}e^{-i(t-\tau)(\theta(\xi+\zeta)-\theta(\xi))}dzd\tau d\xi$$

$$\begin{aligned}\widehat{L_4^{(2)}}(\zeta,y)&=e^{i\zeta y}\overline{\widehat{L_4^{(1)}}(-\zeta,-y)}\\&=-ie^{i\zeta y}\int_0^t\iint f^2(\xi)w(z)\overline{\hat{V}(-\zeta,z,\tau)}e^{-i\xi(z+y)}e^{-i(t-\tau)(\theta(\xi)-\theta(\xi-\zeta))}dzd\tau d\xi\\&=-i\int_0^t\iint f^2(\xi)w(z)\hat{V}(\zeta,-z,\tau)e^{i(\zeta-\xi)(z+y)}e^{-i(t-\tau)(\theta(\xi)-\theta(\xi-\zeta))}dzd\tau d\xi\\&=-i\int_0^t\iint f^2(\xi+\zeta)w(z)\hat{V}(\zeta,z,\tau)e^{i\xi(z-y)}e^{-i(t-\tau)(\theta(\zeta+\xi)-\theta(\xi))}dzd\tau d\xi\end{aligned}$$

$$\frac{2}{p_1}+\frac{d}{q_1}=\frac{d}{2}-\sigma_1$$

$$U\in L^2_t,B_2^{-1/2+\sigma_1,\sigma+\sigma_1-1/2}$$

$$\left\|\int_0^\infty S(t-\tau)[U(\tau)Y(\tau)]d\tau\right\|_{L^{p_1}\left(\mathbb{R},W^{\sigma,q_1}(\mathbb{R}^d,L^2(\Omega))\right)}\leq C_\theta\|\langle\xi\rangle^{2[\sigma]}g\|_{W^{2,1}}\|U\|_{L^2_t,B_2^{-1/2+\sigma_1,\sigma+\sigma_1-1/2}}$$

$$L_1^\infty(U)\coloneqq\int_0^\infty S(t-\tau)Y(\tau)U(\tau)d\tau$$

$$\xi\mapsto e^{-it(|\xi|^2+2\eta\xi+(2\pi)^d(-1)^2\hat{w}*g(\xi+\eta)-\hat{w}*g(\eta))}=e^{it(\theta(\eta)-\theta(\xi+\eta))}$$

$$S(t)(e^{i\eta x}U)=\mathcal{F}^{-1}(e^{-it\theta(\xi)}\hat{U}(\xi-\eta))=e^{i\eta x}\mathcal{F}^{-1}(e^{-it\theta(\xi+\eta)}\hat{U}(\xi))$$

$$S(t)(e^{i\eta x}U)=e^{i\eta x-it\theta(\eta)}\mathcal{F}^{-1}(e^{-it(\theta(\xi+\eta)-\theta(\eta))}\hat{U}(\xi))$$

$$S(t)(e^{i\eta x}U)=e^{i\eta x-it\theta(\eta)}S_\eta(t)U$$

$$\begin{aligned}S(t-\tau)(U(\tau)Y(\tau))&=\int f(\eta)e^{-i\tau\theta(\eta)}S(t-\tau)(e^{i\eta x}U(\tau))dW(\eta)\\&=\int f(\eta)e^{i\eta x}e^{-it\theta(\eta)}S_\eta(t-\tau)U(s)dW(\eta)\end{aligned}$$

$$\mathbb{E}[|L_1^\infty(U)|^2]=\int_{\eta\in\mathbb{R}^d}g(\eta)\left|\int_0^\infty S_\eta(t-\tau)U(\tau)d\tau\right|^2d\eta$$

$$\|L_1^\infty(U)\|_{L_t^{p_1},L_x^{q_1},L_\omega^2}\leq C(\theta)\|g\|_{W^{2,1}}\|U\|_{L_t^2,B_2^{\sigma_1-\frac{1}{2}\sigma_1-\frac{1}{2}}}$$

$$\|L_1^\infty(U)\|_{L_t^{p_1},L_x^{q_1},L_\omega^2}^2\leq \int_{\eta\in\mathbb{R}^d}g(\eta)\left\|\int_0^\infty S_\eta(t-\tau)U(\tau)d\tau\right\|_{L_t^{p_1},L_x^{q_1}}^2d\eta$$

$$\|L_1^\infty(U)\|_{L_t^{p_1}, L_x^{q_1}, L_\omega^2}^2 \leq \int_{\eta \in \mathbb{R}^d} g(\eta) \left\| \int_0^\infty S_\eta(-\tau) U(\tau) d\tau \right\|_{B_2^{\sigma_1, \sigma_1}}^2 d\eta$$

$$\begin{aligned} & \|L_1^\infty(U)\|_{L_t^{p_1}, L_x^{q_1}, L_\omega^2} \\ & \leq \int_{\eta \in \mathbb{R}^d} g(\eta) \int_{\xi \in \mathbb{R}^d} \int_0^\infty \int_0^\infty e^{i(t_1-t_2)(\xi^2-2\xi\cdot\eta-\tilde{\theta}_\xi(\eta))} \hat{U}_1(t_1, \xi) \overline{\hat{U}_1(t_2, \xi)} dt_2 dt_1 d\xi d\eta \end{aligned}$$

$$\tilde{\theta}_\xi(\eta) = \tilde{\theta}(\xi + \eta) - \tilde{\theta}(\eta)$$

$$\eta_\xi = \eta - \tilde{\theta}_\xi(\eta) \frac{\xi}{2|\xi|^2}$$

$$\eta \mapsto \theta_\xi(\eta) \frac{\xi}{2|\xi|^2} \frac{\xi}{2|\xi|} \nabla_\eta \frac{\tilde{\theta}_\xi}{|\xi|} 1 - \left\langle \frac{\xi}{2|\xi|}, \nabla_\eta \frac{\tilde{\theta}_\xi}{|\xi|} \right\rangle$$

$$\nabla \frac{\tilde{\theta}_\xi}{|\xi|} = \int_0^1 \nabla^{\otimes 2} \tilde{\theta}(\eta + t\xi) \frac{\xi}{|\xi|} dt$$

$$\nabla^{\otimes 2} \theta = 2Id + \nabla^{\otimes 2} \tilde{\theta}$$

$$1 - \left\langle \frac{\xi}{2|\xi|}, \nabla_\eta \frac{\tilde{\theta}_\xi}{|\xi|} \right\rangle = \frac{1}{2} \int_0^1 \frac{\xi^T}{|\xi|} \nabla^{\otimes 2} \theta(\eta + t\xi) \frac{\xi}{|\xi|} dt > \frac{1}{2} \lambda_*$$

$$\phi_\xi = \tilde{\eta}_\xi^{-1}$$

$$\begin{aligned} & \|L_1^\infty(U)\|_{L_t^{p_1}, L_x^{q_1}, L_\omega^2} \\ & \leq \int_{\eta \in \mathbb{R}^d} \int_{\xi \in \mathbb{R}^d} g(\phi_\xi(\eta)) jac(\phi_\xi(\eta)) \int_{\mathbb{R}} \int_{D_t} e^{-it(\xi^2-2\xi\eta)} \hat{U}_1(t_1, \xi) \overline{\hat{U}_1(t+t_1, \xi)} dt_1 dt d\xi d\eta \end{aligned}$$

$$D_t = [-t, \infty] jac(\phi_\xi(\eta))$$

$$\begin{aligned} & \|L_1^\infty(U)\|_{L_t^{p_1}, L_x^{q_1}, L_\omega^2} \\ & \leq (2\pi)^{d/2} \int_{\xi \in \mathbb{R}^d} \int_{\mathbb{R}} \int_{D_t} \mathcal{F}_\eta \left(g(\phi_\xi(\eta)) jac(\phi_\xi(\eta)) \right) (-2\xi t) e^{-it\xi^2} \hat{U}_1(t_1, \xi) \overline{\hat{U}_1(t+t_1, \xi)} dt_1 dt d\xi \end{aligned}$$

$$\|L_1^\infty(U)\|_{L_t^{p_1}, L_x^{q_1}, L_\omega^2}^2 \leq \int_{\xi \in \mathbb{R}^d} \int_{\mathbb{R}} \left| \mathcal{F}_\eta \left(g(\phi_\xi(\eta)) jac(\phi_\xi(\eta)) \right) (-2\xi t) \right| \|\hat{U}_1(t_1, \xi)\|_{L_{t_1}^2}^2 dt d\xi$$

$$\|L_1^\infty(U)\|_{L_t^{p_1}, L_x^{q_1}, L_\omega^2} \lesssim \int_{\xi \in \mathbb{R}^d} \int_{\mathbb{R}} \left| \mathcal{F}_\eta \left(g(\phi_\xi(\eta)) jac(\phi_\xi(\eta)) \right) \left(-2\tau \frac{\xi}{|\xi|} \right) \right| |\xi|^{-1} \|\hat{U}_1(t_1, \xi)\|_{L_{t_1}^2}^2 d\tau d\xi$$

$$(\tau, \xi) \mapsto \mathcal{F}_\eta \left(g(\phi_\xi(\eta)) jac(\phi_\xi(\eta)) \right) \left(-2\tau \frac{\xi}{|\xi|} \right) L_\xi^\infty(\mathbb{R}^d, L_\tau^1(\mathbb{R}))$$

$$(\xi, \eta) \mapsto g(\phi_\xi(\eta)) jac(\phi_\xi(\eta))$$

$$L^\infty_\xi\left(\mathbb{R}^d,W^{2,1}_\eta(\mathbb{R}^d)\right)$$

$$g\in W^{2,1}(\mathbb{R}^d)$$

$$\phi_\xi\in L^\infty_\xi W^{3,\infty}$$

$$\tilde{\theta}_\xi\in L^\infty_\xi\left(\mathbb{R}^d,W^3_\eta(\mathbb{R}^d)\right)$$

$$\|L_1^\infty(U)\|_{L_t^{p_1},L_x^{q_1},L_\omega^2}^2\leq C_\theta\|g\|_{W^{2,1}}\int_{\xi\in\mathbb{R}^d}\left\|\xi^{|\sigma_1-\frac{1}{2}|}\hat{U}(t_1,\xi)\right\|_{L_{t_1}^2}^2dtd\xi=C_\theta\|g\|_{W^{2,1}}\|U\|_{L_t^2,\beta_2^{\sigma_1-\frac{1}{2},\sigma_1-\frac{1}{2}}}$$

$$|\alpha|=\sum_{j=1}^d\alpha_j$$

$$\partial^\alpha=\prod_{j=1}^d\partial^{\alpha_j}$$

$$\eta^\alpha=\prod_{j=1}^d\eta_j^{\alpha_j}$$

$$\partial^\alpha L_1^\infty(U)=\sum_{\gamma+\beta=\alpha}C(\alpha,\beta)\int_0^tS(t-s)\partial^\beta Y(s)\partial^\gamma U(s)ds$$

$$\partial^\beta Y(s)=\int_{\mathbb{R}^d}i^{|\beta|}\eta^\beta f(\eta)e^{-is\theta(\eta)+i\eta x}dW(\eta)$$

$$\|L_1^\infty(U)\|_{L_t^{p_1},W_x^{\sigma,q_1},L_\omega^2}\lesssim \|U\|_{L_t^2,B_2^{\sigma_1-\frac{1}{2},\sigma_1+\sigma-\frac{1}{2}}}$$

$$\sup_{|\alpha|\leq \sigma}\left\|\mathcal{F}_\eta\left(\phi_\xi(\eta)^{2\alpha}g(\phi_\xi(\eta))jac(\phi_\xi(\eta))\right)\right\|_{L^1}$$

$$L_1^{\infty,0}\colon U\mapsto \int_0^tS(t-\tau)[U(\tau)Y(\tau)]d\tau, L_1^{\infty,\infty}\colon U\mapsto \int_t^\infty S(t-\tau)[U(\tau)Y(\tau)]d\tau$$

$$L_t^2B_2^{-1/2+\sigma_1,-1/2+\sigma_2+\sigma}L_t^{p_1}W_x^{\sigma,q_1}$$

$$L_1\colon V\mapsto L_1(V)=-i\int_0^tS(t-\tau)[w\ast V(\cdot,0)Y]d\tau$$

$$L_y^\infty L_t^2 B_2^{-1/2, s_c} \text{ to } E_Z$$

$$(p,p,0,s_c), (d+2,d+2,s_c,0), \Big(4,q,\frac{d-3}{4},0\Big) \text{ or } (\infty,2,0,s_c)$$

$$L_2\colon V\mapsto L_2(V)=i\int_0^tS(t-\tau)\left[\int dzw(z)V(x,z)Y(x+z)\right]d\tau$$

$$\|L_2(V)\|_{E_Z}\lesssim \int_{z\in\mathbb{R}^d}\left\|\int_0^tS(t-\tau)V(\cdot,z)T_zYd\tau\right\|_{E_Z}|w|(z)dz$$

$$\left\|\int_0^tS(t-\tau)V(\cdot,z)T_zYd\tau\right\|_{E_Z}=\left\|\int_0^tS(t-\tau)T_{-z}V(\cdot,z)Yd\tau\right\|_{E_Z}$$

$$\left\|\int_0^tS(t-\tau)T_{-z}V(\cdot,z)Yd\tau\right\|_{E_Z}\lesssim \|T_{-z}V(\cdot,z)\|_{L^2_t,B_2^{-\frac{1}{2}s_c}}=\|V(\cdot,z)\|_{L^2_t,B_2^{-\frac{1}{2}s_c}}$$

$$\left\|\int_0^tS(t-\tau)T_{-z}V(\cdot,z)Yd\tau\right\|_{E_Z}\lesssim \|V\|_{E_V}$$

$$\|L_2(V)\|_{E_Z}\lesssim \|w\|_M\|V\|_{E_V}.$$

$$C_y L^2_{t,x} \cap L^\infty_y L^2_{t,x}$$

$$\|L_k(V)\|_{L^\infty_y L^2_{t,x}}\leq C_{\theta,w,g}\|V\|_{L^\infty_y L^2_{t,x}}.$$

$$C_{\theta,w,g}=C_{\theta}\|\langle y\rangle w\|_{L^1}\|\nabla g\|_{W^{2,1}}\|\nabla^{\otimes 3}\tilde{\theta}\|_{L^\infty}$$

$$\left| p.v.\int_{\mathbb{R}} u(\alpha)\frac{e^{i\eta\alpha}}{\tilde{\Omega}(\alpha)}d\alpha\right|\leq \frac{C}{\lambda}\left(1+\frac{\|\tilde{\Omega}''\|_{L^\infty}}{\lambda}\right)\|u\|_{W^{1,q}(\mathbb{R})}$$

$$\frac{e^{i\eta x}}{\hat{\Omega}(\alpha)}=\frac{1}{\alpha}$$

$$\left(\frac{1}{\alpha} * u\right)' \in L^{1,w}$$

$$\int_{\mathbb{R}}\frac{e^{i\eta\alpha}}{\tilde{\Omega}(\alpha)}u(\alpha)d\alpha=I+II+III$$

$$I=\int_{|\alpha-\alpha_0|>1}\left(\frac{e^{i\eta\alpha}}{\tilde{\Omega}(\alpha)}-\frac{e^{i\eta\alpha}}{\tilde{\Omega}'(\alpha_0)(\alpha-\alpha_0)}\right)u(\alpha)d\alpha$$

$$II=\int_{\mathbb{R}}\frac{e^{i\eta\alpha}}{\tilde{\Omega}'(\alpha_0)(\alpha-\alpha_0)}u(\alpha)d\alpha$$

$$III=\int_{|\alpha-\alpha_0|<1}\left(\frac{e^{i\eta\alpha}}{\tilde{\Omega}(\alpha)}-\frac{e^{i\eta\alpha}}{\tilde{\Omega}'(\alpha_0)(\alpha-\alpha_0)}\right)u(\alpha)d\alpha$$

$$|I| \leq 2 \int_{|\alpha - \alpha_0| \geq 1} \frac{|u(\alpha)|}{|\alpha - \alpha_0|} d\alpha \lesssim \|u\|_{L^q}$$

$$II = \frac{e^{i\eta\alpha_0}}{\tilde{\Omega}'(\alpha_0)} v(\alpha_0) \text{ with } v = \left(\alpha \mapsto \frac{e^{i\eta\alpha}}{\alpha}\right) * u$$

$$|v(\tilde{\alpha})| = \left| \int_{\mathbb{R}} \frac{e^{i\eta(\alpha - \tilde{\alpha})}}{\alpha - \tilde{\alpha}} u(\alpha) d\alpha \right| \leq \left| \int_{\mathbb{R}} \frac{1}{\alpha - \tilde{\alpha}} e^{i\eta\alpha} u(\alpha) d\alpha \right|$$

$$|v'(\tilde{\alpha})| = \left| \int_{\mathbb{R}} \frac{e^{i\eta(\alpha - \tilde{\alpha})}}{\alpha - \tilde{\alpha}} u'(\alpha) d\alpha \right| \leq \left| \int_{\mathbb{R}} \frac{1}{\alpha - \tilde{\alpha}} e^{i\eta\alpha} u'(\alpha) d\alpha \right|$$

$$v \in W^{1,q} \text{ with } \|v\|_{W^{1,q}} \lesssim \|u\|_{W^{1,q}}$$

$$|II| \lesssim \|u\|_{W^{1,q}}$$

$$2|\tilde{\Omega}(\alpha) - \tilde{\Omega}'(\alpha_0)(\alpha - \alpha_0)| \leq \|\tilde{\Omega}''\|_{L^\infty} |\alpha - \alpha_0|^2$$

$$|\alpha - \alpha_0| < \frac{|\tilde{\Omega}'(\alpha_0)|}{\|\tilde{\Omega}''\|_{L^\infty}} \|\tilde{\Omega}''\|_{L^\infty}$$

$$\frac{1}{\tilde{\Omega}(\alpha)} = \frac{1}{\tilde{\Omega}'(\alpha_0)(\alpha - \alpha_0)} \frac{1}{1 + \frac{\tilde{\Omega}(\alpha) - \tilde{\Omega}'(\alpha_0)(\alpha - \alpha_0)}{\tilde{\Omega}'(\alpha_0)(\alpha - \alpha_0)}} = \frac{1}{\tilde{\Omega}'(\alpha_0)(\alpha - \alpha_0)} + o\left(\|\tilde{\Omega}''\|_{L^\infty}\right)$$

$$|\tilde{\Omega}(\alpha)| > |\alpha - \alpha_0| \text{ as } \tilde{\Omega}' > 1$$

$$|\alpha - \alpha_0| > \frac{|\tilde{\Omega}'(\alpha_0)|}{\|\tilde{\Omega}''\|_{L^\infty}}$$

$$\frac{1}{|\Omega(\alpha)|} < \|\tilde{\Omega}''\|_{L^\infty}$$

$$\frac{e^{i\eta\alpha}}{\tilde{\Omega}(\alpha)} - \frac{e^{i\eta\alpha}}{\tilde{\Omega}'(\alpha_0)(\alpha - \alpha_0)} = o\left(\|\tilde{\Omega}''\|_{L^\infty}\right)$$

$$|III| \lesssim \|\tilde{\Omega}''\|_{L^\infty} \int_{|\alpha - \alpha_0| \leq 1} |u(\alpha)| d\alpha \lesssim \|\tilde{\Omega}''\|_{L^\infty} \|u\|_{L^q}$$

$$\widehat{L_4(V)}(\zeta,y,t)=-i\int_0^t\int\!\!\!\int (g(\xi+\zeta)-g(\xi))e^{-i(t-\tau)(\theta(\xi+\zeta)-\theta(\xi))}\hat{U}(\zeta,z,\tau)e^{i\xi(z-y)}dzd\xi d\tau$$

$$\widehat{L_4(V)}(\zeta,y,t)=-i(2\pi)^{\frac{d}{2}}\int (g(\xi+\zeta)$$

$$-g(\xi))e^{-i\xi y}\Big(\mathcal{F}_{x,y}U(\zeta,-\xi,\cdot)*\big(\mathbf{1}(\cdot\geq 0)e^{-i(\theta(\xi+\zeta)-\theta(\xi))\cdot}\big)\Big)(t)d\xi$$



$$\widehat{L_3(V)}(\zeta, y, t) \\ = i(2\pi)^{\frac{d}{2}} \int (g(\xi + \zeta) - g(\xi))e^{-i\xi y} \left(\hat{w}(\zeta) \mathcal{F}_x V(\zeta, 0, \cdot) * (\mathbf{1}(\cdot \geq 0) e^{-i(\theta(\xi + \zeta) - \theta(\xi))}) \right) (t) d\xi$$

$$U_4(\zeta, \xi, \omega) = \mathcal{F}_{x,y,t} U(\zeta, -\xi, \omega), U_3(\zeta, \xi, \omega) = \hat{w}(\zeta) \mathcal{F}_{x,t} V(\zeta, 0, \omega).$$

$$\mathcal{F}_t(\mathbf{1}(\cdot \geq 0))(\omega) = \frac{1}{2} \sqrt{2\pi} \delta(\omega) + \frac{1}{\sqrt{2\pi}} \frac{1}{i\omega}$$

$$L_k(V) = (-1)^{k+1} \frac{i(2\pi)^{\frac{d+1}{2}}}{2} L_{k,\delta}(V) + (-1)^{k+1} (2\pi)^{\frac{d-1}{2}} L_{k,p.v.}(V)$$

$$\mathcal{F}_{x,t} L_{k,\delta}(V)(\zeta,y,\omega) = \int (g(\xi+\zeta)-g(\xi))e^{-i\xi y} U_k(\zeta,\xi,\omega) \delta(\omega+\theta(\xi+\zeta)-\theta(\xi)) d\xi$$

$$\mathcal{F}_{x,t} L_{k,p.v.}(V)(\zeta,y,\omega) = \int (g(\xi+\zeta)-g(\xi))e^{-i\xi y} U_k(\zeta,\xi,\omega) \frac{1}{\omega+\theta(\xi+\zeta)-\theta(\xi)} d\xi$$

$$\xi=\xi^\perp+\tilde{\xi} \text{ where } \tilde{\xi}\in \text{Span}\{\zeta\} \text{ and } \xi^\perp\in \{\zeta\}^\perp$$

$$\tilde{\xi}=\sigma\frac{\zeta}{|\zeta|}$$

$$\mathcal{F}_{x,t} L_{k,\delta}(V)(\zeta,y,\omega) = \iint (g(\xi+\zeta)-g(\xi))e^{-i\xi y} U_k(\zeta,\xi,\omega) \delta\left(\Omega\left(\zeta,\xi^\perp+\sigma\frac{\zeta}{|\zeta|},\omega\right)\right) d\xi^\perp d\sigma$$

$$\Omega(\zeta,\xi,\omega)=\omega+\theta(\xi+\zeta)-\theta(\xi)$$

$$\nabla_\xi \Omega = \nabla \theta(\xi + \zeta) - \nabla \theta(\xi)$$

$$\frac{\zeta}{|\zeta|}\cdot \nabla_\xi \Omega(\zeta,\xi,\omega)>\lambda_*|\zeta|$$

$$\xi_0=\xi^\perp+\tilde{\xi}_0 \text{ with } \tilde{\xi}_0=\sigma_0(\zeta,\xi^\perp,\omega)\frac{\zeta}{|\zeta|}$$

$$\mathcal{F}_{x,t} L_{k,\delta}(V)(\zeta,y,\omega) = \int \frac{1}{\frac{\zeta}{|\zeta|}\cdot \nabla_\xi \Omega(\zeta,\xi_0,\omega)} (g(\xi_0+\zeta)-g(\xi_0))e^{-i\xi_0 y} U_k(\zeta,\xi_0,\omega) d\xi^\perp$$

$$g_\zeta(\xi)=\frac{g(\xi+\zeta)-g(\xi)}{|\zeta|}$$

$$\tilde{U}_{1,k}(\zeta,\xi,\omega)=\frac{|\zeta|}{\frac{\zeta}{|\zeta|}\cdot \nabla_\xi \Omega(\zeta,\xi,\omega)} g_\zeta(\xi) U_k(\zeta,\xi,\omega)$$

$$\mathcal{F}_{x,t} L_{k,\delta}(V)(\zeta,y,\omega) = \int e^{-i\xi^\perp y - i\sigma_0 \frac{\zeta}{|\zeta|} y} \tilde{U}_{1,k}\left(\zeta,\xi^\perp + \sigma_0 \frac{\zeta}{|\zeta|},\omega\right) d\xi^\perp$$

$$\left|\tilde{U}_{1,k}\left(\zeta,\xi^\perp+\sigma_0\frac{\zeta}{|\zeta|},\omega\right)\right|\lesssim\|\tilde{U}_{1,k}(\zeta,\xi^\perp+\tilde{\xi},\omega)\|_{L^1_{\tilde{\xi}}}+\|\nabla_{\tilde{\xi}}\tilde{U}_{1,k}(\zeta,\xi^\perp+\tilde{\xi},\omega)\|_{L^1_{\tilde{\xi}}}.$$

$$|\mathcal{F}_{x,t}L_{k,\delta}(V)(\zeta, y, \omega)| \lesssim \|\tilde{U}_{1,k}(\zeta, \cdot, \omega)\|_{L_{\xi}^1} + \|\nabla_{\xi}\tilde{U}_{1,k}(\zeta, \cdot, \omega)\|_{L_{\xi}^1}$$

$$\xi = \xi^{\perp} + \tilde{\xi} \text{ with } \tilde{\xi} = \sigma \frac{\zeta}{|\zeta|} \text{ and } \xi^{\perp} \in \{\zeta\}^{\perp}$$

$$\mathcal{F}_{x,t}L_{k,p.v.}(V)(\zeta, y, \omega) = \iint g_{\zeta}(\xi) e^{-i\xi y} U_k(\zeta, \xi, \omega) \frac{|\zeta|}{\Omega\left(\zeta, \xi^{\perp} + \sigma \frac{\zeta}{|\zeta|}, \omega\right)} d\xi^{\perp} d\sigma$$

$$\tilde{U}_{2,k}(\zeta, \xi, \omega) = g_{\zeta}(\xi) U_k(\zeta, \xi, \omega)$$

$$\mathcal{F}_{x,t}L_{k,p.v.}(V)(\zeta, y, \omega) = \iint \tilde{U}_{2,k}\left(\zeta, \xi^{\perp} + \sigma \frac{\zeta}{|\zeta|}, \omega\right) e^{-i\xi^{\perp} y - i\sigma y \frac{\zeta}{|\zeta|}} \frac{|\zeta|}{\Omega\left(\zeta, \xi^{\perp} + \sigma \frac{\zeta}{|\zeta|}, \omega\right)} d\xi^{\perp} d\sigma$$

$$\begin{aligned} \left| \nabla_{\xi} \left(\frac{\zeta}{|\zeta|} \cdot \nabla_{\xi} \Omega(\zeta, \xi, \omega) \right) \right| &\lesssim \left| \nabla_{\xi} \left(\frac{\zeta}{|\zeta|} \cdot \nabla_{\xi} \theta(\xi + \zeta) \right) - \nabla_{\xi} \left(\frac{\zeta}{|\zeta|} \cdot \nabla_{\xi} \theta(\xi) \right) \right| \\ &\leq C \left(\|\nabla^{\otimes 3} \tilde{\theta}\|_{L^{\infty}, \lambda_*} \right) |\zeta| \end{aligned}$$

$$\begin{aligned} &\left| \int \tilde{U}_{2,k}\left(\zeta, \xi^{\perp} + \sigma \frac{\zeta}{|\zeta|}, \omega\right) e^{-i\xi^{\perp} y - i\sigma y \frac{\zeta}{|\zeta|}} \frac{|\zeta|}{\Omega\left(\zeta, \xi^{\perp} + \sigma \frac{\zeta}{|\zeta|}, \omega\right)} d\sigma \right| \\ &\leq C \left(\|\nabla^{\otimes 3} \tilde{\theta}\|_{L^{\infty}, \lambda_*} \right) \|\tilde{U}_{2,k}(\zeta, \xi^{\perp} + \tilde{\xi}, \omega)\|_{L_{\xi}^2} + \|\nabla_{\xi} \tilde{U}_{2,k}(\zeta, \xi^{\perp} + \tilde{\xi}, \omega)\|_{L_{\xi}^2} \end{aligned}$$

$$|\mathcal{F}_{x,t}L_{k,p.v.}(V)(\zeta, y, \omega)| \lesssim \|\tilde{U}_{2,k}(\zeta, \cdot, \omega)\|_{L_{\xi^{\perp}}^1 L_{\xi}^2} + \|\nabla_{\xi} \tilde{U}_{2,k}(\zeta, \cdot, \omega)\|_{L_{\xi^{\perp}}^1 L_{\xi}^2}$$

$$|\tilde{U}_{1,k}(\zeta, \xi, \omega)| \approx |\tilde{U}_{2,k}(\zeta, \xi, \omega)| = |g_{\zeta}(\xi) U_k(\zeta, \xi, \omega)|.$$

$$\|\tilde{U}_{1,k}(\zeta, \cdot, \cdot)\|_{L_{\xi}^1 L_{\omega}^2} \lesssim \|g_{\zeta}\|_{L_{\xi}^1} \|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2}$$

$$\begin{aligned} \|\tilde{U}_{2,k}(\zeta, \cdot, \cdot)\|_{L_{\xi^{\perp}}^1 L_{\xi}^q L_{\omega}^2} &\lesssim \|g_{\zeta}\|_{L_{\xi^{\perp}}^1 L_{\xi}^q} \|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} \\ &\lesssim \|g_{\zeta}\|_{W_{\xi}^{1,1}} \|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} \end{aligned}$$

$$\nabla_{\xi} \tilde{U}_{2,k}(\zeta, \xi, \omega) = \nabla g_{\zeta}(\xi) U_k(\zeta, \xi, \omega) + g_{\zeta}(\xi) \nabla_{\xi} U_k(\zeta, \xi, \omega)$$

$$\begin{aligned} \|\nabla_{\xi} \tilde{U}_{2,k}(\zeta, \xi, \omega)\|_{L_{\xi^{\perp}}^1 L_{\xi}^q L_{\omega}^2} &\lesssim \|\nabla g_{\zeta}\|_{L_{\xi^{\perp}}^1 L_{\xi}^q} \|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} + \|g_{\zeta}\|_{L_{\xi^{\perp}}^1 L_{\xi}^q} \|\nabla_{\xi} U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} \\ &\lesssim \|g_{\zeta}\|_{W^{2,1}} \left(\|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} + \|\nabla_{\xi} U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} \right). \end{aligned}$$

$$\begin{aligned} |\nabla_{\xi} \tilde{U}_{1,k}(\zeta, \xi, \omega)| &= \left| \frac{|\zeta|}{\frac{\zeta}{|\zeta|} \cdot \nabla_{\xi} \Omega(\zeta, \xi, \omega)} \nabla_{\xi} \tilde{U}_{2,k} + \nabla_{\xi} \left(\frac{|\zeta|}{\frac{\zeta}{|\zeta|} \cdot \nabla_{\xi} \Omega(\zeta, \xi, \omega)} \right) \tilde{U}_{2,k} \right| \\ &\lesssim C \left(\|\nabla^{\otimes 3} \tilde{\theta}\|_{L^{\infty}, \lambda_*} \right) (|\nabla_{\xi} \tilde{U}_{2,k}| + |\tilde{U}_{2,k}|) \end{aligned}$$

$$\left| \frac{|\zeta|}{\left| \frac{\zeta}{|\zeta|} \cdot \nabla_{\xi} \Omega(\zeta, \cdot, \cdot) \right|} \right| + \left| \nabla_{\xi} \left(\frac{|\zeta|}{\left| \frac{\zeta}{|\zeta|} \cdot \nabla_{\xi} \Omega(\zeta, \cdot, \cdot) \right|} \right) \right| \lesssim 1$$

$$\|\nabla_{\xi} \tilde{U}_{1,k}(\zeta, \xi, \omega)\|_{L_{\xi}^1 L_{\omega}^2} \lesssim C \left(\|\nabla^{\otimes 3} \tilde{\theta}\|_{L^{\infty}, \lambda_*} \right) \|g_{\zeta}\|_{W^{2,1}} \left(\|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} + \|\nabla_{\xi} U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} \right)$$

$$|\mathcal{F}_{x,t} L_k(V)(\zeta, y_0, \omega)| \lesssim \sum_{j=0}^1 \left\| \nabla_{\xi}^j \tilde{U}_{1,k}(\zeta, \cdot, \omega) \right\|_{L_{\xi}^1} + \left\| \nabla_{\xi}^j \tilde{U}_{2,k}(\zeta, \cdot, \omega) \right\|_{L_{\xi \perp}^1 L_{\xi}^2}.$$

$$\begin{aligned} \|\mathcal{F}_x L_k(V)(\zeta, y_0, \cdot)\|_{L_t^2} &= \|\mathcal{F}_{x,t} L_k(V)(\zeta, y_0, \cdot)\|_{L_{\omega}^2} \\ &\lesssim \sum_{j=0}^1 \left\| \nabla_{\xi}^j \tilde{U}_{1,k}(\zeta, \cdot, \omega) \right\|_{L_{\omega}^2 L_{\xi}^1} + \left\| \nabla_{\xi}^j \tilde{U}_{2,k}(\zeta, \cdot, \omega) \right\|_{L_{\omega}^2 L_{\xi \perp}^1 L_{\xi}^2} \\ &\lesssim \sum_{j=0}^1 \left\| \nabla_{\xi}^j \tilde{U}_{1,k}(\zeta, \cdot, \omega) \right\|_{L_{\xi}^1 L_{\omega}^2} + \left\| \nabla_{\xi}^j \tilde{U}_{2,k}(\zeta, \cdot, \omega) \right\|_{L_{\xi \perp}^1 L_{\xi}^2 L_{\omega}^2}. \end{aligned}$$

$$\|\mathcal{F}_x L_k(V)(\zeta, y_0, \cdot)\|_{L_t^2} \lesssim C \left(\|\nabla^{\otimes 3} \tilde{\theta}\|_{L^{\infty}, \lambda_*} \right) \|g_{\zeta}\|_{W_{\xi}^{2,1}} \left(\|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} + \|\nabla_{\xi} U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} \right)$$

$$\nabla^j g_{\zeta}(\xi) = \frac{\nabla^j g(\xi + \zeta) - \nabla^j g(\xi)}{|\zeta|} = \int_0^1 \nabla^{j+1} g(\xi + t\zeta) \cdot \frac{\zeta}{|\zeta|} dt$$

$$\|\nabla^j g_{\zeta}\|_{L_{\xi}^1} = \frac{1}{|\zeta|} \|\nabla^j g(\cdot + \zeta) - \nabla^j g(\cdot)\|_{L^1} \leq \|\nabla g\|_{W^{j,1}}$$

$$\|\mathcal{F}_x L_k(V)(\zeta, y_0, \cdot)\|_{L_t^2} \lesssim C \left(\|\nabla^{\otimes 3} \tilde{\theta}\|_{L^{\infty}, \lambda_*} \right) \|\nabla g\|_{W^{2,1}} \left(\|U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} + \|\nabla_{\xi} U_k(\zeta, \cdot, \cdot)\|_{L_{\xi}^{\infty} L_{\omega}^2} \right)$$

$$\begin{aligned} U_4(\zeta, \xi, \omega) &= \mathcal{F}_{x,y,t}(w(y)V(x,y,t))(\zeta, -\xi, \omega) \\ \nabla_{\xi} U_4(\zeta, \xi, \omega) &= \mathcal{F}_{x,y,t}(i y w(y)V(x,y,t))(\zeta, -\xi, \omega) \end{aligned}$$

$$\|U_4\|_{L_{\zeta}^2 L_{\xi}^{\infty} L_{\omega}^2} \leq \|\mathcal{F}_{t,x} V(\zeta, y, \omega)\|_{L_{\zeta}^2 L_{|w(y)|dy}^1} L_{\omega}^2$$

$$\|U_4\|_{L_{\xi}^2 L_{\xi}^{\infty} L_{\omega}^2} \leq \|V\|_{L_{|w(y)|dy}^1} L_{t,x}^2.$$

$$\|\nabla_{\xi} U_4\|_{L_{\zeta}^2 L_{\xi}^{\infty} L_{\omega}^2} \leq \|V\|_{L_{|yw(y)|dy}^1} L_{t,x}^2.$$

$$\|\nabla_{\xi} U_4\|_{L_{\zeta}^2 L_{\xi}^{\infty} L_{\omega}^2} + \|U_4\|_{L_{\zeta}^2 L_{\xi}^{\infty} L_{\omega}^2} \lesssim_w \|V\|_{L_y^{\infty} L_{t,x}^2}.$$

$$U_3(\zeta, \xi, \omega) = \hat{w}(\zeta) \mathcal{F}_{x,t}(V(x, 0, t))(\zeta, \omega), \nabla_{\xi} U_3(\zeta, \xi, \omega) = 0$$

$$\|U_3\|_{L_{\zeta}^2 L_{\xi}^{\infty} L_{\omega}^2}^2 \leq \|\hat{w}\|_{L^{\infty}} \|V(y=0)\|_{L_{t,x}^2}^2$$

$$\begin{aligned} & \mathcal{F}_{t,x}L_{k,\delta}(V)(\zeta,y_0+y,\omega)-\mathcal{F}_{t,x}L_{k,\delta}(V)(\zeta,y_0,\omega) \\ &= \int \left(e^{-i\xi^\perp y-i\sigma_0\frac{\zeta}{|\zeta|}y}-1\right)e^{-i\xi^\perp y_0-i\sigma_0\frac{\zeta}{|\zeta|}y_0}\tilde{U}_{1,k}\left(\zeta,\xi^\perp+\sigma_0\frac{\zeta}{|\zeta|},\omega\right)d\xi^\perp \end{aligned}$$

$$\begin{aligned} & \|L_{k,\delta}(V)(\cdot,y_0+y,\cdot)-L_{k,\delta}(V)(\cdot,y_0,\cdot)\|_{L^2_{t,x}} \\ & \lesssim \|(e^{i\xi y}-1)\tilde{U}_{1,k}\|_{L^2_{\zeta,\omega},L^1_{\xi}}+\|(e^{i\xi y}-1)\nabla_{\xi}\tilde{U}_{1,k}\|_{L^2_{\zeta,\omega},L^1_{\xi}}+|y|\|\tilde{U}_{1,k}\|_{L^2_{\zeta,\omega},L^1_{\xi}}. \end{aligned}$$

$$\|L_{k,\delta}(V)(\cdot,y_0+y,\cdot)-L_{k,\delta}(V)(\cdot,y_0,\cdot)\|_{L^2_{t,x}}\rightarrow 0$$

$$\|\langle y\rangle w\|_{L^1}\|\nabla g\|_{W^{2,1}}\leq C\left(\|\nabla^{\otimes 3}\tilde{\theta}\|_{L_{\infty}},\lambda_*\right)$$

$$C_yL_t^2\dot{H}_x^{-1/2}\cap L_y^\infty L_t^2\dot{H}_x^{-1/2}$$

$$C_yL_t^2\dot{H}_x^{S_c}\cap L_y^\infty L_t^2\dot{H}_x^{S_c}$$

$$C_yL_t^2B_2^{-1/2,S_x}\cap L_y^\infty L_t^2B_2^{-1/2,S_c}$$

$$1-L_3-L_4 \text{ on } C_yL_t^2B_2^{-1/2,S_x}\cap L_y^\infty L_t^2B_2^{-1/2,S_c}$$

$$C_yL_t^2B_2^{-1/2,S_x}\cap L_y^\infty L_t^2B_2^{-1/2,S_c} \text{ to } E_Z$$

$$C_yL_t^2B_2^{-1/2,S_x}\cap L_y^\infty L_t^2B_2^{-1/2,S_c} \text{ to } L_{t,x}^{d+2}L_\omega^2$$

$$\begin{aligned} |L_{k+2}(V)(x,y,t)| &= \left| \mathbb{E}(\bar{Y}(x+y,t)L_1(V)(x,t)) + \mathbb{E}(\overline{L_1(V)}(x+y,t)Y(x,t)) \right| \\ &\leq \left(\int \ g \right) (\|L_k(V)(x,t)\|_{L_\omega^2} + \|L_k(V)(x+y,t)\|_{L_\omega^2}) \end{aligned}$$

$$\|L_{k+2}(V)\|_{L_{t,x}^{d+2}}\lesssim_g \|L_k(V)\|_{E_Z}\lesssim_g \|V\|_{L_y^\infty L_t^2B_2^{-1/2,S_c}}$$

$$\frac{d+2}{2}\in [2,d+2]$$

$$\|L_{k+2}(V)\|_{L_{t,x}^{(d+2)/2}}\lesssim_g \|V\|_{L_y^\infty L_t^2B_2^{-1/2,S_c}}$$

$$C_yL_t^2B_2^{-1/2,S_x}\cap L_y^\infty L_t^2B_2^{-1/2,S_c}$$

$$(1-L_3-L_4)^{-1}=1+(L_3+L_4)(1-L_3-L_4)^{-1}$$

$$\|Q_k(Z,V)\|_Z\leq C\|\langle y\rangle w\|_M\|Z\|_Z\|V\|_V$$

$$\tilde{V}_1=w*V(y=0)Z,\tilde{V}_2(x)=-\int\, dzw(z)V(x,z)Z(x+z)$$

$$Q_k(Z,V)=-i\int_0^tS(t-\tau)\tilde{V}_k(\tau)d\tau$$

$$\|Q_k(Z,V)\|_Z\lesssim\|\tilde{V}_k\|_{L^{p'}(\mathbb{R},W^{s_c,p'}(\mathbb{R}^d,L^2(\Omega)))}.$$

$$\frac{1}{p'} = \frac{1}{p} + \frac{2}{d+2}, \frac{1}{p'} = \frac{1}{d+2} + \frac{1}{2}$$

$$\begin{aligned} & \|\tilde{V}_1\|_{L^{p'}(\mathbb{R}, W^{sc,p'}(\mathbb{R}^d, L^2(\Omega)))} \\ & \lesssim \|w * V(y=0)\|_{L^{(d+2)/2}(\mathbb{R} \times \mathbb{R}^d) \cap L^2(\mathbb{R}, H^{sc}(\mathbb{R}^d))} \|Z\|_{L^p(\mathbb{R}, W^{sc,p}(\mathbb{R}^d, L^2(\Omega))) \cap L^{d+2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))}. \end{aligned}$$

$$\|\tilde{V}_1\|_{L^{p'}(\mathbb{R}, W^{sc,p'}(\mathbb{R}^d, L^2(\Omega)))} \leq \|V\|_V \|Z\|_Z$$

$$\|\tilde{V}_2\|_{L^{p'}(\mathbb{R}, W^{sc,p'}(\mathbb{R}^d, L^2(\Omega)))} \leq \int \left| w(z) \|V(z) T_z Z\|_{L^{p'}(\mathbb{R}, W^{sc,p'}(\mathbb{R}^d, L^2(\Omega)))} \right|$$

$$\|\tilde{V}_2\|_{L^{p'}(\mathbb{R}, W^{sc,p'}(\mathbb{R}^d, L^2(\Omega)))} \lesssim \int \left| w(z) \|V(z)\|_{L^{(d+2)/2}(\mathbb{R} \times \mathbb{R}^d) \cap L^2(\mathbb{R}, H^{sc}(\mathbb{R}^d))} \|T_z Z\|_Z \right|$$

$$\|\tilde{V}_2\|_{L^{p'}(\mathbb{R}, W^{sc,p'}(\mathbb{R}^d, L^2(\Omega)))} \lesssim \int \left| w(z) \|V\|_V \|Z\|_Z \right|$$

$$\begin{aligned} E_Z \times E_Z &\mapsto E_V \\ (Z, Z') &\mapsto ((x, y) \mapsto \mathbb{E}(Z(x+y)Z'(x))) \end{aligned}$$

$$\|\mathbb{E}(T_y ZZ')\|_{L^{(d+2)/2}(\mathbb{R} \times \mathbb{R}^d)} \leq \|T_y Z\|_{L^{d+2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \|Z'\|_{L^{d+2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))}.$$

$$u\in L^{{d+2}}_{t,x}L^2_{\omega}$$

$$\|\mathbb{E}(T_y ZZ')\|_{L^{(d+2)/2}(\mathbb{R} \times \mathbb{R}^d)} \leq \|Z\|_Z \|Z'\|_Z$$

$$\mathbb{E}(T_y ZZ') \in C_y L^{(d+2)/2}_{t,x}$$

$$\|\mathbb{E}(T_y ZZ')\|_{L^\infty(\mathbb{R}^d, L^{(d+2)/2}(\mathbb{R}^d \times \mathbb{R}))} \leq \|Z\|_Z \|Z'\|_Z$$

$$\underline{C_y L_t^2 H_x^{S_c}}$$

$$\frac{1}{2} = \frac{d}{2(d+2)} + \frac{1}{d+2} = \frac{1}{p} + \frac{1}{d+2}$$

$$\begin{aligned} \|\mathbb{E}(T_y ZZ')\|_{L^2(\mathbb{R}, H^{sc}(\mathbb{R}^d))} &\leq \left(\|T_y Z\|_{L^p(\mathbb{R}, W^{sc,p}(\mathbb{R}^d, L^2(\Omega)))} + \|T_y Z\|_{L^{d+2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \right) \\ &\quad \times \left(\|Z'\|_{L^p(\mathbb{R}, W^{sc,p}(\mathbb{R}^d, L^2(\Omega)))} + \|Z'\|_{L^{d+2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \right). \end{aligned}$$

$$\sup_{y \in \mathbb{R}^d} \|\mathbb{E}(T_y ZZ')\|_{L^2(\mathbb{R}, H^{sc}(\mathbb{R}^d))} \leq \|Z\|_Z \|Z'\|_Z$$

$$\mathbb{E}(T_y ZZ') \in C_y L_t^2 H_x^{S_c} L_\omega^2$$

$$C_y L_t^2 B_2^{-1/2, S_c}$$



$$\|\cdot\|_{L^2(\mathbb{R},B_2^{-1/2sc}(\mathbb{R}^d))}\leq \|\cdot\|_{L^2(\mathbb{R},\dot{H}^{-1/2}(\mathbb{R}^d))}+\|\cdot\|_{L^2(\mathbb{R},H^{sc}(\mathbb{R}^d))}$$

$$L^2\left(\mathbb{R},\dot{H}^{-1/2}(\mathbb{R}^d)\right)$$

$$\begin{aligned}\|\mathbb{E}(T_yZZ')\|_{L^2(\mathbb{R},\dot{H}^{-1/2}(\mathbb{R}^d))}&\lesssim\|\mathbb{E}(T_yZZ')\|_{L^2(\mathbb{R},L^{q/2}(\mathbb{R}^d))}\\&\lesssim\|T_yZ\|_{L^4(\mathbb{R},L^q(\mathbb{R}^d,L^2(\Omega)))}\|Z'\|_{L^4(\mathbb{R},L^q(\mathbb{R}^d,L^2(\Omega)))}.\end{aligned}$$

$$\sup_{y\in\mathbb{R}^d}\|\mathbb{E}(T_yZZ')\|_{L^2(\mathbb{R},B_2^{-1/2,0}(\mathbb{R}^d))}\lesssim\|Z\|_Z\|Z'\|_Z$$

$$\mathbb{E}(T_yZZ')\in C_yL_t^2B_2^{-1/2,0}L_\omega^2$$

$$\|Q_k(Z,V)\|_V\leq C\|\langle y\rangle w\|_M\|Z\|_Z\|V\|_V$$

$$\tilde{V}_1=w*V(y=0)Z,\tilde{V}_2(x)=-\int\,dzw(z)V(x,z)Z(x+z)$$

$$Q_k(Z,V)(y)=\mathbb{E}(T_y\bar{Y}Q_{k-2})+\mathbb{E}(T_y\bar{Q}_{k-2}Y)$$

$$C_yL_{t,x}^{\frac{d+2}{2}}Q_{k-2}(Z,V)E_Z\times E_VL^{d+2}(\mathbb{R}\times\mathbb{R}^d)Y\in L^\infty(\mathbb{R}\times\mathbb{R}^d,L^2(\Omega))$$

$$\|Q_k(Z,V)(y)\|_{L^{d+2}(\mathbb{R}\times\mathbb{R}^d)}\lesssim\|Z\|_Z\|V\|_V$$

$$L^{\frac{2(d+2)}{d}}Q_k(Z,V)\in L_y^\infty,L_{t,x}^{(d+2)/2}$$

$$u\in L_{t,x}^{(d+2)/2}$$

$$y\mapsto T_yuL_{t,x}^{(d+2)/2}C_yL_t^2B_x^{-1/2,s_c}$$

$$\|Q_k(Z,V)(y)\|_{L^2(\mathbb{R},B_2^{-1/2,sc}(\mathbb{R}^d))}\leqslant\|Z\|_Z\|V\|_V$$

$$\|\mathbb{E}(T_y\bar{Q}_{k-2}Y)\|_{L^2(\mathbb{R},B_2^{-1/2,sc}(\mathbb{R}^d))}=\|\mathbb{E}(Q_{k-2}T_{-y}\bar{Y})\|_{L^2(\mathbb{R},B_2^{-1/2,sc}(\mathbb{R}^d))}.$$

$$\|\mathbb{E}(T_y\bar{Q}_{k-2}Y)\|_{L^2(\mathbb{R},B_2^{-1/2,sc}(\mathbb{R}^d))}$$

$$U\in L^2\left(\mathbb{R},B_2^{1/2}(\mathbb{R}^d)\right)$$

$$\langle U,\mathbb{E}(T_yQ_{k-2}\bar{Y})\rangle=\mathbb{E}(\langle UY,T_yQ_{k-2}\rangle)$$

$$\langle U,\mathbb{E}(T_yQ_{k-2}\bar{Y})\rangle=\mathbb{E}\left(\left\langle UY,-i\int_0^tS(t-\tau)T_y\tilde{V}_{k-2}(\tau)\right\rangle\right)=\mathbb{E}\left(\left\langle\int_\tau^\infty U(t)Y(t)dt,T_y\tilde{V}_{k-2}\right\rangle\right)$$

$$|\langle U, \mathbb{E}(T_y Q_{k-2} \bar{Y}) \rangle| \leq \left\| \int_{\tau}^{\infty} U(t) Y(t) dt \right\|_{L^{p_1}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \|T_y \tilde{V}_{k-2}(\tau)\|_{L^{p'_1}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))}$$

$$\left\| \int_{\tau}^{\infty} U(t) Y(t) dt \right\|_{L^{p_1}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \lesssim \|U\|_{L^2(\mathbb{R}, B_2^{1/2,1}(\mathbb{R}^d))}$$

$$\left\| \int_{\tau}^{\infty} U(t) Y(t) dt \right\|_{L^{p_1}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \lesssim \|U\|_{L^2(\mathbb{R}, B_2^{1/2,0}(\mathbb{R}^d))}$$

$$\|\tilde{V}_1\|_{L^{p'_1}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \leq \|w * V(y=0)\|_{L^2(\mathbb{R} \times \mathbb{R}^d)} \|Z\|_{L^{(d+2)/2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))}.$$

$$\|w * V(y=0)\|_{L^2(\mathbb{R} \times \mathbb{R}^d)} \lesssim \|V\|_V$$

$$4, \frac{d+2}{2} \in \left[2 \frac{d+2}{d}, d+2 \right]$$

$$\|Z\|_{L^{(d+2)/2}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \leq \|Z\|_Z$$

$$\|\tilde{V}_2\|_{L^{p'_1}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \leq \int dz \, |w(z)| \|V(z)\|_{L^2(\mathbb{R} \times \mathbb{R}^d)} \|Z\|_Z$$

$$\langle U, \nabla^{\otimes n} \mathbb{E}(T_y Q_{k-2} \bar{Y}) \rangle = \sum_{j=0}^n \binom{n}{j} \mathbb{E}(\langle U, \nabla^{\otimes(n-j)} \bar{Y} \otimes \nabla^{\otimes j} T_y Q_{k-2} \rangle).$$

$$\langle U, \nabla^{\otimes n} \mathbb{E}(T_y Q_{k-2} \bar{Y}) \rangle = \sum_{j=0}^n \binom{n}{j} \mathbb{E} \left(\left\langle \int_{\tau}^{\infty} S(\tau-t) U(t) \nabla^{\otimes(n-j)} Y(t) dt, \nabla^{\otimes j} T_y \tilde{V}_{k-2} \right\rangle \right)$$

$$\begin{aligned} & |\langle U, \nabla^{\otimes n} \mathbb{E}(T_y Q_{k-2} \bar{Y}) \rangle| \\ & \leq \sum_{j=0}^n \binom{n}{j} \left\| \int_{\tau}^{\infty} S(\tau-t) U(t) \nabla^{\otimes(n-j)} Y(t) dt \right\|_{L^p(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \|\nabla^{\otimes j} T_y \tilde{V}_{k-2}\|_{L^{p'}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \end{aligned}$$

$$\left\| \int_{\tau}^{\infty} S(\tau-t) U(t) \nabla^{\otimes(n-j)} Y(t) dt \right\|_{L^p(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))} \lesssim \|U\|_{L^2(\mathbb{R}, B_2^{-1/2,0}(\mathbb{R}^d))}$$

$$\tilde{V}_{k-2} \mapsto \Pi \mathbb{E} \left(Y \int_0^t S(t-\tau) \tilde{V}_{k-2}(\tau) d\tau \right)$$

$$L^{p'}\left(\mathbb{R}, W^{n,p'}(\mathbb{R}^d, L^2(\Omega))\right) L^\infty_y, L^2(\mathbb{R}, H^n)$$

$$L^{p'}\left(\mathbb{R}, W^{s_c,p'}(\mathbb{R}^d, L^2(\Omega))\right) L^\infty_y, L^2(\mathbb{R}, H^{s_c})$$

$$\|\tilde{V}_{k-2}\|_{L^{p'}(\mathbb{R}, W^{s_c,p'}(\mathbb{R}^d, L^2(\Omega)))} \leq \|Z\|_Z \|V\|_V$$

$$u \in L^{p'_1}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega))$$

$$v \in L^{p'} \left(\mathbb{R}, W^{s_c, p'}(\mathbb{R}^d, L^2(\Omega)) \right)$$

$$y \mapsto T_y u \text{ and } y \mapsto T_y v$$

$$L^{p_1'}(\mathbb{R} \times \mathbb{R}^d, L^2(\Omega)) L^{p'} \left(\mathbb{R}, W^{s_c, p'}(\mathbb{R}^d, L^2(\Omega)) \right)$$

$$\|S(t)Z_0\|_Z \lesssim \|Z_0\|_{L^2_\omega H^{s_c}_x}$$

$$\left\| \mathbb{E} \left[\overline{Y(x+y)} S(t) Z_0(x) + \overline{S(t) Z_0(x+y)} Y(x) \right] \right\|_{L^\infty_y \frac{d+2}{L^2_{t,x}}} \lesssim \|Z_0\|_{L^2_\omega H^{s_c}_x}$$

$$Z_0 \in L^{\frac{2d}{d+2}}_x L^2_\omega \mathbb{E} \left[\overline{Y(x+y)} S(t) Z_0(x) + \overline{S(t) Z_0(x+y)} Y(x) \right] \in C_y L^2_t B_2^{-\frac{1}{2}, s_c}$$

$$\left\| \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \right\|_{L^\infty_y L^2_t B_2^{-1/2, s_c}} \lesssim \|Z_0\|_{L^{2d/(d+2)}_x L^2_\omega} + \|Z_0\|_{H^{s_c}_x L^2_\omega}$$

$$\mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right]$$

$$\|S(t)Z_0\|_{L^p_{t,x}L^2_\omega} + \|S(t)Z_0\|_{L^{d+2}_{t,x}L^2_\omega} \lesssim \|Z_0\|_{L^2_\omega H^{s_c}_x}$$

$$\|S(t)Z_0\|_{\frac{d+2}{L^2_{t,x}}L^2_\omega} \lesssim \|Z_0\|_{L^2_\omega H^{s_c}_x}$$

$$\left\| \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \right\|_{\frac{d+2}{L^2_{t,x}}} \lesssim \|T_y Z_0\|_{L^2_\omega H^{s_c}}$$

$$L^2_\omega H^{s_c}_x \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \in C_y L^{(d+2)/2}_{t,x}$$

$$\left\| \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \right\|_{L^\infty_y L^2_{t,x}} \lesssim \|T_y Z_0\|_{L^2_\omega H^{s_c}}$$

$$\underline{C_y L^2_t \dot{H}^{-1/2}_x} U \in L^2_t \dot{H}^{1/2}_x \|U\|_{L^2_t \dot{H}^{1/2}_x} = 1$$

$$\int_0^\infty \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \bar{U} dx dt \lesssim \|T_y Z_0\|_{L^{2d/(d+2)}_x L^2_\omega}$$

$$\left\| \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \right\|_{L^2_t \dot{H}^{-1/2}_x} \lesssim \|T_y Z_0\|_{L^{2d/(d+2)}_x L^2_\omega}$$

$$\mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \in C_y L^2_t \dot{H}^{-1/2}_x$$

$$\left\| \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \right\|_{L^\infty_y L^2_t \dot{H}^{-1/2}_x} \lesssim \|Z_0\|_{L^{2d/(d+2)}_x L^2_\omega}$$

$$\int_0^\infty \mathbb{E} \left[\overline{Y(x)} S(t) T_y Z_0(x) \right] \bar{U} dx dt = \int \mathbb{E} \left[T_y Z_0 \int_0^\infty \overline{S(-t) Y U} dt \right] dx$$

$$\int_0^\infty S(-t) Y U dt \in L^{2d/(d-2)}_x L^2_\omega \left\| \int_0^\infty S(-t) Y U \right\|_{L^{2d/(d-2)}_x L^2_\omega} \lesssim 1$$



$$\nabla_x^{\lfloor s_c \rfloor} (YS(t)T_yZ_0),$$

$$\sum_i \alpha_i + \sum_i \beta_i = \lfloor s_c \rfloor$$

$$U\in H_x^{\lfloor s_c \rfloor - s_c} L_\omega^2 \text{ with } \|U\|_{H_x^{\lfloor s \rfloor - s_c} L_\omega^2} = 1$$

$$\int_0^\infty \mathbb{E}[\overline{\partial^\alpha Y(x)} S(t) T_y \partial^\beta Z_0(x)] \bar{U} dx dt \lesssim \|T_y Z_0\|_{H_x^{s_c} L_\omega^2}$$

$$\|\mathbb{E}[\overline{Y(x)}S(t)T_yZ_0(x)]\|_{L_t^\infty H_x^{s_c}}\lesssim \|T_yZ_0\|_{L_x^{2d/(d+2)}L_\omega^2}+\|T_yZ_0\|_{H_x^{s_c}L_\omega^2}$$

$$\mathbb{E}[\overline{Y(x)}S(t)T_yZ_0(x)]\in C_yL_t^2H_x^{s_c}$$

$$\|\mathbb{E}[\overline{Y(x)}S(t)T_yZ_0(x)]\|_{L_y^\infty L_t^2H_x^{s_c}}\lesssim \|Z_0\|_{L_x^{2d/(d+2)}L_\omega^2}+\|T_yZ_0\|_{H_x^{s_c}L_\omega^2}$$

$$\int_0^\infty \mathbb{E}[\overline{\partial^\alpha Y(x)} S(t) T_y \partial^\beta Z_0(x)] \bar{U} dx dt = \int \mathbb{E} \left[T_y \partial^\beta Z_0 \int_0^\infty \overline{S(-t) \partial^\alpha Y U} dt \right] dx$$

$$\partial^\alpha Y(t,x)=\int f_\alpha(\xi)e^{i(\xi x-\theta(\xi)t)}dW(\xi)$$

$$f_\alpha(\xi)=(i\xi_1)^{\alpha_1}\dots(i\xi_d)^{\alpha_d}f(\xi)$$

$$\left\|\int_0^\infty S(-t)\partial^\alpha YU\right\|_{L_{x,\omega}^2}\lesssim \|U\|_{L_t^2H_x^{-1/2}}\lesssim \|U\|_{L_t^2H_x^{[s_c]-s_c}}=1$$

$$C_yL_t^2B_2^{-1/2,s_c}C_yL_t^2\dot{H}_x^{-1/2}C_yL_t^2H_x^{s_c}\mathbb{E}[\overline{Y(x)}S(t)T_yZ_0(x)]\in C_yL_t^2B_2^{-1/2,s_c}$$

$$\|\mathbb{E}[\overline{Y(x)}S(t)T_yZ_0(x)]\|_{L_y^\infty L_t^2B_2^{-1/2,s_c}}\lesssim \|Z_0\|_{L_x^{2d/(d+2)}L_\omega^2}+\|Z_0\|_{H_x^{s_c}L_\omega^2}$$

$$L=\begin{pmatrix} 0 & L_1+L_2 \\ 0 & L_3+L_4 \end{pmatrix}$$

$$\binom{Z}{V}=(1-L)^{-1}\mathcal{B}_{Z_0}\binom{Z}{V}=(1-L)^{-1}\begin{pmatrix} \mathcal{B}_{Z_0}^{(1)}(Z,V)\\ \mathcal{B}_{Z_0}^{(2)}(Z,V) \end{pmatrix}$$

$$\begin{aligned}\mathcal{B}_{Z_0}^{(1)}(Z,V)&=S(t)Z_0+Q_1(Z,V)+Q_2(Z,V),\\ \mathcal{B}_{Z_0}^{(2)}(Z,V)&=\mathbb{E}[\overline{Y(x+y)}S(t)Z_0(x)+\overline{S(t)Z_0(x+y)}Y(x)]\\ &\quad +Q_3(Z,V)+Q_4(Z,V)+\mathbb{E}[\overline{Z(x+y)}Z(x)].\end{aligned}$$

$$\Phi[Z_0]\colon \left\{ \begin{array}{ccc} E_Z\times E_V & \rightarrow & E_Z\times E_V \\ \binom{Z}{V} & \mapsto & (1-L)^{-1}\mathcal{B}_{Z_0}\binom{Z}{V} \end{array} \right.$$

$$B_{E_Z\times E_V}(0,R\|Z_0\|_{E_0})=:B$$

$$\left\|\Phi[Z_0]\left(\frac{Z}{V}\right)\right\|\lesssim\left\|B_{Z_0}\left(\frac{Z}{V}\right)\right\|$$

$$\mathcal{B}_{Z_0} = C_{Z_0} + Q$$

$$C_{Z_0}=\left(\frac{S(t)Z_0}{\mathbb{E}\left[\overline{Y(x+y)}S(t)Z_0(x)+\overline{S(t)Z_0(x+y)}Y(x)\right]}\right)$$

$$Q(Z,V)=\begin{pmatrix} Q_1(Z,V)+Q_2(Z,V)\\ Q_3(Z,V)+Q_4(Z,V) \end{pmatrix}$$

$$\|C_{Z_0}\|\lesssim \|Z_0\|_{Z_0}.$$

$$\|Q(Z,V)\|\lesssim \|Z\|_{E_Z}\|V\|_{E_V}\leq R^2\|Z_0\|_{E_0}^2.$$

$$\|Q(Z,V)-Q(Z',V')\|\lesssim \|(Z,V)-(Z',V')\|(\|(Z,V)\|+\|(Z',V')\|)$$

$$\|Q(Z,V)-Q(Z',V')\|\lesssim R\|Z_0\|_{Z_0}\|(Z,V)-(Z',V')\|.$$

$$B_{E_Z\times E_V}(0,R\|Z_0\|_{E_0})$$

$$\begin{aligned} Z(t)=S(t)\Bigg(& Z_0-i\int_0^\infty S(-\tau)\Big[(w*V(\cdot,0))Y+\int w(z)V(x,z)Y(x+z)dz\Big] \\ & -i\int_0^\infty S(-\tau)\Big[(w*V(\cdot,0))Z+\int w(z)V(x,z)Z(x+z)dz\Big] \\ & +i\int_t^\infty S(-\tau)\Big[(w*V(\cdot,0))Y+\int w(z)V(x,z)Y(x+z)dz\Big] \\ & +i\int_t^\infty S(-\tau)\Big[(w*V(\cdot,0))Z+\int w(z)V(x,z)Z(x+z)dz\Big]\Bigg) \end{aligned}$$

$$\int_0^\infty S(-\tau)\Big[(w*V(\cdot,0))Y+\int w(z)V(x,z)Y(x+z)dz\Big]\in L^2_\omega,H^{Sc}$$

$$\left\|\int_t^\infty S(-\tau)\Big[(w*V(\cdot,0))Y+\int w(z)V(x,z)Y(x+z)dz\Big]\right\|_{L^2_\omega,H^{Sc}}\rightarrow 0$$

$$\int_0^\infty S(-\tau)\Big[(w*V(\cdot,0))Z+\int w(z)V(x,z)Z(x+dz)\Big]\in L^2_\omega,H^{Sc}$$

$$\left\|\int_t^\infty S(-\tau)\Big[(w*V(\cdot,0))Z+\int w(z)V(x,z)Z(x+z)dz\Big]\right\|_{L^2_\omega,H^{Sc}}\rightarrow 0$$

$$Z(t)=S(t)Z_\infty+o_{L^2_\omega,H^{Sc}}$$

$$X(t)=Y+S(t)Z_\infty+o_{L^2_\omega,H^{Sc}}$$

$$\mathcal{L}=\mathcal{L}_\psi+\mathcal{L}_\sigma+\mathcal{L}_\omega+\mathcal{L}_\rho+\mathcal{L}_\pi+\mathcal{L}_A+\mathcal{L}_I,$$

$$T_{ii'} + \sum_{j=1}^A \bar{V}_{iji'j} = \varepsilon_i \delta_{ii'}$$

$$\begin{aligned} T_{ii'} &= \int d\mathbf{x} \bar{\psi}_i(\mathbf{x}) (-i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + M) \psi_{i'}(\mathbf{x}) \\ \bar{V}_{iji'j'} &= \int d\mathbf{x} d\mathbf{x}' \bar{\psi}_i(\mathbf{x}) \bar{\psi}_j(\mathbf{x}') \Gamma_\phi D_\phi \psi_{i'}(\mathbf{x}) \psi_{j'}(\mathbf{x}') \\ &\quad - \int d\mathbf{x} d\mathbf{x}' \bar{\psi}_i(\mathbf{x}) \bar{\psi}_j(\mathbf{x}') \Gamma_\phi D_\phi \psi_{j'}(\mathbf{x}) \psi_{i'}(\mathbf{x}') \end{aligned}$$

$$P=\sum_n\left|\Psi_n\right\rangle\left\langle\Psi_n\right|,\left|\Psi_n\right\rangle=\left|\prod_{i=1}^{N_{\text{val}}}c_{n_i}^{\dagger}\mid\text{core}\right\rangle,$$

$$PH^{\rm eff}P|\Psi\rangle=EP|\Psi\rangle.$$

$$H_n^{\rm eff} = H^{\rm BH}(E_0) + \sum_{k=1}^{\infty} \frac{1}{k!} \frac{d^k \hat{Q}(E_0)}{dE_0^k} \{H_{n-1}^{\rm eff} - E_0\}^k$$

$$H^{\rm BH}(E) = PH_0P + \hat{Q}(E)$$

$$\hat{Q}(E) = PVP + PV\frac{Q}{E-QHQ}VP$$

$$V_n^{\rm eff} = \hat{Q}(E_0) + \sum_{k=1}^{\infty} \frac{1}{k!} \frac{d^k \hat{Q}(E_0)}{dE_0^k} \{V_{n-1}^{\rm eff}\}^k$$

$$\begin{aligned} \hat{Q}(E) = & PVP + PV\frac{Q}{E-H_0}VP \\ & + PV\frac{Q}{E-H_0}V\frac{Q}{E-H_0}VP + \cdots \end{aligned}$$

$$B(E2;\Psi_i\rightarrow\Psi_f)=\frac{1}{2J_i+1}|\langle\Psi_f\|e_{\tau_z}r^2Y_2\|\Psi_i\rangle|^2$$

$$H=\sum_{ii'}T_{ii'}c_i^\dagger c_{i'}+\frac{1}{4}\sum_{ij i' j'}\bar{V}_{ij i' j'}(\rho)c_i^\dagger c_j^\dagger c_{j'}c_{i'},$$

$$\rho_{ii'}=\langle\Psi|c_i^\dagger c_{i'}|\Psi\rangle,\rho_{ij i' j'}=\langle\Psi|c_i^\dagger c_j^\dagger c_{j'}c_{i'}|\Psi\rangle.$$

$$E = \sum_{ii'} T_{ii'} \rho_{ii'} + \frac{1}{4} \sum_{iji'j'} \bar{V}_{iji'j'}(\rho^0) \rho_{iji'j'} + \frac{1}{4} \sum_{iji'j'} \sum_{kl} \bar{V}'_{iji'j'}(\rho^0) \rho_{iji'j'} (\rho_{kl} - \rho_{kl}^0) +$$

$$E \simeq E_0^{\text{re}} + \sum_{ii'} T_{ii'}^{\text{re}} \rho_{ii'} + \frac{1}{4} \sum_{iji'j'} \bar{V}_{iji'j'}(\rho^{\text{HF}}) \rho_{iji'j'}$$

$$E_0^{\text{re}} = -\frac{1}{4} \sum_{iji'j'} \sum_{kl} \bar{V}'_{iji'j'}(kl)(\rho^{\text{HF}}) \rho_{iji'j'}^{\text{HF}} \rho_{kl}^{\text{HF}}, T_{ii'}^{\text{re}} = T_{ii'} + \frac{1}{4} \sum_{kjlj'} \bar{V}'_{kjlj'}(ii')(\rho^{\text{HF}}) \rho_{kjlj'}^{\text{HF}}$$

$$\sum_n H_{mn}^{\text{eff}} C_n = E C_m, H_{mn}^{\text{eff}} = E_c^{\text{eff}} \delta_{mn} + \sum_{ii'} \varepsilon_{ii'}^{\text{eff}} \rho_{ii'}^{mn} + \frac{1}{4} \sum_{iji'j'} \bar{V}_{iji'j'}^{\text{eff}} \rho_{iji'j'}^{mn},$$

$$\rho_{ii'}^{mn} = \langle \Psi_m | c_i^\dagger c_{i'} | \Psi_n \rangle, \rho_{iji'j'}^{mn} = \langle \Psi_m | c_i^\dagger c_j^\dagger c_{j'} c_{i'} | \Psi_n \rangle$$

$$E_c^{\text{eff}} = \sum_{i=1}^{N_c} T_{ii}^{\text{re}} + \frac{1}{2} \sum_{i,j=1}^{N_c} \bar{V}_{ijij}(\rho^{\text{HF}}), \varepsilon_{ii'}^{\text{eff}} = T_{ii'}^{\text{re}} + \sum_{j=1}^{N_c} \bar{V}_{ijij}(\rho^{\text{HF}}),$$

$$V_{abcd;J} = \hat{f}^{-2} \sum_{m_a m_b m_c m_d M} C_{j_a m_a j_b m_b}^{JM} C_{j_c m_c j_d m_d}^{JM} \bar{V}_{\alpha\beta\gamma\delta}$$

$$\begin{aligned} V_{abcd;J}^{3\text{p1 h}} = & f_{adph} \sum_{ph\lambda} \lambda^2 \left\{ \begin{matrix} j_a & j_c & \lambda \\ j_d & j_b & J \end{matrix} \right\} \frac{\bar{V}_{hbpd;\lambda} \bar{V}_{apch;\lambda}}{E_0 - (\varepsilon_a + \varepsilon_d - \varepsilon_h + \varepsilon_p)} \\ & + f_{bcph} \sum_{ph\lambda} \lambda^2 \left\{ \begin{matrix} j_b & j_d & \lambda \\ j_c & j_a & J \end{matrix} \right\} \frac{\bar{V}_{harc;\lambda} \bar{V}_{bpdh;\lambda}}{E_0 - (\varepsilon_b + \varepsilon_c - \varepsilon_h + \varepsilon_p)} \\ & + f_{acph} \sum_{ph\lambda} \lambda^2 \left\{ \begin{matrix} j_a & j_d & \lambda \\ j_c & j_b & J \end{matrix} \right\} \frac{\bar{V}_{hbpc;\lambda} \bar{V}_{apdh;\lambda}}{E_0 - (\varepsilon_a + \varepsilon_c - \varepsilon_h + \varepsilon_p)} \\ & + f_{bdph} \sum_{ph\lambda} \lambda^2 \left\{ \begin{matrix} j_b & j_c & \lambda \\ j_d & j_a & J \end{matrix} \right\} \frac{\bar{V}_{hapd;\lambda} \bar{V}_{bpch;\lambda}}{E_0 - (\varepsilon_b + \varepsilon_d - \varepsilon_h + \varepsilon_p)}, \end{aligned}$$

$$\begin{aligned} f_{adph} &= (-1)^{J+j_c+j_d}, & f_{bcph} &= (-1)^{J+j_a+j_b} \\ f_{acph} &= -1, & f_{bdph} &= -(-1)^{j_a+j_b+j_c+j_d} \end{aligned}$$

$$V_{abcd;\lambda} = \hat{\lambda}^{-2} \sum_{m_a m_b m_c m_d M} (-1)^{j_b+m_b+j_c+m_c} C_{j_a m_a j_c - m_c}^{\lambda M} C_{j_d m_d j_b - m_b}^{\lambda M} \bar{V}_{\alpha\beta\gamma\delta}$$

$$V_{abcd;J}^{4\text{p2 h}} = \sum_{hh'} \frac{\bar{V}_{abh'h';J} \bar{V}_{hh'cd;J}}{E_0 - (\varepsilon_a + \varepsilon_b + \varepsilon_c + \varepsilon_d - \varepsilon_h - \varepsilon_{h'})}$$

$$\Xi(x_1,x_2,\ldots,x_N)=\frac{1}{\sqrt{N}!}\sum_{P\in S_N}(-1)^P\phi_{P_1}(x_1)\phi_{P_2}(x_2)\ldots\phi_{P_N}(x_N)=\frac{1}{\sqrt{N}!}\det\big(\phi_i(x_j)\big),$$

$$\Phi(x_1,x_2,\ldots,x_N)=\frac{1}{\sqrt{N}!}\sum_{P\in S_N}\phi_{P_1}(x_1)\phi_{P_2}(x_2)\ldots\phi_{P_N}(x_N)=\frac{1}{\sqrt{N}!}\text{per}\big(\phi_i(x_j)\big)$$



$$A_{ij} = \langle \phi_i | \phi_j \rangle$$

$$\langle \Xi | \Xi \rangle = \det(A), \langle \Phi | \Phi \rangle = \text{per}(A)$$

$$\mathcal{H}=\text{span}\{|x\rangle,1\leq x\leq L\},$$

$$|\phi\rangle=\sum_x|x\rangle\langle x|\phi\rangle=\sum_x\phi(x)|x\rangle$$

$$\hat{a}_\phi^\dagger=\sum_x\phi(x)\hat{a}_x^\dagger$$

$$|{\bf n}\rangle=\frac{(\hat{a}_1^\dagger)^{n_1}(\hat{a}_2^\dagger)^{n_2}\ldots(\hat{a}_L^\dagger)^{n_L}}{\sqrt{n_1!n_2!\ldots n_L!}}|vac\rangle$$

$$\sum_{x=1}^Ln_x=N$$

$$\mathcal{D}=\binom{N+L-1}{N}=\frac{(N+L-1)!}{N!(L-1)!}$$

$$\hat{H}=\sum_{i=1}^N\hat{K}(i)+\sum_{1\leq i< j\leq N}\hat{W}(i,j)$$

$$\hat{H}=-\sum_{x=1}^L\left(\hat{a}_x^\dagger\hat{a}_{x+1}+\hat{a}_{x+1}^\dagger\hat{a}_x\right)+\frac{U}{2}\sum_{x=1}^L\hat{a}_x^\dagger\hat{a}_x^\dagger\hat{a}_x\hat{a}_x$$

$$\begin{aligned}\hat{K}_{x,x'} &= -(\delta_{x,x'+1} + \delta_{x,x'-1}) \\ \hat{W}_{x_1x_2,x'_1x'_2} &= U\delta_{x_1,x_2}\delta_{x_1,x'_1}\delta_{x_1,x'_2}\end{aligned}$$

$$\Phi=\sum_{\alpha=1}^M\Phi^{(\alpha)}=\sum_{\alpha=1}^M\hat{\mathcal{S}}\left(\phi_1^{(\alpha)},\ldots,\phi_N^{(\alpha)}\right)$$

$$E=\frac{\langle \Phi|\hat{H}|\Phi\rangle}{\langle \Phi\,|\,\Phi\rangle}=\frac{\sum_{\alpha,\beta=1}^M\langle \Phi^{(\alpha)}|\hat{H}|\Phi^{(\beta)}\rangle}{\sum_{\alpha,\beta=1}^M\langle \Phi^{(\alpha)}\,|\,\Phi^{(\beta)}\rangle}$$

$$\phi_{2\leq i\leq N}^{(1\leq\alpha\leq M)}\langle\Phi^{(\alpha)}|\hat{H}|\Phi^{(\beta)}\rangle\langle\Phi^{(\alpha)}\,|\,\Phi^{(\beta)}\rangle\hat{F}^{(\alpha\beta)}\hat{G}^{(\alpha\beta)}\phi_{2\leq i\leq N}^{(\alpha)}\phi_{2\leq i\leq N}^{(\beta)}\left\langle\phi_1^{(\alpha)}\right|\hat{F}^{(\alpha\beta)}\left|\phi_1^{(\beta)}\right\rangle$$

$$=\langle\Phi^{(\alpha)}|\hat{H}|\Phi^{(\beta)}\rangle,\left\langle\phi_1^{(\alpha)}\right|\hat{G}^{(\alpha\beta)}\left|\phi_1^{(\beta)}\right\rangle=\langle\Phi^{(\alpha)}\,|\,\Phi^{(\beta)}\rangle\langle\Phi^{(\alpha)}\,|\,\Phi^{(\beta)}\rangle$$

$$=\langle\Phi^{(\beta)}\,|\,\Phi^{(\alpha)}\rangle^*\left\langle\phi_1^{(\alpha)}\right|\hat{G}^{(\alpha\beta)}\left|\phi_1^{(\beta)}\right\rangle=\left\langle\phi_1^{(\beta)}\right|\hat{G}^{(\beta\alpha)}\left|\phi_1^{(\alpha)}\right\rangle^*\hat{G}^{(\beta\alpha)}\hat{G}^{(\alpha\beta)}(\hat{G}^{(\alpha\beta)})^\dagger$$

$$=\hat{G}^{(\beta\alpha)}(\hat{F}^{(\alpha\beta)})^\dagger=\hat{F}^{(\beta\alpha)}$$

$$E = \frac{\sum_{\alpha,\beta=1}^M \left\langle \phi_1^{(\alpha)} \left| \hat{F}^{(\alpha\beta)} \right| \phi_1^{(\beta)} \right\rangle}{\sum_{\alpha,\beta=1}^M \left\langle \phi_1^{(\alpha)} \left| \hat{G}^{(\alpha\beta)} \right| \phi_1^{(\beta)} \right\rangle} = \frac{\langle \phi_1 | \hat{F} | \phi_1 \rangle}{\langle \phi_1 | \hat{G} | \phi_1 \rangle}$$

$$LM, \phi_1 = \left(\phi_1^{(1)}; \phi_1^{(2)}; \dots; \phi_1^{(M)} \right)$$

$$\hat{F} \equiv \left(\hat{F}^{(\alpha\beta)} \right)_{1 \leq \alpha, \beta \leq M}$$

$$\hat{G} \equiv \left(\hat{G}^{(\alpha\beta)} \right)_{1 \leq \alpha, \beta \leq M}$$

$$\langle \phi_1 | \hat{F} | \phi_1 \rangle = \langle \Phi | H | \Phi \rangle$$

$$\langle \phi_1 | \hat{G} | \phi_1 \rangle = \langle \Phi | \Phi \rangle$$

$$\overline{\hat{F}}^{(\alpha\beta)} \hat{G}^{(\alpha\beta)} \hat{G}^{(\alpha\beta)} \hat{F}^{(\alpha\beta)} \left\langle \phi_1^{(\alpha)} \left| \hat{G}^{(\alpha\beta)} \right| \phi_1^{(\beta)} \right\rangle = \langle \Phi^{(\alpha)} | \Phi^{(\beta)} \rangle$$

$$A_{ij}^{(\alpha\beta)} = \left\langle \phi_i^{(\alpha)} | \phi_j^{(\beta)} \right\rangle \langle \Phi^{(\alpha)} | \Phi^{(\beta)} \rangle = \text{per}(A^{(\alpha\beta)})$$

$$\begin{aligned} \text{per}(A^{(\alpha\beta)}) &= \left\langle \phi_1^{(\alpha)} | \phi_1^{(\beta)} \right\rangle \text{per}(A^{(\alpha\beta)}; 1 | 1) + \sum_{j_1=2}^N \left\langle \phi_1^{(\alpha)} | \phi_{j_1}^{(\beta)} \right\rangle \text{per}(A^{(\alpha\beta)}; 1 | j_1) \\ &= \left\langle \phi_1^{(\alpha)} | \phi_1^{(\beta)} \right\rangle \text{per}(A^{(\alpha\beta)}; 1 | 1) + \sum_{j_1=2}^N \sum_{i_1=2}^N \left\langle \phi_1^{(\alpha)} | \phi_{j_1}^{(\beta)} \right\rangle \left\langle \phi_{i_1}^{(\alpha)} | \phi_1^{(\beta)} \right\rangle \text{per}(A^{(\alpha\beta)}; 1, i_1 | 1, j_1). \end{aligned}$$

$$\begin{aligned} \hat{G}^{(\alpha\beta)} &= \hat{G} \left(\phi_2^{(\alpha)}, \dots, \phi_N^{(\alpha)}; \phi_2^{(\beta)}, \dots, \phi_N^{(\beta)} \right) \\ &= \text{per}(A^{(\alpha\beta)}; 1 | 1) \hat{I} + \sum_{j_1=2}^N \sum_{i_1=2}^N \text{per}(A^{(\alpha\beta)}; 1, i_1 | 1, j_1) \left| \phi_{j_1}^{(\beta)} \right\rangle \left\langle \phi_{i_1}^{(\alpha)} \right| \end{aligned}$$

$$\phi_1 \equiv \left(\phi_1^{(1)}; \phi_1^{(2)}; \dots; \phi_1^{(M)} \right)$$

$$\phi_2 \equiv \left(\phi_2^{(1)}; \phi_2^{(2)}; \dots; \phi_2^{(M)} \right)$$

$$\hat{P}_{ij}^{(\gamma)} = \frac{d_\gamma}{|G|} \sum_{\hat{g} \in G} D_{ij}^{(\gamma)*}(\hat{g}) \hat{g}, 1 \leq i, j \leq d_\gamma$$

$$\Phi_{ij}^{(\gamma)} = \frac{d_\gamma}{|G|} \sum_{\hat{g} \in G} \sum_{\alpha=1}^M D_{ij}^{(\gamma)*}(\hat{g}) \hat{\mathcal{S}} \left(\hat{g} \phi_1^{(\alpha)}, \dots, \hat{g} \phi_N^{(\alpha)} \right)$$

$$\hat{g} \Phi_{ij}^{(\gamma)} = \sum_{k=1}^{d_\gamma} D_{ki}^{(\gamma)}(\hat{g}) \Phi_{kj}^{(\gamma)}$$



$$\bar{\Phi} = \frac{1}{|G|} \sum_{\hat{g} \in G} \hat{g} \Phi = \frac{1}{|G|} \sum_{\hat{g} \in G} \sum_{\alpha=1}^M \hat{\mathcal{S}} \left(\hat{g} \phi_1^{(\alpha)}, \dots, \hat{g} \phi_N^{(\alpha)} \right)$$

$$\Phi_i^{(\gamma)} = \sum_{j=1}^{d_\gamma} w_j \Phi_{ij}^{(\gamma)} = \sum_{j=1}^{d_\gamma} w_j P_{ij}^{(\gamma)} \Phi$$

$$E = \frac{\left\langle \Phi_i^{(\gamma)} \left| \hat{H} \right| \Phi_i^{(\gamma)} \right\rangle}{\left\langle \Phi_i^{(\gamma)} \left| \Phi_i^{(\gamma)} \right\rangle} = \frac{\sum_{j,k} w_j^* \langle \Phi | \hat{P}_{ij}^{(\gamma)\dagger} \hat{H} \hat{P}_{ik}^{(\gamma)} | \Phi \rangle w_k}{\sum_{j,k} w_j^* \langle \Phi | \hat{P}_{ij}^{(\gamma)\dagger} \hat{P}_{ik}^{(\gamma)} | \Phi \rangle w_k} = \frac{\sum_{j,k} w_j^* \langle \Phi | \hat{H} \hat{P}_{jk}^{(\gamma)} | \Phi \rangle w_k}{\sum_{j,k} w_j^* \langle \Phi | \hat{P}_{jk}^{(\gamma)} | \Phi \rangle w_k}.$$

$$\hat{P}_{ij}^{(\gamma)\dagger} = \hat{P}_{ji}^{(\gamma)}, \hat{P}_{mn}^{(\gamma)} \hat{P}_{ij}^{(\gamma)} = \hat{P}_{mj}^{(\gamma)} \delta_{ni} \left[\hat{P}_{ij}^{(\gamma)}, \hat{H} \right]$$

$$\mathcal{N}_{jk} = \langle \Phi | \hat{H} \hat{P}_{jk}^{(\gamma)} | \Phi \rangle \text{ and } \mathcal{D}_{jk} = \langle \Phi | \hat{P}_{jk}^{(\gamma)} | \Phi \rangle$$

$$\phi_1 = \left(\phi_1^{(1)}; \phi_1^{(2)}; \dots; \phi_1^{(M)}\right)$$

$$\hat{F} \equiv \left(\hat{F}^{(\alpha\beta)}\right)_{1\leq\alpha,\beta\leq M} \text{ and } \hat{G} \equiv \left(\hat{G}^{(\alpha\beta)}\right)_{1\leq\alpha,\beta\leq M}$$

$$\hat{F}^{(\alpha\beta)} = \frac{d_\gamma}{|G|} \sum_{\hat{g} \in G} \sum_{j,k=1}^{d_\gamma} w_j^* D_{jk}^{(\gamma)*}(\hat{g}) w_k \hat{\mathcal{F}} \left(\phi_{2 \leq i \leq N}^{(\alpha)}; \hat{g} \phi_{2 \leq i \leq N}^{(\beta)} \right) \hat{g},$$

$$\hat{G}^{(\alpha\beta)} = \frac{d_\gamma}{|G|} \sum_{\hat{g} \in G} \sum_{j,k=1}^{d_\gamma} w_j^* D_{jk}^{(\gamma)*}(\hat{g}) w_k \hat{\mathcal{G}} \left(\phi_{2 \leq i \leq N}^{(\alpha)}; \hat{g} \phi_{2 \leq i \leq N}^{(\beta)} \right) \hat{g}.$$

$$\hat{\mathcal{F}} \left(\phi_{2 \leq i \leq N}^{(\alpha)}; \hat{g} \phi_{2 \leq i \leq N}^{(\beta)} \right) \hat{g} \text{ and } \hat{\mathcal{G}} \left(\phi_{2 \leq i \leq N}^{(\alpha)}; \hat{g} \phi_{2 \leq i \leq N}^{(\beta)} \right) \hat{g}$$

$$\hat{\mathcal{F}} \left(\phi_{2 \leq i \leq N}^{(\alpha)}; \hat{g} \phi_{2 \leq i \leq N}^{(\beta)} \right) \hat{g} = \left[\hat{\mathcal{F}} \left(\phi_{2 \leq i \leq N}^{(\beta)}; \hat{g}^{-1} \phi_{2 \leq i \leq N}^{(\alpha)} \right) \hat{g}^{-1} \right]^\dagger$$

$$\hat{\mathcal{G}} \left(\phi_{2 \leq i \leq N}^{(\alpha)}; \hat{g} \phi_{2 \leq i \leq N}^{(\beta)} \right) \hat{g} = \left[\hat{\mathcal{G}} \left(\phi_{2 \leq i \leq N}^{(\beta)}; \hat{g}^{-1} \phi_{2 \leq i \leq N}^{(\alpha)} \right) \hat{g}^{-1} \right]^\dagger$$

$$\begin{aligned} \left\langle \phi_1^{(\alpha)} \left| \hat{\mathcal{F}} \left(\phi_{2 \leq i \leq N}^{(\alpha)}; \hat{g} \phi_{2 \leq i \leq N}^{(\beta)} \right) \hat{g} \right| \phi_1^{(\beta)} \right\rangle &= \langle \Phi^{(\alpha)} | \hat{H} \hat{g} | \Phi^{(\beta)} \rangle \\ &= \langle \Phi^{(\beta)} | \hat{g}^{-1} \hat{H} | \Phi^{(\alpha)} \rangle^* \\ &= \langle \Phi^{(\beta)} | \hat{H} | g^{-1} \Phi^{(\alpha)} \rangle^* \\ &= \left\langle \phi_1^{(\beta)} \left| \hat{\mathcal{F}} \left(\phi_{2 \leq i \leq N}^{(\beta)}; \hat{g}^{-1} \phi_{2 \leq i \leq N}^{(\alpha)} \right) \hat{g}^{-1} \right| \phi_1^{(\alpha)} \right\rangle^* \end{aligned}$$

$$\tilde{H} = \hat{H} \hat{P}_{ii}^{(\gamma)} + \lambda \left(1 - \hat{P}_{ii}^{(\gamma)} \right)$$

$$\hat{H} = - \sum_{x=-L_1}^{L_1-1} (\hat{a}_x^\dagger \hat{a}_{x+1} + \hat{a}_{x+1}^\dagger \hat{a}_x) + \frac{k}{2} \sum_{x=-L_1}^{L_1} x^2 \hat{a}_x^\dagger \hat{a}_x + \frac{U}{2} \sum_{x=-L_1}^{L_1} \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x \hat{a}_x.$$

$$\Phi^{(\pm)} = \frac{1}{2}(\Phi \pm \hat{P}\Phi) = \frac{1}{2} \sum_{\alpha=1}^M \left[\hat{\mathcal{S}} \left(\phi_1^{(\alpha)}, \dots, \phi_N^{(\alpha)} \right) \pm \hat{\mathcal{S}} \left(\hat{P}\phi_1^{(\alpha)}, \dots, \hat{P}\phi_N^{(\alpha)} \right) \right].$$

$$\mathcal{O} = \left| \langle GS \mid \Phi^{(+)} \rangle \right|^2$$

$$\rho(x,x)=\langle \hat{a}_x^\dagger \hat{a}_x \rangle$$

$$\rho(x,0)=\langle \hat{a}_0^\dagger \hat{a}_x \rangle$$

$$\Phi^{(+)}, \left\{ \Phi_m^{(+)} = (\Phi_m + \hat{P}\Phi_m)/2, 1 \leq m \leq 10 \right\}$$

$$A_{mn} = \frac{|\langle \Phi_m \mid \Phi_n \rangle|^2}{\langle \Phi_m \mid \Phi_m \rangle \langle \Phi_n \mid \Phi_n \rangle}$$

$$\hat{H} = - \sum_{x=1}^L \left(\hat{a}_x^\dagger \hat{a}_{x+1} + \hat{a}_{x+1}^\dagger \hat{a}_x \right) + \frac{U}{2} \sum_{x=1}^L \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x \hat{a}_x$$

$$(\hat{T}\phi)(x)=\phi(x-1) \text{ and } (\hat{S}\phi)(x)=\phi(-x)$$

$$\mathcal{D}_L=\{\hat{I},\hat{T},\ldots,\hat{T}^{L-1},\hat{S},\hat{S}\hat{T},\ldots,\hat{S}\hat{T}^{L-1}\}$$

$$\hat{T}\hat{S}\Psi=\hat{S}\hat{S}\hat{T}\hat{S}\Psi=\hat{S}\hat{T}^{-1}\Psi=e^{-i2\pi q/L}\hat{S}\Psi$$

$$D^{(q)}(\hat{T}^n)=\begin{pmatrix} e^{i2\pi qn/L} & 0 \\ 0 & e^{-i2\pi qn/L} \end{pmatrix}, D^{(q)}(\hat{S}\hat{T}^n)=\begin{pmatrix} 0 & e^{-i2\pi qn/L} \\ e^{i2\pi qn/L} & 0 \end{pmatrix}$$

$$D^{(q,s)}(\hat{T}^n)=e^{i2\pi qn/L}, D^{(q,s)}(\hat{S}\hat{T}^n)=se^{i2\pi qn/L}$$

$$\Phi_1^{(q)} = \frac{1}{L} \sum_{n=0}^{L-1} \sum_{\alpha=1}^M e^{-i2\pi qn/L} \hat{\mathcal{S}} \left(\hat{T}^n \phi_1^{(\alpha)}, \dots, \hat{T}^n \phi_N^{(\alpha)} \right)$$

$$\Phi^{(q,s)} = \frac{1}{L} \sum_{n=0}^{L-1} \sum_{\alpha=1}^M e^{-i2\pi qn/L} \left[\hat{\mathcal{S}} \left(\hat{T}^n \phi_1^{(\alpha)}, \dots, \hat{T}^n \phi_N^{(\alpha)} \right) + s \hat{\mathcal{S}} \left(\hat{S}\hat{T}^n \phi_1^{(\alpha)}, \dots, \hat{S}\hat{T}^n \phi_N^{(\alpha)} \right) \right].$$

$$\begin{aligned} \hat{H} = & - \sum_{x=1}^L \left(\hat{a}_x^\dagger \hat{a}_{x+1} + \hat{a}_{x+1}^\dagger \hat{a}_x \right) + \frac{U_{bb}}{2} \sum_{x=1}^L \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x \hat{a}_x \\ & - J_i \sum_{x=1}^L \left(\hat{b}_x^\dagger \hat{b}_{x+1} + \hat{b}_{x+1}^\dagger \hat{b}_x \right) + U_{bi} \sum_{x=1}^L \hat{a}_x^\dagger \hat{a}_x \hat{b}_x^\dagger \hat{b}_x \end{aligned}$$

$$|\Psi^{(q)}\rangle = \sum_{n=0}^{L-1} e^{-i2\pi qn/L} |n\rangle_b \otimes \hat{T}^n |\varphi\rangle_a$$

$$|n\rangle_b = \hat{b}_n^\dagger | \text{vac} \rangle$$

$$E|\varphi\rangle_a = [\hat{H}_a + U_{bi}\hat{a}_0^\dagger\hat{a}_0 - J_i(e^{-i2\pi q/L}\hat{T} + e^{i2\pi q/L}\hat{T}^\dagger)]|\varphi\rangle_a.$$

$$\hat{H} = - \sum_{x=1}^L \left(e^{i\theta/L} \hat{a}_x^\dagger \hat{a}_{x+1} + e^{-i\theta/L} \hat{a}_{x+1}^\dagger \hat{a}_x \right) + \frac{U}{2} \sum_{x=1}^L \hat{a}_x^\dagger \hat{a}_x^\dagger \hat{a}_x \hat{a}_x.$$

$$\Phi^{(q)} = \frac{1}{L} \sum_{n=0}^{L-1} \sum_{\alpha=1}^M e^{-i2\pi qn/L} \hat{\mathcal{S}} \left(\hat{T}^n \phi_1^{(\alpha)}, \dots, \hat{T}^n \phi_N^{(\alpha)} \right).$$

$$\hat{H} = - \sum_{x=1}^{L-1} \left(\hat{a}_{x,y}^\dagger \hat{a}_{x+1,y} + h.c. \right) - \sum_{y=1}^{L-1} \left(\hat{a}_{x,y}^\dagger \hat{a}_{x,y+1} + h.c. \right) + \frac{U}{2} \sum_{x,y=1}^L \hat{a}_{x,y}^\dagger \hat{a}_{x,y}^\dagger \hat{a}_{x,y} \hat{a}_{x,y}.$$

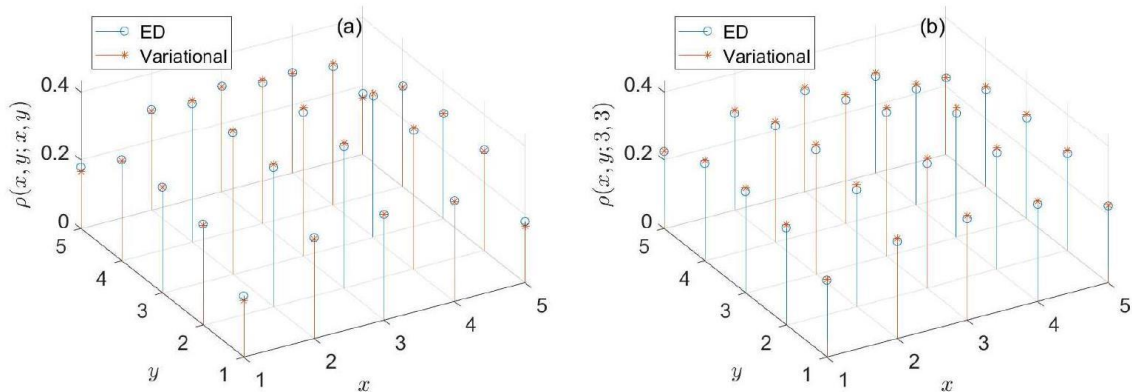
$$D_4 = \{\hat{T}^n, \hat{\mathcal{S}}\hat{T}^n \mid 0 \leq n \leq 3\}$$

$$(\hat{T}\phi)(x,y)=\phi(y,L+1-x)$$

$$(\hat{\mathcal{S}}\phi)(x,y)=\phi(x,L+1-y)$$

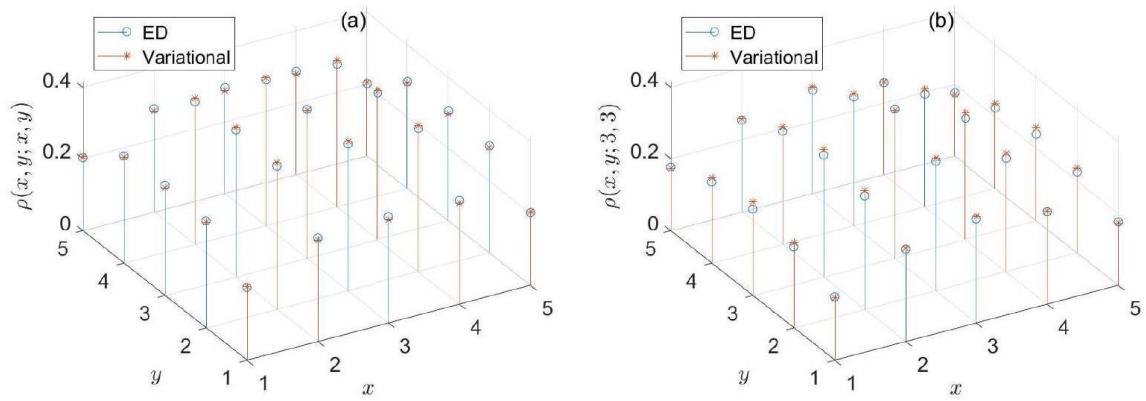
$$\rho(x,y;x,y)=\langle \hat{a}_{x,y}^\dagger \hat{a}_{x,y} \rangle$$

$$\rho(x,y;3,3)=\langle \hat{a}_{3,3}^\dagger \hat{a}_{x,y} \rangle$$



$$\rho(x,y;x,y)=\langle \hat{a}_{x,y}^\dagger \hat{a}_{x,y} \rangle$$

$$\rho(x,y;3,3)=\langle \hat{a}_{3,3}^\dagger \hat{a}_{x,y} \rangle$$



$$\rho(x,y;x,y)=\langle \hat{a}_{x,y}^{\dagger}\hat{a}_{x,y}\rangle$$

$$\rho(x,y;3,3)=\langle \hat{a}_{3,3}^{\dagger}\hat{a}_{x,y}\rangle$$

$$\begin{aligned} H &= H_1 + H_2 \\ &= \sum_{ij} h_{ij} a_i^{\dagger} a_j + \frac{1}{2} \sum_{ijkl} h_{ijkl} a_i^{\dagger} a_j^{\dagger} a_k a_l \end{aligned}$$

$$E_{HF}=\min_{\Psi\in F_1}\langle\Psi|H|\Psi\rangle$$

$$|\Psi_{HF}\rangle=b_1^{\dagger}b_2^{\dagger}\cdots b_N^{\dagger}|vac\rangle.$$

$$b_i^{\dagger}=\sum_j a_j^{\dagger}C_{ji}$$

$$\psi_i(x)=\sum_j\phi_j(x)C_{ji}$$

$$\begin{aligned} [a_i,a_j^{\dagger}]_+ &= \langle \phi_i \mid \phi_j \rangle \mathbb{1}, [a_i,a_j]_+ = 0 \\ [b_i,b_j^{\dagger}] &= \delta_{i,j} \mathbb{1}, [b_i,b_j]_+ = 0 \end{aligned}$$

$$P_{pq}=\sum_i^{occ}C_{pi}C_{qi}^*$$

$$\begin{aligned} E_{HF} &= \min_P \sum_{pq} P_{qp} h_{pq} + \frac{1}{2} \sum_{pqrs} P_{qp} P_{sr} (h_{prsq} - h_{prqs}) \\ &= \min_P \frac{1}{2} \text{Tr}[P(F + H_1)] \end{aligned}$$

$$F=F(P)=H_1+G(P)$$

$$G_{pq}=G(P)_{pq}=\sum_{rs}P_{sr}(h_{prsq}-h_{prqs})$$

$$A_{pqrs}=h_{pqrs}-h_{pqsr}$$

$$h_{s_1s_2}^{o_1o_2}=h_{(s_1+1)(s_2+1)}^{o_1o_2} \text{ and } h_{s_1s_2s_3s_4}^{o_1o_2o_3o_4}=h_{(s_1+1)(s_2+1)(s_3+1)(s_4+1)}^{o_1o_2o_3o_4}$$

$$h_{(i+1)(j+1)}=h_{ij} \text{ and } h_{(i+1)(j+1)(k+1)(l+1)}=h_{ijkl},$$

$$\mathcal{F}[a]_m=\hat{a}_m=\frac{1}{\sqrt{M}}\sum_x e^{-2\pi i m x/M}a_x$$

$$\mathcal{F}^{-1}[\hat{a}]_x=a_x=\frac{1}{\sqrt{M}}\sum_m e^{2\pi i m x/M}\hat{a}_m$$

$$H_I=-\sum_{ij}J_{ij}S_iS_j$$

$$H=\sum_{i=1}^M\sum_{j=1}^MJ_{ij}(\hat{a}_i^\dagger\hat{a}_{M-i}+\hat{a}_{M-i}^\dagger\hat{a}_i)(\hat{a}_{M-j}^\dagger\hat{a}_j+\hat{a}_j^\dagger\hat{a}_{M-j}),$$

$$\hat{a}_{k_1}^\dagger\hat{a}_{k_2}\hat{a}_{k_3}^\dagger\hat{a}_{k_4}+\text{h.c}$$

$$k_1+k_3-(k_2+k_4)=0\,\mathrm{mod}M,$$

$$\begin{aligned}\langle \Psi | \hat{a}_{k_1}^\dagger \hat{a}_{k_2} \hat{a}_{k_3}^\dagger \hat{a}_{k_4} | \Psi \rangle &= \langle \Psi | \hat{a}_{k_1}^\dagger \hat{a}_{k_2} | \Psi \rangle \langle \Psi | \hat{a}_{k_3}^\dagger \hat{a}_{k_4} | \Psi \rangle \\ &\quad - \langle \Psi | \hat{a}_{k_1}^\dagger \hat{a}_{k_4} | \Psi \rangle \langle \Psi | \hat{a}_{k_3}^\dagger \hat{a}_{k_2} | \Psi \rangle.\end{aligned}$$

$$H=\sum_{i,j}J_{ij}\left[\left(n_i^{(+)}-n_i^{(-)}\right)\left(n_j^{(+)}-n_j^{(-)}\right)\right],$$

$$n_k^{(\pm)}=c_k^{(\pm)\dagger}c_k^{(\pm)}\text{ and }c_i^{(\pm)}=(\hat{a}_i\pm\hat{a}_{-i})/\sqrt{2}$$

$$\left[c_m^{(+)},\left(c_n^{(-)}\right)^\dagger\right]_+=\left(n_i^{(+)}-n_i^{(-)}\right)$$

$$|s\rangle=\prod_{i=1}^M\left(c_i^{(+)\dagger}\right)^{\sigma_i}\left(c_i^{(-)\dagger}\right)^{\tau_i}|vac\rangle,$$

$$\langle s|H|s\rangle=\sum_{i,j}J_{ij}(\sigma_i\sigma_j+\tau_i\tau_j-\sigma_i\tau_j-\sigma_i\tau_j).$$

$$\langle s|H|s\rangle\leq 4E_{\mathrm{min}}\,.$$

$$\prod_{i=1}^M\left(c_i^{(+)\dagger}\right)^{\sigma_i}\left(c_i^{(-)\dagger}\right)^{1-\sigma_i}|vac\rangle,$$

$$J_{i\beta,j\beta}=J_{i\alpha,j\alpha}=-J_{i\alpha,j\beta}=-J_{i\beta,j\alpha}=J_{ij}.$$

$$E'=4E-NC.$$

$$\{h_{ij}:h_{ij}=h_{i+1,j+1}\}\text{ and }\{h_{ijkl}:h_{ijkl}=h_{i+1,j+1,k+1,l+1}\}$$

$$P_{pq}=\sum_{i=1}^MC_{pi}R_iC_{qi}^*=\frac{1}{2}\sum_{i=1}^MS_iC_{pi}C_{qi}^*+\frac{1}{2}\delta_{pq}.$$

$$\begin{aligned} E(P)= & -\sum_{ij}\left[\frac{1}{8}\sum_{pqrs}C_{pi}^*C_{qi}C_{rj}^*C_{sj}A_{prqs}\right]S_iS_j\\ & +\sum_j\left[\frac{1}{4}\sum_{pq}C_{qj}C_{pj}^*\left(2h_{pq}+\sum_rA_{prrq}\right)\right]S_j\\ & +\frac{1}{2}\sum_ph_{pp}+\frac{1}{8}\sum_{pr}A_{prrp}. \end{aligned}$$

$$H(\{J_{ij}\})=-\sum_{ij}J_{ij}S_iS_j$$

$$h_{pq\dot{}}=-\sum_rA_{prrq}/2$$

$$G_{pq}=\sum_{rs}P_{sr}A_{prsq}=\sum_{rs}P_{s+1,r+1}A_{p+1,r+1,s+1,q+1}=G_{p+1,q+1}$$

$$|\hat{k}\rangle=\frac{1}{\sqrt{M}}\sum_{x=1}^Me^{-2\pi ikx/M}|x\rangle$$

$$C_{kn}=\exp{(-i2\pi kn/M)}/\sqrt{M} \text{ as } CFC^{\dagger}=\Lambda$$

$$J_{ij}=\sum_{pqrs}C_{pi}^*C_{qi}C_{rj}^*C_{sj}A_{prsq}/8$$

$$A_{pqrs}=-\frac{8}{M}\sum_{tu}C_{pt}C_{qu}(C_{ru}C_{st}-C_{su}C_{rt})^*J_{tu}.$$

$$h_{pq}=-\sum_rA_{prrq}/2$$

$$E_{HF}(S)=H_I(S)+\sum_{mn}J_{mn}$$

$$J=\begin{bmatrix}0&-1&-1&-1&0&-1\\&0&1&0&1&1\\&&0&1&1&0\\&&&0&1&1\\&&&&0&-1\\&&&&&0\end{bmatrix}$$

$$i\frac{\partial |\psi(t)\rangle}{\partial t}=\hat{H}(t)|\psi(t)\rangle,$$



$$|\psi(t)\rangle = |\phi_1(t)\phi_2(t)\cdots\phi_N(t)\rangle$$

$$|\phi_i(t)\rangle = \sum_k^M C_{ki}(t)|\chi_k\rangle$$

$$F_{pq}(t) = h_{pq} + \sum_k^M \sum_{rs}^M C_{rk}^*(t)C_{sk}(t) \left(\langle \chi_p \chi_s | \frac{1}{r_{ee}} | \chi_q \chi_s \rangle - \langle \chi_p \chi_r | \frac{1}{r_{ee}} | \chi_s \chi_q \rangle \right),$$

$$h_{pq} = \langle \chi_p | -\frac{1}{2} \nabla^2 - \sum_i^{nuc} \frac{Z_i}{r_{ei}} | \chi_q \rangle$$

$$\rho_{rs}(t) = \sum_k C_{rk}^*(t)C_{sk}(t) = |\phi_r\rangle\langle\phi_s|$$

$$F_{pq}(t) = h_{pq} + \sum_{rs} \rho_{rs}(t) \left(\langle \chi_p \chi_s | \frac{1}{r_{ee}} | \chi_q \chi_s \rangle - \langle \chi_p \chi_r | \frac{1}{r_{ee}} | \chi_s \chi_q \rangle \right).$$

$$\hat{h}(t) = \hat{F}(t) + \hat{D} \cdot E(t)$$

$$i\frac{\partial |\phi_i(t)\rangle}{\partial t} = \hat{h}(t)|\phi_i(t)\rangle.$$

$$|\psi(t+\delta t)\rangle = \hat{U}(t+\delta t,t)|\psi(t)\rangle$$

$$\hat{U}(t+\delta t,t) \approx e^{-i\hat{h}(t)\delta t}$$

$$\rho(t+\delta t) = |\psi(t+\delta t)\rangle\langle\psi(t+\delta t)|$$

$$(\mathcal{R}\otimes\mathbb{1})(\mathbb{1}\otimes\mathcal{R})(\mathcal{R}\otimes\mathbb{1})=(\mathbb{1}\otimes\mathcal{R})(\mathcal{R}\otimes\mathbb{1})(\mathbb{1}\otimes\mathcal{R}),$$

$$\hat{F} = \sum_{ij} F_{ij} \hat{a}_i^\dagger \hat{a}_j$$

$$F_{ij} = \langle \phi_i | \hat{F} | \phi_j \rangle$$

$$\hat{D} = \sum_{ij} D_{ij} \hat{a}_i^\dagger \hat{a}_j$$

$$D_{ij} = \langle \phi_i | \hat{r} | \phi_j \rangle$$

$$\hat{a}_i^\dagger \hat{a}_i = (I \otimes I - Z \otimes I)/2$$

$$\hat{a}_{i+1}^\dagger \hat{a}_{i+1} = (I \otimes I - I \otimes Z)/2$$

$$\hat{a}_i^\dagger \hat{a}_{i+1} = [X \otimes X + Y \otimes Y + i(X \otimes Y - Y \otimes X)]/4$$

$$\hat{a}_{i+1}^\dagger \hat{a}_i = [X \otimes X + Y \otimes Y + i(Y \otimes X - X \otimes Y)]/4.$$

$$\begin{aligned}
a_i^\dagger a_i &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\
a_{i+1}^\dagger a_{i+1} &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \\
a_i^\dagger a_{i+1} &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \\
a_{i+1}^\dagger a_i &= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}
\end{aligned}$$

$$\hat{h}(t) = \sum_{i,i+1} [F_{ij}(t) + D_{ij}E(t)] \hat{a}_i^\dagger \hat{a}_j$$

$$\hat{h} = \hat{h}_1 + \hat{h}_2,$$

$$\hat{h}_1 = \sum_i G_{ii} \hat{n}_i$$

$$G_{ij} = F_{ij}(t) + D_{ij}E(t)$$

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

$$\hat{h}_2 = \sum_{i \neq j} G_{ij} \hat{a}_i^\dagger \hat{a}_j.$$

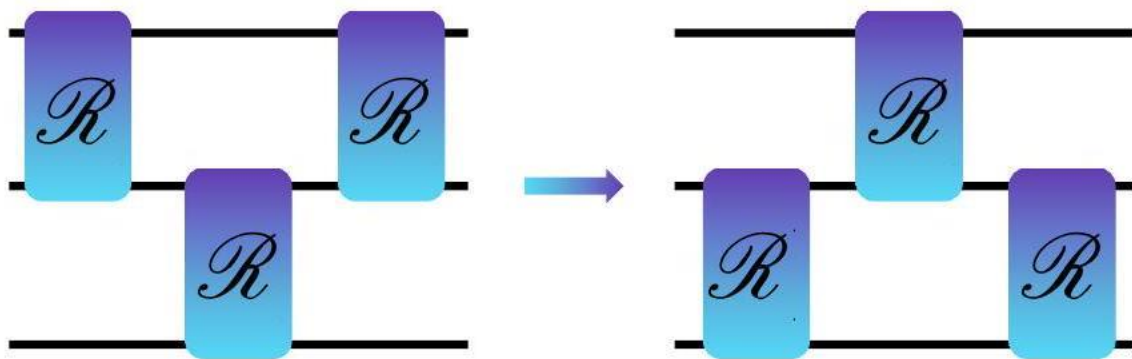
$$e^{-it\hat{h}_2} = e^{-it(G_{i,i+1}a_i^\dagger a_{i+1} + G_{i+1,i}a_{i+1}^\dagger a_i)}$$

$$e^{-it\hat{h}_2} = e^{-itG_{i,i+1}(X \otimes X + Y \otimes Y)}.$$

$$e^{-it\hat{h}_1} = e^{-it(G_{i,i}\hat{n}_i + G_{i+1,i+1}\hat{n}_{i+1})};$$

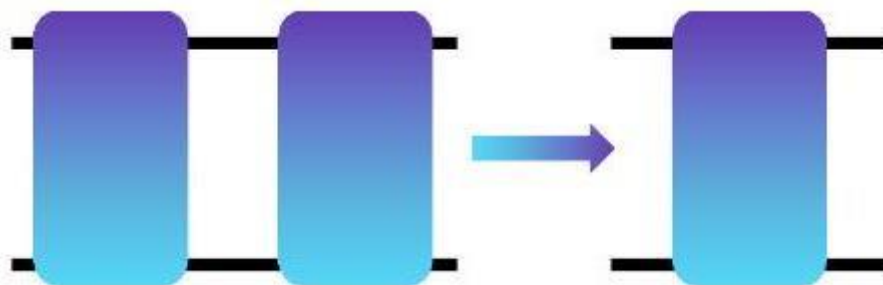
$$e^{-it\hat{h}_1} = e^{-it[G_{i,i}(Z \otimes I) + G_{i+1,i+1}(I \otimes Z)]}.$$



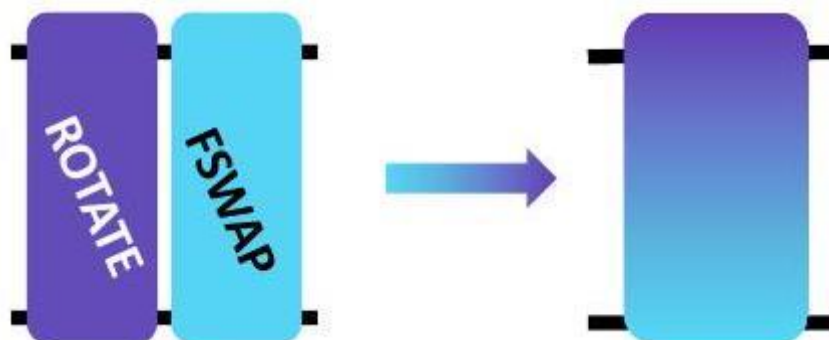


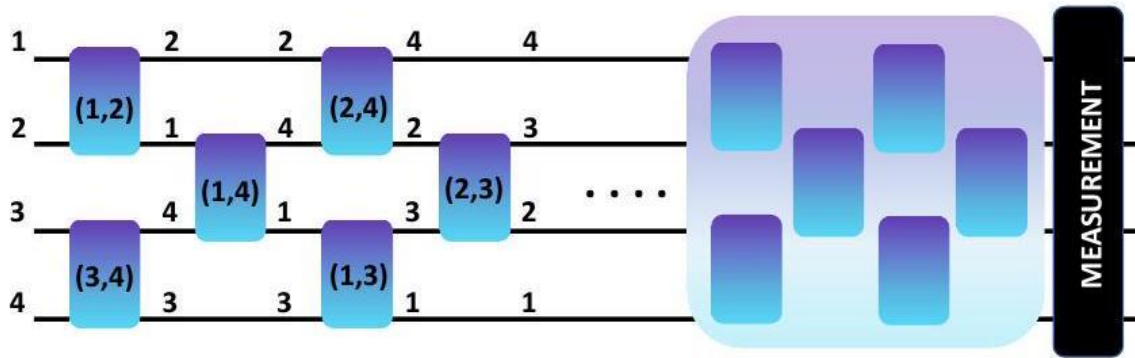
$$(\mathcal{R} \otimes \mathbb{1})(\mathbb{1} \otimes \mathcal{R})(\mathcal{R} \otimes \mathbb{1}) = (\mathbb{1} \otimes \mathcal{R})(\mathcal{R} \otimes \mathbb{1})(\mathbb{1} \otimes \mathcal{R})$$

$$\mathcal{R}_1(\theta_1, \theta_2) \times \mathcal{R}_2(\alpha_1, \alpha_2) = \mathcal{R}'(\theta_1 + \alpha_1, \theta_2 + \alpha_2),$$



$$\text{FSWAP}(\theta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & e^{i\theta} & 0 \\ 0 & e^{i\theta} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$





$$e^{-it(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i)} =$$

$$-R_x(\pi/2) \cdot R_x(t/2) \cdot R_x(-\pi/2)$$

$$-R_x(\pi/2) - R_z(t/2) - R_x(-\pi/2)$$

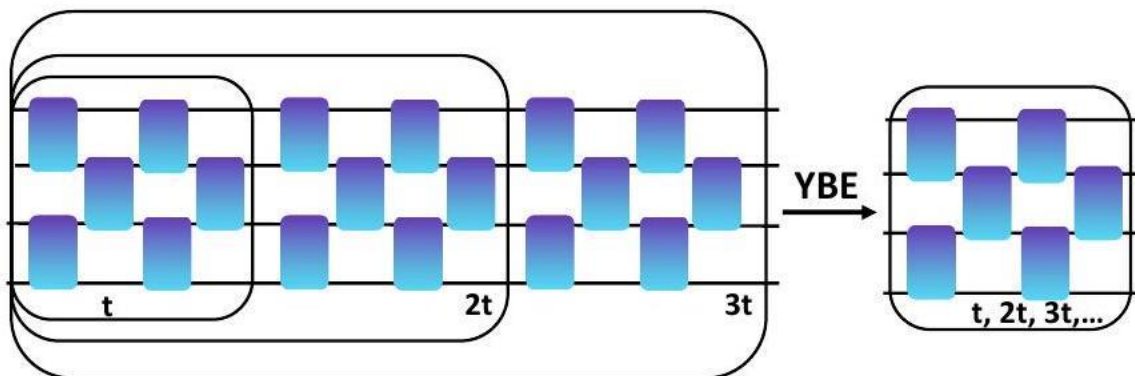
$$\text{FSWAP} = -R_x(\pi/2) - R_x(\pi/2) - R_x(-\pi/2) -$$

$$-R_x(\pi/2) - R_z(\pi/2) - R_x(-\pi/2)$$

$$\text{FSWAP} \times e^{-it(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i)} =$$

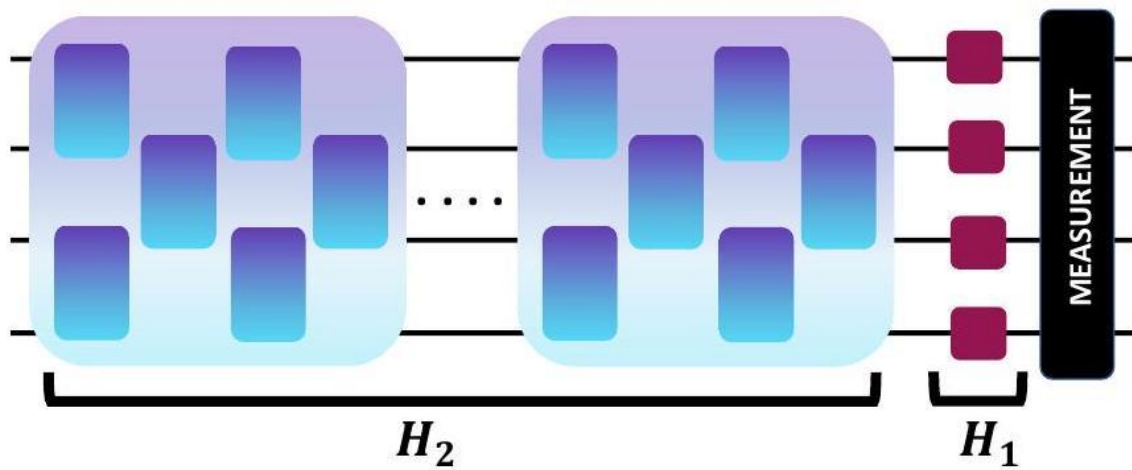
$$-R_x(\pi/2) \cdot R_x(t/2 + \pi/2) \cdot R_x(-\pi/2)$$

$$-R_x(\pi/2) - R_z(t/2 + \pi/2) - R_x(-\pi/2)$$

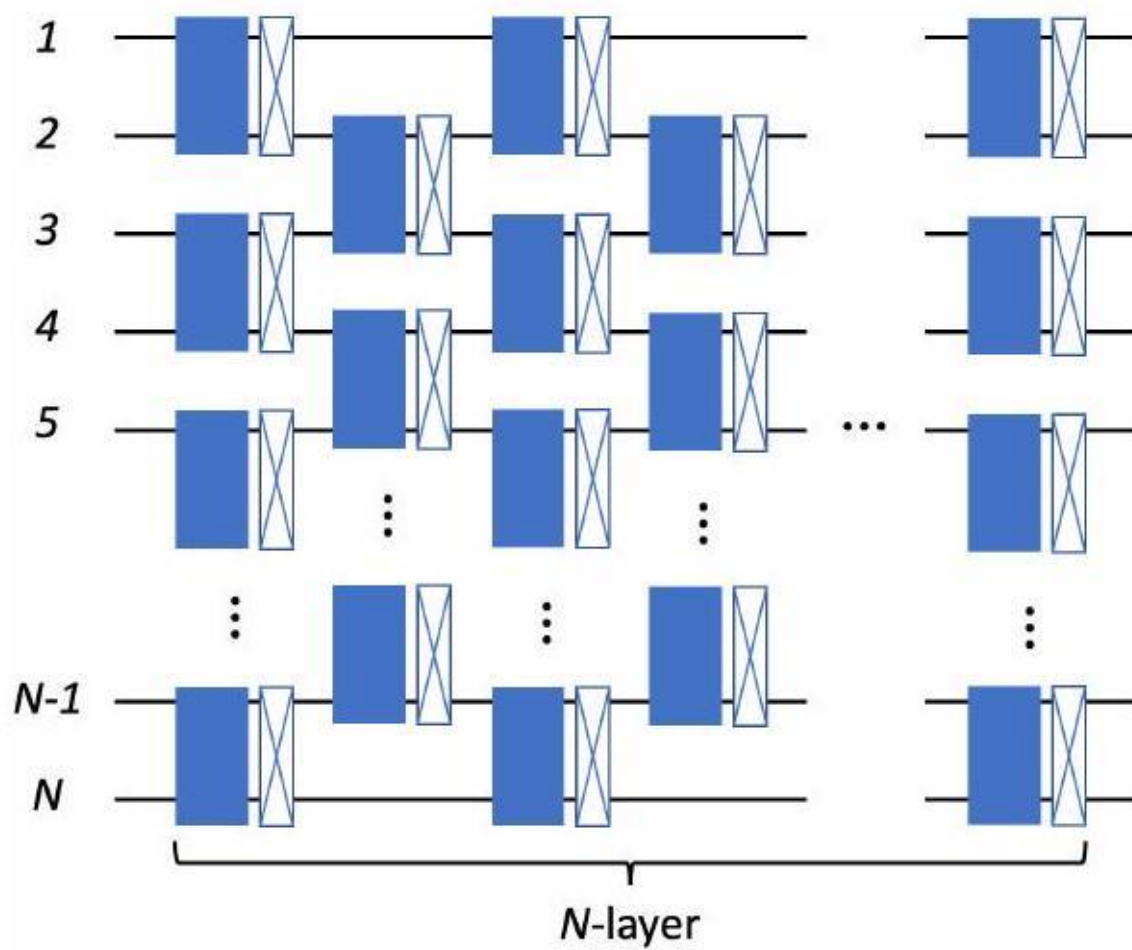


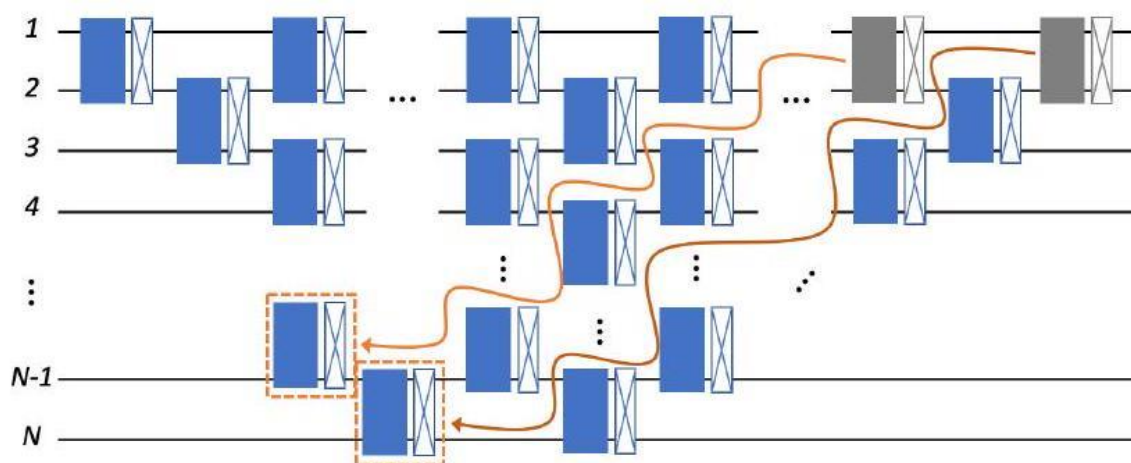
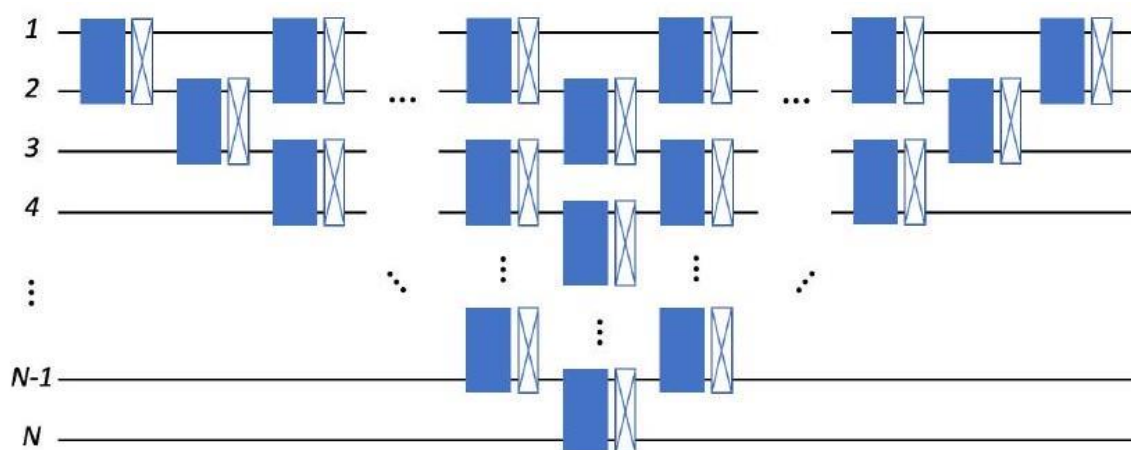
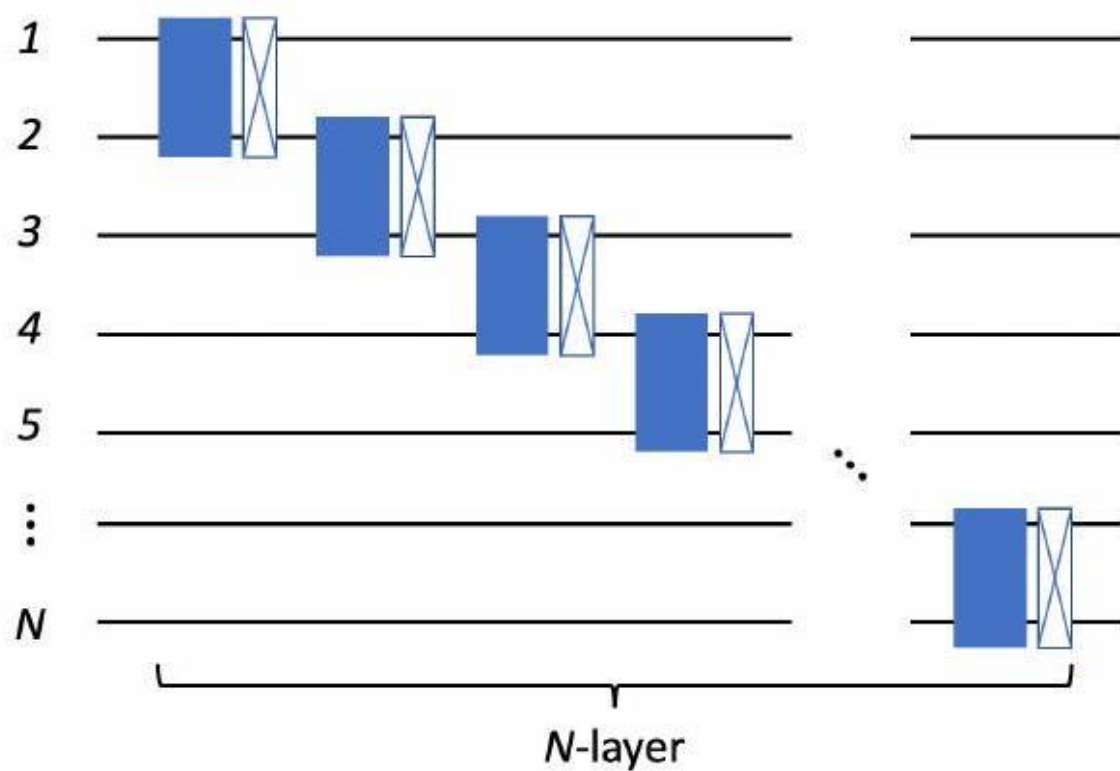
$$e^{-it(G_{11}\hat{n}_1 + G_{22}\hat{n}_2 + \dots)} = e^{-it(G_{11}\hat{n}_1)} \times e^{-it(G_{22}\hat{n}_2)} \times \dots$$

$$e^{-it(G_{ii}\hat{n}_i)} = P(tG_{ii}),$$



$$\begin{aligned}
 E(t) &= (\omega t/2\pi)\sin(\omega t)E_{\max} & \text{for } 0 \leq t \leq 2\pi/\omega \\
 E(t) &= \sin(\omega t)E_{\max} & \text{for } 2\pi/\omega \leq t \leq 4\pi/\omega \\
 E(t) &= (3 - \omega t/2\pi)\sin(\omega t)E_{\max} & \text{for } 4\pi/\omega \leq t \leq 6\pi/\omega \\
 E(t) &= 0 & \text{for } t \leq 0 \text{ and } t \geq 6\pi/\omega
 \end{aligned}$$





$$i\dot{\psi}_k(t) = H(t)\Psi_k(t), k = 1, \dots, N; \langle \Psi_k(t), \Psi_l(t) \rangle = \delta_{kl}.$$

$$\psi_k(t) \in L^2:=L^2(\mathbb{R}^3)$$

$$H(t) \mathop{:}= -\Delta + eV_n(x) + eV_e(x,t)$$

$$V_e(x,t)=\int\frac{\rho(y,t)}{|x-y|}dy,\rho(y,t)\mathop{:}=e\sum_1^N|\psi_k(y,t)|^2\leq 0,$$

$$i\dot{K}(t)=[H(t),K(t)]$$

$$K(t)\mathop{:}=\sum_1^N|\psi_k(t)\rangle\langle\psi_k(t)|$$

$$K^*(t)=K(t)\geq 0, K(t)\leq 1, \mathrm{tr}K=N$$

$$\rho(y,t)\mathop{:}=eK(y,y,t)\leq 0$$

$$i\dot{\Psi}(\bar{x},t)={\bf H}\Psi(\bar{x},t)\mathop{:}=-\sum_1^N\Delta_{x_k}\Psi(\bar{x},t)+e\left[\sum_1^NV_n(x_k)+V_e(\bar{x})\right]\Psi(\bar{x},t),\bar{x}\in\mathbb{R}^{3N}$$

$$V_n(x)\mathop{:}=\sum_1^M\frac{|e|Z_j}{|x-x_j|},V_e(\bar{x})\mathop{:}=\sum_{k<l}\frac{e}{|x_k-x_l|}$$

$$E\mathop{:}=\min\Big\{\frac{1}{2}\langle\Psi,{\bf H}\Psi\rangle\mathop{:}\|\Psi\|_{L^2(R^{3N})}=1\Big\}.$$

$$\Psi(\bar{x})=\frac{1}{\sqrt{N!}}\det\psi_k(x_l)$$

$$\langle \Psi_k, \Psi_l \rangle = \delta_{kl}$$

$$\begin{aligned}\frac{1}{2}\langle\Psi,{\bf H}\Psi\rangle=\mathcal{E}^{HF}(\Psi_N)\mathop{:}=&\frac{1}{2}\sum_1^N\int|\nabla\psi_k(x)|^2dx+\frac{1}{2}\int V_n(x)\rho(x)dx\\&+\frac{1}{4}\int\frac{\rho(x)\rho(y)}{|x-y|}dxdy-\frac{1}{4}\iint\frac{|\tau(x,y)|^2}{|x-y|}dxdy\end{aligned}$$

$$\rho(x)=eK(x,x),\tau(x,y)=eK(x,y),K(x,y)\mathop{:}=\sum_1^N\psi_k(x)\overline{\psi_k(y)}$$

$$K^*=K\geq 0, K\leq 1, \mathrm{tr}K=N.$$

$$\mathcal{E}^{HF}(K)=-\frac{1}{2}\mathrm{tr}\Delta K+\frac{1}{2}\int V_n(x)\rho(x)dx+\frac{1}{4}\int\frac{\rho(x)\rho(y)}{|x-y|}dxdy-\frac{1}{4}\iint\frac{|\tau(x,y)|^2}{|x-y|}dxdy$$

$$\Psi_N=(\Psi_1,\ldots,\Psi_N)\in\oplus_1^NX$$

$$E^{HF}\mathop{:}=\min\{\mathcal{E}^{HF}(\Psi_N)\mathop{:}\Psi_N\in\mathcal{S}(N)\}\geq E$$



$$K=K(\Psi_N)=\sum|\Psi_k\rangle\langle\Psi_k|$$

$$\Psi_N=(\Psi_k\colon k=1,\ldots,N)\mapsto \Phi_N=\Big(\varphi_k=\sum_{l=1}^N U_{kl}\Psi_l\colon k=1,\ldots,N\Big), (U_{kl})\in U(N)$$

$$D_{\Psi_k}\mathcal{E}^{HF}(\Psi_N)=\sum_{l=1}^N\lambda_{kl}\Psi_l, k=1,\ldots,N$$

$$D_{\Psi_k(x)}\coloneqq D_{p_k(x)}+iD_{q_k(x)}$$

$$p_k(x)=\operatorname{Re}\Psi_k(x) \text{ and } q_k(x)=\operatorname{Im}\Psi_k(x)$$

$$D_{\bar{\psi}_k}\mathcal{E}^{HF}(\Psi_N)=H\Psi_k,$$

$$\mathcal{D}\colon=C_0^\infty(\mathbb{R}^3)$$

$$H(\Phi_N)=-\Delta+eV_n(x)+eV_e(x)+e\mathcal{T}.$$

$$V_e(x)=\int\frac{\rho(y)}{|x-y|}dy,\mathcal{T}\psi(x)=-\int\frac{\tau(x,y)}{|x-y|}\psi(y)dy$$

$$H(\Psi_N)\Psi_k=\sum_{l=1}^N\lambda_{kl}\Psi_l, k=1,\ldots,N$$

$$H(\Phi_N)\varphi_k=\varepsilon_k\varphi_k, k=1,\ldots,N$$

$$K(x,y)=\sum\lambda_nu_n(x)\overline{u_n(y)},\langle u_k,u_l\rangle=\delta_{kl},0\leq\lambda_n\leq1,\sum\lambda_n=N$$

$$E^{HF}=\min\{\mathcal{E}^{HF}(K)\colon K^*=K,0\leq K\leq 1,\mathrm{tr}K=N\}$$

$$i\dot{\Psi}_k(x,t)=H(t)\psi_k(\cdot,t), k=1,\ldots,N.)$$

$$H(t)=H(\Psi(t))$$

$$H(t)\coloneqq -\Delta+eV_n(x)+eV_e(x,t)+e\mathcal{T}(t)$$

$$V_e(x,t)=\int\frac{\rho(y,t)}{|x-y|}dy,\mathcal{T}(t)\psi(x)=-\int\frac{\tau(x,y,t)}{|x-y|}\psi(y)dy$$

$$K(x,y,t)\coloneqq\sum_1^N\psi_k(x,t)\overline{\psi_k(y,t)}$$

$$i\dot{K}(t)=[H(t),K(t)]$$

$$K=ww^*, \text{ or equivalently, } K(x,y)=\int w(x,z)w^*(z,y)dz=\int w(x,z)\overline{w(y,z)}dz$$

$$\tilde{\mathcal{E}}^{HF}(w) := \frac{1}{4} \iint \left[|\nabla_x w(x, y)|^2 + |\nabla_y w(x, y)|^2 \right] dx dy + \frac{e}{4} \iint [V_n(x) + V_n(y)] |w(x, y)|^2 dx dy \\ + \frac{1}{4} \iint \frac{\tilde{\rho}(x) \tilde{\rho}(y)}{|x - y|} dx dy - \frac{1}{4} \iint \frac{|\tilde{\tau}(x, y)|^2}{|x - y|} dx dy$$

$$\tilde{\rho}(x) = e\tilde{K}(x, x), \tilde{\tau}(x, y) = e\tilde{K}(x, y), \tilde{K}(x, y) := \frac{1}{2} \int [w(x, z) \overline{w(y, z)} + \overline{w(z, x)} w(z, y)] dz$$

$$\tilde{K} = \frac{1}{2} \{w, w^*\} = \frac{1}{2} [ww^* + w^*w]$$

$$\tilde{\mathcal{E}}^{HF}(w) = -\frac{1}{2} \text{tr} \Delta \tilde{K} + \frac{1}{2} \int V_n(x) \tilde{\rho}(x) dx + \frac{1}{4} \int \frac{\tilde{\rho}(x) \tilde{\rho}(y)}{|x - y|} dx dy - \frac{1}{4} \iint \frac{|\tilde{\tau}(x, y)|^2}{|x - y|} dx dy = \mathcal{E}^{HF}(\tilde{K})$$

$$K = \sum_1^N |\psi_k\rangle \langle \psi_k|$$

$$\tilde{K} = w = K, \tilde{\rho} = \rho, \tilde{\tau} = \tau, \tilde{\mathcal{E}}^{HF}(w) = \mathcal{E}^{HF}(K).$$

$$i\dot{w}(x,y,t)=2D_{\bar{w}(x,y)}\tilde{\mathcal{E}}^{HF}(w(\cdot,t))=-[\Delta_x+\Delta_y]w(x,y,t)+\cdots$$

$$D_{\bar{w}(x,y)}:=D_{w_1(x,y)}+iD_{w_2(x,y)}$$

$$w_1(x,y) = \text{Re} w(x,y) \text{ and } w_2(x,y) = \text{Im} w(x,y)$$

$$\tilde{H}(t) := -\Delta + eV_n(x) + e\tilde{V}_e(x,t) + e\tilde{\mathcal{T}}(t) \\ \tilde{V}_e(x,t) = \int \frac{\tilde{\rho}(y,t)}{|x-y|} dy, \tilde{\mathcal{T}}(t)\psi(x) = -\int \frac{\tilde{\tau}(x,y,t)}{|x-y|} \Psi(y) dy$$

$$i\dot{w}(t)=\{\tilde{H}(t),w(t)\}:=\tilde{H}(t)w(t)+w(t)\tilde{H}(t)$$

$$\tilde{H}(t):=H_0+\tilde{V}(t), H_0:=-\Delta+eV_n(x) \; \tilde{V}(t):=e\tilde{V}_e(x,t)$$

$$\tilde{\mathcal{E}}^{RHF}(w) = \frac{1}{2} \text{tr}[H_0 \tilde{K}(t)] + \frac{1}{4} \int \frac{\tilde{\rho}(x) \tilde{\rho}(y)}{|x - y|} dx dy$$

$$i\dot{w}(t)=2D_{\bar{w}}\tilde{\mathcal{E}}^{RHF}(w(\cdot,t)), t\in\mathbb{R}$$

$$\|w\|_{\mathbf{H}^s}^2 = \sum_{|\alpha|\leq s} \int \left| \partial_{(x,y)}^\alpha w(x,y) \right|^2 dx dy$$

$$\partial_x^\alpha w \in \mathcal{L}^2 w \partial_x^\alpha \in \mathcal{L}^2 |\alpha| \leq s$$

$$w(\cdot) \in X := C^1_S(\mathbb{R}, \mathbf{H}^0) \cap C(\mathbb{R}, \mathbf{H}^2)$$

$$i\dot{w}(t)=\{\tilde{H}(t),w(t)\}, t\in\mathbb{R}$$

$$2D_{\bar{w}}\tilde{\mathcal{O}}^{RHF}(w)=\{\tilde{H},w\}\in\mathbf{H}^0, w\in\mathbf{H}^2$$

$$\tilde{H}=H_0+e\tilde{V}_e(x)$$

$$\tilde{V}_e(x) := \int \frac{\tilde{\rho}(y)}{|x-y|} dy$$

$$K(t) := w(t)w^*(t)$$

$$w(\cdot) \in X$$

$$-i\dot{w}^*(t) = w^*(t)\tilde{H}(t) + \tilde{H}(t)w^*(t)$$

$$i\dot{K}(t) = i[\dot{w}(t)w^*(t) + w(t)\dot{w}^*(t)] = [\tilde{H}w + w\tilde{H}]w^* - w[w^*\tilde{H} + \tilde{H}w^*] = [\tilde{H}(t), K(t)]$$

$$\tilde{V}_e(x) = \int \frac{\tilde{\rho}(y)}{|x-y|} dy = \frac{1}{2} \int \frac{[w(y,z)\bar{w}(y,z) + \bar{w}(z,y)w(z,y)]dz}{|x-y|} dy$$

$$\sup_{x \in \mathbb{R}^3} |\tilde{V}_e(x)| \leq C \|w\|_{\mathbf{H}^0} \|w\|_{\mathbf{H}^1}$$

$$\tilde{V}_e(x,z) = \frac{1}{2} \int \frac{w(y,z)\bar{w}(y,z) + \bar{w}(z,y)w(z,y)}{|x-y|} dy$$

$$|\tilde{V}_e(x,z)| \leq C(\|w(\cdot,z)\| \cdot \|\nabla_1 w(\cdot,z)\| + \|w(z,\cdot)\| \cdot \|\nabla_2 w(z,\cdot)\|)$$

$$F(w) = \{\tilde{V}_e, w\}$$

$$\|F(w) - F(w')\|_{\mathbf{H}^0} \leq C(\|w\|_{\mathbf{H}^1}^2 + \|w'\|_{\mathbf{H}^1}^2) \|w - w'\|_{\mathbf{H}^0}.$$

$$F_1(w) = w \int \frac{\int w(y,z)\bar{w}(y,z)dz}{|x-y|} dy$$

$$F_1(w) - F_1(w') = (w - w') \int \frac{\int w(y,z)\bar{w}(y,z)dz}{|x-y|} dy + w' \int \frac{[w(y,z)\bar{w}(y,z) - w'(y,z)\bar{w}'(y,z)]dz}{|x-y|} dy$$

$$\begin{aligned} I(x,z) &= \int \frac{w(y,z)\bar{w}(y,z) - w'(y,z)\bar{w}'(y,z)}{|x-y|} dy \\ &= \int \frac{w(y,z)\bar{w}(y,z) - w'(y,z)\bar{w}(y,z) + w'(y,z)\bar{w}(y,z) - w'(y,z)\bar{w}'(y,z)}{|x-y|} dy \\ &\leq C(\|\nabla_1 w(\cdot,z)\| \cdot \|w(\cdot,z) - w'(\cdot,z)\| + \|\nabla_1 w'(\cdot,z)\| \cdot \|w(\cdot,z) - w'(\cdot,z)\|) \end{aligned}$$

$$\sup_{x \in \mathbb{R}^3} \int |I(x,z)| dz \leq C(\|w\|_{\mathbf{H}^1} + \|w'\|_{\mathbf{H}^1}) \|w - w'\|_{\mathbf{H}^0}.$$

$$\begin{aligned} \|F(w)\|_{\mathbf{H}^2} &\leq C_F \|w\|_{\mathbf{H}^1}^2 \|w\|_{\mathbf{H}^2} \\ \|F(w) - F(w')\|_{\mathbf{H}^2} &\leq C_F (\|w\|_{\mathbf{H}^2}^2 + \|w'\|_{\mathbf{H}^2}^2) \|w - w'\|_{\mathbf{H}^2} \end{aligned}$$

$$\|F_1(w)\|_{\mathbf{H}^0} \|\Delta F_1(w)\|_{\mathbf{H}^0} \|F_1(w) \Delta\|_{\mathbf{H}^0}$$

$$F_z = w \int \frac{w(y,z)\bar{w}(y,z)}{|x-y|} dy.$$

$$F_z(x, y') = w(x, y') \int \frac{w(y, z) \bar{w}(y, z)}{|y' - y|} dy$$

$$\Delta_{y'} F_z(x, y') = \Delta_z F_z(x, y')$$

$$\begin{aligned} \Delta_z F_z(x, y') = & 4\pi w(x, y') \cdot w(y', z) \bar{w}(y', z) \\ & + 2\nabla_z w \int \frac{\nabla_1 w(y, z) \bar{w}(y, z)}{|x - y|} dy + 2\nabla_z w \int \frac{w(y, z) \nabla_1 \bar{w}(y, z)}{|x - y|} dy + \Delta_z w \int \frac{w(y, z) \bar{w}(y, z)}{|x - y|} dy. \end{aligned}$$

$$K_z(x, y') = 4\pi w(x, y') w(y', z) \bar{w}(y', z).$$

$$\begin{aligned} \int |K_z(x, y')|^2 dy' &\leq C \|w(x, \cdot)\|_{L^6}^2 \|w(\cdot, z)\|_{L^6(\mathbb{R}^3)}^2 \|\bar{w}(\cdot, z)\|_{L^6(\mathbb{R}^3)}^2 \\ &\leq C \|w(x, \cdot)\|_{H^1(\mathbb{R}^3)}^2 \|w(\cdot, z)\|_{H^1(\mathbb{R}^3)}^2 \|\bar{w}(\cdot, z)\|_{H^1(\mathbb{R}^3)}^2. \end{aligned}$$

$$\|K_z\|_{\mathbf{H}^0} \leq C \|w\|_{\mathbf{H}^1(\mathbb{R}^3)} \|w(\cdot, z)\|_{H^1(\mathbb{R}^3)} \|\bar{w}(\cdot, z)\|_{H^1(\mathbb{R}^3)}.$$

$$\|F_1(w) - F_1(w')\|_{\mathbf{H}^2} \sim \|F_1(w) - F_1(w')\|_{\mathbf{H}^0} + \|\Delta[F_1(w) - F_1(w')]\|_{\mathbf{H}^0} + \|[F_1(w) - F_1(w')]\Delta\|_{\mathbf{H}^0}.$$

$$i\dot{w}(t) = \{H_0, w(t)\} + \{\tilde{V}(t), w(t)\}.$$

$$w(t) = U_0(t)C(t)U_0(t), t \in \mathbb{R},$$

$$U_0(t) := \exp(-iH_0t)$$

$$\dot{w}(t) = \{H_0, w(t)\} + U_0(t)\dot{C}(t)U_0(t).$$

$$iU_0(t)\dot{C}(t)U_0(t) = \{\tilde{V}(t), w(t)\}.$$

$$C(t) = C(0) - i \int_0^t U_0(-s) \{ \tilde{V}(s), w(s) \} U_0(-s) ds$$

$$w(t) = U_0(t)w(0)U_0(t) - i \int_0^t U_0(t-s) \{ \tilde{V}(s), w(s) \} U_0(t-s) ds, t \in \mathbb{R}$$

$$\{\tilde{V}(t), w(t)\} \in \mathcal{C}(\mathbb{R}, \mathbf{H}^2)$$

$$X_\varepsilon := C^1_S(-\varepsilon, \varepsilon; \mathbf{H}^0) \cap C(-\varepsilon, \varepsilon; \mathbf{H}^2)$$

$$\varepsilon = \varepsilon(C_F, \|w(0)\|_{\mathbf{H}^2}) > 0$$

$$\varepsilon = \varepsilon(C_F, \|w(0)\|_{\mathbf{H}^2}) > 0$$

$$w(\cdot) \in C^1_S(-\varepsilon, \varepsilon; \mathbf{H}^0).$$

$$\|\dot{U}_0(t)w(0)U_0(t)\|_{\mathbf{H}^0} + \|U_0(t)w(0)\dot{U}_0(t)\|_{\mathbf{H}^0} \sim \|U_0(t)\tilde{H}_0w(0)U_0(t)\|_{\mathbf{H}^0} + \|U_0(t)w(0)\tilde{H}_0U_0(t)\|_{\mathbf{H}^0}$$

$$\{\tilde{V}(t), w(t)\} \in \mathcal{C}(-\varepsilon, \varepsilon; \mathbf{H}^2)$$



$$\tilde{\mathcal{E}}^{HF}(w(t)) = \text{const}, t \in \mathbb{R}$$

$$\tilde{\mathcal{E}}^{RHF}(w(t)) = \frac{1}{4} \text{tr}[H_0 w(t) w^*(t) + H_0 w^*(t) w(t)] + \frac{1}{4} \int \frac{\tilde{\rho}(x, t) \tilde{\rho}(y, t)}{|x - y|} dx dy$$

$$\begin{aligned} \dot{\mathcal{E}}^{RHF}(w(t)) &= \frac{1}{4} \text{tr}[w^*(t) H_0 \dot{w}(t) + H_0 w(t) \dot{w}^*(t) + w(t) H_0 \dot{w}^*(t) + H_0 w^*(t) \dot{w}(t)] + \frac{1}{2} \langle \tilde{V}_e(x, t), \dot{\tilde{\rho}}(x, t) \rangle \\ &= \frac{1}{4} \text{tr}[\{H_0, w(t)\} \dot{w}^*(t) + \{H_0, w^*(t)\} \dot{w}(t)] + \frac{1}{2} \langle \tilde{V}_e(x, t), \dot{\tilde{\rho}}(x, t) \rangle \end{aligned}$$

$$\begin{aligned} \frac{1}{2} \langle \tilde{V}_e(x, t), \dot{\tilde{\rho}}(x, t) \rangle &= \frac{1}{4} \text{tr}[\tilde{V}(t)(\dot{w}(t) w^*(t) + w(t) \dot{w}^*(t) + \dot{w}^*(t) w(t) + w^*(t) \dot{w}(t))] \\ &= \frac{1}{4} \text{tr}[\{\tilde{V}(t), w(t)\} \dot{w}^*(t) + \{\tilde{V}(t), w^*(t)\} \dot{w}(t)] \end{aligned}$$

$$\Delta \tilde{\mathcal{E}}^{RHF}(t) := \tilde{\mathcal{E}}^{RHF}(w(t + \Delta t)) - \tilde{\mathcal{E}}^{RHF}(w(t))$$

$$\Delta w(t) := w(t + \Delta t) - w(t)$$

$$\dot{\mathcal{E}}^{RHF}(w(t)) = \frac{1}{4} \text{tr}[\{H_0 + \tilde{V}(t), w^*(t)\} \dot{w}(t) + \{H_0 + \tilde{V}(t), w(t)\} \dot{w}^*(t)]$$

$$\dot{w}(t) = -i\{H_0 + \tilde{V}(t), w(t)\}$$

$$\dot{w}^*(t) = i\{H_0 + \tilde{V}(t), w^*(t)\}$$

$$\{H_0 + \tilde{V}(t), w(t)\} \text{ and } \{H_0 + \tilde{V}(t), w^*(t)\}$$

$$Q(t) := \int \tilde{\rho}(x, t) dx = \text{const}, t \in \mathbb{R}$$

$$Q(t) = \text{etr} \tilde{K}(t) = \text{etr} w(t) w^*(t) = \text{etr} C(t) C^*(t)$$

$$i\dot{C}(t) = V_L(t)C(t) + C(t)V_R(t), V_L(t) = U_0^*(t)\tilde{V}(t)U_0(t), V_R(t) = U_0(t)\tilde{V}(t)U_0^*(t)$$

$$V_L(t), V_R(t) \in \mathcal{C}_s(\mathbb{R}, \mathcal{L})$$

$$\tilde{V}_e(x, t + \Delta t) - \tilde{V}_e(x, t)$$

$$\mathcal{L} = \mathcal{L}(L^2, L^2) - i\dot{C}^*(t) = C^*(t)V_L(t) + V_R(t)C^*(t)$$

$$i\frac{d}{dt}[C(t)C^*(t)] = [V_L(t), C(t)C^*(t)]$$

$$\|w(t)\|_{\mathbf{H}^0} = \text{const}$$

$$\|w(t)\| = \text{const}, t \in \mathbb{R}$$

$$\begin{aligned} i\dot{U}_L(t, s) &= V_L(t)U_L(t, s), \quad t, s \in \mathbb{R}; \quad U_L(s, s) = I \\ i\dot{U}_R(t, s) &= U_R(t, s)V_R(t), \quad t, s \in \mathbb{R}; \quad U_R(s, s) = I \end{aligned}$$

$$U_L(t, s)U_L(s, r) = U_L(t, r), U_R(t, s)U_R(s, r) = U_R(t, r), t, s, r \in \mathbb{R}$$



$$V_L(t), V_R(t) \in \mathcal{C}(\mathbb{R}, \mathcal{L})$$

$$V_L(t), V_R(t) \dot{U}_L^*(t, s) = i U_L^*(t, s) V_L(t)$$

$$\begin{aligned} \frac{d}{dt} [U_L^*(t, s) U_L(t, s)] &= \dot{U}_L^*(t, s) U_L(t, s) + U_L^*(t, s) \dot{U}_L(t, s) \\ &= i U_L^*(t, s) V_L(t, s) U_L(t, s) - i U_L^*(t, s) V_L(t) U_L(t, s) = 0, t, s \in \mathbb{R} \end{aligned}$$

$$U_L^*(t, s) U_L(t, s) = U_L^*(s, s) U_L(s, s) = I$$

$$w(t) = U_0(t) U_L(t) U_0^*(t) w(0) U_0^*(t) U_R(t) U_0(t), t \in \mathbb{R}$$

$$\begin{aligned} \|w(t)\|_{\mathbf{H}^1} &\leq C_1, \\ \|w(t)\|_{\mathbf{H}^2} &\leq C_2 e^{C_3|t|}, t \in (-\varepsilon, \varepsilon) \\ t &\in (-\varepsilon, \varepsilon) \end{aligned}$$

$$\|w(t)\|_{\mathbf{H}^2} \leq C \left[\|w(0)\|_{\mathbf{H}^2} + \int_0^t \|\{\tilde{V}(s), w(s)\}\|_{\mathbf{H}^2} ds \right], t \in (-\varepsilon, \varepsilon)$$

$$\|w(t)\|_{\mathbf{H}^2} \leq C \left[\|w(0)\|_{\mathbf{H}^2} + C_F \int_0^t \|w(s)\|_{\mathbf{H}^1}^2 \|w(s)\|_{\mathbf{H}^2} ds \right], t \in (-\varepsilon, \varepsilon)$$

$$w(t) = \sum_1^N |\psi_k(t)\rangle \langle \psi_k(t)|$$

$$E^{HF} = \min\{\tilde{\mathcal{E}}^{HF}(w): \|w\| \leq 1, \text{tr} w w^* = N\}$$

$$\tilde{\mathcal{E}}^{HF}(w) = \mathcal{E}^{HF}(\tilde{K})$$

$$\tilde{K}:=\frac{1}{2}[ww^*+w^*w]\geq 0$$

$$\text{tr}\tilde{K}:=\text{tr}ww^*=\text{tr}w^*w=N$$

$$\|w(0)\| \leq 1$$

$$\tilde{K}(t):=\frac{1}{2}[w(t)w^*(t)+w^*(t)w(t)]$$

$$K(t):=w(t)w^*(t)$$

$$\tilde{K}(t)\geq 0, K(t)\geq 0$$

$$\text{tr}\tilde{K}(t)=\text{tr}K(t)$$

$$\text{tr}\tilde{K}(t)=\text{tr}K(t)=N$$

$$\|\tilde{K}(t)\| \leq 1, \|K(t)\| \leq 1, t \in \mathbb{R}$$

$$\|w(t)\|K(t):=w(t)w^*(t)$$

$$I_1 = -\frac{1}{4} [\langle \Delta_x w(x, y), w(x, y) \rangle + \langle \Delta_y w(x, y), w(x, y) \rangle]$$

$$D_{\bar{w}(x,y)} I_1 = -\frac{1}{2} [\Delta_x w(x, y) + \Delta_y w(x, y)]$$

$$I_2 = \frac{e}{4} \iint [V_n(x) + V_n(y)] |w(x, y)|^2 dx dy$$

$$D_{\bar{w}(x,y)} I_2 = \frac{e}{2} [V_n(x) + V_n(y)] w(x, y)$$

$$I_3 = \frac{1}{4} \iint \frac{\tilde{\rho}(x') \tilde{\rho}(y')}{|x' - y'|} dx' dy'$$

$$D_{\bar{w}(x,y)} I_2 = \frac{1}{2} \iint \frac{\tilde{\rho}(y')}{|x' - y'|} D_{\bar{w}(x,y)} \tilde{\rho}(x') dx' dy'$$

$$\begin{aligned} D_{\bar{w}(x,y)} [\tilde{\rho}(x')] &= \frac{e}{2} D_{\bar{w}(x,y)} \int [w(x', z) \overline{w(x', z)} + \overline{w(z, x')} w(z, x')] dz \\ &= e [\delta(x' - x) w(x', y) + \delta(x' - y) w(x, x')] \end{aligned}$$

$$\begin{aligned} D_{\bar{w}(x,y)} I_2 &= \frac{e}{2} \iint \frac{\tilde{\rho}(y')}{|x' - y'|} [\delta(x' - x) w(x', y) + \delta(x' - y) w(x, x')] dx' dy' \\ &= \frac{e}{2} \int \frac{\tilde{\rho}(y')}{|x - y'|} w(x, y) dy' + \frac{e}{2} \int \frac{\tilde{\rho}(y')}{|y - y'|} w(x, y) dx' \end{aligned}$$

$$\tilde{V}(x) = \int \frac{\tilde{\rho}(y)}{|x - y|} dy$$

$$I_4 = -\frac{1}{4} \iint \frac{|\tilde{\tau}(x', y')|^2}{|x' - y'|} dx' dy'$$

$$D_{\bar{w}(x,y)} I_4 = -\frac{1}{4} \iint \frac{\tilde{\tau}(x', y') D_{\bar{w}(x,y)} \tilde{\tau}(y', x') + \tilde{\tau}(y', x') D_{\bar{w}(x,y)} \tilde{\tau}(x', y')}{|x' - y'|} dx' dy'$$

$$\begin{aligned} D_{\bar{w}(x,y)} \tilde{\tau}(x', y') &= \frac{e}{2} D_{\bar{w}(x,y)} \int [w(x', z) \overline{w(y', z)} + \overline{w(z, x')} w(z, y')] dz \\ &= e [\delta(y' - x) w(x', y) + \delta(x' - y) w(x, y')] \end{aligned}$$

$$\begin{aligned} D_{\bar{w}(x,y)} I_4 &= -\frac{e}{4} \iint \frac{\tilde{\tau}(x', y') [\delta(x' - x) w(y', y) + \delta(y' - y) w(x, x')]}{|x' - y'|} dx' dy' \\ &\quad - \frac{e}{4} \iint \frac{\tilde{\tau}(y', x') [\delta(y' - x) w(x', y) + \delta(x' - y) w(x, y')]}{|x' - y'|} dx' dy' \\ &= -\frac{e}{4} \iint \frac{\tilde{\tau}(x, y') w(y', y)}{|x - y'|} dy' - \frac{e}{4} \iint \frac{\tilde{\tau}(x', y) w(x, x')}{|x' - y|} dx' \\ &\quad - \frac{e}{4} \iint \frac{\tilde{\tau}(x, x') w(x', y)}{|x' - x|} dx' - \frac{e}{2} \iint \frac{\tilde{\tau}(y', y) w(x, y')}{|y - y'|} dy' \\ &= -\frac{e}{2} \iint \frac{\tilde{\tau}(x, y') w(y', y)}{|x - y'|} dy' - \frac{e}{2} \iint \frac{\tilde{\tau}(x', y) w(x, x')}{|x' - y|} dx' \end{aligned}$$



$$E_{gs}:=\inf\{\omega(\mathbb{H})\colon \omega\in\mathcal{Z}\}.$$

$$E_{HFB}:=\inf\{\omega(\mathbb{H})\colon \omega\in\mathcal{Z}_{\mathrm{qf}}\}.$$

$$\mathcal{D} \mathop{:=} \left\{ \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbf{1} - \bar{\gamma} \end{pmatrix} \in \mathrm{B}(\mathfrak{H} \oplus \mathfrak{H}) \colon 0 \leq \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbf{1} - \bar{\gamma} \end{pmatrix} \leq \mathbf{1}_{\mathfrak{H} \oplus \mathfrak{H}}, \gamma = \gamma^* \in \mathrm{B}_1(\mathfrak{H}), \alpha^T = -\alpha \right\},$$

$$E_{HFB}=\inf\{\mathcal{E}(\Gamma)\colon \Gamma\in\mathcal{D}\}$$

$$\mathrm{U}_{\mathrm{Bog}}:=\left\{\begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix}\in\mathrm{U}(\mathfrak{H}\oplus\mathfrak{H})\colon v\in\mathrm{B}_2(\mathfrak{H})\right\}$$

$$\mathrm{U}_{\mathrm{Bog}}\times\mathcal{D}\rightarrow\mathcal{D}, U\cdot\Gamma=U\Gamma U^*, U\in\mathrm{U}_{\mathrm{Bog}}, \Gamma\in\mathcal{D}$$

$$\mathcal{O}(\Gamma) \mathop{:=} \{U\Gamma U^* \colon U \in \mathrm{U}_{\mathrm{Bog}}\}$$

$$\mathfrak{u}_{\mathrm{Bog}} \mathop{:=} \left\{ \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \in \mathrm{B}(\mathfrak{H} \oplus \mathfrak{H}) \colon x_1 = -x_1^*, x_2 = -x_2^T \in \mathrm{B}_2(\mathfrak{H}) \right\}$$

$$\left\|\begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix}\right\|_{\mathrm{res}}:=2\max\{\|x_1\|,\|x_2\|_2\}$$

$$\mathcal{O}(\Gamma)\simeq \mathrm{U}_{\mathrm{Bog}}/\mathrm{U}_{\mathrm{Bog}}^\Gamma$$

$$\mathcal{O}(\Gamma)\subseteq i\mathfrak{u}_{\mathrm{Bog}}+\begin{pmatrix}0&0\\0&1\end{pmatrix}:=i\mathfrak{u}_{\mathrm{Bog}}+P_-$$

$$s_\Gamma(X,Y):=\mathrm{Tr}(X[i\Gamma,Y])$$

$$\mathrm{U}_{\mathrm{Bog}}:=\left\{\begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix}\in\mathrm{U}(\mathfrak{H}\oplus\mathfrak{H})\colon v\in\mathrm{B}_2(\mathfrak{H})\right\}.$$

$$I_0\left(\sum_{k\geq 1}\mu_k\varphi_k\right)=\sum_{k\geq 1}\bar{\mu}_k\varphi_k$$

$$D\mathop{:=} P_+-P_-=\begin{pmatrix}\mathbf{1}&0\\0&-\mathbf{1}\end{pmatrix}$$

$$\begin{aligned} \mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H},D) &\mathop{:=} \{X\in\mathrm{B}(\mathfrak{H}\oplus\mathfrak{H})\colon [X,D]\in\mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H})\}\\ &= \left\{ \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \in \mathrm{B}(\mathfrak{H}\oplus\mathfrak{H}) \colon x_{12}, x_{21} \in \mathrm{B}_2(\mathfrak{H}) \right\}. \end{aligned}$$

$$\|X\|_{\mathrm{res}}:=2\max\{\|x_{11}\|,\|x_{22}\|,\|x_{12}\|_2,\|x_{21}\|_2\},$$

$$\mathrm{U}_{\mathrm{Bog}}\subseteq\mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\|UX\|_{\mathrm{res}}\neq\|X\|_{\mathrm{res}}\text{ and }\|XU\|_{\mathrm{res}}\neq\|X\|_{\mathrm{res}}$$

$$U\in\mathrm{U}_{\mathrm{Bog}}\text{ and }X\in\mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$I\mathop{:=} \begin{pmatrix} 0 & I_0 \\ I_0 & 0 \end{pmatrix}.$$

$$\langle (f_1,f_2),I(g_1,g_2)\rangle=\langle (g_1,g_2),I(f_1,f_2)\rangle$$

$$(f_1, f_2), (g_1, g_2) \in \mathfrak{H} \oplus \mathfrak{H}$$

$$\begin{aligned} \mathrm{GL}_2(\mathfrak{H} \oplus \mathfrak{H}, I, D) &:= \{G \in \mathrm{GL}(\mathfrak{H} \oplus \mathfrak{H}): G^{-1} = IG^*I, [G, D] \in \mathrm{B}_2(\mathfrak{H} \oplus \mathfrak{H})\} \\ &= \left\{ \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \in \mathrm{GL}(\mathfrak{H} \oplus \mathfrak{H}): \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}^{-1} = \begin{pmatrix} g_{22}^T & g_{12}^T \\ g_{21}^T & g_{11}^T \end{pmatrix}, g_{12}, g_{21} \in \mathrm{B}_2(\mathfrak{H}) \right\} \end{aligned}$$

$$\begin{aligned} \mathrm{U}_{\mathrm{Bog}} &= \{U \in \mathrm{U}(\mathfrak{H} \oplus \mathfrak{H}): U = IUI, [U, D] \in \mathrm{B}_2(\mathfrak{H} \oplus \mathfrak{H})\} \\ &= \mathrm{U}(\mathfrak{H} \oplus \mathfrak{H}) \cap \mathrm{GL}_2(\mathfrak{H} \oplus \mathfrak{H}, I, D) \end{aligned}$$

$$\begin{aligned} \mathrm{gl}_2(\mathfrak{H} \oplus \mathfrak{H}, I, D) &:= \{X \in \mathrm{B}(\mathfrak{H} \oplus \mathfrak{H}): X = -IX^*I, [X, D] \in \mathrm{B}_2(\mathfrak{H} \oplus \mathfrak{H})\} \\ &= \left\{ \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & -x_{11}^T \end{pmatrix} \in \mathrm{B}(\mathfrak{H} \oplus \mathfrak{H}): x_{12} = -x_{12}^T \in \mathrm{B}_2(\mathfrak{H}), x_{21} = -x_{21}^T \in \mathrm{B}_2(\mathfrak{H}) \right\}. \end{aligned}$$

$$\mathrm{gl}_2(\mathfrak{H} \oplus \mathfrak{H}, I, D)_{\mathbb{R}} := \{X \in \mathrm{gl}_2(\mathfrak{H} \oplus \mathfrak{H}, I, D): X^* = -X\}.$$

$$\mathrm{gl}_2(\mathfrak{H} \oplus \mathfrak{H}, I, D)$$

$$J_0: \mathfrak{H}^{\mathbb{R}} \rightarrow \mathfrak{H}^{\mathbb{R}}, J_0 f = if \mathrm{GL}(\mathfrak{H}^{\mathbb{R}})$$

$$\mathrm{O}_{\mathrm{res}}(\mathfrak{H}^{\mathbb{R}}) := \{O \in \mathrm{GL}(\mathfrak{H}^{\mathbb{R}}): O^{\tau} = O^{-1}, [O, J_0] \in \mathrm{B}_2(\mathfrak{H}^{\mathbb{R}})\}.$$

$$\|O\|_{\mathrm{res}} := \max\{\|O\|, \|[J_0, O]\|_2\}, O \in \mathrm{O}_{\mathrm{res}}(\mathfrak{H}^{\mathbb{R}})$$

$$\mathfrak{o}_{\mathrm{res}}(\mathfrak{H}^{\mathbb{R}}) := \{A \in \mathrm{B}(\mathfrak{H}^{\mathbb{R}}): A^{\tau} = -A, [A, J_0] \in \mathrm{B}_2(\mathfrak{H}^{\mathbb{R}})\}.$$

$$A \in \mathrm{B}(\mathfrak{H}^{\mathbb{R}})$$

$$A \in \mathfrak{o}_{\mathrm{res}}(\mathfrak{H}^{\mathbb{R}})$$

$$A_a \in \mathrm{B}_2(\mathfrak{H}^{\mathbb{R}})$$

$$\mathrm{G}:=\mathrm{GL}_2(\mathfrak{H}\oplus\mathfrak{H},I,D)\text{ and }\mathfrak{g}:=\mathrm{gl}_2(\mathfrak{H}\oplus\mathfrak{H},I,D)$$

$$\begin{aligned} \mathfrak{u}_{\mathrm{Bog}} &:= \{X \in \mathfrak{u}(\mathfrak{H} \oplus \mathfrak{H}): X = IXI, [X, D] \in \mathrm{B}_2(\mathfrak{H} \oplus \mathfrak{H})\} \\ &= \left\{ \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \in \mathrm{B}(\mathfrak{H} \oplus \mathfrak{H}): x_1 = -x_1^*, x_2 = -x_2^T \in \mathrm{B}_2(\mathfrak{H}) \right\} = \mathfrak{g}_{\mathbb{R}} \end{aligned}$$

$$\left\| \begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix} \right\|_{\mathrm{res}} = 2\max\{\|u\|, \|v\|_2\}$$

$$U=\begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix} \in \mathrm{U}_{\mathrm{Bog}}$$

$$\Xi: \mathrm{O}_{\mathrm{res}}(\mathfrak{H}^{\mathbb{R}}) \rightarrow \mathrm{U}_{\mathrm{Bog}}$$

$$\Xi(O)=\begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix} \text{ if and only if } O=u+vI_0, u=O_c, vI_0=O_a$$

$$i\mathfrak{g}_{\mathbb{R}}:=\{X\in\mathfrak{g}:X=X^*\}$$

$$\mathrm{U}_{\mathrm{Bog}} \times i\mathfrak{g}_{\mathbb{R}} \rightarrow \mathrm{G}, (U, X) \mapsto Ue^X$$

$$\pi_0(\mathrm{U}_{\mathrm{Bog}}) = \mathbb{Z}_2$$



$$\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}:\mathrm{U}_{\mathrm{Bog}}\rightarrow\mathbb{Z}_2,\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}\left(\begin{pmatrix}u&v\\ \bar{v}&\bar{u}\end{pmatrix}\right)=\dim\ker(u)(\mathrm{mod}2).$$

$$\mathfrak{u}_{\mathrm{Bog}}=\{X\in\mathfrak{g}:e^{tX}\in\mathrm{U}_{\mathrm{Bog}},\forall t\in\mathbb{R}\}$$

$$\mathfrak{u}_{\mathrm{Bog}}=\mathfrak{g}_{\mathbb{R}}:=\{X\in\mathfrak{g}:X^*=-X\}$$

$$i\mathfrak{g}_{\mathbb{R}}:=\{X\in\mathfrak{g}:X^*=X\}$$

$$0\in\mathcal{W}\subseteq\mathfrak{g},1=\mathbf{1}_{\mathfrak{H}\oplus\mathfrak{H}}\in\mathcal{V}\subseteq G$$

$$\exp\left(\mathcal{W}\cap\mathfrak{u}_{\mathrm{Bog}}\right)=\mathcal{V}\cap\mathrm{U}_{\mathrm{Bog}}$$

$$X=\log\left(U\right)=\sum_{n\geq1}\left(-1\right)^{n+1}\frac{\left(U-\mathbf{1}\right)^n}{n}\in\mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\mathfrak{H}_{\mathbb{C}}:=\left(\mathfrak{H}^{\mathbb{R}}\right)_{\mathbb{C}}$$

$$\mathfrak{H}_{\mathbb{C}}=\mathfrak{H}^{\mathbb{R}}\times\mathfrak{H}^{\mathbb{R}}$$

$$\mathfrak{H}_{\mathbb{C}}=\mathfrak{H}_{\mathbb{C}}^{+}\oplus\mathfrak{H}_{\mathbb{C}}^{-}$$

$$U\colon\mathfrak{H}\rightarrow\mathfrak{H}_{\mathbb{C}}^{+},Uf=\frac{1}{\sqrt{2}}(f,-if)$$

$$C\colon\mathfrak{H}_{\mathbb{C}}\rightarrow\mathfrak{H}_{\mathbb{C}},C((f,g))=(f,-g)$$

$$\mathfrak{H}^{\mathbb{R}}\cong\mathfrak{H}^{\mathbb{R}}\times\{0\}=\{(f,g)\in\mathfrak{H}_{\mathbb{C}}:C((f,g))=(f,g)\}$$

$$C\mathfrak{H}_{\mathbb{C}}^{\pm}=\mathfrak{H}_{\mathbb{C}}^{\mp}$$

$$\mathfrak{H}\oplus\mathfrak{H}\text{ and }\mathfrak{H}_{\mathbb{C}}=\mathfrak{H}_{\mathbb{C}}^{+}\oplus\mathfrak{H}_{\mathbb{C}}^{-}$$

$$T\colon\mathfrak{H}\oplus\mathfrak{H}\rightarrow\mathfrak{H}_{\mathbb{C}},T((f,g))=Uf+CUI_0g=\frac{1}{\sqrt{2}}(f+\bar{g},i(\bar{g}-f))$$

$$\mathrm{B}(\mathfrak{H}\oplus\mathfrak{H})\rightarrow\mathrm{B}(\mathfrak{H}_{\mathbb{C}}),X\mapsto\mathrm{Ad}_TX=TXT^{-1}$$

$$\mathrm{O}_{\mathrm{res}}(\mathfrak{H}^{\mathbb{R}})\rightarrow\{U\in\mathrm{U}(\mathfrak{H}_{\mathbb{C}})\colon UC=CU,[U,J]\in\mathrm{B}_2(\mathfrak{H}_{\mathbb{C}})\},O\mapsto O_{\mathbb{C}}.$$

$$\Xi:\mathrm{O}_{\mathrm{res}}(\mathfrak{H}^{\mathbb{R}})\rightarrow\mathrm{U}_{\mathrm{Bog}},\Xi(O)=T^{-1}O_{\mathbb{C}}T$$

$$\mathrm{ind}_{\mathrm{O}_{\mathrm{res}}}:\mathrm{O}_{\mathrm{res}}\left(\mathfrak{H}^{\mathbb{R}}\right)\rightarrow\mathbb{Z}_2,\mathrm{ind}_{\mathrm{O}_{\mathrm{res}}}\left(O\right)=\dim_{\mathbb{C}}\ker\left(O-J_0OJ_0\right)(\mathrm{mod}2)$$

$$\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}\left(U\right)=\mathrm{ind}_{\mathrm{O}_{\mathrm{res}}}\left(\Xi^{-1}(U)\right)$$

$$W\Gamma W^*=\begin{pmatrix}\Lambda&0\\0&\mathbf{1}-\Lambda\end{pmatrix}$$

$$p_i p_j = \delta_{ij} p_i, \dim(\mathrm{ran}(p_i))\colon = m_i < \infty$$



$$\Lambda=\sum_{i=1}^r\lambda_i p_i$$

$$\lambda_i\in\left(0,\frac{1}{2}\right], i\geq 1, \lambda_i\neq\lambda_j \text{ if } i\neq j \text{ and } \sum_{i=1}^r m_i\lambda_i<\infty$$

$$\sigma(\Gamma)=\{0,1\}\cup\{\lambda_i\}_{i=1}^r\cup\{1-\lambda_i\}_{i=1}^r$$

$$\sigma(\Gamma)=\sigma_p(\Gamma)\cup\sigma_{ess}(\Gamma)$$

$$\sigma_p(\Gamma)=\{\lambda_i\}_{i=1}^r\cup\{1-\lambda_i\}_{i=1}^r \text{ and } \sigma_{\text{ess}}\left(\Gamma\right)=\{0,1\}$$

$$U\cdot\Gamma=U\Gamma U^*, U\in\mathsf{U}_{\mathrm{Bog}}, \Gamma\in\mathcal{D}$$

$$\Gamma=\Gamma[\gamma,\alpha],\,U=\begin{pmatrix}u&v\\ \bar{v}&\bar{u}\end{pmatrix}$$

$$U\cdot\Gamma=\begin{pmatrix}u\gamma u^*+v\alpha^*u^*+u\alpha v^*+v(\mathbf{1}-\bar{\gamma})v^*&u\gamma\bar{v}^*+v\alpha^*\bar{v}^*+u\alpha\bar{u}^*+v(\mathbf{1}-\bar{\gamma})\bar{u}^*\\ \bar{v}\gamma u^*+\bar{u}\alpha^*u^*+\bar{v}\alpha v^*+\bar{u}(\mathbf{1}-\bar{\gamma})v^*&\bar{v}\gamma\bar{v}^*+\bar{u}\alpha^*\bar{v}^*+\bar{v}\alpha\bar{u}^*+\bar{u}(\mathbf{1}-\bar{\gamma})\bar{u}^*\end{pmatrix}$$

$$\mathcal{O}(\Gamma)=\{U\Gamma U^*:U\in\mathsf{U}_{\mathrm{Bog}}\}$$

$$\mathsf{U}_{\mathrm{Bog}}^\Gamma=\{U\in\mathsf{U}_{\mathrm{Bog}}\colon U\Gamma U^*=\Gamma\}$$

$$\mathfrak{u}_{\mathrm{Bog}}^\Gamma=\{X\in\mathfrak{u}_{\mathrm{Bog}}\colon e^{tX}\in\mathsf{U}_{\mathrm{Bog}}^\Gamma,\forall t\in\mathbb{R}\},$$

$$\mathfrak{u}_{\mathrm{Bog}}^\Gamma=\{X\in\mathfrak{u}_{\mathrm{Bog}}\colon X\Gamma=\Gamma X\}$$

$$(tX)^n\Gamma=\Gamma(tX)^n, n\geq 0$$

$$e^{tX}\Gamma=\Gamma e^{tX}$$

$$\exp\left(\mathcal{W}\cap\mathfrak{u}_{\mathrm{Bog}}^\Gamma\right)=\mathcal{V}\cap\mathsf{U}_{\mathrm{Bog}}^\Gamma$$

$$U=e^X\in\mathsf{U}_{\mathrm{Bog}}^\Gamma$$

$$\mathsf{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$X=\log\left(U\right)=\sum_{n\geq 1}(-1)^{n+1}\frac{(U-\mathbf{1})^n}{n}$$

$$(U-\mathbf{1})^n\Gamma=\Gamma(U-\mathbf{1})^n, n\geq 1$$

$$(U)\Gamma=\Gamma\log\left(U\right)$$

$$W\mathsf{U}_{\mathrm{Bog}}^\Gamma W^*=\mathsf{U}_{\mathrm{Bog}}^{W\Gamma W^*}$$

$$\Lambda=\sum_{i=1}^r\lambda_i p_i$$

$$\sigma(\Gamma)=\{0,1\}\cup\{\lambda_i\}_{i=1}^r\cup\{1-\lambda_i\}_{i=1}^r$$

$$X = \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}}$$

$$x_1\Lambda = \Lambda x_1, x_2(\mathbf{1} - \Lambda) = \Lambda x_2$$

$$x_1 = \sum_{i=0}^r p_i x_1 p_i$$

$$\mathfrak{u}_{\text{Bog}}^\Gamma = \left\{ \begin{pmatrix} x_1 & 0 \\ 0 & \bar{x}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}} : x_1 = \sum_{i=0}^r p_i x_1 p_i \right\},$$

$$\mathfrak{u}_{\text{Bog}}^\Gamma = \left\{ \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}} : x_1 = \sum_{i=0}^r p_i x_1 p_i, x_2 = p_1 x_2 p_1 \right\}.$$

$$\mathcal{E}_\Gamma \left(\begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \right) = \begin{cases} \begin{pmatrix} \sum_{i=0}^r p_i x_1 p_i & 0 \\ 0 & \sum_{i=0}^r p_i \bar{x}_1 p_i \end{pmatrix} & \text{if } \frac{1}{2} \notin \sigma(\Gamma), \end{cases}$$

$$\mathsf{U}_{\text{Bog}}^\Gamma = \left\{ \begin{pmatrix} u & 0 \\ 0 & \bar{u} \end{pmatrix} \in \mathsf{U}_{\text{Bog}} : u = \sum_{i=0}^r p_i u p_i \right\}$$

$$\mathsf{U}_{\text{Bog}}^\Gamma = \left\{ \begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix} \in \mathsf{U}_{\text{Bog}} : u = \sum_{i=0}^r p_i u p_i, v = p_1 v p_1 \right\}$$

$$\mathcal{E}_\Gamma \left(\begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \right) = \begin{cases} \begin{pmatrix} \sum_{i=0}^r p_i x_1 p_i & 0 \\ 0 & \sum_{i=0}^r p_i \bar{x}_1 p_i \end{pmatrix} & \text{if } \frac{1}{2} \notin \sigma(\Gamma), \end{cases}$$

$$\mathcal{E}_\Gamma^2 = \mathcal{E}_\Gamma, \text{ran}(\mathcal{E}_\Gamma) = \mathfrak{u}_{\text{Bog}}^\Gamma, \|\mathcal{E}_\Gamma\| = \sup_{\|X\|_{\text{res}}=1} \|\mathcal{E}_\Gamma(X)\|_{\text{res}} = 1, \text{ and } \mathcal{E}_\Gamma(UZU^*) = U\mathcal{E}_\Gamma(Z)U^*,$$

$$T_{\Gamma_1}\mathcal{O}(\Gamma)=\{[X,\Gamma_1]:X\in\mathfrak{u}_{\text{Bog}}\}$$

$$\|[X,\Gamma_1]\|_{\Gamma_1}:=\inf\{\|X+Y\|_{\text{res}}:Y\Gamma_1=\Gamma_1Y\}$$

$$\mathsf{U}_{\text{Bog}}^+ := \left\{ U \in \mathsf{U}_{\text{Bog}} : \text{ind}_{\mathsf{U}_{\text{Bog}}} (U) = 0 \right\}, \mathsf{U}_{\text{Bog}}^- := \left\{ U \in \mathsf{U}_{\text{Bog}} : \text{ind}_{\mathsf{U}_{\text{Bog}}} (U) = 1 \right\}$$

$$\mathcal{O}(\Gamma) = \mathsf{U}_{\text{Bog}}^+ \cdot \Gamma \cup \mathsf{U}_{\text{Bog}}^- \cdot \Gamma$$

$$\mathcal{O}(\Gamma) = \mathsf{U}_{\text{Bog}}^+ \cdot \Gamma = \mathsf{U}_{\text{Bog}}^- \cdot \Gamma$$

$$\mathcal{O}(\Gamma) \rightarrow \mathsf{U}_{\text{Bog}}/\mathsf{U}_{\text{Bog}}^{\Gamma}, W\Gamma W^* \mapsto W\mathsf{U}_{\text{Bog}}^{\Gamma}$$

$$\pi\colon \mathsf{U}_{\text{Bog}} \rightarrow \mathcal{O}(\Gamma), \pi(U) = U\Gamma U^*$$

$$T_{\Gamma_1}\mathcal{O}(\Gamma) = \text{ran}(T_U\pi) \cong \mathfrak{u}_{\text{Bog}}/\mathfrak{u}_{\text{Bog}}^{\Gamma_1} \cong \{[X,\Gamma_1]\colon X \in \mathfrak{u}_{\text{Bog}}\}$$

$$\mathfrak{m}_{\Gamma} = \ker(\mathcal{E}_{\Gamma})$$

$$\mathfrak{u}_{\text{Bog}}^{\Gamma} \oplus \mathfrak{m}_{\Gamma} = \mathfrak{u}_{\text{Bog}}$$

$$\mathcal{E}_{\Gamma}(UXU^*) = U\mathcal{E}_{\Gamma}(X)U^*$$

$$\text{Ad}_U(\mathfrak{m}_{\Gamma}) = \mathfrak{m}_{\Gamma}$$

$$\mathcal{E}_{\Gamma} = \text{Ad}_{W^*U} \circ \mathcal{E}_{\Gamma} \circ \text{Ad}_{U^*W}$$

$$U\mathfrak{m}_{\Gamma}U^* = W\mathfrak{m}_{\Gamma}W^*$$

$$\{\mathfrak{m}_{\Gamma_1}\}_{\Gamma_1 \in \mathcal{O}(\Gamma)} \mathfrak{u}_{\text{Bog}} = \mathfrak{m}_{\Gamma_1} \oplus \mathfrak{u}_{\text{Bog}}^{\Gamma_1}$$

$$\text{Ad}_U(\mathfrak{m}_{\Gamma_1}) = \mathfrak{m}_{\Gamma_1}$$

$$\text{ran}(\mathcal{E}_{\Gamma_1}) = \mathfrak{u}_{\text{Bog}}^{\Gamma_1}$$

$$\ker(\mathcal{E}_{\Gamma_1}) = \mathfrak{m}_{\Gamma_1}$$

$$\pi_{\Gamma_1}\colon \mathsf{U}_{\text{Bog}} \rightarrow \mathcal{O}(\Gamma), \pi_{\Gamma_1}(U) = U\Gamma_1U^*$$

$$\mathcal{V}_{\Gamma_1} \subseteq \mathcal{O}(\Gamma), \Gamma_1 \in \mathcal{V}_{\Gamma_1}$$

$$s_{\Gamma_1}\colon \mathcal{V}_{\Gamma_1} \rightarrow \mathsf{U}_{\text{Bog}}$$

$$\pi_{\Gamma_1} \circ s_{\Gamma_1} = \text{id}|_{\mathcal{V}_{\Gamma_1}}$$

$$F\colon \mathsf{U}_{\text{Bog}} \rightarrow \mathsf{B}(\mathfrak{u}_{\text{Bog}}), F(U) = \mathbf{1}_{\mathsf{B}(\mathfrak{u}_{\text{Bog}})} - U\mathcal{E}_{\Gamma}(U^* \cdot U)U^*$$

$$f\colon \mathcal{O}(\Gamma_1) \rightarrow \mathsf{B}(\mathfrak{u}_{\text{Bog}}), f(\Gamma') = \mathbf{1}_{\mathsf{B}(\mathfrak{u}_{\text{Bog}})} - \mathcal{E}_{\Gamma'}$$

$$\mathsf{U}_{\text{Bog}}^+ \cdot \Gamma = \{U\Gamma U^*\colon U \in \mathsf{U}_{\text{Bog}}^+\}$$

$$\pi_{\Gamma}\colon \mathsf{U}_{\text{Bog}} \rightarrow \mathcal{O}(\Gamma), \pi_{\Gamma}(U) = U\Gamma U^*$$

$$\mathsf{U}_{\text{Bog}}^+ \cdot \Gamma \mathcal{O}(\Gamma)$$

$$\delta\colon [0,1] \rightarrow \mathcal{O}(\Gamma), \delta(0) = \Gamma \text{ and } \delta(1) = \Gamma_1$$

$$\Gamma_1 \in \mathsf{U}_{\text{Bog}}^+ \cdot \Gamma$$



$$\pi_{\Gamma'}\colon \mathsf{U}_{\mathrm{Bog}} \rightarrow \mathcal{O}(\Gamma), \pi_{\Gamma'}(U) = U\Gamma'U^*$$

$$\mathcal{V}_{\Gamma'}\subseteq \mathcal{O}(\Gamma), \Gamma'\in \mathcal{V}_{\Gamma'}$$

$$s_{\Gamma'}\colon \mathcal{V}_{\Gamma'} \rightarrow \mathsf{U}_{\mathrm{Bog}}$$

$$\pi_{\Gamma'}\circ s_{\Gamma'}=\mathrm{id}|_{\mathcal{V}_{\Gamma'}}$$

$$\mathcal{V}_i\coloneqq \mathcal{V}_{\delta(t_i)}$$

$$s_i\coloneqq s_{\delta(t_i)}\text{ of }\pi_{\delta(t_i)},\,i=0,\ldots,n$$

$$\delta([0,1])\subseteq \bigcup_{i=0}^n \mathcal{V}_i$$

$$\delta(t_i)\coloneqq \Gamma^{(i)}, i=0,\ldots,n$$

$$\mathrm{ind}_{\mathrm{Bog}}\left(s_0(\Gamma)\right)=0\text{ or }\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}\left(s_0(\Gamma)\right)=1$$

$$\tilde{s}_0(\Gamma')=s_0(\Gamma')s_0(\Gamma)$$

$$\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}(\tilde{s}_0(\Gamma))=0$$

$$\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}\left(\tilde{s}_0\big(\Gamma^{(1)}\big)\right)=0$$

$$\tilde{s}_0\big(\Gamma^{(1)}\big)\Gamma\tilde{s}_0\big(\Gamma^{(1)}\big)^*=\Gamma^{(1)}$$

$$\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}\left(\tilde{s}_i\big(\Gamma^{(i+1)}\big)\right)=0$$

$$\tilde{s}_{n-1}\big(\Gamma^{(n)}\big)\ldots\tilde{s}_1\big(\Gamma^{(2)}\big)\tilde{s}_0\big(\Gamma^{(1)}\big)\Gamma\tilde{s}_0\big(\Gamma^{(1)}\big)^*\tilde{s}_1\big(\Gamma^{(2)}\big)^*\ldots\tilde{s}_{n-1}\big(\Gamma^{(n)}\big)^*=\Gamma^{(n)}=\Gamma_1$$

$$\Gamma_1\in \mathsf{U}_{\mathrm{Bog}}^+\cdot\Gamma$$

$$\mathsf{U}_{\mathrm{Bog}}^+\cdot\Gamma$$

$$\mathcal{O}(\Gamma)=\mathsf{U}_{\mathrm{Bog}}^+\cdot\Gamma\cup\mathsf{U}_{\mathrm{Bog}}^-\cdot\Gamma$$

$$\mathsf{U}_{\mathrm{Bog}}^+\cdot\Gamma\rightarrow\mathsf{U}_{\mathrm{Bog}}^-\cdot\Gamma,\,U\Gamma U^*\rightarrow R U\Gamma U^*R^*$$

$$\mathsf{U}_{\mathrm{Bog}}^+\cdot\Gamma\cap\mathsf{U}_{\mathrm{Bog}}^-\cdot\Gamma=\emptyset$$

$$W\mathsf{U}_{\mathrm{Bog}}^\pm W^*=\mathsf{U}_{\mathrm{Bog}}^\pm$$

$$P_+(V^*U)|_{\mathfrak{H}\oplus\{0\}}\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}(V^*U)$$

$$\varphi_1\in \mathrm{ran}(p_1)=\ker\left(\Lambda-\frac{1}{2}\mathbf{1}\right)\left(\lambda_1=\frac{1}{2}\right)$$



$$S((\varphi_1,0))=(0,\varphi_1), S((0,\varphi_1))=(\varphi_1,0)$$

$$\{(\varphi_i,0)\}_{i\geq 1}\cup\{(0,\varphi_j)\}_{j\geq 1}$$

$$S\Gamma S^*=\Gamma$$

$$\mathrm{U}^+_{\mathrm{Bog}}\,S=\mathrm{U}^-_{\mathrm{Bog}}\,\mathrm{ind}_{\mathrm{U}_{\mathrm{Bog}}}(S)=1$$

$$\mathrm{U}^+_{\mathrm{Bog}}\cdot\Gamma=\mathrm{U}^+_{\mathrm{Bog}}\,S\cdot\Gamma=\mathrm{U}^-_{\mathrm{Bog}}\cdot\Gamma=\mathcal{O}(\Gamma)$$

$$\mathbb{U}=\mathbb{U}_U\colon\mathfrak{F}\rightarrow\mathfrak{F}$$

$$\mathrm{U}_{\mathrm{Bog}}\times\mathcal{Z}_{\mathrm{qf}}\rightarrow\mathcal{Z}_{\mathrm{qf}},(U,\omega)\mapsto U\cdot\omega=\omega_U$$

$$\mathbb{U}_{UV}=\lambda\mathbb{U}_U\mathbb{U}_V, \text{ for } U,V\in\mathrm{U}_{\mathrm{Bog}}$$

$$\mathcal{O}(\omega)\colon=\left\{\omega_U\colon U\in\mathrm{U}_{\mathrm{Bog}}\right\}$$

$$\Phi\colon\mathcal{Z}_{\mathrm{qf}}\rightarrow\mathcal{D},\Phi(\omega)=\Gamma_\omega$$

$$\Gamma_{\omega_U}=\Phi(\omega_U)=U^*\Gamma_\omega U$$

$$\{U\in\mathrm{U}_{\mathrm{Bog}}\colon\omega_U=\omega\}=\{U\in\mathrm{U}_{\mathrm{Bog}}\colon U\Gamma_\omega=\Gamma_\omega U\}=\mathrm{U}_{\mathrm{Bog}}^{\Gamma_\omega}$$

$$\mathcal{O}(\omega)\cong \mathrm{U}_{\mathrm{Bog}}/\mathrm{U}_{\mathrm{Bog}}^{\Gamma_\omega}$$

$$\Phi\colon\mathcal{O}(\omega)\rightarrow\mathcal{O}(\Gamma_\omega)$$

$$\mathrm{U}_{\mathrm{Bog}}/\mathrm{U}_{\mathrm{Bog}}^{\Gamma_\omega}$$

$$\phi^{-1}=\pi_\omega\circ\exp$$

$$\pi_\omega\colon\mathrm{U}_{\mathrm{Bog}}\rightarrow\mathcal{O}(\omega),\pi_\omega(U)=\omega_U$$

$$\mathcal{W}\subseteq\mathcal{O}(\omega),\omega\in\mathcal{W},\text{ and }\phi(\mathcal{W})$$

$$\mathfrak{m}_{\Gamma_\omega}\cong \mathfrak{u}_{\mathrm{Bog}}/\mathfrak{u}_{\mathrm{Bog}}^{\Gamma_\omega}$$

$$\psi^{-1}=\pi_{\Gamma_\omega}\circ\exp$$

$$(\psi\circ\Phi\circ\phi^{-1})(X)=(\psi\circ\Phi)(\omega_{e^X})=\psi(e^{-X}\Gamma e^X)=-X$$

$$P_-=\begin{pmatrix}0&0\\0&1\end{pmatrix}\omega_-(A)=\langle\Omega,A\Omega\rangle,A\in\mathrm{B}(\mathfrak{F})$$

$$\mathcal{O}(P_-)=\left\{U\begin{pmatrix}0&0\\0&1\end{pmatrix}U^*\colon U\in\mathrm{U}_{\mathrm{Bog}}\right\}$$

$$\mathrm{O}_{\mathrm{res}}\left(\mathfrak{H}^{\mathbb{R}}\right)\mathcal{C}(W)=W^{\perp}(\mathfrak{H}^{\mathbb{R}},\mathfrak{H}_{\mathbb{C}}^{-})$$

$$\mathcal{I}_{\mathrm{res}}:=\{W\colon W\text{ is maximal isotropic, }P_W-P_{\mathfrak{H}_{\mathbb{C}}}\in\mathrm{B}_2(\mathfrak{H}_{\mathbb{C}})\}.$$



$$\mathcal{O}(P_-) \rightarrow \mathcal{I}_{\text{res}}, UP_-U^* \mapsto \text{Ad}_T(U)(\mathfrak{H}_{\mathbb{C}}^-)$$

$$[X,P_-], \text{ for } X=\begin{pmatrix} 0 & y \\ \bar{y} & 0 \end{pmatrix} \in \mathfrak{m}_{P_-}, y=-y^T \in \text{B}_2(\mathfrak{H})$$

$$\delta(t)=e^{tX}P_-e^{-tX}=\begin{pmatrix} \cos(|ty^*|) & ts\text{inc}(|ty|) \\ ty^*\text{sinc}(|ty^*|) & \cos(|ty|) \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1} \end{pmatrix}\begin{pmatrix} \cos(|ty^*|) & t\text{sinc}(|ty^*|)y \\ t\text{sinc}(|ty|)y^* & \cos(|ty|) \end{pmatrix}.$$

$$i\mathfrak{u}_{\text{Bog}}=\left\{\begin{pmatrix} x_1 & x_2 \\ -\bar{x}_2 & -\bar{x}_1 \end{pmatrix}\in \text{B}(\mathfrak{H}\oplus\mathfrak{H})\colon x_1=x_1^*, x_2=-x_2^T\in \text{B}_2(\mathfrak{H})\right\}\subseteq \text{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\|X\|_{\text{res}}=2\text{max}\{\|x_1\|,\|x_2\|_2\}$$

$$\Gamma=\Gamma[\gamma,\alpha]\in\mathcal{D}$$

$$\Gamma=\begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbf{1}-\bar{\gamma} \end{pmatrix}=\begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & -\bar{\gamma} \end{pmatrix}+\begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1} \end{pmatrix}:=\Gamma_0+P_-, \Gamma_0\in i\mathfrak{u}_{\text{Bog}},$$

$$\mathcal{O}(\Gamma)\subseteq i\mathfrak{u}_{\text{Bog}}+P_-$$

$$T_\Gamma\mathcal{O}(\Gamma)=\{X\Gamma-\Gamma X\colon X\in\mathfrak{u}_{\text{Bog}}\}\subseteq i\mathfrak{u}_{\text{Bog}}$$

$$\delta_\Gamma\colon \mathfrak{u}_{\text{Bog}}\rightarrow \mathfrak{u}_{\text{Bog}}, \delta_\Gamma(X)=[i\Gamma,X]$$

$$\Gamma=\Gamma_0+P_-, \Gamma_0\in i\mathfrak{u}_{\text{Bog}}$$

$$[i\Gamma,X]=[i\Gamma_0,X]+[iP_-,X]\in\mathfrak{u}_{\text{Bog}}$$

$$\text{iran}(\delta_\Gamma)=T_\Gamma\mathcal{O}(\Gamma)$$

$$E=\ker(T)\oplus\mathcal{M}$$

$$\text{ran}(\mathcal{E})=\ker(T) \text{ and } \ker(\mathcal{E})=\mathcal{M}$$

$$\|Te\|\geq c\|e-\mathcal{E}e\|, \text{ for all } e\in E$$

$$T_0\mathrel{\mathop:}=T|_{\mathcal{M}}\colon\mathcal{M}\rightarrow\text{ran}(T)$$

$$\|Te\|=\|T_0(e-\mathcal{E}e)\|\geq \|T_0\|^{-1}\|e-\mathcal{E}e\|$$

$$\|Te_n - Te_m\| \geq \|T((e_n - e_m) - \mathcal{E}(e_n - e_m))\| \geq c\|e_n - \mathcal{E}e_n - (e_m - \mathcal{E}e_m)\|$$

$$Te_n=T(e_n-\mathcal{E}e_n)$$

$$i\mathfrak{u}_{\text{Bog}}=i\mathfrak{u}_{\text{Bog}}^\Gamma\oplus T_\Gamma\mathcal{O}(\Gamma)$$

$$\sigma(\Gamma)=\sigma(\Lambda)\cup\sigma(\mathbf{1}-\Lambda)=\{\lambda_k\colon k=0,\ldots,r\}\cup\{1-\lambda_k\colon k=0,\ldots,r\}$$

$$X=\begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}}$$

$$[i\Lambda,x_1]=\sum_{i,j=0}^ri\big(\lambda_i-\lambda_j\big)p_ix_1p_j,i\Lambda x_2-x_2i(\mathbf{1}-\Lambda)=\sum_{i,j=0}^ri\big(\lambda_i+\lambda_j-1\big)p_ix_2p_j$$



$$\frac{1}{2} \in \sigma(\Gamma), p_1(\Lambda x_2 - x_2(\mathbf{1} - \Lambda))p_1 = \frac{1}{2} \notin \sigma(\Gamma)$$

$$\text{ran}(\delta_\Gamma) = \left\{ \begin{pmatrix} \sum_{\substack{i,j=0 \\ i \neq j}}^r p_j x_1 p_i & x_2 \\ \bar{x}_2 & \sum_{\substack{i,j=0 \\ i \neq j}}^r p_j \bar{x}_1 p_i \end{pmatrix} : x_1 = -x_1^* \in B(\mathfrak{H}), x_2 = -x_2^T \in B_2(\mathfrak{H}) \right\}.$$

$$\text{ran}(\delta_\Gamma) = \left\{ \begin{pmatrix} \sum_{\substack{i,j=0 \\ i \neq j}}^r p_j x_1 p_i & \sum_{\substack{i,j=0 \\ (i,j) \neq (1,1)}}^r p_j x_2 p_i \\ \sum_{\substack{i,j=0 \\ (r,j) \neq (1,1)}}^r p_j \bar{x}_2 p_i & \sum_{\substack{i,j=0 \\ i \neq j}}^r p_j \bar{x}_1 p_i \end{pmatrix} : x_1 = -x_1^* \in B(\mathfrak{H}), x_2 = -x_2^T \in B_2(\mathfrak{H}) \right\}.$$

$$\|\delta_\Gamma(X)\|_{\text{res}} \geq c\|X - \mathcal{E}_\Gamma(X)\|_{\text{res}}, X \in \mathfrak{u}_{\text{Bog}}.$$

$$\text{ran}(\mathcal{E}_\Gamma) = \ker(\delta_\Gamma) = \mathfrak{u}_{\text{Bog}}^\Gamma$$

$$\delta_\Lambda^{\text{sk}}\colon=\delta_\Lambda|_{\text{B}(\mathfrak{H})_{\text{sk}}}\colon\text{B}(\mathfrak{H})_{\text{sk}}\rightarrow\text{B}(\mathfrak{H})_{\text{sk}},\,\delta_\Lambda^{\text{sk}}(x)=[i\Lambda,x]$$

$$X=\text{diag}(x,\bar{x}), x^*=-x$$

$$\|\delta_\Lambda^{\text{sk}}(x)\|\geq c\|x-\mathcal{E}_\Lambda(x)\|$$

$$\text{ran}(\mathcal{E}_\Lambda)=\ker(\delta_\Lambda^{\text{sk}})$$

$$\ker(\mathcal{E}_\Lambda) = (\mathfrak{m}_\Lambda)_{\text{sk}}\colon=\left\{x\in \text{B}(\mathfrak{H})_{\text{sk}}\colon x=x-\sum_{i=0}^r p_i x_1 p_i\right\}\ker(\delta_\Lambda^{\text{sk}})$$

$$\delta_\Lambda\colon\text{B}(\mathfrak{H})\rightarrow\text{B}(\mathfrak{H}),\,\delta_\Lambda(x)=[i\Lambda,x]$$

$$\text{ran}(\delta_\Gamma) = \ker(\mathcal{E}_\Gamma)$$

$$\mathfrak{u}_{\text{Bog}} = \text{ran}(\mathcal{E}_\Gamma) \oplus \ker(\mathcal{E}_\Gamma) = \mathfrak{u}_{\text{Bog}}^\Gamma \oplus \text{ran}(\delta_\Gamma)$$

$$i\mathfrak{u}_{\text{Bog}}=i\mathfrak{u}_{\text{Bog}}^\Gamma\oplus T_\Gamma\mathcal{O}(\Gamma)$$

$$\mathcal{O}(\Gamma)\subseteq i\mathfrak{u}_{\text{Bog}}+P_-$$

$$d(\Gamma_0,\Gamma_1)=\|\Gamma_0-\Gamma_1\|_{\text{res}}$$

$$\mathcal{O}(\Gamma) \cong \mathfrak{U}_{\text{Bog}}/\mathfrak{U}_{\text{Bog}}^\Gamma$$

$$\pi_\Gamma\colon \mathfrak{U}_{\text{Bog}} \rightarrow \mathcal{O}(\Gamma), \pi_\Gamma(U) = U\Gamma U^*$$

$$\pi_\Gamma\colon \mathfrak{U}_{\text{Bog}} \rightarrow \mathcal{O}(\Gamma), \pi_\Gamma(U) = U\Gamma U^*$$

$$\tilde{\delta}_{\Gamma}: B_2(\mathfrak{H} \oplus \mathfrak{H}, D) \rightarrow B_2(\mathfrak{H} \oplus \mathfrak{H}, D), \tilde{\delta}_{\Gamma}(X) = [i\Gamma, X].$$

$$B_2(\mathfrak{H} \oplus \mathfrak{H}, D)$$

$$\tilde{\mathcal{E}}_{\Gamma}: B_2(\mathfrak{H} \oplus \mathfrak{H}, D) \rightarrow B_2(\mathfrak{H} \oplus \mathfrak{H}, D), \quad \tilde{\mathcal{E}}_{\Gamma} \left(\begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \right) = \begin{cases} \begin{pmatrix} \left(\sum_{i=0}^r p_i x_{11} p_i & 0 \\ 0 & \sum_{i=0}^r p_i x_{22} p_i \end{pmatrix} \end{cases}$$

$$\begin{pmatrix} \sum_{i=0}^r p_i x_{11} p_i & p_1 x_{12} p_1 \\ p_1 x_{21} p_1 & \sum_{i=0}^r p_i x_{22} p_i \end{pmatrix} \quad \text{if } \frac{1}{2} \notin \sigma(\Gamma),$$

$$\tilde{\mathfrak{m}}_{\Gamma} = \ker(\tilde{\mathcal{E}}_{\Gamma})$$

$$B(\mathfrak{H} \oplus \mathfrak{H})$$

$$\mathfrak{m}_{\Gamma}^0 = \ker(\delta_{\Gamma}^0)$$

$$X \in B_2(\mathfrak{H} \oplus \mathfrak{H}, D)$$

$$\|\tilde{\delta}_{\Gamma}(X)\|_{\text{res}} \geq \tilde{c}_{\Gamma} \|X - \tilde{\mathcal{E}}_{\Gamma}(X)\|_{\text{res}}$$

$$\tilde{c}_{\Gamma} = \begin{cases} \min \left\{ \left(\sum_{i \neq j} |\lambda_i - \lambda_j|^{-1} \right)^{-1}, \left(\sum_{i,j=0}^r |\lambda_i + \lambda_j - 1|^{-1} \right)^{-1} \right\} & \text{if } \frac{1}{2} \notin \sigma(\Gamma), \\ \min \left\{ \left(\sum_{i \neq j} |\lambda_i - \lambda_j|^{-1} \right)^{-1}, \left(\sum_{i,j=0, (i,j) \neq (1,1)}^r |\lambda_i + \lambda_j - 1|^{-1} \right)^{-1} \right\} & \text{if } \frac{1}{2} \in \sigma(\Gamma). \end{cases}$$

$$X \in B(\mathfrak{H} \oplus \mathfrak{H})$$

$$\|\delta_{\Gamma}^0(X)\| \geq \tilde{c}_{\Gamma}^0 \|X - \tilde{\mathcal{E}}_{\Gamma}^0(X)\|$$

$$c_{\Gamma}^0 = \begin{cases} \left(\frac{1}{2} \left(\sum_{i \neq j} |\lambda_i - \lambda_j|^{-1} + \sum_{i,j=0}^r |\lambda_i + \lambda_j - 1|^{-1} \right) \right)^{-1} & \text{if } \frac{1}{2} \notin \sigma(\Gamma), \\ \left(\frac{1}{2} \left(\sum_{i \neq j} |\lambda_i - \lambda_j|^{-1} + \sum_{i,j=0, (i,j) \neq (1,1)}^r |\lambda_i + \lambda_j - 1|^{-1} \right) \right)^{-1} & \text{if } \frac{1}{2} \in \sigma(\Gamma). \end{cases}$$

$$X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \in B_2(\mathfrak{H} \oplus \mathfrak{H}, D)$$

$$[i\Lambda, x_{11}] = \sum_{i,j=0}^r i(\lambda_i - \lambda_j) p_i x_{11} p_j, i\Lambda x_{12} - x_{12} i(\mathbf{1} - \Lambda) = \sum_{i,j=0}^r i(\lambda_i + \lambda_j - 1) p_i x_{12} p_j$$

$$i(\mathbf{1} - \Lambda) x_{21} - x_{21} i\Lambda = \sum_{i,j=0}^r i(1 - \lambda_i - \lambda_j) p_j x_{21} p_i, [i(\mathbf{1} - \Lambda), x_{22}] = \sum_{i,j=0}^r i(\lambda_j - \lambda_i) p_i x_{22} p_j$$

$$A_x = - \sum_{\substack{i,j=0 \\ i \neq j}}^r i(\lambda_i - \lambda_j)^{-1} p_i x p_j, B_x = - \sum_{i,j=0}^r i(\lambda_i + \lambda_j - 1)^{-1} p_i x p_j$$

$$B_x = - \sum_{\substack{i,j=0 \\ (i,j) \neq (1,1)}}^r i(\lambda_i + \lambda_j - 1)^{-1} p_i x p_j$$

$$\beta_\Gamma\colon \mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)\rightarrow \mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\beta_\Gamma\left(\begin{pmatrix}x_{11}&x_{12}\\x_{21}&x_{22}\end{pmatrix}\right)=\begin{pmatrix}A_{x_{11}}&B_{x_{12}}\\-B_{x_{21}}&-A_{x_{22}}\end{pmatrix}$$

$$\beta_\Gamma\circ\tilde{\delta}_\Gamma=\tilde{\delta}_\Gamma\circ\beta_\Gamma=\mathbf{1}-\tilde{\mathcal{E}}_\Gamma(\text{here }\mathbf{1}=\mathbf{1}_{\mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)})$$

$$\|X-\tilde{\mathcal{E}}_\Gamma(X)\|_{\mathrm{res}}=\|(\beta_\Gamma\circ\tilde{\delta}_\Gamma)(X)\|_{\mathrm{res}}\leq\|\beta_\Gamma\|\|\tilde{\delta}_\Gamma(X)\|_{\mathrm{res}}$$

$$\|\tilde{\delta}_\Gamma(X)\|_{\mathrm{res}}\geq\|\beta_\Gamma\|^{-1}\|X-\tilde{\mathcal{E}}_\Gamma(X)\|_{\mathrm{res}}$$

$$\|\beta_\Gamma\|\leq \max\left\{\sum_{i\neq j}|\lambda_i-\lambda_j|^{-1},\sum_{i,j=0}^r|\lambda_i+\lambda_j-1|^{-1}\right\}$$

$$\tilde{c}_\Gamma=\min\left\{\left(\sum_{i\neq j}|\lambda_i-\lambda_j|^{-1}\right)^{-1},\left(\sum_{i,j=0}^r|\lambda_i+\lambda_j-1|^{-1}\right)^{-1}\right\}$$

$$\sum_{i,j=0,(i,j)\neq(1,1)}^r|\lambda_i+\lambda_j-1|^{-1}\sum_{i,j=0}^r|\lambda_i+\lambda_j-1|^{-1}$$

$$\|U\Gamma U^*-\Gamma\|_{\mathrm{res}}\leq \frac{c_\Gamma^0}{3}$$

$$U=\begin{pmatrix}u&v\\ \bar{v}&\bar{u}\end{pmatrix}, U\Gamma U^*=\begin{pmatrix}*&u\Lambda\bar{v}^*+v(\mathbf{1}-\Lambda)\bar{u}^*\\ *&*\end{pmatrix}$$

$$\Lambda=\sum_{i=0}^r\lambda_i p_i$$

$$\sum_{i=0}^r p_i = \mathbf{1}$$

$$v = p_0 v p_0 + (\mathbf{1} - p_0) v p_0 + v(\mathbf{1} - p_0)$$

$$\|U\Gamma U^* - \Gamma\|_{\text{res}} \leq \frac{c_\Gamma^0}{3}$$

$$\|u\Lambda\bar{v}^* + v(\mathbf{1} - \Lambda)\bar{u}^*\|_2 \leq \frac{c_\Gamma^0}{6}$$

$$\begin{aligned} \|p_0 v p_0 \bar{u}^*\|_2 &\leq \frac{c_\Gamma^0}{6} + \|u\Lambda\bar{v}^*\|_2 + \|v\Lambda\bar{u}^*\|_2 + \|(\mathbf{1} - p_0) v p_0 + v(\mathbf{1} - p_0)\bar{u}^*\|_2 \\ &\leq \frac{c_\Gamma^0}{6} + \|u\| \|\bar{v}^*\| \|\Lambda\|_2 + \|v\| \|\bar{u}^*\| \|\Lambda\|_2 + \|(\mathbf{1} - p_0)\|_2 \|v p_0\| + \|v\| \|(\mathbf{1} - p_0)\|_2 \|\bar{u}^*\| \\ &\leq \frac{c_\Gamma^0}{6} + 2\|\Lambda\|_2 + 2\|\mathbf{1} - p_0\|_2 =: C_1 \end{aligned}$$

$$\begin{aligned} \|p_0 v p_0 \bar{u}^*\|_2^2 &= \|\bar{u} p_0 v^* p_0\|_2^2 = \text{Tr}(p_0 v p_0 \bar{u}^* \bar{u} p_0 v^* p_0) \\ &= \text{Tr}(p_0 v p_0 (\mathbf{1} - \bar{v}^* \bar{v}) p_0 v^* p_0) \geq (1 - \|p_0 \bar{v}^* \bar{v} p_0\|) \|p_0 v p_0\|_2^2 \end{aligned}$$

$$(1 - \|p_0 \bar{v}^* \bar{v} p_0\|) \|p_0 v p_0\|_2^2 \leq \|p_0 v p_0 \bar{u}^*\|_2^2 \leq C_1^2$$

$$\|p_0 \bar{v}^* \bar{v} p_0\| = \|p_0 v^* v p_0\| \leq C < 1$$

$$\|p_0 v p_0\|_2 \leq (1 - C^2)^{-1/2} C_1$$

$$\begin{aligned} \|X\| &\leq \|P_+ X P_+\| + \|P_+ X P_-\| + \|P_- X P_+\| + \|P_- X P_-\| \\ &\leq \|P_+ X P_+\| + \|P_+ X P_-\|_2 + \|P_- X P_+\|_2 + \|P_- X P_-\| \leq 2\|X\|_{\text{res}}. \end{aligned}$$

$$\begin{aligned} \|v p_0\| \leq \|v\| &= \|P_+(U - \mathcal{E}_\Gamma^0(U))P_-\| \leq \|U - \mathcal{E}_\Gamma^0(U)\| \leq (c_\Gamma^0)^{-1} \|\delta_\Gamma^0(U)\| \\ &= (c_\Gamma^0)^{-1} \|U\Gamma U^* - \Gamma\| \leq 2(c_\Gamma^0)^{-1} \|U\Gamma U^* - \Gamma\|_{\text{res}} \leq \frac{2}{3} \end{aligned}$$

$$P_+(U - \mathcal{E}_\Gamma^0(U))P_- = v - p_1 v p_1$$

$$\|v p_0\| = \|(v - p_1 v p_1) p_0\| \leq \|v - p_1 v p_1\| = \|P_+(U - \mathcal{E}_\Gamma^0(U))P_-\| \leq \frac{2}{3}$$

$$\|p_0 v^* v p_0\| = \|v p_0\|^2 < \frac{4}{9}$$

$$\|p_0 v p_0\|_2 \leq \frac{9}{\sqrt{65}} C_1$$

$$\|v\|_2 = \|p_0 v p_0 + (\mathbf{1} - p_0) v p_0 + v(\mathbf{1} - p_0)\|_2 \leq \frac{9}{\sqrt{65}} C_1 + 2\|\mathbf{1} - p_0\|_2 =: K$$

$$\delta_\Gamma\colon \mathfrak{u}_{\text{Bog}} \rightarrow \mathfrak{u}_{\text{Bog}}, \delta_\Gamma(X) = [i\Gamma, X]$$

$$\|X_n\|_{\text{res}} = \|\delta_\Gamma(X_n)\|_{\text{res}} \leq 1/n$$

$$e^Z \Gamma e^{-Z} = \text{Ad}_{e^Z}(\Gamma) = e^{\delta_Z}(\Gamma) = (\mathbf{1}_{\mathbf{B}(\mathfrak{g} \oplus \mathfrak{h})} + \delta_Z + \delta_Z^2/2 + \delta_Z^3/3! + \cdots)(\Gamma)$$

$$\delta_Z(X) = [iZ, X] \|\delta_{X_n}\| \leq 2$$



$$\begin{aligned}\|e^{X_n}\Gamma e^{-X_n}-\Gamma\|_{\text{res}} &= \|e^{\delta_{X_n}}(\Gamma)-\Gamma\|_{\text{res}}\leq \sum_{k=1}^{\infty}\frac{\|\delta_{X_n}^k(\Gamma)\|_{\text{res}}}{k!}\\ &\leq \sum_{k=1}^{\infty}\frac{\|\delta_{X_n}\|^{k-1}\|\delta_{\Gamma}(X_n)\|_{\text{res}}}{k!}\leq \frac{1}{n}\sum_{k=1}^{\infty}\frac{2^{k-1}}{k!}\leq \frac{e^2}{n}.\end{aligned}$$

$$\phi\colon \mathcal{V}_\Gamma\rightarrow \mathcal{W}_\Gamma, \phi(Z)=e^Z\Gamma e^{-Z}$$

$$\pi_\Gamma\colon \mathsf{U}_{\text{Bog}}\rightarrow \mathcal{O}(\Gamma), \pi_\Gamma(U)=U\Gamma U^*$$

$$\Omega(G)=G|G|^{-1}$$

$$r_\Gamma\!:=\frac{1}{2}\min\!\left\{\frac{c_\Gamma^0}{3},K^{-2}\tilde{c}_\Gamma\right\}$$

$$s\colon \{U\Gamma U^*\in \mathcal{O}(\Gamma)\colon \|U\Gamma U^*-\Gamma\|_{\text{res}}< r_\Gamma\}\rightarrow \mathsf{U}_{\text{Bog}}, s(U\Gamma U^*)=U\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right).$$

$$U\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)\in \mathsf{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\|U\Gamma U^*-\Gamma\|_{\text{res}}< r_\Gamma, \text{ then } \tilde{\mathcal{E}}_\Gamma(U^*)$$

$$\mathsf{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\|U^*\|_{\text{res}}\leq K\mathbf{1}=\mathbf{1}_{\mathfrak{H}\oplus\mathfrak{H}}$$

$$\begin{aligned}\|\mathbf{1}-U\tilde{\mathcal{E}}_\Gamma(U^*)\|_{\text{res}} &\leq \|U\|_{\text{res}}\|U^*-\tilde{\mathcal{E}}_\Gamma(U^*)\|_{\text{res}}\leq K\tilde{c}_\Gamma^{-1}\|\tilde{\delta}_\Gamma(U^*)\|_{\text{res}}\\ &\leq K\tilde{c}_\Gamma^{-1}\|U^*\|_{\text{res}}\|U\Gamma U^*-\Gamma\|_{\text{res}}\leq K^2\tilde{c}_\Gamma^{-1}\|U\Gamma U^*-\Gamma\|_{\text{res}}<1\end{aligned}$$

$$\begin{aligned}s(U\Gamma U^*) &= U\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)=U\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*VV^*)\right)=U\Omega\left(U^*V\tilde{\mathcal{E}}_\Gamma(V^*)\right)\\ &=UU^*V\Omega\left(\tilde{\mathcal{E}}_\Gamma(V^*)\right)=V\Omega\left(\tilde{\mathcal{E}}_\Gamma(V^*)\right)=s(V\Gamma V^*)\end{aligned}$$

$$\tilde{\mathcal{E}}_\Gamma(ZX)=Z\tilde{\mathcal{E}}_\Gamma(X)$$

$$X,Z\in \mathsf{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\tilde{\mathcal{E}}_\Gamma,\tilde{\mathcal{E}}_\Gamma(U^*)I=I\tilde{\mathcal{E}}_\Gamma(U^*)$$

$$\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)I=I\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)$$

$$\mathsf{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)\in \mathsf{B}_2(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\mathsf{B}_2(\mathfrak{H}\oplus\mathfrak{H})$$

$$\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)\in \mathsf{U}_{\text{Bog}}$$

$$s(U\Gamma U^*)\in \mathsf{U}_{\text{Bog}}$$



$$\Gamma_1=U\Gamma U^*$$

$$\tilde{\mathcal{E}}_\Gamma(U^*)\Gamma=\Gamma\tilde{\mathcal{E}}_\Gamma(U^*)$$

$$\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)\Gamma=\Gamma\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)$$

$$s(\Gamma_1)\Gamma s(\Gamma_1)^*=U\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)\Gamma\Omega\left(\tilde{\mathcal{E}}_\Gamma(U^*)\right)^*U^*=U\Gamma U^*=\Gamma_1$$

$$\{U_n\Gamma U_n^*\}_{n\geq 1}\|U_n\Gamma U_n^*-\Gamma\|_{\mathrm{res}}\rightarrow 0$$

$$\left\|\mathbf{1}-U_n\tilde{\mathcal{E}}_\Gamma(U_n^*)\right\|_{\mathrm{res}}\leq K^2c_\Gamma^{-1}\|U_n\Gamma U_n^*-\Gamma\|_{\mathrm{res}}\rightarrow 0$$

$$\Omega(G)=G|G|^{-1}$$

$$\mathrm{B}_2(\mathfrak{H}\oplus\mathfrak{H})$$

$$s(U_n\Gamma U_n^*)=U_n\Omega\left(\tilde{\mathcal{E}}_\Gamma(U_n^*)\right)=\Omega(U_n\mathcal{E}_\Gamma(U_n^*))\rightarrow\Omega(\mathbf{1})=\mathbf{1}=s(\Gamma)$$

$$s_{\Gamma_1}=\mathrm{Ad}_U\circ s_\Gamma\circ \mathrm{Ad}_{U^*}\Gamma_1=U\Gamma U^*$$

$$\mathfrak{g}=\mathfrak{gl}_2(\mathfrak{H}\oplus\mathfrak{H},I,D)$$

$$H_c^2(\mathfrak{g},\mathbb{C})\cong\mathbb{C}$$

$$\mathfrak{g}_{\mathbb{R}}=\{X\in\mathfrak{g}:X^*=-X\}=\mathfrak{u}_{\mathrm{Bog}}$$

$$H_c^2\big(\mathfrak{u}_{\mathrm{Bog}}\,,\,\mathbb{R}\big)\cong\mathbb{R}$$

$$s_+(X,Y)\!:=\!\mathrm{Tr}(X[iP_+,Y]), X,Y\in\mathfrak{u}_{\mathrm{Bog}}\,.$$

$$s_+\left(\begin{pmatrix}x_1&x_2\\ \bar{x}_2&\bar{x}_1\end{pmatrix},\begin{pmatrix}y_1&y_2\\ \bar{y}_2&\bar{y}_1\end{pmatrix}\right)=2\Im\mathrm{Tr}(x_2\bar{y}_2).$$

$$\alpha\colon \mathfrak{o}_{\mathrm{res}}\left(\mathfrak{H}^{\mathbb{R}}\right)\times \mathfrak{o}_{\mathrm{res}}\left(\mathfrak{H}^{\mathbb{R}}\right)\rightarrow \mathbb{R}, \alpha(A,B)=\mathrm{Tr}([A_a,B_a]J_0)=2\mathrm{Tr}(A_aB_aJ_0),$$

$$(d\Xi)_1\colon \mathfrak{o}_{\mathrm{res}}\left(\mathfrak{H}^{\mathbb{R}}\right)\rightarrow \mathfrak{u}_{\mathrm{Bog}}\,(d\Xi)_1(A)=T^{-1}A_{\mathbb{C}}T$$

$$(\Xi_*\alpha)(X,Y)\!:=\!\alpha\big((d\Xi)_1^{-1}(X),(d\Xi)_1^{-1}(Y)\big).$$

$$(\Xi_*\alpha)\left(\begin{pmatrix}x_1&x_2\\ \bar{x}_2&\bar{x}_1\end{pmatrix},\begin{pmatrix}y_1&y_2\\ \bar{y}_2&\bar{y}_1\end{pmatrix}\right)=-4\Im\mathrm{Tr}(x_2\bar{y}_2).$$

$$\mathrm{B}_{1,2}(\mathfrak{H}\oplus\mathfrak{H},D)\!:=\!\left\{\begin{pmatrix}x_{11}&x_{12}\\ x_{21}&x_{22}\end{pmatrix}\in\mathrm{B}(\mathfrak{H}\oplus\mathfrak{H})\!:\!x_{11},x_{22}\in\mathrm{B}_1(\mathfrak{H}),x_{12},x_{21}\in\mathrm{B}_2(\mathfrak{H})\right\},$$

$$\|X\|_{1,2}\!:=\!2\max\{\|x_{11}\|_1,\|x_{22}\|_1,\|x_{12}\|_2,\|x_{21}\|_2\}.$$

$$\begin{aligned} \left(\mathfrak{u}_{\mathrm{Bog}}\right)_* &:= \mathfrak{u}_{\mathrm{Bog}}\cap \mathrm{B}_{1,2}(\mathfrak{H}\oplus\mathfrak{H},D) \\ &= \left\{\begin{pmatrix}x_1&x_2\\ \bar{x}_2&\bar{x}_1\end{pmatrix}\!:\!x_1^*=-x_1\in\mathrm{B}_1(\mathfrak{H}),x_2^T=-x_2\in\mathrm{B}_2(\mathfrak{H})\right\}. \end{aligned}$$



$$\langle \cdot, \cdot \rangle: (\mathfrak{u}_{\text{Bog}})_* \times \mathfrak{u}_{\text{Bog}} \rightarrow \mathbb{R}, \langle X, Y \rangle := \Re \text{Tr}(XY)$$

$$\left((\mathfrak{u}_{\text{Bog}})_* \right)^* \cong \mathfrak{u}_{\text{Bog}}$$

$$\mathfrak{u}_{\text{res}} := \left\{ \begin{pmatrix} x_{11} & x_{12} \\ -x_{12}^* & x_{22} \end{pmatrix} \in \text{B}(\mathfrak{H} \oplus \mathfrak{H}) : x_{11} = -x_{11}^*, x_{22} = -x_{22}^*, x_{12} \in \text{B}_2(\mathfrak{H}) \right\}$$

$$(\mathfrak{u}_{\text{res}})_* := \left\{ \begin{pmatrix} x_{11} & x_{12} \\ -x_{12}^* & x_{22} \end{pmatrix} \in \text{B}(\mathfrak{H} \oplus \mathfrak{H}) : x_{11} = -x_{11}^* \in \text{B}_1(\mathfrak{H}), x_{22} = -x_{22}^* \in \text{B}_1(\mathfrak{H}), x_{12} \in \text{B}_2(\mathfrak{H}) \right\}$$

$$((\mathfrak{u}_{\text{res}})_*)^* \cong \mathfrak{u}_{\text{res}}$$

$$\langle X, Y \rangle = \text{Tr}(XY) = \Re \text{Tr}(XY)$$

$$\left((\mathfrak{u}_{\text{Bog}})_* \right)^* \cong \mathfrak{u}_{\text{Bog}} \quad f \in \left((\mathfrak{u}_{\text{Bog}})_* \right)^*$$

$$f(X) = \Re \text{Tr}(XY)$$

$$X \in (\mathfrak{u}_{\text{Bog}})_*$$

$$X \in (\mathfrak{u}_{\text{Bog}})_*$$

$$f(X) = f(IXI) = \Re \text{Tr}((IXI)Y) = \Re \text{Tr}(X(IYI))$$

$$f(X) = f\left(\frac{X+IXI}{2}\right) = \Re \text{Tr}\left(X\left(\frac{Y+IYI}{2}\right)\right), \text{ where } \frac{Y+IYI}{2} \in \mathfrak{u}_{\text{Bog}}$$

$$s_{\Gamma}(X, Y) := \text{Tr}(X[i\Gamma, Y]) = \text{Tr}(X\delta_{\Gamma}(Y)).$$

$$X = \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}}, Y = \begin{pmatrix} y_1 & y_2 \\ \bar{y}_2 & \bar{y}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}}, \Gamma = \Gamma[\gamma, \alpha]$$

$$[\Gamma, Y] = \begin{pmatrix} [\gamma, y_1] + \alpha \bar{y}_2 - y_2 \alpha^* & \gamma y_2 - y_2 (\mathbf{1} - \bar{\gamma}) + \alpha \bar{y}_1 - y_1 \alpha \\ \alpha^* y_1 - \bar{y}_1 \alpha^* + (\mathbf{1} - \bar{\gamma}) \bar{y}_2 - \bar{y}_2 \gamma & \alpha^* y_2 - \bar{y}_2 \alpha + [\mathbf{1} - \bar{\gamma}, \bar{y}_1] \end{pmatrix} := \begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & -\bar{z}_1 \end{pmatrix}$$

$$z_1 \in \text{B}_1(\mathfrak{H}), z_2 \in \text{B}_2(\mathfrak{H}).$$

$$\begin{aligned} s_{\Gamma}(X, Y) &= i(\text{Tr}(x_1 z_1) - \text{Tr}(\bar{x}_1 \bar{z}_1)) + i(\text{Tr}(\bar{x}_2 z_2) - \text{Tr}(x_2 \bar{z}_2)) \\ &= -2\Im(\text{Tr}(x_1 z_1) + \text{Tr}(\bar{x}_2 z_2)) < \infty \end{aligned}$$

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & -\bar{\gamma} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1} \end{pmatrix} =: \Gamma_0 + P_-$$

$$s_{\Gamma}(X, Y) = \text{Tr}(X[i\Gamma_0, Y]) + \text{Tr}(X[iP_-, Y]) =: s_{\Gamma_0}(X, Y) + s_-(X, Y)$$



$$\begin{aligned}
|s_{\Gamma_0}(X, Y)| &= \left| \text{Tr} \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \begin{pmatrix} [\gamma, y_1] + \alpha \bar{y}_2 - y_2 \alpha^* & \gamma y_2 + y_2 \bar{\gamma} + \alpha \bar{y}_1 - y_1 \alpha \\ \alpha^* y_1 - \bar{y}_1 \alpha^* - \bar{\gamma} \bar{y}_2 - \bar{y}_2 \gamma & \alpha^* y_2 - \bar{y}_2 \alpha - [\bar{\gamma}, \bar{y}_1] \end{pmatrix} \right| \\
&\leq 4(\|\gamma\|_1 + \|\alpha\|_2) \|X\|_{\text{res}} \|Y\|_{\text{res}} \\
&\leq 4\|\Gamma_0\|_{1,2} \|X\|_{\text{res}} \|Y\|_{\text{res}}
\end{aligned}$$

$$|s_-(X, Y)| = 2|\Im \text{Tr}(\bar{x}_2 y_2)| \leq 2\|x_2\|_2 \|y_2\|_2 \leq \|X\|_{\text{res}} \|Y\|_{\text{res}}$$

$$\text{Tr}((X\Gamma_{00})Y) = \text{Tr}(Y(X\Gamma_{00}))$$

$$s_{\Gamma_{00}}(X, Y) = -\text{Tr}([X, Y]i\Gamma_{00}) := f_{\Gamma_{00}}([X, Y])$$

$$f_{\Gamma_0}(Z) = -\text{Tr}(Zi\Gamma_0)$$

$$\Gamma_0 \in \mathcal{B}_{1,2}(\mathfrak{H} \oplus \mathfrak{H}, D)$$

$$|f_{\Gamma_0}(Z)| \leq \|\Gamma_0\|_{1,2} \|Z\|_{\text{res}}$$

$$s_{\Gamma_0}(X, Y) = f_{\Gamma_0}([X, Y])$$

$$\mathfrak{u}_{\text{Bog}}^\Gamma = \{X \in \mathfrak{u}_{\text{Bog}} : s_\Gamma(X, Y) = 0, \forall Y \in \mathfrak{u}_{\text{Bog}}\}$$

$$s_\Gamma(\text{Ad}_V(X), \text{Ad}_V(Y)) = s_{\text{Ad}_{V^*(\Gamma)}}(X, Y), V \in \text{U}_{\text{Bog}}, X, Y \in \mathfrak{u}_{\text{Bog}}$$

$$X = \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}}^\Gamma, Y = \begin{pmatrix} y_1 & y_2 \\ \bar{y}_2 & \bar{y}_1 \end{pmatrix} \in \mathfrak{u}_{\text{Bog}}, \Gamma = \begin{pmatrix} \Lambda & 0 \\ 0 & \mathbf{1} - \Lambda \end{pmatrix}$$

$$\begin{aligned}
s_\Gamma(X, Y) &= i\text{Tr} \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix} \begin{pmatrix} [\Lambda, y_1] & \{\Lambda, y_2\} - y_2 \\ \bar{y}_2 - \{\Lambda, \bar{y}_2\} & [\bar{y}_1, \Lambda] \end{pmatrix} \\
&= -2\Im \left(\text{Tr}(x_1[\Lambda, y_1]) + \text{Tr}(x_2(\bar{y}_2 - \{\Lambda, \bar{y}_2\})) \right)
\end{aligned}$$

$$X = \begin{pmatrix} x_1 & x_2 \\ \bar{x}_2 & \bar{x}_1 \end{pmatrix}, Y = \begin{pmatrix} y_1 & y_2 \\ \bar{y}_2 & \bar{y}_1 \end{pmatrix}$$

$$0 = s_\Gamma(X, Y) = -2\Im \left(\text{Tr}(x_1[\Lambda, y_1]) + \text{Tr}(x_2(\bar{y}_2 - \{\Lambda, \bar{y}_2\})) \right)$$

$$0 = \Im \text{Tr}(x_1[\Lambda, y_1]) = \Im \text{Tr}([x_1, \Lambda]y_1)$$

$$0 = \Im \text{Tr}(ziz) = \|z\|_2^2$$

$$0 = \Im \text{Tr}(x_2(\bar{y}_2 - \{\Lambda, \bar{y}_2\})) = \Im \text{Tr}((x_2(\mathbf{1} - \Lambda) - \Lambda x_2)\bar{y}_2)$$

$$-y_2^T = y_2 \in \mathcal{B}_2(\mathfrak{H})$$

$$z := x_2(\mathbf{1} - \Lambda) - \Lambda x_2$$

$$-z^T = z \in \mathcal{B}_2(\mathfrak{H})$$

$$0 = \Im \text{Tr}(z(-i\bar{z})) = \Im i \text{Tr}(zz^*) = \|z\|_2^2$$

$$M = \mathcal{O}(\Gamma), G = \text{U}_{\text{Bog}}, K = \text{U}_{\text{Bog}}^\Gamma \text{ and } s = s_\Gamma$$

$$T_{\Gamma}\mathcal{O}(\Gamma)=\{[X,\Gamma]:X\in\mathfrak{u}_{\mathrm{Bog}}\}$$

$$\omega_{\Gamma}([X,\Gamma],[Y,\Gamma]):=s_{\Gamma}(X,Y),X,Y\in\mathfrak{u}_{\mathrm{Bog}}.$$

$$\omega_{U\Gamma U^*}([X,U\Gamma U^*],[Y,U\Gamma U^*]):=\omega_{\Gamma}([U^*XU,\Gamma],[U^*YU,\Gamma]),X,Y\in\mathfrak{u}_{\mathrm{Bog}}.$$

$$\omega=\Sigma(s_{\Gamma})$$

$$\omega\colon=\{\omega_{U\Gamma U^*}\}_{U\in\mathcal{U}_{\mathrm{Bog}}}$$

$$(\mathcal{O}(\Gamma),\Sigma(s_{\Gamma}))$$

$$T_{\Gamma}\mathcal{O}(\Gamma)\rightarrow T_{\Gamma}^*\mathcal{O}(\Gamma),[X,\Gamma]\mapsto\mathrm{Tr}(X[i\Gamma,\cdot])$$

$$\mathrm{ran}(\delta_{\Gamma})=T_{\Gamma}\mathcal{O}(\Gamma)\subseteq i\big(\mathfrak{u}_{\mathrm{Bog}}\big)_*\subseteq \mathrm{B}_{1,2}(\mathfrak{H}\oplus\mathfrak{H},D)$$

$$\| [X,\Gamma]\|_{\Gamma} = \inf\{\|X+Y\|_{\mathrm{res}}: Y\Gamma = \Gamma Y\} \leq \| [X,\Gamma]\|_{\mathrm{res}} \leq \| [X,\Gamma]\|_{1,2}.$$

$$\tilde{f}\in\left(i\big(\mathfrak{u}_{\mathrm{Bog}}\big)_*\right)^*$$

$$\tilde{f}|_{T_{\Gamma}\mathcal{O}(\Gamma)}=f$$

$$\left(i\big(\mathfrak{u}_{\mathrm{Bog}}\big)_*\right)^*\cong i\mathfrak{u}_{\mathrm{Bog}}$$

$$\tilde{f}=\mathrm{Tr}(Z_0\cdot)$$

$$f([Y,\Gamma])=\tilde{f}([Y,\Gamma])=\mathrm{Tr}(Z_0[Y,\Gamma])=\mathrm{Tr}(iZ_0[i\Gamma,Y])$$

$$\big(\mathfrak{u}_{\mathrm{Bog}}\big)_{\mathbb{C}}=\mathfrak{gl}_2(\mathfrak{H}\oplus\mathfrak{H},I,D)=:\mathfrak{g}$$

$$\Gamma=\begin{pmatrix}\Lambda&0\\0&\mathbf{1}-\Lambda\end{pmatrix},\Lambda=\sum_{i=1}^r\lambda_ip_i$$

$$\{p_i\}_{i=1}^{r+1}(r<\infty)$$

$$\mathfrak{p}:=\left\{\begin{pmatrix}x&0\\y&-x^T\end{pmatrix}\in\mathfrak{g}:p_ixp_j=0\text{ if }i=1,\ldots,r+1,j<i\right\}$$

$$\mathfrak{p}:=\left\{\begin{pmatrix}x&z\\y&-x^T\end{pmatrix}\in\mathfrak{g}:p_ixp_j=0\text{ if }i=1,\ldots,r+1,j<i,z=p_1zp_1\right\}$$

$$\left[\begin{pmatrix}x_1&0\\y_1&-x_1^T\end{pmatrix},\begin{pmatrix}x_2&0\\y_2&-x_2^T\end{pmatrix}\right]=\begin{pmatrix}[x_1,x_2]&0\\w&-[x_1,x_2]^T\end{pmatrix},$$

$$\mathfrak{n}:=\left\{\begin{pmatrix}x&z\\0&-x^T\end{pmatrix}\in\mathfrak{g}:p_ixp_j=0\text{ if }i=1,\ldots,r+1,j\geq i\right\}$$

$$\big(\mathfrak{u}_{\mathrm{Bog}}^{\Gamma}\big)_{\mathbb{C}}=\left\{\begin{pmatrix}x&0\\0&-x^T\end{pmatrix}\in\mathfrak{g}:x=\sum_{i=1}^{r+1}p_ixp_i\right\}$$

$$\mathfrak{p} + \bar{\mathfrak{p}} = \mathfrak{g}, \mathfrak{p} \cap \bar{\mathfrak{p}} = (\mathfrak{u}_{\text{Bog}}^\Gamma)_{\mathbb{C}}$$

$$\text{Ad}_U \mathfrak{p} \subseteq \mathfrak{p} \text{ for all } U \in \text{U}_{\text{Bog}}^\Gamma$$

$$X_i = \begin{pmatrix} x_i & 0 \\ y_i & -x_i^T \end{pmatrix} \in \mathfrak{p}, i = 1, 2$$

$$\text{Tr}(x) = \text{Tr}(x^T) \text{ for any } x \in \text{B}_1(\mathfrak{H})$$

$$\begin{aligned} s_\Gamma(X_1, X_2) &= i\text{Tr}(X_1[\Gamma, X_2]) = i\text{Tr}\left(\begin{pmatrix} x_1[\Lambda, x_2] & 0 \\ * & -x_1^T[\Lambda, x_2^T] \end{pmatrix}\right) \\ &= i\text{Tr}(x_1[\Lambda, x_2] - x_1^T[\Lambda, x_2^T]) \\ &= i\left(\text{Tr}(x_1\Lambda x_2 - x_2\Lambda x_1) = i\sum_{i=1}^r \lambda_i(\text{Tr}(p_i x_1 p_i x_2 p_i) - \text{Tr}(p_i x_2 p_i x_1 p_i))\right) = 0. \end{aligned}$$

$$-is_\Gamma(X, \bar{X}) > 0, X = \begin{pmatrix} x & 0 \\ y & -x^T \end{pmatrix} \in \mathfrak{p} \setminus (\mathfrak{u}_{\text{Bog}}^\Gamma)_{\mathbb{C}}$$

$$\Lambda = \sum_{i=1}^{r+1} \lambda_i p_i = \sum_{i=1}^r \lambda_i p_i$$

$$\begin{aligned} -is_\Gamma(X, \bar{X}) &= -\text{Tr}(X[\Gamma, X^*]) = -\text{Tr}\left(\begin{pmatrix} x & 0 \\ y & -x^T \end{pmatrix} \begin{pmatrix} [\Lambda, x^*] & \Lambda y^* - y^*(\mathbf{1} - \Lambda) \\ 0 & [\Lambda, \bar{x}] \end{pmatrix}\right) \\ &= -\text{Tr}\left(\begin{pmatrix} x[\Lambda, x^*] & * \\ * & y\Lambda y^* - yy^*(\mathbf{1} - \Lambda) - x^T[\Lambda, \bar{x}] \end{pmatrix}\right) \\ &= -2\text{Tr}(x[\Lambda, x^*]) + \text{Tr}(yy^* - (y^*y + yy^*)\Lambda) =: A + B \end{aligned}$$

$$\text{Tr}(x[\Lambda, x^*]) = -\text{Tr}(x^T[\Lambda, \bar{x}])$$

$$\{p_i\}_{i=1}^{r+1}x = \sum_{i=1}^{r+1} \sum_{j \geq i} p_i x p_j$$

$$\begin{aligned} A &= -2\text{Tr}(x[\Lambda, x^*]) = 2\text{Tr}((xx^* - x^*x)\Lambda) \\ &= \text{Tr}\left(\sum_{i=1}^r \sum_{j \geq i} \lambda_i p_i x p_j x^* p_i\right) - \text{Tr}\left(\sum_{i=1}^{r+1} \sum_{j \geq i} \lambda_j p_j x^* p_i x p_j\right) \\ &= 2 \sum_{i=1}^r \sum_{j > i} (\lambda_i - \lambda_j) \|p_i x p_j\|_2^2 \end{aligned}$$

$$\begin{aligned} B &= \text{Tr}(yy^* - (y^*y + yy^*)\Lambda) = \|y\|_2^2 - \sum_{i=1}^r (\lambda_i \text{Tr}(y^* y p_i) + \lambda_i \text{Tr}(y y^* p_i)) \\ &\geq \|y\|_2^2 - \lambda_1 \left(\sum_{i=1}^r \text{Tr}(p_i y^* y p_i) + \text{Tr}(p_i y y^* p_i) \right) \\ &\geq (1 - 2\lambda_1) \|y\|_2^2 \end{aligned}$$

$$\left\| \sum_{i=1}^r p_i z p_i \right\|_1 \leq \|z\|_1$$

$$\left\| \sum_{i=1}^r p_i z p_i \right\|_1 = \text{Tr} \left(\sum_{i=1}^r p_i z p_i \right)$$

$$\lambda_1 = \max_{i=1,\dots,r} \lambda_i < \frac{1}{2}$$

$$X \in \mathfrak{p} \setminus (\mathfrak{u}_{\text{Bog}}^\Gamma)_{\mathbb{C}}$$

$$[X_1,X_2]=\begin{pmatrix}x_1&z_1\\y_1&-x_1^T\end{pmatrix}\begin{pmatrix}x_2&z_2\\y_2&-x_2^T\end{pmatrix}-\begin{pmatrix}x_2&z_2\\y_2&-x_2^T\end{pmatrix}\begin{pmatrix}x_1&z_1\\y_1&-x_1^T\end{pmatrix}$$

$$[X_1,X_2]_{11}=[x_1,x_2]+p_1(z_1p_1y_2-z_2p_1y_1)$$

$$\begin{aligned} [X_1,X_2]_{12} &= x_1z_2-z_1x_2^T-(x_2z_1-z_2x_1^T) \\ &= p_1(x_1p_1z_2+x_2p_1z_1-z_1p_1x_2^T-z_2p_1x_1^T)p_1:=p_1wp_1 \end{aligned}$$

$$[X_1,X_2]_{21}=y_1x_2-x_1^Ty_2-(y_2x_1-x_2^Ty_1)$$

$$[X_1,X_2]_{22}=[x_1^T,x_2^T]+(y_1p_1z_2-y_2p_1z_1)p_1=-[X_1,X_2]_{11}^T$$

$$\mathfrak{n}:=\left\{\begin{pmatrix}x&z\\0&-x^T\end{pmatrix}\in\mathfrak{g}:p_ixp_j=0\text{ if }i=1,\dots,r+1,j\geq i,\text{ and }p_1zp_1=0\right\}$$

$$(\mathfrak{u}_{\text{Bog}}^\Gamma)_{\mathbb{C}}=\left\{\begin{pmatrix}x&z\\y&-x^T\end{pmatrix}\in\mathfrak{g}:x=\sum_{i=1}^{r+1}p_ixp_i,z=p_1zp_1,z=-z^T,y=p_1yp_1,y=-y^T\right\}.$$

$$\mathfrak{p}+\overline{\mathfrak{p}}=\mathfrak{g},\mathfrak{p}\cap\overline{\mathfrak{p}}=(\mathfrak{u}_{\text{Bog}}^\Gamma)_{\mathbb{C}}$$

$$\mathrm{Ad}_U\mathfrak{p}\subseteq\mathfrak{p}$$

$$\begin{aligned} s_\Gamma(X_1,X_2) &= \text{Tr} \left(\begin{pmatrix} x_1 & z_1 \\ y_1 & -x_1^T \end{pmatrix} \left[i \begin{pmatrix} \Lambda & 0 \\ 0 & \mathbf{1} - \Lambda \end{pmatrix}, \begin{pmatrix} x_2 & z_2 \\ y_2 & -x_2^T \end{pmatrix} \right] \right) \\ &= i \text{Tr} (x_1 [\Lambda, x_2] - x_1^T [\Lambda, x_2^T]) + i \text{Tr} (z_1 ((\mathbf{1} - \Lambda) y_2 - y_2 \Lambda)) + i \text{Tr} (y_1 (\Lambda z_2 - z_2 (\mathbf{1} - \Lambda))) \\ &= 0 \end{aligned}$$

$$\text{Tr}(z_1((\mathbf{1}-\Lambda)y_2-y_2\Lambda))=\text{Tr}(z_1p_1((\mathbf{1}-\Lambda)y_2-y_2\Lambda)p_1)=0$$

$$\Lambda z_2-z_2(\mathbf{1}-\Lambda)=\frac{1}{2}(p_1z_2p_1-p_1z_2p_1)=0$$

$$X\in\mathfrak{p}\setminus(\mathfrak{u}_{\text{Bog}}^\Gamma)_{\mathbb{C}}$$

$$\begin{aligned}
-is_{\Gamma}(X, \bar{X}) &= -\text{Tr}(X[\Gamma, X^*]) = -\text{Tr}\left(\begin{pmatrix} x & z \\ y & -x^T \end{pmatrix} \left[\begin{pmatrix} \Lambda & 0 \\ 0 & \mathbf{1} - \Lambda \end{pmatrix}, \begin{pmatrix} x^* & y^* \\ z^* & -\bar{x} \end{pmatrix} \right] \right) \\
&= -2\text{Tr}(x[\Lambda, x^*]) + \text{Tr}(yy^* - (y^*y + yy^*)\Lambda) - \text{Tr}(z((\mathbf{1} - \Lambda)z^* - z^*\Lambda)) \\
&:= A + B + C
\end{aligned}$$

$$X \in \mathfrak{p} \setminus (\mathfrak{u}_{\text{Bog}}^{\Gamma})_{\mathbb{C}}$$

$$\|y\|_2^2 = \|p_1 y\|_2^2 + \|(\mathbf{1} - p_1)y\|_2^2$$

$$\begin{aligned}
B &= \text{Tr}(yy^* - (y^*y + yy^*)\Lambda) = \|(\mathbf{1} - p_1)y\|_2^2 - \sum_{i=2}^r (\lambda_i \text{Tr}(y^* y p_i) + \lambda_i \text{Tr}(y y^* p_i)) \\
&\geq \|(\mathbf{1} - p_1)y\|_2^2 - \lambda_2 \left(\sum_{i=2}^r \text{Tr}(p_i (y(\mathbf{1} - p_1))^* y (\mathbf{1} - p_1) p_i) + \text{Tr}(p_i (\mathbf{1} - p_1) y ((\mathbf{1} - p_1) y)^* p_i) \right) \\
&\geq (1 - 2\lambda_2) \|(\mathbf{1} - p_1)y\|_2^2
\end{aligned}$$

$$\lambda_2 = \max_{i=2,\dots,r} \lambda_i < \frac{1}{2} \text{ and } (\mathbf{1} - p_1)y \neq 0, \text{ for } y \neq p_1 y p_1$$

$$-is_{\Gamma}(X, \bar{X}) > 0 \text{ for } X \in \mathfrak{p} \setminus (\mathfrak{u}_{\text{Bog}}^{\Gamma})_{\mathbb{C}}$$

$$\Gamma = \begin{pmatrix} \Lambda & 0 \\ 0 & \mathbf{1} - \Lambda \end{pmatrix}, \Lambda = \sum_{i=1}^{\infty} \lambda_i p_i$$

$$\mathfrak{p} := \left\{ \begin{pmatrix} x & 0 \\ y & -x^T \end{pmatrix} \in \mathfrak{g} : p_i x p_j = 0 \text{ if } i \geq 1, j < i \right\}$$

$$\mathfrak{p} := \left\{ \begin{pmatrix} x & z \\ y & -x^T \end{pmatrix} \in \mathfrak{g} : p_i x p_j = 0 \text{ if } i \geq 1, j < i, z = p_1 z p_1 \right\}$$

$$x = \sum_{i,j \geq 1} p_i x p_j$$

$$\left\| \sum_{i=1}^N \sum_{j=1}^M p_i x p_j \right\| \leq \|x\|$$

$$x = \sum_{i=1}^{\infty} \sum_{j \geq i} p_i x p_j$$

$$x = \sum_{i=1}^{\infty} \sum_{j \geq i} p_i x p_j + \sum_{i=1}^{\infty} \sum_{j < i} p_i x p_j$$

$$\mathfrak{n} := \left\{ \begin{pmatrix} x & z \\ 0 & -x^T \end{pmatrix} \in \mathfrak{g} : p_i x p_j = 0 \text{ if } i \geq 1, j \geq i \right\}$$

$$-is_{\Gamma}(X, \bar{X}) = -2\text{Tr}(x[\Lambda, x^*]) + \text{Tr}(yy^* - (y^*y + yy^*)\Lambda) > 0$$

$$X \in \mathfrak{p} \setminus (\mathfrak{u}_{\text{Bog}}^{\Gamma})_{\mathbb{C}}$$

$$\mathrm{Tr}\big((xx^*-x^*x)\Lambda\big)$$

$$x=\sum_{i=1}^{\infty}\sum_{j\geq i}p_ixp_j$$

$$f(y)=\mathrm{Tr}(yz), z\in \mathrm{B}_1(\mathfrak{H}), y\in \mathrm{B}(\mathfrak{H})$$

$$\begin{aligned}\mathrm{Tr}(xx^*\Lambda)&=\sum_{i=1}^{\infty}\sum_{j\geq i}\mathrm{Tr}(p_ixp_jx^*\Lambda)\\&=\sum_{i=1}^{\infty}\sum_{j\geq i}\mathrm{Tr}\left(p_ixp_j\left(\sum_{k=1}^{\infty}\sum_{l\geq k}p_lx^*p_k\right)\left(\sum_{s=1}^{\infty}\lambda_sp_s\right)\right)\\&=\sum_{i=1}^{\infty}\sum_{j\geq i}\lambda_i\mathrm{Tr}(p_ixp_jx^*p_i)\end{aligned}$$

$$-2\mathrm{Tr}(x[\Lambda,x^*])=2\sum_{i=1}^{\infty}\sum_{j>i}(\lambda_i-\lambda_j)\|p_ixp_j\|_2^2$$

$$\ker(\Gamma)=\{0\}(\mathcal{O}(\Gamma),\Sigma(s_\Gamma))$$

$$\mathbf{g}1-\mathbf{pdm}\Gamma=\Gamma[\Lambda,0]$$

$$\alpha_U\colon \mathcal{O}(\Gamma)\rightarrow \mathcal{O}(\Gamma), \alpha_U(\Gamma_1)=U\Gamma_1U^*, \Gamma_1\in \mathcal{O}(\Gamma)$$

$$\mathfrak{F}\colon=\mathfrak{F}[\mathfrak{H}]=\bigoplus_{N=0}^{\infty}\mathfrak{F}^{(N)},$$

$$\mathfrak{F}^{(N)}=\bigwedge_{n=1}^N\mathfrak{H}$$

$$\mathfrak{F}^{(0)}=\mathbb{C}\Omega$$

$$f_1\wedge\ldots\wedge f_N\colon=\frac{1}{\sqrt{N!}}\sum_{\pi\in S_N}\mathrm{sign}(\pi)f_{\pi(1)}\otimes f_{\pi(2)}\otimes\ldots\otimes f_{\pi(N)},f_i\in\mathfrak{H},$$

$$\langle f_1\wedge\ldots\wedge f_N,g_1\wedge\ldots\wedge g_N\rangle_{\mathfrak{F}^{(N)}}=\det(\langle f_i,g_j\rangle)_{1\leq i,j\leq N},f_i,g_i\in\mathfrak{H}.$$

$$\langle \Psi_1,\Psi_2\rangle_{\mathfrak{F}}\colon=\sum_{N=0}^{\infty}\left\langle f_1^{(N)},f_2^{(N)}\right\rangle_{\mathfrak{F}^{(N)}},\Psi_i=\left(f_i^{(0)},f_i^{(1)},\ldots\right),i=1,2$$

$$c^*(f)\Omega=f;\;c^*(f)(f_1\wedge\ldots\wedge f_N)\colon=f\wedge f_1\wedge\ldots\wedge f_N$$

$$\begin{aligned}\{c(f),c^*(g)\}&=\langle f,g\rangle\mathbf{1}_{\mathfrak{F}}\\ \{c^*(f),c^*(g)\}&=\{c(f),c(g)\}=0\end{aligned}$$

$$c(f),c^*(f)\in\mathrm{B}(\mathfrak{F})$$

$$\|c(f)\|=\|f\| \text{ and } \|c^*(f)\|=\|f\|$$

$$\{c(f)\colon f\in\mathfrak{H}\}\text{ in }\mathsf{B}(\mathfrak{F})$$

$$\mathcal{A}=\mathcal{A}(\mathfrak{H})\text{ of }\mathfrak{H}$$

$$\widehat{\mathbb{N}}\!:=\bigoplus_{N\geq 0}N\mathbf{1}_{\mathfrak{F}^{(N)}}$$

$$\Psi=(f^{(0)},f^{(1)},\ldots)$$

$$\sum_{N=1}^\infty N^2\|f^{(N)}\|_{\mathfrak{F}^{(N)}}^2<\infty$$

$$I_0f\colon=\bar{f}\colon=\sum_{k\geq 1}\bar{\mu}_k\varphi_k$$

$$f=\sum_{k\geq 1}\mu_k\varphi_k$$

$$\bar{x}\colon=I_0xI_0, \text{ and } x^T\colon=(\bar{x})^*=\overline{x^*}$$

$$\begin{array}{l}uu^*+vv^*=\mathbf{1}=u^*u+v^T\bar{v}\\u^*v+v^T\bar{u}=0=uv^T+vu^T\end{array}$$

$$U=\begin{pmatrix}u&v\\ \bar{v}&\bar{u}\end{pmatrix}$$

$$d^*(f)\colon=c^*(uf)+c(v\bar{f}),\,d(f)\colon=(d^*(f))^*$$

$$\beta_U(c(f))=d(f)$$

$$\mathbb{U}\colon=\mathbb{U}_U\colon\mathfrak{F}\rightarrow\mathfrak{F}$$

$$\mathbb{U}c^*(f)\mathbb{U}^*=c^*(uf)+c(v\bar{f})$$

$$\omega(\mathbf{1}_{\mathfrak{F}})=1 \text{ and } \omega(A^*A)\geq 0, \text{ for all } A\in\mathsf{B}(\mathfrak{F})$$

$$\mathfrak{F},\rho\geq 0 \text{ and } \mathrm{Tr}(\rho)=1$$

$$\omega(A)=\mathrm{Tr}_{\mathfrak{F}}(\rho A)$$

$$\omega(A)=\langle \Psi, A\Psi\rangle_{\mathfrak{F}}$$

$$e_1,\ldots,e_{2n}\in\{c^*(h_1),c(h_1),\ldots,c^*(h_{2n}),c(h_{2n})\}$$

$$\omega(e_1\ldots e_{2n})=\sum_{\pi\in P_{2n}}\mathrm{sign}(\pi)\omega(e_{\pi(1)}e_{\pi(2)})\ldots\omega(e_{\pi(2n-1)}e_{\pi(2n)})$$

$$\omega(e_1e_2e_3e_4)=\omega(e_1e_4)\omega(e_2e_3)-\omega(e_1e_3)\omega(e_2e_4)+\omega(e_1e_2)\omega(e_3e_4)$$



$$\omega(\widehat{\mathbb{N}}):=\sum_{N=1}^{\infty}N\omega(\Pi^{(N)})<\infty$$

$$\Psi\in\mathfrak{F}^{(N)}$$

$$\Psi=f_1\wedge...\wedge f_N$$

$$\left\langle \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \Gamma_\omega \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \right\rangle_{\mathfrak{H} \oplus \mathfrak{H}} = \omega([c^*(g_1) + c(\bar{g}_2)][c(f_1) + c^*(\bar{f}_2)]), f_i, g_i \in \mathfrak{H}.$$

$$0\leq \Gamma_\omega\leq \mathbf{1}_{\mathfrak{H}\oplus\mathfrak{H}}$$

$$\Gamma_\omega=\begin{pmatrix} \gamma_\omega & \alpha_\omega \\ \alpha_\omega^* & \mathbf{1}-\bar{\gamma}_\omega \end{pmatrix} =: \Gamma_\omega[\gamma_\omega,\alpha_\omega]$$

$$c_k^{\ast}:=c^{\ast}(\varphi_k) \text{ and } c_k:=c(\varphi_k)$$

$$\langle \varphi_m, \gamma_\omega \varphi_k \rangle = \omega(c_k^* c_m), \langle \varphi_m, \alpha_\omega^* \varphi_k \rangle = \omega(c_k^* c_m^*)$$

$$\gamma_\omega^*=\gamma_\omega, \alpha_\omega^T=-\alpha_\omega.$$

$$\omega_\Psi(A)=\langle \Psi,A\Psi\rangle_{\mathfrak{F}}$$

$$\Psi\in\mathfrak{F}^{(N)}$$

$$\widehat{\mathbb{N}}=\sum_{k\geq 1}c_k^*c_k$$

$$\omega(\widehat{\mathbb{N}})=\sum_{k\geq 1}\omega(c_k^*c_k)=\mathrm{Tr}(\gamma_\omega)$$

$$\omega(A)=\langle \Psi,A\Psi\rangle$$

$$\Psi=(f^{(0)},f^{(1)},\ldots)\in\mathfrak{F}$$

$$\omega(\widehat{\mathbb{N}}^2)-\omega(\widehat{\mathbb{N}})^2=\sum_{n\geq 0}(n-N)^2\|f^{(N)}\|_{\mathfrak{F}^{(N)}}^2=2\mathrm{Tr}(\alpha_\omega^*\alpha_\omega)$$

$$\Gamma=\Gamma[\gamma,\alpha]=\begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbf{1}-\bar{\gamma} \end{pmatrix}\in\mathrm{B}(\mathfrak{H}\oplus\mathfrak{H})$$

$$\mathcal{D}:=\left\{\begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbf{1}-\bar{\gamma} \end{pmatrix}\in\mathrm{B}(\mathfrak{H}\oplus\mathfrak{H}):0\leq\begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbf{1}-\bar{\gamma} \end{pmatrix}\leq\mathbf{1}_{\mathfrak{H}\oplus\mathfrak{H}},\gamma=\gamma^*\in\mathrm{B}_1(\mathfrak{H}),\alpha^T=-\alpha\right\}.$$

$$\Phi\colon Z_{\mathrm{qf}}\rightarrow\mathcal{D}, \Phi(\omega)=\Gamma_\omega$$

$$U\colon \mathfrak{H}\oplus \mathfrak{H}\rightarrow \mathfrak{H}\oplus \mathfrak{H}$$

$$\omega_U(A):=\omega(\mathbb{U}_UA\mathbb{U}_U^*)$$

$$\Phi(\omega_U)=U^*\Gamma_\omega U$$

$$\Gamma=\Gamma[\gamma,\alpha]\in\mathcal{D}$$

$$0\leq \Gamma-\Gamma^2=\begin{pmatrix} \gamma-\gamma^2-\alpha\alpha^* & (\mathbf{1}-\gamma)\alpha+\alpha(\mathbf{1}-\bar\gamma) \\ \alpha^*(\mathbf{1}-\gamma)+(\mathbf{1}-\bar\gamma)\alpha^* & \bar\gamma-\bar\gamma^2-\alpha^*\alpha \end{pmatrix}$$

$$W\Gamma W^*=\begin{pmatrix} \Lambda & 0 \\ 0 & \mathbf{1}-\Lambda \end{pmatrix}$$

$$E_{gs}:=\inf\{\omega(\mathbb{H})\colon \omega\in\mathcal{Z}\}.$$

$$E_{HF}\!:=\!\inf\!\{\langle\Psi,\mathbb{H}\Psi\rangle_{\mathfrak{F}}\!:\!N\in\mathbb{N},\Psi=f_1\wedge\ldots\wedge f_N,\langle f_i,f_j\rangle=\delta_{ij}\}$$

$$\begin{aligned} E_{HFB} &:= \inf\{\omega(\mathbb{H})\colon \omega\in\mathcal{Z}_{\text{qf}}\}\\ &= \inf\{\mathcal{E}(\Gamma)\colon \Gamma\in\mathcal{D}\} \end{aligned}$$

$$\mathcal{E}(\Gamma_\omega)\colon=\omega(\mathbb{H})$$

$$\mathbb{H}=\bigoplus_{N\geq 0}\left(\sum_{i=1}^Nh_i+\sum_{1\leq i,j\leq N}W_{ij}\right).$$

$$h=-\Delta-\sum_{k=1}^K\frac{Z_k}{|x-r_k|}-\mu$$

$$\mathfrak{H}=L^2(\mathbb{R}^3,\mathbb{C}^2),\text{ and }W=\frac{1}{|x-y|}$$

$$\mathfrak{H}\otimes\mathfrak{H}\cong L^2(\mathbb{R}^6,\mathbb{C}^2)$$

$$h=\sqrt{-\Delta+m^2}-m, m>0$$

$$G\times M\rightarrow M, (g,p)\mapsto g\cdot p$$

$$(gh)\cdot p=g\cdot (h\cdot p)$$

$$\pi_p\colon G\rightarrow M, \pi_p(g)=g\cdot p$$

$$\mathcal{O}(p)\colon=\{g\cdot p\colon g\in G\}$$

$$G_p\colon=\{g\in G\colon g\cdot p=p\}$$

$$\mathcal{O}(p)\rightarrow G/G_p, g\cdot p\mapsto gG_p$$

$$T_p f\colon T_p M\rightarrow T_{f(p)}N$$

$$\pi_p\colon G\rightarrow M, \pi_p(g)=g\cdot p$$

$$(\mathcal{W},\phi)\text{ at }p,\phi:\mathcal{W}\subseteq E\rightarrow M,\phi(0)=p$$

$$\phi(\mathcal{W}\cap (F\oplus \{0\}))=\phi(\mathcal{W})\cap N$$



$$T_p f\colon T_p M\rightarrow T_{f(p)}N$$

$$\mathbf{L}(K)\colon=\{X\in\mathfrak{g}\colon\exp_G\left(tX\right)\in K,\forall t\in\mathbb{R}\}$$

$$\exp_K=\exp_G|_{\mathbf{L}(K)}\colon\mathbf{L}(K)\rightarrow K$$

$$\pi\colon G\rightarrow M, \pi(g)=gK$$

$$G\times M\rightarrow M, \, g\cdot hK=ghK$$

$$\{\mathfrak{m}_p\}_{p\in M}\mathfrak{g}_p\oplus \mathfrak{m}_p=\mathfrak{g}\mathrm{Ad}_g(\mathfrak{m}_p)=\mathfrak{m}_p$$

$$T_pM\rightarrow T_p^*M, v\rightarrow \omega_p(v,\cdot)$$

$$\alpha_g(hK)=ghK$$

$$(\alpha_g)^*\omega=\omega$$

$$s(X,[Y,Z])+s(Z,[X,Y])+s(Y,[Z,X])=0$$

$$s(X,Y)=f([X,Y])$$

$$H_c^2(\mathfrak{g},\mathfrak{z})\colon=Z_c^2(\mathfrak{g},\mathfrak{z})/B_c^2(\mathfrak{g},\mathfrak{z})$$

$$\mathfrak{k}=\{X\in\mathfrak{g}:s(X,Y)=0,\forall Y\in\mathfrak{g}\}$$

$$T_pM\cong \mathfrak{g}/\mathfrak{k}$$

$$\omega_p(X+\mathfrak{k},Y+\mathfrak{k})\colon=s(X,Y),X,Y\in\mathfrak{g}.$$

$$\omega_{g\cdot p}(v,w)\colon=\omega_p\big(T_{g\cdot p}\big(\alpha_{g^{-1}}\big)(v),T_{g\cdot p}\big(\alpha_{g^{-1}}\big)(w)\big),v,w\in T_{g\cdot p}M$$

$$\omega=\Sigma(s)$$

$$\omega\colon=\left\{\omega_{g\cdot p}\right\}_{g\in G}$$

$$\mathfrak{k}=\{X\in\mathfrak{g}:s(X,Y)=0,\forall Y\in\mathfrak{g}\}$$

$$\alpha_g\colon M\rightarrow M, \alpha_g(hK)=ghK$$

$$g\in G; \omega_p(v,w)=\omega_p(J_p v,J_p w)$$

$$\mathfrak{p}+\overline{\mathfrak{p}}=\mathfrak{g}_{\mathbb{C}},\mathfrak{p}\cap\overline{\mathfrak{p}}=\mathfrak{k}_{\mathbb{C}},\text{ and }\mathrm{Ad}_h\mathfrak{p}\subseteq\mathfrak{p},h\in K.$$

$$\omega=\Sigma(s)$$

$$s\colon \mathfrak{g}_{\mathbb{C}}\times \mathfrak{g}_{\mathbb{C}}\rightarrow \mathbb{C}$$

$$s(\mathfrak{p}\times \mathfrak{p})=0, \text{ and } \quad -is(a,\bar{a})>0, a\in \mathfrak{p}\setminus \mathfrak{k}_{\mathbb{C}}$$



$$\mathfrak{g}/\mathfrak{k} \rightarrow (\mathfrak{g}/\mathfrak{k})^* \simeq T_p^*M, X + \mathfrak{k} \mapsto \omega_p(X + \mathfrak{k}, \cdot)$$

$$H=\sum_jt_jc_j^\dagger c_{j+1}+\text{ h.c. }+U\sum_jn_jn_{j+1},$$

$$j,t_j=-t-V_2\cos\left(2\pi\tau\left(j+\frac{1}{2}\right)+\phi\right)$$

$$L_M=\left(\tau-\frac{1}{2}\right)^{-1}=\delta^{-1}$$

$$H_{MF}=H_0+\sum_{ij}\epsilon_{ij}c_i^\dagger c_j$$

$$H_{MF}=H_0+\sum_i\epsilon_ic_i^\dagger c_i+\sum_i\Delta_ic_i^\dagger c_{i+1}+h.c.,$$

$$\begin{aligned}\epsilon_i&=U(\langle n_{i-1}\rangle_{MF}+\langle n_{i+1}\rangle_{MF})\\ \Delta_i&=-U\langle c_{i+1}^\dagger c_i\rangle_{MF}\end{aligned}$$

$$\begin{aligned}\langle n_i\rangle_{MF}&=\sum_{\alpha occ}|\mathcal{U}_{i,\alpha}|^2\\ \langle c_{i+1}^\dagger c_i\rangle_{MF}&=\sum_{\alpha occ}\mathcal{U}_{i+1,\alpha}^*\mathcal{U}_{i,\alpha},\end{aligned}$$

$$H=\sum_aE_a^{(\mathrm{MF})}d_a^\dagger d_a+\sum_{abcd}U_{cd}^{ab}d_a^\dagger d_b^\dagger d_c d_d$$

$$A_p(t)=F(t)\sum_{ab}A_{ab}d_a^\dagger d_b$$

$$\rho_{ba}(t)=\langle d_a^\dagger(t)d_b(t)\rangle$$

$$\boldsymbol{\rho}^{(1)}(\omega)=(\hbar\omega\boldsymbol{I}-\boldsymbol{H}_{eh})^{-1}\boldsymbol{V}_p(\omega),$$

$$\boldsymbol{H}_{eh}=\left(\begin{array}{cc}\boldsymbol{R} & \boldsymbol{C} \\ -\boldsymbol{C}^* & -\boldsymbol{R}^*\end{array}\right),$$

$$\boldsymbol{R}_{e'o'}^{eo}=(E_o-E_e)\delta_{ee'}\delta_{oo'}+\left(U_{eo'o}^{e'o}+U_{o'e}^{oe'}-U_{o'e}^{e'o}-U_{eo'}^{oe'}\right)$$

$$\boldsymbol{C}_{o'e'}^{eo}=U_{ee'}^{oo'}+U_{e'e}^{o'o}-U_{ee'}^{o'o}-U_{e'e}^{oo'}$$

$$\chi_{BA}(\omega)=[\boldsymbol{B}_{eo} \quad \boldsymbol{B}_{oe}]\left[\begin{array}{cc}\hbar\omega\boldsymbol{I}-\boldsymbol{R} & -\boldsymbol{C} \\ \boldsymbol{C}^* & \hbar\omega\boldsymbol{I}+\boldsymbol{R}^*\end{array}\right]^{-1}\left[\begin{array}{c}\boldsymbol{A}_{eo} \\ -\boldsymbol{A}_{oe}\end{array}\right]$$

$$\langle \delta n_m \rangle = \langle n_m \rangle - \frac{1}{2}$$



$$\langle \delta n_k \rangle = \frac{1}{\sqrt{N}} \sum_m e^{ikm} \langle \delta n_m \rangle,$$

$$\mathcal{O}_{CDW} = \max_i \langle n_i \rangle - \min \langle n_i \rangle.$$

$$\text{IPR}(\langle \delta \mathbf{n} \rangle) = \left(\sum_k |\langle \delta n_k \rangle|^4 \right) / \left(\sum_k |\langle \delta n_k \rangle|^2 \right)^2.$$

$$\Delta \sim \exp\left(-\frac{1}{U}\right)$$

$$K_n=\pi+2\pi\tau n,$$

$$\Delta(U) \sim \exp\left(-\frac{U_{\rm typ}}{U}\right), \text{ with } U_{\rm typ}^{-1} = 2\rho_F$$

$$K_n=\pi+2\pi\tau_cn.$$

$$\Psi_X^{eo}(r_1,r_2)=\psi_e(r_1)\psi_o(r_2),$$

$$\chi_{BA}(t,t',\boldsymbol{r},\boldsymbol{r}')=-\frac{i}{\hbar}\langle [B(\boldsymbol{r},t),A(\boldsymbol{r}',t')]\rangle,$$

$$\langle B \rangle(\boldsymbol{r},t) = \langle B \rangle_0(\boldsymbol{r},t) + \int \, d\boldsymbol{r}' \int_{-\infty}^{\infty} \chi_{BA}(\boldsymbol{r},\boldsymbol{r}';t-t') F(t')$$

$$\langle B \rangle = \sum_{ab} B_{ab} \langle c_a^\dagger(t) c_b(t) \rangle,$$

$$\langle c_a^\dagger(t) c_b(t) \rangle \equiv \rho_{ba}(t)$$

$$|\psi_i\rangle = d_i^\dagger |0\rangle$$

$$H=H_0+H_{\rm int}+\hat{A}F(t),$$

$$H_0=\sum_{ij}t_{ij}d_i^\dagger d_j$$

$$H_{\rm int}=\sum_{ijkl}U_{kl}^{ij}d_i^\dagger d_j^\dagger d_k d_l$$

$$\hat{A}=\sum_{ij}A_{ij}d_i^\dagger d_j$$

$$\frac{d}{dt}\rho_{ba}=\left\langle d_a^\dagger\frac{d}{dt}d_b\right\rangle+\left\langle\frac{d}{dt}d_a^\dagger d_b\right\rangle$$

$$\frac{d}{dt}\mathcal{O}(t) = \frac{i}{\hbar}[H, \mathcal{O}(t)].$$

$$\frac{d}{dt}\rho_{ba} = \frac{i}{\hbar}\langle d_a^\dagger[H, d_b] \rangle + \frac{i}{\hbar}\langle [H, d_a^\dagger]d_b \rangle.$$

$$\begin{aligned} [H, d_b] = & -\sum_j (t_{bj} + A_{bj}F(t))d_j \\ & + \sum_{jkl} (U_{kl}^{jb} - U_{kl}^{bj})d_j^\dagger d_k d_l \end{aligned}$$

$$\begin{aligned} [H, d_a^\dagger] = & \sum_i (t_{ia} + A_{ia}F(t))d_i^\dagger \\ & + \sum_{ijk} (U_{ka}^{ij} - U_{ka}^{ji})d_i^\dagger d_j^\dagger d_k. \end{aligned}$$

$$\begin{aligned} -i\hbar \frac{d}{dt}\rho_{ba} = & -\sum_j (t_{bj} + A_{bj}F(t))\rho_{ja} \\ & + \sum_i (t_{ia} + A_{ia}F(t))\rho_{bi} \\ & + \sum_{jkl} (U_{kl}^{jb} - U_{kl}^{bj})\langle d_a^\dagger d_j^\dagger d_k d_l \rangle \\ & + \sum_{ijk} (U_{ka}^{ij} - U_{ka}^{ji})\langle d_i^\dagger d_j^\dagger d_k d_b \rangle. \end{aligned}$$

$$\langle d_a^\dagger d_j^\dagger d_k d_l \rangle = \langle d_a^\dagger d_l \rangle \langle d_j^\dagger d_k \rangle - \langle d_a^\dagger d_k \rangle \langle d_j^\dagger d_l \rangle,$$

$$\begin{aligned} -i\hbar \frac{d}{dt}\rho_{ba}(t) = & \sum_i (t_{ia} + A_{ia}F(t))\rho_{bi} \\ & - \sum_j (t_{bj} + A_{bj}F(t))\rho_{ja} \\ & + \sum_l \Sigma_{bl}[\boldsymbol{\rho}]\rho_{la} + \rho_{bi}\Sigma_{ia}[\boldsymbol{\rho}] \end{aligned}$$

$$\Sigma_{bl}[\boldsymbol{\rho}] = \sum_{kl} (U_{kl}^{jb} + U_{lk}^{bj} - U_{kl}^{bj} - U_{lk}^{jb})\rho_{kj},$$

$$\boldsymbol{\rho}(t) = \sum_n \boldsymbol{\rho}^{(n)}(t),$$

$$\Sigma[\boldsymbol{\rho}] \rightarrow \Sigma[\boldsymbol{\rho} - \boldsymbol{\rho}^{(0)}]$$

$$\begin{aligned}
i\hbar \frac{d}{dt} \rho_{ba}^{(1)}(t) = & \sum_i \left(t_{bi} \rho_{ia}^{(1)} - \rho_{bi}^{(1)} t_{ia} \right) \\
& + \sum_i \left(A_{bi} \rho_{ia}^{(0)} - \rho_{bi}^{(0)} A_{ia} \right) F(t) \\
& + \sum_{ijk} \left(U_{ki}^{bj} + U_{ik}^{jb} - U_{ki}^{jb} - U_{ik}^{bj} \right) \rho_{kj}^{(1)} \rho_{ia}^{(0)} \\
& - \sum_{ijk} \rho_{bi}^{(0)} \left(U_{ka}^{ij} + U_{ak}^{ji} - U_{ak}^{ij} - U_{ka}^{ji} \right) \rho_{kj}^{(1)}.
\end{aligned}$$

$$\sum_{cd} \left(\hbar \omega \delta_{c\alpha} \delta_{\beta d} - H_{\alpha\beta}^{cd} \right) \rho_{cd}^{(1)}(\omega) = J_{\alpha\beta}(\omega)$$

$$\begin{aligned}
H_{\alpha\beta}^{cd} = & t_{\alpha c} \delta_{d\beta} - t_{d\beta} \delta_{\alpha c} \\
& + \sum_e \left(U_{ce}^{\alpha d} + U_{ec}^{d\alpha} - U_{ce}^{d\alpha} - U_{ec}^{\alpha d} \right) \rho_{e\beta}^{(0)} \\
& - \sum_e \rho_{\alpha e}^{(0)} \left(U_{c\beta}^{ed} + U_{\beta c}^{de} - U_{\beta c}^{ed} - U_{c\beta}^{de} \right)
\end{aligned}$$

$$J_{\alpha\beta}(\omega) = \sum_e \left(A_{\alpha e} \rho_{e\beta}^{(0)} - \rho_{\alpha e}^{(0)} A_{e\beta} \right) F(\omega).$$

$$\rho_{\alpha\beta}^{(0)} = f_{\alpha} \delta_{\alpha\beta}$$

$$t_{\alpha\beta} = E_{\alpha}^{(MF)} \delta_{\alpha\beta}$$

$$\begin{aligned}
H_{\alpha\beta}^{cd} = & \left(E_{\alpha}^{(MF)} - E_{\beta}^{(MF)} \right) \delta_{\alpha c} \delta_{\beta d} \\
& + \left(U_{c\beta}^{\alpha d} + U_{\beta c}^{d\alpha} - U_{c\beta}^{d\alpha} - U_{\beta c}^{\alpha d} \right) (f_{\beta} - f_{\alpha}),
\end{aligned}$$

$$J_{\alpha\beta}(\omega) = (f_{\beta} - f_{\alpha}) A_{\alpha\beta} F(\omega).$$

$$\begin{pmatrix} H_{oo}^{o'o'} & H_{oo}^{o'e'} & H_{oo}^{e'o'} & H_{oo}^{e'e'} \\ H_{oe}^{o'o'} & H_{oe}^{o'e'} & H_{oe}^{e'o'} & H_{oe}^{e'e'} \\ H_{eo}^{o'o'} & H_{eo}^{o'e'} & H_{eo}^{e'o'} & H_{eo}^{e'e'} \\ H_{ee}^{o'o'} & H_{ee}^{o'e'} & H_{ee}^{e'o'} & H_{ee}^{e'e'} \end{pmatrix} \begin{pmatrix} \rho_{o'o'}^{(1)} \\ \rho_{o'e'}^{(1)} \\ \rho_{e'o'}^{(1)} \\ \rho_{e'e'}^{(1)} \end{pmatrix} = \begin{pmatrix} J_{oo}(\omega) \\ J_{oe}(\omega) \\ J_{eo}(\omega) \\ J_{ee}(\omega) \end{pmatrix}.$$

$$\begin{pmatrix} R_{oe}^{o'e'} & C_{oe}^{e'o'} \\ C_{eo}^{o'e'} & R_{eo}^{e'o'} \end{pmatrix} \begin{pmatrix} \rho_{o'e'}^{(1)} \\ \rho_{e'o'}^{(1)} \end{pmatrix} = \begin{pmatrix} J_{oe}(\omega) \\ J_{eo}(\omega) \end{pmatrix},$$

$$R_{oe}^{o'e'} = (E_o - E_e) \delta_{ee'} \delta_{oo'} + \left(U_{oe}^{o'e'} + U_{eo}^{e'o} - U_{oe}^{e'o} - U_{eo}^{o'e'} \right) C_{oe}^{e'o'} = U_{ee'}^{o'o} + U_{ee'}^{o'o} - U_{ee'}^{o'o} - U_{ee'}^{o'o}$$



$$\begin{aligned}\delta\langle B\rangle(\omega) &= \text{Tr}[\rho^{(1)}(\omega)B] \\ &= [\mathbf{B}_{eo} \quad \mathbf{B}_{oe}] \begin{bmatrix} \hbar\omega\mathbf{I} - \mathbf{R} & -\mathbf{C} \\ \mathbf{C}^\dagger & \hbar\omega\mathbf{I} + \mathbf{R}^* \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{A}_{eo} \\ -\mathbf{A}_{oe} \end{bmatrix}\end{aligned}$$

$$H_{\text{Hub}}=-t\sum_{i\sigma}c_{i\sigma}^\dagger c_{i+1\sigma}+\text{h.c.}+U\sum_n n_{i\uparrow}n_{i\downarrow},$$

$$i,n_{i\sigma}=c_{i\sigma}^\dagger c_{i\sigma}$$

$$\begin{aligned}H_{\text{MF}} = & -t \sum_{i\sigma} c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.} + U \sum_{i\sigma} \langle n_{i-\sigma} \rangle n_{i\sigma} \\ & - U \sum_{i\sigma} \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle c_{i\downarrow}^\dagger c_{i\downarrow} + \text{h.c.}.\end{aligned}$$

$$\omega(q)=\frac{4}{U}|\sin{(q)}|,$$

$$\begin{aligned}S_c = & \lambda \int_{k,q} [\bar{c}_{k-q} \boldsymbol{s} \cdot \boldsymbol{N}_q \tau_z c_k \\ & + (\bar{c}_{k-q} \boldsymbol{s} \cdot \boldsymbol{d}_q i s_y \tau_y \bar{c}_{-k} + \text{H.c.})]\end{aligned}$$

$$S_b=\int_q\left[\chi_N^{-1}(q)\boldsymbol{N}_q\cdot\boldsymbol{N}_{-q}+\chi_{\bar{d}}^{-1}(q)\bar{\boldsymbol{d}}_q\cdot\boldsymbol{d}_q\right]$$

$$\chi_\mu=\bar{\chi}_\mu/(r_\mu^2+\Omega_n^2+v_\mu^2\boldsymbol{q}^2), \mu=d,N$$

$$S_e = \int_k \bar{c}_{k,s,\tau} (-i\omega_n + \epsilon_{k,\tau}) c_{k,s,\tau}$$

$$S_B^{\rm eff} = S_b + S_V$$

$$S_V = \int_x V(\boldsymbol{d}(x), \boldsymbol{N}(x))$$

$$V=b_1(\overline{\boldsymbol{d}}\boldsymbol{d})^2-b_2|\boldsymbol{d}\boldsymbol{d}|^2+b_3\boldsymbol{N}^4-c_1|\boldsymbol{d}\boldsymbol{N}|^2+c_2(\overline{\boldsymbol{d}}\boldsymbol{d})\boldsymbol{N}^2.$$

$$\begin{aligned}S_B^{\text{HS}} = S_b + \int_x [& \frac{b_3\psi_d^2 + b_1\psi_N^2 + c_2\psi_d\psi_N}{4b_1b_3 - c_2^2} + \frac{|\phi_{da}|^2}{b_2} \\ & + \frac{|\phi_{dN}|^2}{c_1} + i\psi_d\overline{\boldsymbol{d}}\boldsymbol{d} + i\psi_N\boldsymbol{N}^2 \\ & + (\phi_{da}\boldsymbol{d}\boldsymbol{d} + \phi_{dN}\boldsymbol{d}\boldsymbol{N} + \text{H.c.})]\end{aligned}$$

$$\begin{aligned}S_{\psi\phi}^{\text{HS}} = & \int_q \left\{ \frac{\psi_d^2}{4b_1} + \frac{\psi_N^2}{4b_3} + \frac{|\phi_{da}|^2}{b_2} + \frac{|\phi_{dN}|^2}{c_1} \right. \\ & + \frac{3}{2} \ln [(\chi_N^{-1} + i\psi_d)[(\chi_d^{-1} + i\psi_d) - 4|\phi_{da}|^2] \\ & \left. - (\chi_d^{-1} + i\psi_d)|\phi_{dN}|^2 + \bar{\phi}_{da}\phi_{dN}^2 + \phi_{da}\bar{\phi}_{dN}^2 \right\}\end{aligned}$$

$$\begin{aligned}\frac{\psi_d^0}{b_1} &= \int_q \frac{-2i(\chi_d^{-1} + i\psi_d^0)(\chi_N^{-1} + i\psi_N) + i|\phi_{dN}^0|^2}{Q[\chi_d, \chi_N, \psi_d^0, \psi_N^0, \phi_{dd}^0, \phi_{dN}^0]} \\ \frac{\psi_N^0}{b_3} &= \int_q \frac{-i(\chi_d^{-1} + i\psi_d^0)^2 + 4i|\phi_{dd}^0|^2}{Q[\chi_d, \chi_N, \psi_d^0, \psi_N^0, \phi_{dd}^0, \phi_{dN}^0]} \\ \frac{\phi_{dd}^0}{b_2} &= \int_q \frac{2\phi_{dd}^0(\chi_N^{-1} + i\psi_N^0) - (\phi_{dN}^0)^2/2}{Q[\chi_d, \chi_N, \psi_d^0, \psi_N^0, \phi_{dd}^0, \phi_{dN}^0]} \\ \frac{\phi_{dN}^0}{c_1} &= \int_q \frac{\phi_{dN}^0(\chi_d^{-1} + i\psi_d^0)/2 - \phi_{dd}^0\bar{\phi}_{dN}^0}{Q[\chi_d, \chi_N, \psi_d^0, \psi_N^0, \phi_{dd}^0, \phi_{dN}^0]}\end{aligned}$$

$$\begin{aligned}Q &= (\chi_N^{-1} + i\psi_N^0) \left[(\chi_d^{-1} + i\psi_d^0)^2 - 4|\phi_{dd}^0|^2 \right] \\ &\quad - (\chi_d^{-1} + i\psi_d^0)|\phi_{dN}^0|^2 + \bar{\phi}_{dd}^0(\phi_{dN}^0)^2 + \phi_{dd}^0(\bar{\phi}_{dN}^0)^2\end{aligned}$$

$$r_\mu \rightarrow \tilde{r}_\mu = r_\mu + i\psi_\mu^0$$

$$S_B^{\text{HS},0} = \int_q \overline{\mathbf{B}}_q \underline{\chi}(q) \mathbf{B}_q$$

$$\mathbf{B}_q = \left(\mathbf{N}_q, \mathbf{d}_q, \overline{\mathbf{d}}_{-q}^T \right)^T \quad \overline{\mathbf{B}}_q = \left(\mathbf{N}_{-q}, \overline{\mathbf{d}}_q, \mathbf{d}_{-q}^T \right)$$

$$\underline{\chi}(q) = \begin{pmatrix} \tilde{\chi}_N^{-1}(q) & \phi_{dN}^0/2 & \bar{\phi}_{dN}^0/2 \\ \bar{\phi}_{dN}^0/2 & \tilde{\chi}_d^{-1}(q)/2 & \bar{\phi}_{dd}^0 \\ \phi_{dN}^0/2 & \phi_{dd}^0 & \tilde{\chi}_d^{-1}(q)/2 \end{pmatrix}.$$

$$\tilde{\chi}_\mu^{-1} = \chi_\mu^{-1} + i\psi_\mu^0$$

$$\int_q \rightarrow \int \mathrm{d}^2\mathbf{q}/(2\pi)^2$$

$$r_d \rightarrow r'_d = r_d + \frac{b_1}{(2\pi)^2} \int \frac{2}{q^2 + q_0^2} q \, \mathrm{d}q$$

$$\hat{\tilde{r}}_\mu = \frac{\tilde{r}_\mu}{(v_\mu q_0)^2}, \hat{\phi}_{dN}^0 = \frac{\phi_{dN}^0}{v_N q_0 v_d q_0}, \hat{\phi}_{dd}^0 = \frac{\phi_{dd}^0}{(v_d q_0)^2}$$

$$\hat{b}_1 = \frac{b_1}{2\pi v_d^4 q_0^2}, \hat{b}_2 = \frac{b_2}{2\pi v_d^4 q_0^2}, \hat{b}_3 = \frac{b_3}{2\pi v_N^4 q_0^2}, \hat{c}_1 = \frac{c_1}{2\pi v_N^2 v_d^2 q_0^2},$$

$$\tilde{r}_d = r'_d + b_1 \int_0^\infty \left[\frac{2(\tilde{r}_N + p^2)(\tilde{r}_d + p^2) - (\phi_{dN}^0)^2}{P(p, \tilde{r}_d, \tilde{r}_N, \phi_{dd}^0, \phi_{dN}^0)} - \frac{2}{p^2 + 1} \right] p \, \mathrm{d}p$$

$$\tilde{r}_N = r'_N + b_3 \int_0^\infty \left[\frac{(\tilde{r}_d + p^2)^2 - 4(\phi_{dd}^0)^2}{P(p, \tilde{r}_d, \tilde{r}_N, \phi_{dd}^0, \phi_{dN}^0)} - \frac{1}{p^2 + 1} \right] p \, \mathrm{d}p$$

$$\phi_{dd}^0 = b_2 \int_0^\infty \frac{2\phi_{dd}^0(\tilde{r}_N + p^2) - (\phi_{dN}^0)^2/2}{P(p, \tilde{r}_d, \tilde{r}_N, \phi_{dd}^0, \phi_{dN}^0)} p \, \mathrm{d}p$$

$$\phi_{dN}^0 = c_1 \int_0^\infty \frac{2\phi_{dN}^0(\tilde{r}_d + p^2)/2 - \phi_{dd}^0\phi_{dN}^0}{P(p, \tilde{r}_d, \tilde{r}_N, \phi_{dd}^0, \phi_{dN}^0)} p \, \mathrm{d}p$$

$$P(p,\tilde{r}_d,\tilde{r}_N,\phi_{dd}^0,\phi_{dN}^0)=(\tilde{r}_N+p^2)\left[(\tilde{r}_d+p^2)^2-4(\phi_{dd}^0)^2\right]-(\tilde{r}_d+p^2)(\phi_{dN}^0)^2+2\phi_{dd}^0(\phi_{dN}^0)^2$$

$$\tilde{r}_d=r'_d-\frac{b_1}{2}\ln\left(\tilde{r}_d^2-4(\phi_{dd}^0)^2\right)$$

$$\tilde{r}_N=r'_N-\frac{b_3}{2}\ln\tilde{r}_N$$

$$\phi_{dd}^0=\phi_{dd}^0\frac{b_2}{2|\phi_{dd}^0|}\operatorname{arccoth}\left(\frac{\tilde{r}_d}{2|\phi_{dd}^0|}\right)$$

$$|\phi_{dd}^0|<\tilde{r}_d/2$$

$$r'_d=2|\phi_{dd}^0|\coth\left(\frac{2|\phi_{dd}^0|}{b_2}\right)+b_1\ln\left(\frac{2|\phi_{dd}^0|}{\sinh\left(2|\phi_{dd}^0|/b_2\right)}\right)$$

$$S_V^0=\int_q\left[\phi_{dN}^0\boldsymbol{d}_q\cdot\boldsymbol{N}_{-q}+\phi_{dd}^0\boldsymbol{d}_q\cdot\boldsymbol{d}_{-q}+\text{H.c.}\right]$$

$$\tilde{S}^{(A/B)}=S_e+S_1^{(A/B)}+S_2^{(A/B)}+S_{\phi}^{(A/B)}$$

$$S_1^{(A/B)}=\int_q p_1^{(A/B)}(q)(\boldsymbol{S}_q\boldsymbol{S}_{-q}+\text{H.c.})$$

$$S_2^{(A/B)}=\int_q p_2^{(A/B)}(q)(\overline{\boldsymbol{D}}_q\boldsymbol{D}_q+\text{H.c.})$$

$$\boldsymbol{S}_q\!=\!\int_k\bar{c}_{k+q}\boldsymbol{s}\tau_zc_k=\int_k\bar{\psi}_{k+q}\boldsymbol{s}\psi_k$$

$$\boldsymbol{D}_q=\int_kc_{k+q}(-is_y\boldsymbol{s})\tau_y c_{-k}=-2i\int_k\bar{\psi}_{k+q}\boldsymbol{s}\gamma_-\psi_k$$

$$\overline{\boldsymbol{D}}_q=\int_k\bar{c}_{k+q}\boldsymbol{s}is_y\tau_y\bar{c}_{-k}=2i\int_k\bar{\psi}_{k+q}\boldsymbol{s}\gamma_+\psi_k$$

$$\psi_k=(c_{k,+},is_y\bar{c}_{-k,-})^T$$

$$\gamma_{\pm}=(\gamma_x\pm i\gamma_y)/2$$

$$p_1^{(A)}(q)=-\frac{\lambda^2}{4\chi_N^{-1}(q)},p_2^{(A)}=-\frac{\lambda^2\chi_d^{-1}(q)}{2\left(\chi_d^{-2}(q)-4|\phi_{dd}^0|^2\right)},$$

$$p_1^{(B)}(q)=-\frac{\lambda^2\chi_d^{-1}(q)}{4\left(\chi_d^{-1}(q)\chi_N^{-1}(q)-|\phi_{dN}^0|^2\right)}$$

$$p_2^{(B)}(q)=-\frac{\lambda^2\chi_N^{-1}(q)}{2\left(\chi_d^{-1}(q)\chi_N^{-1}(q)-|\phi_{dN}^0|^2\right)}$$

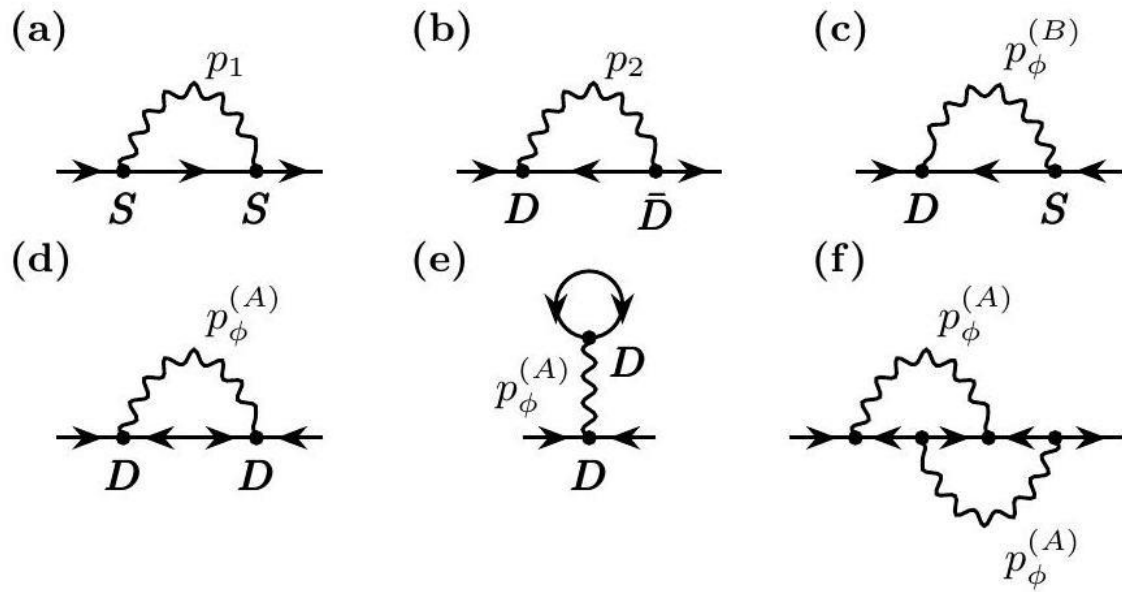
$$S_{\phi}^{(A)}=\int_q\left[p_{\phi}^{(A)}(q)\boldsymbol{D}_{-q}\boldsymbol{D}_q+\text{H.c.}\right]$$

$$p_{\phi}^{(A)}(q) = \frac{\lambda^2 \phi_{dd}^0}{(\chi_d^{-2}(q) - 4|\phi_{dd}^0|^2)}$$

$$\mathbf{D}_{-q} \mathbf{D}_q \rightarrow e^{4i\varphi} \mathbf{D}_{-q} \mathbf{D}_q$$

$$S_{\phi}^{(B)} = \int_q \left[p_{\phi}^{(B)}(q) \mathbf{S}_q \mathbf{D}_q + \text{H.c.} \right]$$

$$p_{\phi}^{(B)}(q) = \frac{\lambda^2 \phi_{dN}^0}{2(\chi_d^{-1}(q) \chi_N^{-1}(q) - 4|\phi_{dN}^0|^2)}$$



$$\Sigma_1(k) = 6 \int_q p_1^{(A,B)}(q) \gamma_z G_{0,k+q} \gamma_z$$

$$G_{0,k}^{-1} = i\omega_n \gamma_0 - \epsilon_k \gamma_z$$

$$\Sigma_2(k) = -24 \int_q p_2^{(A,B)}(q) (\gamma_- G_{0,k+q} \gamma_+ + \gamma_+ G_{0,k+q} \gamma_-).$$

$$\Sigma_{\phi}(k) = 24 \int_q p_{\phi}^{(A)}(q) (\gamma_+ G_{0,k+q} \gamma_+ + \gamma_- G_{0,k+q} \gamma_-) = 0$$

$$\tilde{p}_2^{(A)}(\boldsymbol{q}) = \left(p_2^{(A)}(q) \right)_{\Omega_n=0} = -\frac{\lambda}{2} \frac{R_d(\boldsymbol{q})}{R_d^2(\boldsymbol{q}) - 4(\phi_{dd}^0)^2}$$

$$R_d(\boldsymbol{q}) = r_d + (v_d \boldsymbol{q})^2$$

$$\left(\Sigma_{\boldsymbol{k}}^{(2)}\right)_{11} = -24T \int_q \tilde{p}_2^{(A)}(\boldsymbol{q}) \frac{1}{\omega + \epsilon_{\boldsymbol{k}+\boldsymbol{q}} + i0^+}$$

$$\begin{aligned}\mathcal{I}m\left[\Sigma_{\mathbf{k}}^{(2)}(\omega)\right] &= 24\pi T\int_{\mathbf{q}}\tilde{p}_2^{(A)}(\mathbf{q})\delta(\omega+\epsilon_{\mathbf{k}+\mathbf{q}}) \\ &= \tilde{g}T\sum_{p=\pm}\frac{1}{\sqrt{\beta_p+(\omega+\epsilon_{\mathbf{k}})^2}}\end{aligned}$$

$$\epsilon_{\mathbf{k}+\mathbf{q}}\simeq\epsilon_{\mathbf{k}}+v_Fq_{||}$$

$$q_{||}=\mathbf{k}\cdot\mathbf{q}/|\mathbf{k}|$$

$$\beta_{\pm}=(v_F/v_d)^2(\tilde{r}_d\pm2\phi_{dd}^0)$$

$$\begin{aligned}\mathcal{R}e\left[\Sigma_{\mathbf{k}}^{(2)}(\omega)\right] &= \frac{1}{\pi}\int_{-\infty}^{\infty}d\omega'\frac{\mathcal{I}m\left[\Sigma_{\mathbf{k}}^{(3)}(\omega')\right]}{\omega'-\omega} \\ &\propto \sum_{p=\pm}\frac{\tilde{g}T}{\sqrt{\beta_p+(\omega+\epsilon_{\mathbf{k}})^2}}\ln\left|\frac{\omega+\epsilon_{\mathbf{k}}+\sqrt{\beta_p+(\omega+\epsilon_{\mathbf{k}})^2}}{\omega+\epsilon_{\mathbf{k}}-\sqrt{\beta_p+(\omega+\epsilon_{\mathbf{k}})^2}}\right|\end{aligned}$$

$$\mathcal{R}e[\Sigma^{(2)}] \sim 2 \sum_p \tilde{g}T(\omega+\epsilon_{\mathbf{k}})/\beta_p$$

$$\mathcal{R}e[\Sigma^{(2)}] \sim 2 \Sigma_p \tilde{g}T(\omega+\epsilon_{\mathbf{k}})/\beta_p$$

$$-\mathcal{I}m[\Sigma_{\text{AFM}}] \propto T \int_{\mathbf{q}} \delta(\omega-\epsilon_{\mathbf{k}+\mathbf{q}}) \frac{1}{(\mathbf{q}-\mathbf{Q})^2+\xi^{-2}}$$

$$\begin{aligned}H_{\phi} &= 4g_{\phi}\int_{\mathbf{k}_1,\mathbf{k}_2}(\psi_{\mathbf{k}_1}^{\dagger}\boldsymbol{s}\gamma_{+}\psi_{\mathbf{k}_1})\cdot(\psi_{\mathbf{k}_2}^{\dagger}\boldsymbol{s}\gamma_{+}\psi_{\mathbf{k}_2})+\text{H.c.}\\ H_2 &= 8g_2\int_{\mathbf{k}_1,\mathbf{k}_2}(\psi_{\mathbf{k}_1}^{\dagger}\boldsymbol{s}\gamma_{+}\psi_{\mathbf{k}_1})\cdot(\psi_{\mathbf{k}_2}^{\dagger}\boldsymbol{s}\gamma_{-}\psi_{\mathbf{k}_2})\end{aligned}$$

$$\psi_{\mathbf{k}} = \left(c_{\mathbf{k},+}, i s_y c_{-\mathbf{k},-}^{\dagger}\right)^T$$

$$g_{\phi}=p_{\phi}^{(A)}(q=0) \text{ and } g_2=p_2^{(A)}(q=0)$$

$$p_{\phi}^{(A)}\propto\phi_{dd}^0$$

$$H_0=\int_{\mathbf{k}}\psi_{\mathbf{k}}^{\dagger}\epsilon_{\mathbf{k}}\gamma_z\psi_{\mathbf{k}}$$

$$(\underline{\mathcal{C}}_{\mathbf{k}})_{ij}=\left\langle (\psi_{\mathbf{k}}^{\dagger})_j(\psi_{\mathbf{k}})_i\right\rangle$$

$$H_{\text{MF}} = H_0 - 24 \int_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger (g_\phi [\gamma_+ \cdot \underline{\mathbf{C}}_{\mathbf{k}} \cdot \gamma_+ + \text{H.c.}] + g_2 ([\gamma_- \cdot \underline{\mathbf{C}}_{\mathbf{k}} \cdot \gamma_+ + \text{H.c.}] - \gamma_+ \cdot \gamma_-)) \psi_{\mathbf{k}}$$

$$\underline{\mathbf{C}}_{\mathbf{k}} = \frac{1}{2} \gamma_0 + C_{\mathbf{k}}^z \gamma_z - \text{Im}[C_{\mathbf{k}}] \gamma_y + \text{Re}[C_{\mathbf{k}}] \gamma_x$$

$$H_{\text{MF}} = \int_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger \begin{pmatrix} \tilde{\epsilon}_{\mathbf{k}} & -\Delta_{\mathbf{k}}^* \\ -\Delta_{\mathbf{k}} & -\tilde{\epsilon}_{\mathbf{k}} \end{pmatrix} \psi_{\mathbf{k}}$$

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \delta\epsilon_{\mathbf{k}} + 12g_2$$

$$\delta\epsilon_{\mathbf{k}} = 24g_2C_{\mathbf{k}}^z$$

$$\Delta_{\mathbf{k}} = 24g_\phi C_{\mathbf{k}}$$

$$(\underline{\mathbf{C}}_{\mathbf{k}})_{ij} = \mathbb{I}_{ij} - \frac{\text{Tr}[(\psi_{\mathbf{k}})_i (\psi_{\mathbf{k}}^\dagger)_j] e^{-\beta H_{\text{MF}}}}{\text{Tr}[e^{-\beta H_{\text{MF}}}]}$$

$$\underline{\mathbf{C}}_{\mathbf{k}} = \frac{1}{2} \gamma_0 + \frac{1}{4} t(\beta E_{\mathbf{k}}/2) \beta \begin{pmatrix} -\tilde{\epsilon}_{\mathbf{k}} & \Delta_{\mathbf{k}}^* \\ \Delta_{\mathbf{k}} & \tilde{\epsilon}_{\mathbf{k}} \end{pmatrix}$$

$$t(x) = \tanh(x)/x$$

$$E_{\mathbf{k}} = \sqrt{\tilde{\epsilon}_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$$

$$\Delta_{\mathbf{k}} = 6\beta g_\phi t(\beta E_{\mathbf{k}}/2) \Delta_{\mathbf{k}}^*$$

$$\delta\epsilon_{\mathbf{k}} = -6\beta g_2 t(\beta E_{\mathbf{k}}/2) (\epsilon_{\mathbf{k}} + \delta\epsilon_{\mathbf{k}})$$

$$\frac{1}{6\beta g_\phi} = t(\beta E_{\mathbf{k}}/2)$$

$$\delta\epsilon_{\mathbf{k}} = -12g_2 \tanh(\beta \tilde{\epsilon}_{\mathbf{k}}/2)$$

$$\tilde{\epsilon}_{\mathbf{k}} \sim \left(1 + \frac{6\beta |g_2|}{1 - 6\beta |g_2|}\right) \epsilon_{\mathbf{k}}, \epsilon_{\mathbf{k}} \rightarrow 0$$

$$\frac{1}{6\beta |g_2|} = t(\beta \delta\epsilon_{\mathbf{k}}/2)$$

$$T^*/T_c = |g_2/g_\phi|$$

$$|g_2/g_\phi| > 1 \text{ and } |g_2/g_\phi| < 1$$

$$\begin{aligned} \Delta_{\mathbf{k}} &= \beta \tilde{g}_\phi t(\beta E_{\mathbf{k}}/2) \tilde{\epsilon}_{\mathbf{k}} \\ \tilde{\epsilon}_{\mathbf{k}} &= \epsilon_{\mathbf{k}} + \beta \tilde{g}_\phi t(\beta E_{\mathbf{k}}/2) \Delta_{\mathbf{k}} \end{aligned}$$

$$p_\phi^{(A)}(q)\Big|_{i\Omega_n\rightarrow 0} \bar{p}_\phi^{(A)}(q)$$

$$H_{\text{MF}}^{(A)}=H_0-24\int_{\boldsymbol{q},\boldsymbol{k}}\bar{p}_{\phi}^{(A)}(\boldsymbol{q})\psi_{\boldsymbol{k}}^{\dagger}(\boldsymbol{\gamma}_+\cdot\boldsymbol{\underline{C}}_{\boldsymbol{k}+\boldsymbol{q}}\cdot\boldsymbol{\gamma}_++\text{H.c.})\psi_{\boldsymbol{k}}.$$

$$\Delta_{\boldsymbol{k}}=6\int_{\boldsymbol{q}}\beta\bar{p}_{\phi}^{(A)}(\boldsymbol{q})t(\beta E_{\boldsymbol{k}}/2)\Delta_{\boldsymbol{k}+\boldsymbol{q}}^*$$

$$E_{\boldsymbol{k}}=\sqrt{\epsilon_{\boldsymbol{k}}^2+\left(\sum_{\boldsymbol{q}}24p_{\phi}^{(A)}(\boldsymbol{q})\Delta_{\boldsymbol{k}+\boldsymbol{q}}\right)^2}$$

$$\bar{p}_{\phi}^{(A)}(\boldsymbol{q})=\delta(\boldsymbol{q})g_{\phi}$$

$$\sum_{\boldsymbol{q}}\bar{p}_{\phi}^{(A)}(\boldsymbol{q})=g_{\phi}.$$

$$\bar{p}_{\phi}^{(A)}(\boldsymbol{q})\in\mathbb{R}^+$$

$$p_{\phi}^{(B)}(q)\big|_{i\Omega_n\rightarrow 0}$$

$$\Delta_{\boldsymbol{k}}=\frac{1}{4}\int_{\boldsymbol{q}}\beta\bar{p}_{\phi}^{(B)}(\boldsymbol{q})t(\beta E_{\boldsymbol{k}+\boldsymbol{q}}/2)\tilde{\epsilon}_{\boldsymbol{k}+\boldsymbol{q}}$$

$$\tilde{\epsilon}_{\boldsymbol{k}}=\epsilon_{\boldsymbol{k}}+\frac{1}{4}\int_{\boldsymbol{q}}\beta\bar{p}_{\phi}^{(B)}(\boldsymbol{q})t(\beta E_{\boldsymbol{k}+\boldsymbol{q}}/2)\Delta_{\boldsymbol{k}+\boldsymbol{q}}$$

$$E_{\boldsymbol{k}}=\sqrt{\tilde{\epsilon}_{\boldsymbol{k}}+\Delta_{\boldsymbol{k}}}$$

$$\bar{p}_{\phi}^{(B)}(\boldsymbol{q})=\delta(\boldsymbol{q})\tilde{g}_{\phi}$$

$$\boldsymbol{M}=-\frac{ie}{2\hbar V}\sum_{n\boldsymbol{k}}f_{n\boldsymbol{k}}\Big\langle\frac{\partial u_{n\boldsymbol{k}}}{\partial\boldsymbol{k}}\Big|\times\big[\hat{H}_0(\boldsymbol{k})+\epsilon_n(\boldsymbol{k})-2\mu\big]\Big|\frac{\partial u_{n\boldsymbol{k}}}{\partial\boldsymbol{k}}\Big\rangle,$$

$$\left|\delta\phi_{\alpha}^{(1)}\right\rangle=\sum_{\beta\neq\alpha}\frac{\left|\phi_{\beta}\right\rangle\left\langle\phi_{\beta}\right|\hat{V}_{\text{ext}}|\phi_{\alpha}\rangle}{\epsilon_{\alpha}-\epsilon_{\beta}}$$

$$\left|\delta\phi_{\alpha}^{(2)}\right\rangle=\sum_{\beta\neq\alpha}\frac{\left|\phi_{\beta}\right\rangle\left\langle\phi_{\beta}\right|\delta\hat{H}_{\text{HF}}|\phi_{\alpha}\rangle}{\epsilon_{\alpha}-\epsilon_{\beta}}$$

$$\boldsymbol{B}(\boldsymbol{r})=B\text{cos}\left(\boldsymbol{q}\cdot\boldsymbol{r}\right)\boldsymbol{e}_z$$

$$\boldsymbol{A}(\boldsymbol{r})=-B\text{sin}\left(\boldsymbol{q}\cdot\boldsymbol{r}\right)\boldsymbol{e}_x/q$$

$$\hat{V}_B=e[\hat{\boldsymbol{v}}_0\cdot\boldsymbol{A}(\boldsymbol{r})+\boldsymbol{A}(\boldsymbol{r})\cdot\hat{\boldsymbol{v}}_0]/2$$

$$\hat{\boldsymbol{v}}_0=-i[\hat{\boldsymbol{r}},\hat{H}]/\hbar=-i[\hat{\boldsymbol{r}},\hat{H}_0]/\hbar$$

$$\delta K(\boldsymbol{r}) = -\boldsymbol{M} \cdot \boldsymbol{B}(\boldsymbol{r}),$$

$$\delta K(\boldsymbol{r}) = \frac{1}{2} \left[\sum_{\alpha} f_{\alpha} \langle \phi_{\alpha} | \{ (\hat{H}_{\text{HF}} - \mu \hat{N}), \delta(\hat{\boldsymbol{r}} - \boldsymbol{r}) \} | \delta \phi_{\alpha} \rangle + c.c. \right] \\ + \frac{1}{2} \sum_{nk} f_{\alpha} \langle \phi_{\alpha} | \{ \hat{V}_B, \delta(\hat{\boldsymbol{r}} - \boldsymbol{r}) \} | \phi_{\alpha} \rangle.$$

$$M_z^{(1)} = \lim_{q \rightarrow 0} \frac{e}{4qV} \text{Im} \sum_{nn'k} [(\epsilon_{nk} + \epsilon_{n'k+q} - 2\mu) \langle u_{nk} | u_{n'k+q} \rangle \\ \langle u_{n'k+q} | \hat{v}_{0,x}(\boldsymbol{k} + \boldsymbol{q}) + \hat{v}_{0,x}(\boldsymbol{k}) | u_{nk} \rangle \left[\frac{f_{nk} - f_{n'k+q}}{\epsilon_{nk} - \epsilon_{n'k+q}} \right],$$

$$\hat{v}_{0,x}(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \hat{v}_{0,x} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$\left| \delta \phi_{nk}^{(2)} \right\rangle \delta \hat{H}_{\text{HF}} = e \hat{\boldsymbol{v}}_{\text{MF}} \cdot \boldsymbol{A}$$

$$\hat{\boldsymbol{v}}_{\text{MF}} = -i[\hat{\boldsymbol{r}}, \hat{H}_{\text{MF}}]/\hbar$$

$$\boldsymbol{A}(\boldsymbol{r}), \delta \hat{H}_{\text{HF}} \approx e[\hat{\boldsymbol{v}}_{\text{MF}} \cdot \boldsymbol{A}(\hat{\boldsymbol{r}}) + \boldsymbol{A}(\hat{\boldsymbol{r}}) \cdot \hat{\boldsymbol{v}}_{\text{MF}}]/2$$

$$\hat{\boldsymbol{v}}_{\text{HF}} = \hat{\boldsymbol{v}}_0 + \hat{\boldsymbol{v}}_{\text{MF}} = -i[\hat{\boldsymbol{r}}, \hat{H}_{\text{HF}}]/\hbar$$

$$\boldsymbol{M} = -\frac{ie}{2\hbar V} \sum_{nk} f_{nk} \left\langle \frac{\partial u_{nk}}{\partial \boldsymbol{k}} \right| \times [\hat{H}_{\text{HF}}(\boldsymbol{k}) + \epsilon_{nk} - 2\mu] \left| \frac{\partial u_{nk}}{\partial \boldsymbol{k}} \right\rangle.$$

$$\delta \hat{H}_{\text{HF}} \approx e[\hat{\boldsymbol{v}}_{\text{MF}} \cdot \boldsymbol{A}(\hat{\boldsymbol{r}}) + \boldsymbol{A}(\hat{\boldsymbol{r}}) \cdot \hat{\boldsymbol{v}}_{\text{MF}}]/2$$

$$\hat{H}^{\text{KMH}} = \sum_{\langle i,j \rangle, \sigma} t_1 \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{\langle\langle i,j \rangle\rangle, \sigma} t_2 e^{i\sigma v_{ij}\theta} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \\ + \sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{\langle i,j \rangle, \sigma} V \hat{n}_{i\sigma} \hat{n}_{j\sigma'}$$

$$\Delta M/\Delta\mu=Ce/h$$

$$\boldsymbol{M} = -\partial K(\boldsymbol{B})/\partial \boldsymbol{B}$$

$$t_{ij} \rightarrow t_{ij} \exp \left[i(e/\hbar) \int_{r_i}^{r_j} \boldsymbol{A}(\boldsymbol{r}) d\boldsymbol{r} \right]$$

$$|v\rangle = Q_v^\dagger |0\rangle = \sum_{ph} [X_{ph}^\nu B_{ph}^\dagger - Y_{ph}^\nu B_{ph}] |0\rangle.$$

$$B_{ph}^\dagger = D_{ph}^{-1/2} a_p^\dagger a_h$$

$$D_{ph} = n_h - n_p,$$

$$n_r = \langle 0 | a_r^\dagger a_r | 0 \rangle$$

$$Q_\nu|0\rangle=0.$$

$$\left(\begin{array}{cc} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{array}\right)\left(\begin{array}{c} X^\nu \\ Y^\nu \end{array}\right)=\hbar\omega_\nu\left(\begin{array}{c} X^\nu \\ Y^\nu \end{array}\right),$$

$$\begin{aligned}\mathcal{A}_{ph,p'h'} &= \langle 0| \left[B_{ph}, H, B_{p'h'}^\dagger \right] |0\rangle \\ \mathcal{B}_{ph,p'h'} &= -\langle 0| \left[B_{ph}^\dagger, H, B_{p'h'}^\dagger \right] |0\rangle\end{aligned}$$

$$[A,B,C]=\frac{1}{2}([A,[B,C]]+[[A,B],C]).$$

$$\begin{aligned}\mathcal{A}_{ph,p'h'}=&\mathcal{D}_{php'h'}(\epsilon_{pp'}\delta_{hh'}-\epsilon_{hh'}\delta_{pp'})\\&+D_{ph}^{1/2}D_{p'h'}^{1/2}\langle hp'|V|ph'\rangle\\ \mathcal{B}_{ph,p'h'}=&D_{ph}^{1/2}D_{p'h'}^{1/2}\langle hh'|V|pp'\rangle\end{aligned}$$

$$\begin{aligned}\mathcal{D}_{php'h'}&=\frac{1}{2}\Big(D_{ph}^{1/2}D_{p'h'}^{-1/2}+D_{ph}^{-1/2}D_{p'h'}^{1/2}\Big)\\ \epsilon_{pp'}&=\langle p'|t|p\rangle+\sum_r n_r\langle p'r|V|pr\rangle\\&+\frac{1}{2}\sum_{r,s} n_r n_s\langle p'rs|V|prs\rangle\\ \epsilon_{hh'}&=\langle h|t|h'\rangle+\sum_r n_r\langle hr|V|h'r\rangle\\&+\frac{1}{2}\sum_{r,s} n_r n_s\langle hrs|V|h'rs\rangle\end{aligned}$$

$$\begin{aligned}\langle 0|a_p^\dagger a_{p'}|0\rangle &= \sum_{\nu,\mu,h}\left[\delta_{\nu\mu}-\frac{1}{2}\sum_{q,g}D_{qg}X_{qg}^\mu X_{qg}^{\nu*}\right.\\&\quad\cdot D_{ph}^{1/2}D_{p'h}^{1/2}Y_{ph}^\nu Y_{p'h}^{\mu*}+\mathcal{O}(|Y|^6)\\ \langle 0|a_h^\dagger a_{h'}|0\rangle &= \delta_{hh'}-\sum_{\nu,\mu,p}\left[\delta_{\nu\mu}-\frac{1}{2}\sum_{q,g}D_{qg}X_{qg}^\mu\right.\\&\quad\cdot X_{qg}^{\nu*}]D_{ph}^{1/2}D_{ph'}^{1/2}Y_{ph}^\nu Y_{ph'}^{\mu*}+\mathcal{O}(|Y|^6)\\ \langle \nu|F|0\rangle &= \sum_{p,h}D_{ph}^{1/2}(X_{ph}^{\nu*}\langle p|F|h\rangle+Y_{ph}^{\nu*}\langle h|F|p\rangle).\end{aligned}$$

$$E_0=E_{\rm HF}+E_{\rm corr}\,,$$

$$E_{\rm corr}=-\sum_\nu\hbar\omega_\nu\sum_{p,h}|Y_{ph}|^2$$

$$\langle r_\tau^2 \rangle = \frac{1}{N_\tau} \langle 0 | \sum_{i=1}^{N_\tau} \left(\vec{r}_\tau(i) - \vec{R}_{\rm c.m.} \right)^2 | 0 \rangle$$

$$\dot{\rho} = -i[H_0 + u_a H_a]\rho + D_{ab}\left(H_a \rho H_b - \frac{1}{2}\{H_a H_b, \rho\}\right).$$

$$C[u] = \frac{Q}{2} \text{Tr}(H_{\text{target}} \, \rho(T)) + \frac{1}{2} \int_0^T u(t)^\top R u(t) dt$$

$$d\psi(t) = -iH_0\psi(t)dt - iH_a\psi(t)(u_a(t)dt + dW_a(t)) \\ - \frac{1}{2}D_{ab}H_aH_b\psi(t)dt$$

$$\mathbb{E}(dW_a(t)dW_b(t))=D_{ab}dt$$

$$d\|\psi(t)\|^2=0$$

$$\rho(t) = \mathbb{E}(\psi(t)\psi(t)^\dagger)$$

$$C[u] = \mathbb{E}(S^u)$$

$$S^u = \frac{Q}{2} \langle \psi(T) | H_{\text{target}} | \psi(T) \rangle + \frac{1}{2} \int_0^T u(t)^\top R u(t)$$

$$+ \frac{1}{2} \int_0^T u(t)^\top R dW(t)$$

$$\rho(T) = \mathbb{E}(\psi(T)\psi(T)^\dagger)$$

$$u_a(t) = \sum_{k=1}^K u_{ak} \mathbf{1}_{I_k}(t) \; a = 1, \ldots, n_c$$

$$u_{ak}^{(p+1)} = u_{ak}^{(p)} + \mathbb{E}\Big(\omega^{(p)}\frac{\Delta W_{ak}}{\Delta t_k}\Big), k = 1, \ldots, K$$

$$\Delta W_{ak}\!:=\!\int_{I_k}dW_a(t), \Delta t_k=t_k-t_{k-1}$$

$$\omega^{(p)}\!:=\!\frac{e^{-S^{(p)}/\lambda}}{\mathbb{E}(e^{-S^{(p)}/\lambda})}$$

$$D_j \leftarrow D_{\text{init}} \times \left(\frac{D_{\text{final}}}{D_{\text{init}}}\right)^{j/(n_D-1)}$$

$$E^{(i)} = \langle \psi(T)^{(i)} | H | \psi(T)^{(i)} \rangle \text{ for } i = 1, \ldots, N_{\text{traj}}$$

$$E = \min_i E^{(i)}$$



$$E(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | H_{\text{target}} | \psi(\boldsymbol{\theta}) \rangle$$

$$U(\boldsymbol{\theta}) = \prod_{\ell=1}^L [V^{(\ell)} R^{(\ell)}(\boldsymbol{\theta}_{\ell})]$$

$$R^{(\ell)}(\boldsymbol{\theta}_{\ell}) = \prod_{m=1}^M \prod_{q=1}^n R_{q,m}^{(\ell)}(\theta_{q,m}^{(\ell)})$$

$$d\psi(t) = -i \sum_{\ell} f^{(\ell)}(t) H_0^{(\ell)} \psi(t) dt$$

$$f^{(\ell)}(t) \text{ and } g_m^{(\ell)}(t) \text{ are}$$

$$f^{(\ell)}(t) = \begin{cases} 1, & \text{if } t \in J^{(\ell)} \\ 0, & \text{otherwise} \end{cases}$$

$$g_m^{(\ell)}(t) = \begin{cases} 1, & \text{if } t \in I_m^{(\ell)} \\ 0, & \text{otherwise,} \end{cases}$$

$$R_{q,m}^{(\ell)}(\theta_{q,m}^{(\ell)}) = e^{-i\theta_{q,m}^{(\ell)} H_{q,m}^{(\ell)}/2}$$

$$H_{q,m}^{(\ell)} \in \{\sigma_q^x, \sigma_q^y, \sigma_q^z\}$$

$$I_m^{(\ell)} = [(\ell-1)(M+1) + m - 1, \\ (\ell-1)(M+1) + m],$$

$$J^{(\ell)} = [(\ell-1)(M+1) + M, \\ (\ell-1)(M+1) + M + 1].$$

$$dW_q(t)\mathbb{E}(dW_q(t)dW_{q'}(t))=\delta_{q,q'}Ddt$$

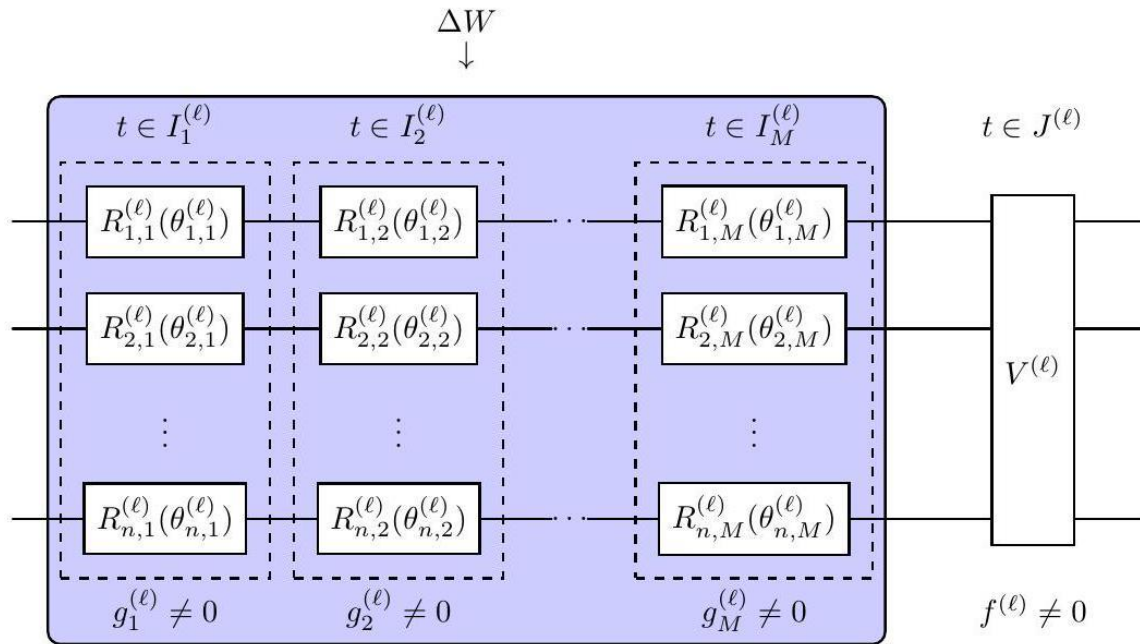
$$\tilde{\theta}_{q,m}^{(\ell)} = \theta_{q,m}^{(\ell)} + \Delta W_{q,m}^{(\ell)}$$

$$V^{(\ell)} = e^{-iH_0^{(\ell)}}$$

$$\Delta W_{q,m}^{(\ell)} = \int_{I_m^{(\ell)}} dW_q(t)$$

$$H_{eff}(t) = \frac{1}{2} \int_{t_m^{(\ell)}}^t \sum_q \left(\theta_{q,m}^{(\ell)} dt + dW_q(t) \right) H_{q,m}^{(\ell)}$$





$$\psi(t)=e^{-iH_{\text{eff}}\left(t-t_m^{(\ell)}\right)}\psi\left(t_m^{(\ell)}\right)$$

$$d\psi(t)=-\sum_q\left[\frac{i}{2}\Big(\theta_{q,m}^{(\ell)}dt+dW_q(t)\Big)H_{q,m}^{(\ell)}\psi(t)+\frac{1}{8}D\psi(t)dt\right]$$

$$\prod_{q=1}^n e^{-i\tilde{\theta}_{q,m}^{(\ell)}H_{q,m}^{(\ell)}/2}$$

$$I^{(\ell)}\!:=\bigcup_{m=1}^M I_m^{(\ell)}$$

$$R^{(\ell)}(\tilde{\boldsymbol{\theta}}_l)J^{(\ell)}I^{(\ell)}f^{(\ell)}(t)g_m^{(\ell)}(t)$$

$$\boldsymbol{\theta}=\left\{\theta_{q,m}^{(\ell)}\right\}$$

$$S^{\boldsymbol{\theta}} = \frac{Q}{2} \langle \psi(\boldsymbol{\theta}) | H_{\text{target}} | \psi(\boldsymbol{\theta}) \rangle + \frac{R}{2} \boldsymbol{\theta}^\top \boldsymbol{\theta} + \frac{R}{2} \boldsymbol{\theta}^\top \Delta \boldsymbol{W}.$$

$$\boldsymbol{\theta}^{(p+1)} = \boldsymbol{\theta}^{(p)} + \mathbb{E}\big(\omega^{(p)}\Delta\boldsymbol{W}\big),$$

$$\boldsymbol{\Delta W} = \left\{ \Delta W_{q,m}^{(\ell)} \right\}$$

$$\omega^{(p)}=\frac{e^{-S^{(p)}/\lambda}}{\mathbb{E}\big(e^{-S^{(p)}/\lambda}\big)}$$

$$|\psi(\boldsymbol{\theta}+\Delta\boldsymbol{W})\rangle\Delta W_{q,m}^{(\ell)}=\int_{I_m^{(\ell)}}dW_q(t)$$

$$D\left|I_m^{(\ell)}\right|=D$$

$$\boldsymbol{\theta}^{(j+1)}=\boldsymbol{\theta}^{(j)}-a_j\hat{\boldsymbol{g}}_j$$

$$\hat{\boldsymbol{g}}_j=\frac{E(\boldsymbol{\theta}^{(j)}+c_j\boldsymbol{\Delta}_j)-E(\boldsymbol{\theta}^{(j)}-c_j\boldsymbol{\Delta}_j)}{2c_j}\boldsymbol{\Delta}_j^{-1}$$

$$H_0=\sum_{i< j}\frac{C_6}{r_{ij}^6}|11\rangle_{ij}\langle 11|$$

$$\frac{\Omega(t)}{2}(e^{i\phi(t)}|0\rangle\langle 1|+e^{-i\phi(t)}|1\rangle\langle 0|).$$

$$H_c(t)=\sum_{q=1}^n\left(u_{qx}(t)\sigma_q^x+u_{qy}(t)\sigma_q^y\right)$$

$$V^{(\ell)}=e^{-i\tau_VH_0}$$

$$H_{q,m}^{(\ell)}=\sigma_q^z,\sigma_q^x,\sigma_q^z$$

$$T_{\rm GB}=L(\tau_g+\tau_V)$$

$$u_a(t)=\sum_{k=1}^KA_{ak}h_k(t)\;a=1,\ldots,n_c$$

$$A^{(p+1)}=A^{(p)}+C^{(p)}B^{-1}$$

$$B_{kk'}\,=\,\int_0^T\,h_k(t)h_{k'}(t)dt$$

$$C_{ak}^{(p)}=\mathbb{E}\left(\omega^{(p)}\int_0^Th_k(t)dW_a(t)\right)$$

$$u_q(t)=\sum_{m,\ell}\theta_{q,m}^{(\ell)}g_m^{(\ell)}(t)\;q=1,\ldots,n$$

$$a_k=\frac{a}{(A+k+1)^\alpha}$$

$$c_k=\frac{c}{(k+1)^\gamma}$$

$$d\psi_t=f(t,\psi_t)dt+g(t,\psi_t)(u(t)dt+dW(t))$$

$$2\hbar\omega+[0]\rightarrow 1s(n,x)p+\hbar\omega\rightarrow 1s\varepsilon l.$$

$$\hat{C} \sim \sum_{n=1}^N (\hat{A}_n \cdot \hat{A}_n)$$

$$\hat{A}_n \rightarrow \sum_{\mathbf{k}} \sum_{\rho=1,2} \mathbf{e}_{\mathbf{k}\rho} (\hat{a}_{\mathbf{k}\rho}^+ + \hat{a}_{\mathbf{k}\rho}^-)$$

$$(\mathbf{k}\cdot\mathbf{r}_n)\ll1\Rightarrow\exp\left[\pm i(\mathbf{k}\cdot\mathbf{r}_n)\right]\cong1,\\r_{1s}/\lambda_{\omega}\ll1.$$

$$\begin{aligned} A_l &= A_l^{(1)} + A_l^{(2)} \\ A_l^{(1)} &= \sum_{M'} \sum_{N=2}^{\infty} \frac{\langle 0|\hat{R}|\Phi_n\rangle \langle \Phi_n|\hat{R}|\Psi_{\varepsilon l}\rangle}{\omega - I_{1snp} + i\gamma_{1s,n}} \\ A_l^{(2)} &= \sum_{M'} \int_0^{\infty} dx \frac{\langle 0|\hat{R}|\Phi_x\rangle \langle \Phi_x|\hat{R}|\Psi_{\varepsilon l}\rangle}{\omega - I_{1s} - x + i\gamma_{1s}} \\ |0\rangle &= [0] \otimes (a_{\omega}^+)^2 |0_{ph}\rangle \\ |\Phi_{n,x}\rangle &= |1s(n,x)p(^1P_1),M'\rangle \otimes \hat{a}_{\omega}^+ |0_{ph}\rangle \\ |\Psi_{\varepsilon l}\rangle &= |1scl(^1l_{j=l}),M\rangle \otimes |0_{ph}\rangle \\ \hat{R} &= -\frac{1}{c} \sum_{n=1}^N (\hat{p}_n \cdot \hat{A}_n) \end{aligned}$$

$$(x-\varepsilon)\langle xp_+|\hat{r}|\varepsilon l_+\rangle\cong i\sqrt{2x}\cdot\delta(x-\varepsilon)$$

$$\begin{aligned} A_s &= \zeta \left(\mu + \sum_{n=2}^{\infty} \beta_n \langle np_+ | \hat{r} | \bar{\varepsilon} s_+ \rangle \right) \\ A_d &= \sqrt{6} \zeta \left(\mu + \sum_{n=2}^{\infty} \beta_n \langle np_+ | \hat{r} | \bar{\varepsilon} d_+ \rangle \right) \cdot Q_M \\ \mu &= i \cdot 2 \sqrt{2} \bar{\varepsilon} \langle 1s_0 \| \hat{r} \| \bar{\varepsilon} p_+ \rangle \\ \beta_n &= \frac{I_{1snp} (2\omega - I_{1snp})}{\omega - I_{1snp} + i\gamma_{1s,n}} \langle 1s_0 \| \hat{r} \| np_+ \rangle \end{aligned}$$

$$Q_M=-\frac{4\pi}{3}\sum_{M'}\sum_p(-1)^{M'}Y_{1,M'}(\mathbf{e}_\omega)Y_{1,p}^*(\mathbf{e}_\omega)\begin{pmatrix}1&1&2\\-M'&p&M\end{pmatrix}$$

$$\begin{aligned}\langle 1s_0\|\hat{r}\|np_+\rangle &= \langle 1s_0\mid 1s_+\rangle\langle 2s_0\mid 2s_+\rangle^2\langle 1s_0|\hat{r}|np_+\rangle \\ \langle 1s_0|\hat{r}|np_+\rangle &= \int_0^\infty P_{1s_0}(r)rP_{np_+}(r)dr\end{aligned}$$

$$d\sigma_g^{(l)}=(V/2c)d\sigma_l$$

$$d\sigma_l=(\pi V/c)|A_l|^2\cdot\delta(\varepsilon-\bar{\varepsilon})d\varepsilon$$

$$\sigma_g(\text{cm}^4 \cdot \text{s}) = (\eta/\omega)^2 \sum_{l=s,d} \sum_{i=1,2} al \cdot L_{il}^2,$$

$$L_{1l}=\sum_{n=2}^{\infty} \left(\omega-I_{1snp}\right)B_{ln},$$

$$L_{2l}=D-\sum_{n=2}^{\infty}\gamma_{1s,np}B_{ln},$$

$$D=2\sqrt{2\bar{\varepsilon}}\cdot\langle 1s_0||\hat{r}||np_+\rangle$$

$$B_{ln}=\frac{\beta_n}{\omega-I_{1snp}-i\gamma_{1s,n}}\langle np_+|\hat{r}|\overline{\varepsilon l_+}\rangle.$$

$$a_d=6\cdot\sum_{M=-2}^2|Q_M|^2$$

$$Y_{1,0}(\mathbf{e}_\omega)=0, Y_{1,\pm 1}(\mathbf{e}_\omega)=\mp 3/(4\pi\sqrt{2}).$$

$$\begin{array}{l} \Gamma_{1s,n}=\Gamma_A+\Gamma_{R,n},\\ \Gamma_{R,n}=\alpha n^{-(\beta+\gamma/n)},\\ \lim_{n\rightarrow\infty}\Gamma_{1s,n}=\Gamma_A. \end{array}$$

$$\frac{\Gamma_{R,n}}{\Gamma_{R,n+1}}=\left(\frac{I_{1snp}}{I_{1s(n+1)p}}\right)^3\left(\frac{\langle 1s|\hat{r}|np\rangle}{\langle 1s|\hat{r}|(n+1)p\rangle}\right)^2,n\geq 2.$$

$$\Gamma_{R,n}\sim n^{-\beta}.$$

$$I_{1snp}=I_{1s}-\frac{1}{n^2}\Big(a-\frac{b}{n}\Big),\lim_{n\rightarrow\infty}I_{1snp}=I_{1s}$$

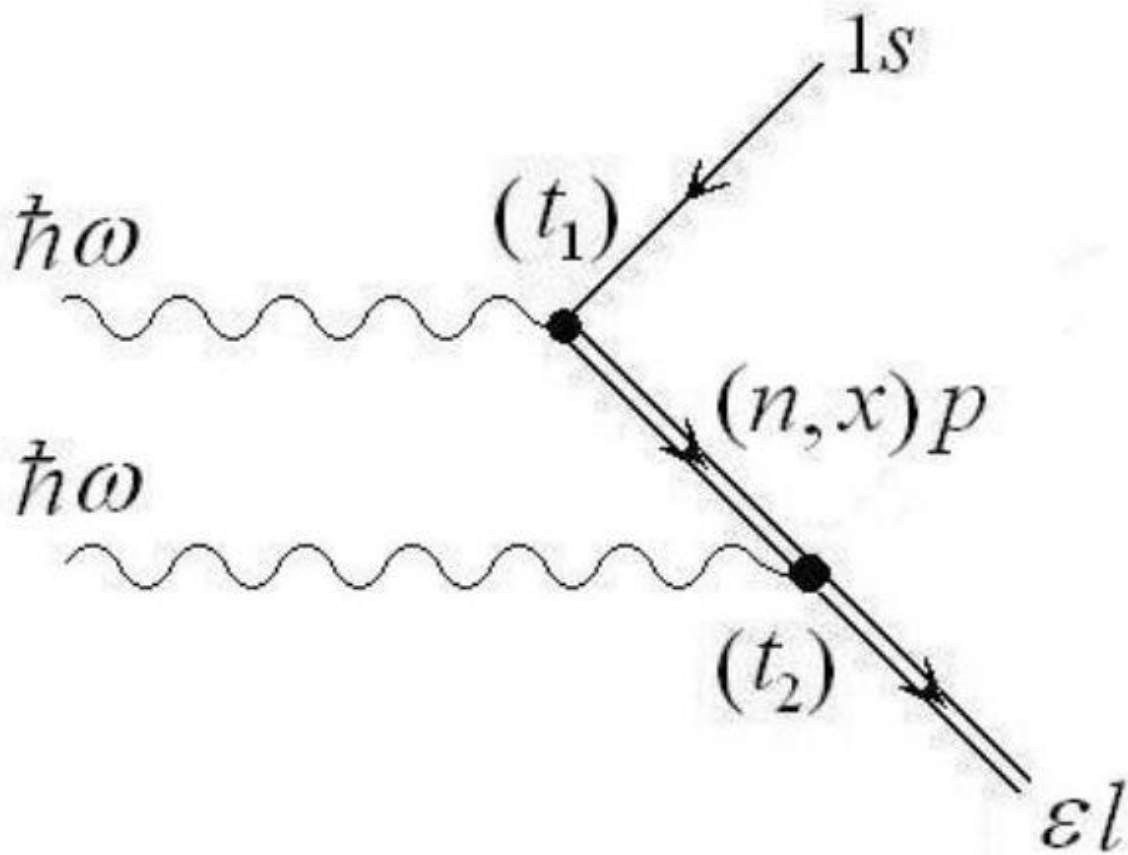
$$J_n=\frac{1}{n^2}\Big(c+\frac{d}{n}+\frac{f}{n^2}\Big),\lim_{n\rightarrow\infty}J_n=0$$

$$\alpha=\langle 1s_+ \mid \bar{\varepsilon}s_+\rangle\neq 0,\beta=\langle 2s_+ \mid \bar{\varepsilon}s_+\rangle\neq 0$$

$$\begin{array}{l} |\bar{\varepsilon}s_+\rangle\rightarrow|\tilde{\varepsilon}s_+\rangle=|\bar{\varepsilon}s_+\rangle-\alpha\cdot|1s_+\rangle-\beta\cdot|2s_+\rangle\\ \langle 1s_+ \mid \tilde{\varepsilon}s_+\rangle=\langle 2s_+ \mid \tilde{\varepsilon}s_+\rangle=0 \end{array}$$

$$\langle np_+|\hat{r}|\tilde{\varepsilon}s_+\rangle=\langle np_+|\hat{r}|\bar{\varepsilon}s_+\rangle-\alpha\langle np_+|\hat{r}|1s_+\rangle-\beta\langle np_+|\hat{r}|2s_+\rangle.$$

$$\langle np_+|\hat{r}|\bar{\varepsilon}d_+\rangle>\langle np_+|\hat{r}|\bar{\varepsilon}s_+\rangle.$$



$$N_{\tau} = \langle \hat{N}_{\tau} \rangle (\tau = n, p)$$

$$E = \text{Tr}(\hat{D} \hat{H})$$

$$Q = \text{Tr}(\hat{D} \hat{Q})$$

$$N_{\tau} = \text{Tr}(\hat{D} \hat{N}_{\tau})$$

$$S = -\text{Tr}(\hat{D} \ln \hat{D})$$

$$\hat{D} = \frac{1}{Z} e^{-\beta \hat{H} + \alpha_n \hat{N}_n + \alpha_p \hat{N}_p + \lambda \hat{Q}}$$

$$Z = \text{Tr}(e^{-\beta \hat{H} + \alpha_n \hat{N}_n + \alpha_p \hat{N}_p + \lambda \hat{Q}})$$

$$\frac{\partial}{\partial \beta} \ln Z = -E$$

$$\frac{\partial}{\partial \alpha_{\tau}} \ln Z = N_{\tau}$$

$$\frac{\partial}{\partial \lambda} \ln Z = Q$$

$$S = \ln Z + \beta E - \alpha_n N_n - \alpha_p N_p - \lambda Q$$

$$dS = \beta dE - \alpha_n dN_n - \alpha_p dN_p - \lambda dQ$$

$$dE = T dS + \kappa dQ$$

$$\kappa(Q,T)=\frac{\partial F(Q,T)}{\partial Q}$$

$$\kappa(Q,S)=\frac{\partial E(Q,S)}{\partial Q}$$

$$\kappa(Q,E)=-T(Q,E)\frac{\partial S(Q,E)}{\partial Q}$$

$$\kappa(Q,T)=\kappa(Q,S)=\kappa(Q,E)$$

$$V_S(Q)=E(Q,S)$$

$$dV_E=-T\frac{dS}{dq}dq$$

$$V_E(Q)=E-\int_{Q_b}^QT(q,E)\frac{dS(q,E)}{dq}dq$$

$$S(Q)=2\sqrt{a(Q)U(Q)}$$

$$T(Q)=\sqrt{U(Q)/a(Q)}$$

$$V_T(Q)=V(Q)-a(Q)T^2$$

$$V_S(Q)=V(Q)+a(Q)T^2(Q),\left(T(Q)=\frac{S}{2a(Q)}\right),$$

$$V_E(Q)=V(Q)-\int_{Q_b}^QT^2(q)\frac{da(q)}{dq}dq.$$

$$\hat{D}_{\text{HFB}}=\frac{e^{-\beta\hat{K}}}{Z_{\text{HFB}}}, Z_{\text{HFB}}=\text{Tr}(e^{-\beta\hat{K}}),$$

$$V_E(Q)=E+\int_{Q_b}^Q\kappa(q,E)dq$$

$$S=-\sum_i\left[f_i\ln f_i+(1-f_i)\ln (1-f_i)\right],$$

$$T\frac{dS}{dq}=\sum_i\varepsilon_i\frac{df_i}{dq},$$

$$U_E(Q)=\sum_i f_i\varepsilon_i-\int_{Q_b}^Q\sum_i f_i\frac{d\varepsilon_i}{dq}dq$$

$$\frac{dB_f(E)}{dE}\approx\int_{Q_{\rm gs}^*}^{Q_{\rm sp}}\frac{\partial\kappa(Q,E)}{\partial E}dQ<0$$

$$E(Q_{\rm gs}^*,X)=U+E_{\rm gs},\,(X=T,S,E).$$

$$\begin{aligned}\Delta B_f &= B_f(E' = \text{const}) - B_f(S' = \text{const}) \\ &= \int_{Q_{\text{gs}}^*}^{Q_{\text{sp}}} [\kappa(Q, E') - \kappa(Q, S')] dQ\end{aligned}$$

$$\begin{aligned}\Delta B_f &= \int_{Q_{\text{gs}}^*}^{Q_{\text{sp}}} [\kappa(Q, E') - \kappa(Q, E(Q, S'))] dQ \\ &\approx \int_{Q_{\text{gs}}^*}^{Q_{\text{sp}}} \left. \frac{\partial \kappa(Q, E)}{\partial E} \right|_{E=E'} [E' - E(Q, S')] dQ\end{aligned}$$

$$\frac{\partial \kappa(Q, E)}{\partial E} < 0 \text{ for } Q_{\text{gs}}^* < Q < Q_{\text{sp}},$$

$$B_f \propto e^{-\gamma_D U},$$

$$a(Q,E)=\frac{S^2(Q,E)}{4U(Q)}, U(Q)=E-V(Q),$$

$$a(Q_{\text{sp}})/a(Q_{\text{gs}}^*)$$

$$a(Q_{\text{sp}})/a(Q_{\text{gs}}^*) \approx 1.18$$

$$\tilde{a}(Q,E)=\frac{S^2(Q,E)}{4U_E(Q)}, U_E(Q)=E-V_E(Q).$$

$$\begin{aligned}\mathcal{H} &= \int \mathrm{d}\mathbf{r} \psi_a^\dagger(\mathbf{r}) \left(\hat{H}_{ab} \left(p_\mu + \frac{e}{c} A_\mu(\mathbf{r}) \right) + U_{ab}(\mathbf{r}) \right) \psi_b(\mathbf{r}) + \mathcal{V} \\ \mathcal{V} &= \frac{1}{2} \int \mathrm{d}\mathbf{r} \mathrm{d}\mathbf{r}' V_{ab,cd}(\mathbf{r} - \mathbf{r}') \psi_a^\dagger(\mathbf{r}) \psi_c^\dagger(\mathbf{r}') \psi_d(\mathbf{r}') \psi_b(\mathbf{r})\end{aligned}$$

$$\hat{H}_{ab}(p_\mu)=\sum_n\Lambda_{n,ab}^{\mu_1\mu_2\cdots\mu_n}p_{\mu_1}p_{\mu_2}\cdots p_{\mu_n}$$

$$p_\mu=\frac{\hbar}{i}\frac{\partial}{\partial r_\mu}$$

$$\nabla\times\mathbf{A}(\mathbf{r})=B\hat{\mathbf{z}}$$

$$V_{ab,cd}(\mathbf{r})=V_{ba,dc}^*(\mathbf{r})$$

$$V_{ab,cd}(\mathbf{r})=V_{cd,ab}(-\mathbf{r})$$

$$\begin{aligned}\langle \mathcal{H} \rangle &= \\ &\int \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \left[\delta(\mathbf{r} - \mathbf{r}') (\hat{H}_{ab}(p_\mu + \frac{e}{c} A_\mu(\mathbf{r})) + U_{ab}(\mathbf{r})) P_{ba}(\mathbf{r}, \mathbf{r}') \right. \\ &\quad \left. + \frac{1}{2} V_{ab,cd}(\mathbf{r} - \mathbf{r}') (P_{ba}(\mathbf{r}, \mathbf{r}) P_{dc}(\mathbf{r}', \mathbf{r}') - P_{da}(\mathbf{r}', \mathbf{r}) P_{bc}(\mathbf{r}, \mathbf{r}')) \right]\end{aligned}$$

$$\Phi(\mathbf{r},\mathbf{r}')=\frac{e}{c\hbar}\int_{\mathbf{r}}^{\mathbf{r}'}\mathbf{A}(\mathbf{r}'')\cdot d\mathbf{r}''$$

$$G(\mathbf{r},\mathbf{r}';z)=e^{i\Phi(\mathbf{r},\mathbf{r}')}\tilde{G}(\mathbf{r},\mathbf{r}';z)$$

$$P_{ab}(\mathbf{r},\mathbf{r}')=\langle\psi_b^\dagger(\mathbf{r}')\psi_a(\mathbf{r})\rangle$$

$$N=\int\,d\mathbf{r}P_{aa}(\mathbf{r},\mathbf{r})$$

$$\frac{\delta\langle\mathcal{H}\rangle}{\delta P_{ba}(\mathbf{y},\mathbf{x})}$$

$$\hat{\mathcal{H}}_{ab}^{\rm HF}\psi_b(\mathbf{x})=\hat{H}_{ab}\left(p_\mu+\frac{e}{c}A_\mu(\mathbf{x})\right)\psi_b(\mathbf{x})\\ +\int\,d\mathbf{r}V_{ab}^{\rm HF}(\mathbf{x},\mathbf{r})\psi_b(\mathbf{r})$$

$$V_{ab}^{\rm HF}(\mathbf{x},\mathbf{r})=-V_{ad,cb}(\mathbf{x}-\mathbf{r})P_{dc}(\mathbf{x},\mathbf{r})+\\ \delta(\mathbf{x}-\mathbf{r})\left(U_{ab}(\mathbf{r})+\int\,d^2\mathbf{y}V_{ab,cd}(\mathbf{x}-\mathbf{y})P_{dc}(\mathbf{y},\mathbf{y})\right)$$

$$P_{ab}(\mathbf{r},\mathbf{r}')=\oint\,c\,\frac{\mathrm{d}z}{2\pi i}G_{ab}(\mathbf{r},\mathbf{r}';z)$$

$$G_{ab}(\mathbf{r},\mathbf{r}';z)=\langle\mathbf{r}|(z-\hat{\mathcal{H}}^{\rm HF})_{ab}^{-1}|\mathbf{r}'\rangle$$

$$\Phi(\mathbf{r},\mathbf{r}')=\frac{eB}{2c\hbar}(r_x+r'_x)(r'_y-r_y)$$

$$\tilde{P}(\mathbf{r},\mathbf{r}')=\oint\,c\,\frac{\mathrm{d}z}{2\pi i}\tilde{G}(\mathbf{r},\mathbf{r}';z)$$

$$\langle\mathcal{H}\rangle=\int\,d\mathbf{r}d\mathbf{r}'\Big[\delta(\mathbf{r}-\mathbf{r}')(\hat{H}_{ab}(p_\mu)+U_{ab}(\mathbf{r}))\tilde{P}_{ba}(\mathbf{r},\mathbf{r}')+\\ \frac{1}{2}V_{ab,cd}(\mathbf{r}-\mathbf{r}')\Big(\tilde{P}_{ba}(\mathbf{r},\mathbf{r})\tilde{P}_{dc}(\mathbf{r}',\mathbf{r}')-\tilde{P}_{da}(\mathbf{r}',\mathbf{r})\tilde{P}_{bc}(\mathbf{r},\mathbf{r}')\Big)\Big]$$

$$\hat{H}_{ab}\left(p_\mu+\frac{e}{c}A_\mu(\mathbf{r})\right)e^{i\Phi(\mathbf{r},\mathbf{r}')}=e^{i\Phi(\mathbf{r},\mathbf{r}')}\hat{H}_{ab}\left(p_\mu-\epsilon_{\mu\nu}\frac{eB}{2c}(r_\nu-r'_\nu)\right)$$

$$\Lambda_{n,ab}^{\mu_1\mu_2\cdots\mu_n}d\langle\mathcal{H}\rangle/dB|_{B=0}$$

$$\mathrm{d}\tilde{P}/\mathrm{d}B|_{B=0}$$

$$\begin{aligned}
-M &= \frac{d\langle \mathcal{H} \rangle}{dB} \Big|_{B=0} - \mu \frac{d\langle \hat{N} \rangle}{dB} \Big|_{B=0} \\
&= \int d\mathbf{r} \langle \mathbf{r} | \left(\hat{\mathcal{H}}_{ab}^{(0)\text{HF}} - \mu \delta_{ab} \right) \frac{d\hat{\tilde{P}}_{ba}}{dB} \Big|_{B=0} | \mathbf{r} \rangle \\
&= \sum_n \oint_c \frac{dz}{2\pi i} (E_n - \mu) \langle n | \frac{d\hat{G}(z)}{dB} \Big|_{B=0} | n \rangle, \\
&\langle \mathbf{r} | (z - \hat{\mathcal{H}}^{\text{HF}}) \hat{G}(z) | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}')
\end{aligned}$$

$$\begin{aligned}
&\int d\mathbf{x} (z\delta(\mathbf{r} - \mathbf{x})\delta_{ab} - \tilde{V}_{ab}^{\text{HF}}(\mathbf{r}, \mathbf{x})) e^{i\varphi(\mathbf{r}', \mathbf{r}, \mathbf{x})} \tilde{G}_{ba'}(\mathbf{x}, \mathbf{r}'; z) - \\
&\hat{H}_{ab} \left(p_\mu - \epsilon_{\mu\nu} \frac{eB}{2c} (r_\nu - r'_\nu) \right) \tilde{G}_{ba'}(\mathbf{r}, \mathbf{r}'; z) = \delta_{aa'} \delta(\mathbf{r} - \mathbf{r}')
\end{aligned}$$

$$\begin{aligned}
&\tilde{V}_{ab}^{\text{HF}}(\mathbf{r}, \mathbf{x}) = -V_{ad,cb}(\mathbf{r} - \mathbf{x}) \tilde{P}_{dc}(\mathbf{r}, \mathbf{x}) + \\
(13)) \quad &\delta(\mathbf{r} - \mathbf{x}) \left(U_{ab}(\mathbf{r}) + \int d^2\mathbf{y} V_{ab,cd}(\mathbf{r} - \mathbf{y}) \tilde{P}_{dc}(\mathbf{y}, \mathbf{y}) \right)
\end{aligned}$$

$$e^{i\varphi(\mathbf{r}', \mathbf{r}, \mathbf{x})} = e^{i\Phi(\mathbf{r}', \mathbf{r})} e^{i\Phi(\mathbf{r}, \mathbf{x})} e^{i\Phi(\mathbf{x}, \mathbf{r}')}$$

$$e^{i\varphi(\mathbf{r}', \mathbf{r}, \mathbf{x})} = \exp \left(i \frac{eB}{2\hbar c} \hat{\mathbf{z}} \cdot (\mathbf{x} - \mathbf{r}) \times (\mathbf{r}' - \mathbf{x}) \right)$$

$$i \frac{e}{2\hbar c} \epsilon_{\mu\nu} (x_\mu - r_\mu) (r'_\nu - x_\nu)$$

$$-\frac{i}{\hbar} [\hat{H}_{ab}(p_\mu), r_\mu] \epsilon_{\mu\nu} \frac{e}{2c} (r_\nu - r'_\nu)$$

$$(r'_\nu - x_\nu) \tilde{G}_{ba'}(\mathbf{x}, \mathbf{r}'; z) = -\langle \mathbf{x} | [\hat{x}_\nu, \hat{\tilde{G}}_{ba'}(z)] | \mathbf{r}' \rangle$$

$$\tilde{V}_{ab}^{\text{HF}}(\mathbf{r}, \mathbf{x}) (x_\mu - r_\mu) = \langle \mathbf{r} | [\hat{\tilde{V}}_{ab}^{\text{HF}}, \hat{x}_\mu] | \mathbf{x} \rangle$$

$$\epsilon_{\mu\nu} [\hat{H}_{ab}(p_\mu), r_\mu] (r_\nu - r'_\nu) \tilde{G}_{ba'}(\mathbf{r}, \mathbf{r}'; z) = \epsilon_{\mu\nu} \int d\mathbf{x} \langle \mathbf{r} | [\hat{H}_{ab}(\hat{p}_\mu), \hat{x}_\mu] | \mathbf{x} \rangle \langle \mathbf{x} | [\hat{x}_\nu, \hat{\tilde{G}}_{ba'}(z)] | \mathbf{r}' \rangle$$

$$[\hat{G}^{(0)}(z), \hat{x}] = \hat{G}^{(0)}(z) [\hat{\mathcal{H}}^{(0)\text{HF}}, \hat{x}] \hat{G}^{(0)}(z)$$

$$\hat{G}^{(0)} = (z - \hat{\mathcal{H}}^{(0)\text{HF}})^{-1}$$

$$\begin{aligned}
&\frac{d\hat{\tilde{G}}_{b'a'}(z)}{dB} \Big|_{B=0} = \hat{G}_{b'a}^{(0)}(z) \frac{d\hat{\tilde{V}}_{ab}^{\text{HF}}}{dB} \Big|_{B=0} \hat{G}_{ba'}^{(0)}(z) + \\
&\frac{ie}{2\hbar c} \epsilon_{\mu\nu} \hat{G}_{b'a}^{(0)}(z) [\hat{\mathcal{H}}_{ab}^{(0)\text{HF}}, \hat{x}_\mu] \hat{G}_{bc}^{(0)}(z) [\hat{\mathcal{H}}_{cc'}^{(0)\text{HF}}, \hat{x}_\nu] \hat{G}_{c'a'}^{(0)}(z) \mathcal{O}^{(2)}
\end{aligned}$$

$$\oint_{\mathcal{C}} \frac{dz}{2\pi i} (E_n - \mu) \langle n | \hat{G}^{(0)}(z) \frac{d\hat{V}^{\text{HF}}}{dB} \Big|_{B=0} \hat{G}^{(0)}(z) | n \rangle$$

$$\langle \mathbf{r} | \frac{d\hat{V}_{ab}^{\text{HF}}}{dB} \Big|_{B=0} | \mathbf{x} \rangle \equiv \delta(\mathbf{r} - \mathbf{x}) \int d\mathbf{y} V_{ab,cd}(\mathbf{r} - \mathbf{y}) \frac{d\tilde{P}_{dc}(\mathbf{y}, \mathbf{y})}{dB} \Big|_{B=0}$$

$$- V_{ad,cb}(\mathbf{r} - \mathbf{x}) \frac{d\tilde{P}_{dc}(\mathbf{r}, \mathbf{x})}{dB} \Big|_{B=0}$$

$$\hat{v}_{\mu}^{\text{HF}} = \frac{i}{\hbar} [\hat{\mathcal{H}}^{(0)\text{HF}}, \hat{x}_{\mu}]$$

$$\frac{ie\hbar}{2c} \epsilon_{\alpha\beta} \sum_{nn'} \oint_{\mathcal{C}} \frac{dz}{2\pi i} (E_n - \mu) \frac{\langle n | \hat{v}_{\alpha}^{\text{HF}} | n' \rangle \langle n' | \hat{v}_{\beta}^{\text{HF}} | n \rangle}{(z - E_n)^2 (z - E_{n'})} = \frac{ie\hbar}{2c} \times$$

$$\epsilon_{\alpha\beta} \sum_{n \neq n'} (E_n - \mu) \langle n | \hat{v}_{\alpha}^{\text{HF}} | n' \rangle \langle n' | \hat{v}_{\beta}^{\text{HF}} | n \rangle \frac{n_F(E_{n'}) - n_F(E_n)}{(E_{n'} - E_n)^2}$$

$$n_F(E_n) = \lim_{T \rightarrow 0} 1/(e^{(E_n - \mu)/T} + 1)$$

$$\langle \mathbf{r} \mid n, \mathbf{k} \rangle = e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})$$

$$\langle n, \mathbf{k} | \hat{v}_{\mu}^{\text{HF}} | n', \mathbf{k}' \rangle = \delta_{\mathbf{k}\mathbf{k}'} \frac{1}{\hbar} (E_{n'}(\mathbf{k}) - E_n(\mathbf{k})) \left\langle u_{n,\mathbf{k}} \left| \frac{\partial u_{n',\mathbf{k}}}{\partial k_{\mu}} \right. \right\rangle$$

$$M = \frac{e}{2i\hbar c} \epsilon_{\alpha\beta} \sum_{\mathbf{k}} \sum_{n \neq n'} (E_n(\mathbf{k}) - \mu) \left\langle u_{n,\mathbf{k}} \left| \frac{\partial u_{n',\mathbf{k}}}{\partial k_{\alpha}} \right. \right\rangle \times$$

$$\left\langle u_{n',\mathbf{k}} \left| \frac{\partial u_{n,\mathbf{k}}}{\partial k_{\beta}} \right. \right\rangle (n_F(E_{n'}(\mathbf{k})) - n_F(E_n(\mathbf{k})))$$

$$\epsilon_{\alpha\beta} \left\langle u_{n,\mathbf{k}} \left| \frac{\partial u_{n',\mathbf{k}}}{\partial k_{\alpha}} \right. \right\rangle \left\langle u_{n',\mathbf{k}} \left| \frac{\partial u_{n,\mathbf{k}}}{\partial k_{\beta}} \right. \right\rangle$$

$$n_F(E_{n'}(\mathbf{k})) - n_F(E_n(\mathbf{k}))$$

$$\frac{1}{2} (E_n(\mathbf{k}) + E_{n'}(\mathbf{k}) - 2\mu)$$

$$\hat{\mathcal{H}}^{(0)\text{HF}}(\mathbf{k}) = e^{-i\mathbf{k} \cdot \mathbf{r}} \hat{\mathcal{H}}^{(0)\text{HF}} e^{i\mathbf{k} \cdot \mathbf{r}}$$

$$M = \frac{e}{2i\hbar c} \epsilon_{\alpha\beta} \sum_{\mathbf{k}} \sum_n \left\langle \frac{\partial u_{n,\mathbf{k}}}{\partial k_{\alpha}} \right| \hat{\mathcal{H}}^{(0)\text{HF}}(\mathbf{k}) + E_n(\mathbf{k}) - 2\mu \left| \frac{\partial u_{n,\mathbf{k}}}{\partial k_{\beta}} \right\rangle n_F(E_n(\mathbf{k}))$$

$$\chi = \frac{\partial M(B, N)}{\partial B} \Big|_{B=0} = \chi_1 + \chi_2 + \chi_3,$$

$$\begin{aligned}\chi_1 &= \frac{\hbar^2 e^2}{12c^2} \sum_n \oint_c \frac{dz}{2\pi i} \langle n | \hat{G}^{(0)}(z) (\hat{\mathcal{M}}^{\text{HF}})^{-1}_{xx} \hat{G}^{(0)}(z) (\hat{\mathcal{M}}^{\text{HF}})^{-1}_{yy} - \hat{G}^{(0)}(z) (\hat{\mathcal{M}}^{\text{HF}})^{-1}_{xy} \hat{G}^{(0)}(z) (\hat{\mathcal{M}}^{\text{HF}})^{-1}_{xy} \\ &\quad - 4(\hat{G}^{(0)}(z) \hat{v}_x^{\text{HF}} \hat{G}^{(0)}(z) \hat{v}_x^{\text{HF}} \hat{G}^{(0)}(z) \hat{v}_y^{\text{HF}} \hat{G}^{(0)}(z) \hat{v}_y^{\text{HF}} - \hat{G}^{(0)}(z) \hat{v}_x^{\text{HF}} \hat{G}^{(0)}(z) \hat{v}_y^{\text{HF}} \hat{G}^{(0)}(z) \hat{v}_x^{\text{HF}} \hat{G}^{(0)}(z) \hat{v}_y^{\text{HF}}) | n \rangle, \\ \chi_2 &= \sum_n \oint_c \frac{dz}{2\pi i} \langle n | \hat{G}^{(0)}(z) \left. \frac{d\hat{V}^{\text{HF}}}{dB} \right|_{B=0} \hat{G}^{(0)}(z) \left. \frac{d\hat{V}^{\text{HF}}}{dB} \right|_{B=0} | n \rangle, \\ \chi_3 &= - \int d\mathbf{r} d\mathbf{r}' V_{ab,cd}(\mathbf{r} - \mathbf{r}') \left(\left. \frac{d\tilde{P}_{ba}(\mathbf{r}, \mathbf{r}')}{dB} \right|_{B=0} \left. \frac{d\tilde{P}_{dc}(\mathbf{r}', \mathbf{r}')}{dB} \right|_{B=0} - \left. \frac{d\tilde{P}_{da}(\mathbf{r}', \mathbf{r}')}{dB} \right|_{B=0} \left. \frac{d\tilde{P}_{bc}(\mathbf{r}, \mathbf{r}')}{dB} \right|_{B=0} \right),\end{aligned}$$

$$(\hat{\mathcal{M}}^{\text{HF}})^{-1}_{\mu\nu} = \left(\frac{i}{\hbar}\right)^2 \left[[\hat{\mathcal{H}}^{(0)\text{HF}}, \hat{x}_\mu], \hat{x}_\nu \right].$$

$$\hat{H}_{ab}(\mathbf{p}) = \begin{pmatrix} m_0 + b_2 \mathbf{p}^2 & b_1(p_x - ip_y) \\ b_1(p_x + ip_y) & -m_0 + b_2 \mathbf{p}^2 \end{pmatrix}$$

$$V_{ab,cd}(\mathbf{r}-\mathbf{r}')=\delta_{ab}\delta_{cd}\frac{e^2}{4\pi\epsilon}\sum_{n=-\infty}^{\infty}\frac{(-1)^n}{\sqrt{|\mathbf{r}-\mathbf{r}'|^2+(2nd)^2}}$$

$$\Delta = m_0 b_2/b_1^2$$

$$\phi/\phi_0=eB\hbar^2b_2^2/(\hbar b_1^2)$$

$$\langle \sigma_z \rangle \equiv \int d\mathbf{r} \langle \psi^\dagger_\uparrow(\mathbf{r}) \psi_\uparrow(\mathbf{r}) - \psi^\dagger_\downarrow(\mathbf{r}) \psi_\downarrow(\mathbf{r}) \rangle / N$$

$$\{\Delta, e^2/(4\pi\epsilon), d, \rho\} = \{1/4, 10\hbar b_1, \hbar b_2/(2\pi b_1), b_1^2/(5\hbar^2 b_2^2)\}$$

$$\langle n, \boldsymbol{k} | \hat{v}_\mu^{\text{HF}} | n', \boldsymbol{k}' \rangle$$

$$\langle n, \boldsymbol{k} | \hat{v}_\mu^{\text{HF}} | n', \boldsymbol{k}' \rangle \propto \delta_{\boldsymbol{k}, \boldsymbol{k}'}$$

$$\hat{\mathcal{H}}^{(0)\text{HF}}(\boldsymbol{k})=e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\hat{\mathcal{H}}^{(0)\text{HF}}e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}$$

$$\begin{aligned}\hat{\mathcal{H}}^{(0)\text{HF}}|n,\boldsymbol{k}\rangle &= E_n(\boldsymbol{k})|n,\boldsymbol{k}\rangle = e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}E_n(\boldsymbol{k})|u_{n,\boldsymbol{k}}\rangle \\ \hat{\mathcal{H}}^{(0)\text{HF}}|n,\boldsymbol{k}\rangle &= e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\hat{\mathcal{H}}^{(0)\text{HF}}e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}|u_{n,\boldsymbol{k}}\rangle = e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\hat{\mathcal{H}}^{(0)\text{HF}}(\boldsymbol{k})|u_{n,\boldsymbol{k}}\rangle\end{aligned}$$

$$\begin{aligned}\langle n, \boldsymbol{k} | \hat{v}_\mu^{\text{HF}} | n', \boldsymbol{k} \rangle &= \frac{i}{\hbar} \langle n, \boldsymbol{k} | [\hat{\mathcal{H}}^{(0)\text{HF}}, \hat{r}_\mu] | n', \boldsymbol{k} \rangle = \frac{i}{\hbar} \langle u_{n,\boldsymbol{k}} | e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} [\hat{\mathcal{H}}^{(0)\text{HF}}, \hat{r}_\mu] e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} | u_{n',\boldsymbol{k}} \rangle \\ &= \frac{1}{\hbar} \langle u_{n,\boldsymbol{k}} | \frac{\partial}{\partial k_\mu} (e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} \hat{\mathcal{H}}^{(0)\text{HF}} e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}) | u_{n',\boldsymbol{k}} \rangle = \frac{1}{\hbar} \langle u_{n,\boldsymbol{k}} | \frac{\partial \hat{\mathcal{H}}^{(0)\text{HF}}(\boldsymbol{k})}{\partial k_\mu} | u_{n',\boldsymbol{k}} \rangle \\ &= \frac{1}{\hbar} \left(\frac{\partial}{\partial k_\mu} \langle u_{n,\boldsymbol{k}} | \hat{\mathcal{H}}^{(0)\text{HF}}(\boldsymbol{k}) | u_{n',\boldsymbol{k}} \rangle - \left\langle \frac{\partial u_{n,\boldsymbol{k}}}{\partial k_\mu} \right| \hat{\mathcal{H}}^{(0)\text{HF}}(\boldsymbol{k}) | u_{n',\boldsymbol{k}} \rangle - \langle u_{n,\boldsymbol{k}} | \hat{\mathcal{H}}^{(0)\text{HF}}(\boldsymbol{k}) \left| \frac{\partial u_{n',\boldsymbol{k}}}{\partial k_\mu} \right\rangle \right) \\ &= \frac{1}{\hbar} \frac{\partial E_n(\boldsymbol{k})}{\partial k_\mu} \delta_{nn'} - \frac{E_{n'}(\boldsymbol{k})}{\hbar} \left\langle \frac{u_{n,\boldsymbol{k}}}{\partial k_\mu} \middle| u_{n',\boldsymbol{k}} \right\rangle - \frac{E_n(\boldsymbol{k})}{\hbar} \left\langle u_{n,\boldsymbol{k}} \middle| \frac{u_{n',\boldsymbol{k}}}{\partial k_\mu} \right\rangle\end{aligned}$$

$$\left\langle \frac{u_{n,\boldsymbol{k}}}{\partial k_\mu} \middle| u_{n',\boldsymbol{k}} \right\rangle = \frac{\partial}{\partial k_\mu} \langle u_{n,\boldsymbol{k}} | u_{n',\boldsymbol{k}} \rangle - \left\langle u_{n,\boldsymbol{k}} \middle| \frac{u_{n',\boldsymbol{k}}}{\partial k_\mu} \right\rangle = - \left\langle u_{n,\boldsymbol{k}} \middle| \frac{u_{n',\boldsymbol{k}}}{\partial k_\mu} \right\rangle.$$

$$\langle n, \mathbf{k} | \hat{v}_\mu^{\text{HF}} | n', \mathbf{k}' \rangle = \delta_{\mathbf{k}, \mathbf{k}'} \left(\frac{1}{\hbar} \frac{\partial E_n(\mathbf{k})}{\partial k_\mu} \delta_{nn'} + \frac{E_n(\mathbf{k}) - E_{n'}(\mathbf{k})}{\hbar} \left\langle u_{n, \mathbf{k}} \left| \frac{u_{n', \mathbf{k}}}{\partial k_\mu} \right. \right\rangle \right)$$

$$M = \frac{e}{2i\hbar c} \epsilon_{\alpha\beta} \sum_{\mathbf{k}} \sum_{n \neq n'} (E_n(\mathbf{k}) - \mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n', \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle (n_F(E_{n'}(\mathbf{k})) - n_F(E_n(\mathbf{k})))$$

$$\begin{aligned} M &= \frac{e}{4i\hbar c} \epsilon_{\alpha\beta} \sum_{\mathbf{k}} \sum_{n \neq n'} (E_n(\mathbf{k}) + E_{n'}(\mathbf{k}) - 2\mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n', \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle (n_F(E_{n'}(\mathbf{k})) - n_F(E_n(\mathbf{k}))) \\ &= \frac{e}{4i\hbar c} \epsilon_{\alpha\beta} \sum_{\mathbf{k}} \sum_{n \neq n'} (E_n(\mathbf{k}) + E_{n'}(\mathbf{k}) - 2\mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n', \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle n_F(E_{n'}(\mathbf{k})) \\ &\quad - \frac{e}{4i\hbar c} \epsilon_{\alpha\beta} \sum_{\mathbf{k}} \sum_{n \neq n'} (E_n(\mathbf{k}) + E_{n'}(\mathbf{k}) - 2\mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n', \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle n_F(E_n(\mathbf{k})) \end{aligned}$$

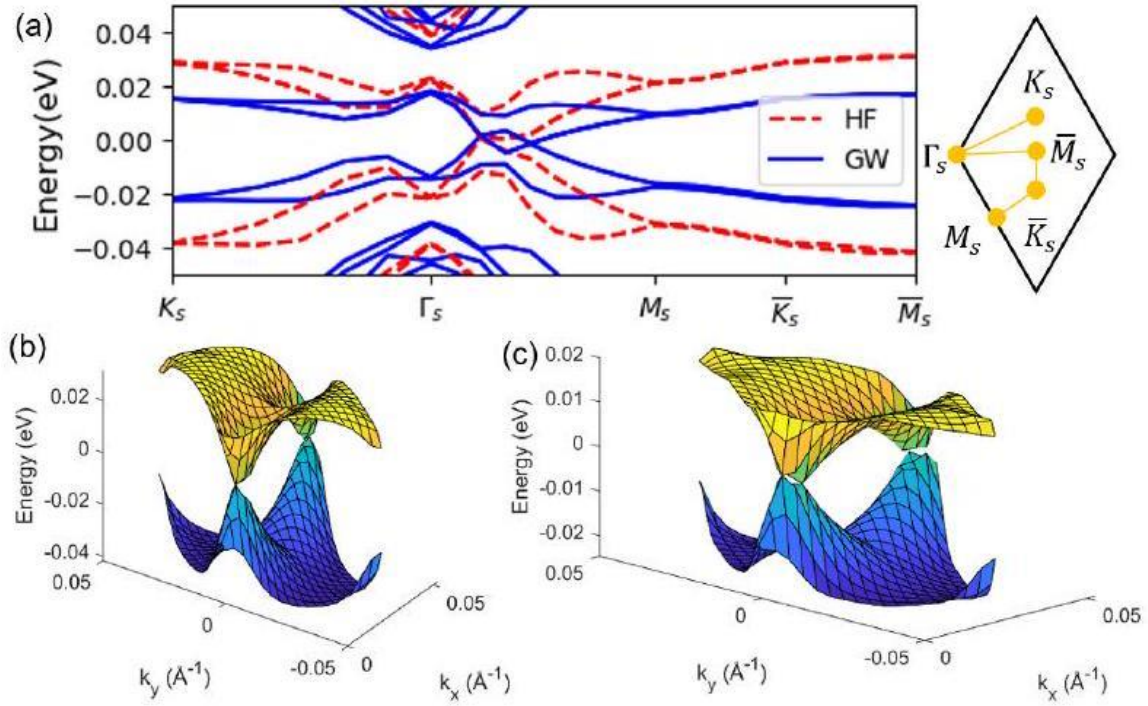
$$\begin{aligned} &\sum_{n \neq n'} (E_n(\mathbf{k}) + E_{n'}(\mathbf{k}) - 2\mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n', \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle n_F(E_{n'}(\mathbf{k})) \\ &= - \sum_{n, n'} (E_n(\mathbf{k}) + E_{n'}(\mathbf{k}) - 2\mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle \frac{\partial u_{n', \mathbf{k}}}{\partial k_\beta} \left| u_{n, \mathbf{k}} \right. \right\rangle n_F(E_{n'}(\mathbf{k})) \\ &\quad - \sum_n 2(E_n(\mathbf{k}) - \mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle n_F(E_n(\mathbf{k})) \\ &= - \sum_{n'} \left\langle \frac{\partial u_{n', \mathbf{k}}}{\partial k_\beta} \left| (E_{n'}(\mathbf{k}) + \hat{\mathcal{H}}^{(0)\text{HF}}(\mathbf{k}) - 2\mu) \right| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right\rangle n_F(E_{n'}(\mathbf{k})) \\ &\quad - \sum_n 2(E_n(\mathbf{k}) - \mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle n_F(E_n(\mathbf{k})). \end{aligned}$$

$$\begin{aligned} &\sum_{n \neq n'} (E_n(\mathbf{k}) + E_{n'}(\mathbf{k}) - 2\mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n', \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n', \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle n_F(E_n(\mathbf{k})) \\ &= - \sum_n \left\langle \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \left| (E_n(\mathbf{k}) + \hat{\mathcal{H}}^{(0)\text{HF}}(\mathbf{k}) - 2\mu) \right| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\alpha} \right\rangle n_F(E_n(\mathbf{k})) \\ &\quad - \sum_n 2(E_n(\mathbf{k}) - \mu) \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\alpha} \right. \right\rangle \left\langle u_{n, \mathbf{k}} \left| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right. \right\rangle n_F(E_n(\mathbf{k})). \end{aligned}$$

$$M = \frac{e}{2i\hbar c} \epsilon_{\alpha\beta} \sum_{\mathbf{k}} \sum_n \left\langle \frac{\partial u_{n, \mathbf{k}}}{\partial k_\alpha} \left| \mathcal{H}^{(0)\text{HF}}(\mathbf{k}) + E_n(\mathbf{k}) - 2\mu \right| \frac{\partial u_{n, \mathbf{k}}}{\partial k_\beta} \right\rangle n_F(E_n(\mathbf{k}))$$

$$I = \oint c \frac{dz}{2\pi i} (E_n - \mu) \langle n | \hat{G}^{(0)}(z) \frac{d\hat{V}^{\text{HF}}}{dB} \Big|_{B=0} \hat{G}^{(0)}(z) | n \rangle$$

$$\begin{aligned}
I &= (E_n - \mu) \lim_{\delta \rightarrow 0^+} \left(\int_{-\infty - i\delta}^{\mu - i\delta} \frac{dz}{2\pi i} + \int_{\mu + i\delta}^{\infty + i\delta} \frac{dz}{2\pi i} \right) \frac{1}{(z - E_n)^2} \langle n | \frac{d\hat{V}^{\text{HF}}}{dB} \Big|_{B=0} | n \rangle \\
&= \frac{E_n - \mu}{2\pi i} \lim_{\delta \rightarrow 0^+} \left(-\frac{1}{\mu - i\delta - E_n} + \frac{1}{\mu + i\delta - E_n} \right) \langle n | \frac{d\hat{V}^{\text{HF}}}{dB} \Big|_{B=0} | n \rangle \\
&= (E_n - \mu) \lim_{\delta \rightarrow 0^+} \frac{1}{2\pi i} \frac{2i\delta}{(\mu - E_n)^2 + \delta^2} \langle n | \frac{d\hat{V}^{\text{HF}}}{dB} \Big|_{B=0} | n \rangle = (E_n - \mu) \delta(E_n - \mu) \langle n | \frac{d\hat{V}^{\text{HF}}}{dB} \Big|_{B=0} | n \rangle = 0
\end{aligned}$$



$$H^{0,\mu} = \begin{pmatrix} h_{\text{intra}}^{0,\mu} + V_{\text{hBN}} & (h_{\text{inter}}^{0,\mu})^\dagger & 0 & 0 & 0 \\ h_{\text{inter}}^{0,\mu} & h_{\text{intra}}^{0,\mu} & (h_{\text{inter}}^{0,\mu})^\dagger & 0 & 0 \\ 0 & h_{\text{inter}}^{0,\mu} & h_{\text{intra}}^{0,\mu} & (h_{\text{inter}}^{0,\mu})^\dagger & 0 \\ 0 & 0 & h_{\text{inter}}^{0,\mu} & h_{\text{intra}}^{0,\mu} & (h_{\text{inter}}^{0,\mu})^\dagger \\ 0 & 0 & 0 & h_{\text{inter}}^{0,\mu} & h_{\text{intra}}^{0,\mu} \end{pmatrix}$$

$$h_{\text{intra}}^{0,\mu} = -\hbar v_F^0 \mathbf{k} \cdot \boldsymbol{\sigma}_\mu$$

$$h_{\text{inter}}^{0,\mu} = \begin{pmatrix} \hbar v_\perp (\mu k_x + i k_y) & t_\perp \\ \hbar v_\perp (\mu k_x - i k_y) & \hbar v_\perp (\mu k_x + i k_y) \end{pmatrix}$$

$$V_{\text{hBN}} = V^{\text{eff}}(\mathbf{r}) + M^{\text{eff}}(\mathbf{r})\sigma_z + e v_F \mathbf{A}^{\text{eff}}(\mathbf{r}) \cdot \boldsymbol{\sigma}_\mu.$$

$$V^{\text{eff}}(\mathbf{r}) = V_0 - V_1 \sum_{j=1}^3 \cos \alpha_j(\mathbf{r})$$

$$M^{\text{eff}}(\mathbf{r}) = \sqrt{3}V_1 \sum_{j=1}^3 \sin \alpha_j(\mathbf{r})$$

$$ev_F \mathbf{A}^{\text{eff}}(\mathbf{r}) = 2\mu V_1 \sum_{j=1}^3 \begin{pmatrix} \cos [2\pi(j+1)/3] \\ \sin [2\pi(j+1)/3] \end{pmatrix} \cos \alpha_j(\mathbf{r})$$

$$\alpha_j(\mathbf{r}) = \mathbf{G}_j \cdot \mathbf{r} + \psi + \frac{2\pi}{3} \text{ with } \mathbf{G}_3 = -\mathbf{G}_1 - \mathbf{G}_2$$

$$\hat{V} = \frac{1}{2N_s} \sum_{\substack{\alpha\alpha',l,l' \\ \mu\mu',\sigma\sigma'}} \sum_{\substack{\mathbf{k}\mathbf{k}',\tilde{\mathbf{q}} \\ \mathbf{G}\mathbf{G}'\mathbf{Q}}} V_{ll'}(\tilde{\mathbf{q}} + \mathbf{Q}) \hat{c}_{\sigma\mu\alpha,\mathbf{G}+\mathbf{Q}}^\dagger(\tilde{\mathbf{k}} + \tilde{\mathbf{q}}) \\ \times \hat{c}_{\sigma'\mu'l'\alpha',\mathbf{G}'-\mathbf{Q}}^\dagger(\tilde{\mathbf{k}}' - \tilde{\mathbf{q}}) \hat{c}_{\sigma'\mu'l'\alpha',\mathbf{G}'}(\tilde{\mathbf{k}}') \hat{c}_{\sigma\mu\alpha,\mathbf{G}}(\tilde{\mathbf{k}})$$

$$V_{ll}(\mathbf{q}) = \frac{e^2}{2\Omega_0\epsilon_r\epsilon_0\sqrt{q^2+\kappa^2}}$$

$$\Omega_0 = \sqrt{3}L_s^2/2$$

$$V_{ll'}(\mathbf{q}) = \frac{e^2}{2\Omega_0\epsilon_r\epsilon_0q} e^{-q|l-l'|d_0}$$

$$E_{\text{tot.}} = E_{\text{kin.}} + E_{\text{HF}} + E_c^{\text{RPA}}$$

$$E_c^{\text{RPA}} = \int_{-\infty}^{\infty} \frac{d\omega}{4\pi} \sum_{\tilde{\mathbf{q}}, \mathbf{Q}, \mathbf{Q}'} \left\{ \ln \left[\delta_{\mathbf{Q}\mathbf{Q}'} - V_{\mathbf{Q}}(\tilde{\mathbf{q}}) \delta_{\mathbf{Q}\mathbf{Q}'} \chi_{\mathbf{Q}'\mathbf{Q}}^0(\tilde{\mathbf{q}}, i\omega) \right] \right. \\ \left. + V_{\mathbf{Q}}(\tilde{\mathbf{q}}) \delta_{\mathbf{Q}\mathbf{Q}'} \chi_{\mathbf{Q}'\mathbf{Q}}^0(\tilde{\mathbf{q}}, i\omega) \right\}$$

$$\chi_{\mathbf{Q}\mathbf{Q}'}^0(\tilde{\mathbf{q}}, \nu) = \frac{1}{N_s\Omega_0} \sum_{n', n, \tilde{\mathbf{k}}} \left[\sum_{\lambda, \mathbf{G}} C_{\lambda\mathbf{G}+\mathbf{Q}, n'\mathbf{k}+\tilde{\mathbf{q}}}^* C_{\lambda\mathbf{G}, n\tilde{\mathbf{k}}} \right]^* \left[\sum_{\lambda', \mathbf{G}'} C_{\lambda'\mathbf{G}'+\mathbf{Q}', n'\mathbf{k}+\tilde{\mathbf{q}}}^* C_{\lambda'\mathbf{G}', n\tilde{\mathbf{k}}} \right] \\ \times \left[\frac{\theta(\varepsilon_{n'}\tilde{\mathbf{k}}+\tilde{\mathbf{q}}}{\nu-\varepsilon_{n'}\tilde{\mathbf{k}}+\tilde{\mathbf{q}}} + \varepsilon_{n\tilde{\mathbf{k}}} + i\delta(\varepsilon_F - \varepsilon_{n\tilde{\mathbf{k}}}) \right. \\ \left. - \frac{\theta(\varepsilon_F - \varepsilon_{n'\mathbf{k}+\tilde{\mathbf{q}}})\theta(\varepsilon_{n\tilde{\mathbf{k}}} - \varepsilon_F)}{\nu - \varepsilon_{n'\mathbf{k}+\tilde{\mathbf{q}}} + \varepsilon_{n\tilde{\mathbf{k}}} - i\delta} \right]$$

$$\Sigma(12) = i \int d^3G(13)W(14)\Gamma(342)$$

$$G(12) = G_0(12) + \int d^3G_0(13)\Sigma(34)G(42)$$

$$\Gamma(123) = \delta(12)\delta(13) + \int d^4 d^5 \frac{\delta \Sigma(12)}{\delta G(45)} G(46)G(75)\Gamma(673)$$

$$P(12) = -i \int d^3 d^4 G(13)G(42)\Gamma(342)$$

$$W(12) = V(12) + \int d^3V(13)P(34)W(42)$$

$$\Gamma(123) = \delta(12)\delta(13)$$

$$\Sigma(12) = iG(12)W(12)$$

$$P(12) = -iG(12)G(21)$$

$$V(12) = \int d^3\epsilon(13)W(32)$$

$$\epsilon(12) = \delta(12) - \int d^3V(13)P(32)$$

$$G_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{n\mathbf{k}} \frac{\psi_{n\mathbf{k}}(\mathbf{r})\psi_{n\mathbf{k}}^*(\mathbf{r}')}{\omega - \varepsilon_{n\mathbf{k}} + i\delta \text{sgn}(\varepsilon_{n\mathbf{k}} - \varepsilon_F)}$$

$$\chi^0(\mathbf{r},\mathbf{r}',\nu) = -i \int \frac{d\omega}{2\pi} e^{i\omega\delta^+} G_0(\mathbf{r},\mathbf{r}',\omega+\nu)G_0(\mathbf{r}',\mathbf{r},\omega).$$

$$\epsilon_{\text{RPA}}(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r},\mathbf{r}') - \int d\mathbf{r}'' V(\mathbf{r},\mathbf{r}'')\chi^0(\mathbf{r}'',\mathbf{r}',\omega)$$

$$W_{\text{RPA}}(\mathbf{r},\mathbf{r}',\omega) = \int d\mathbf{r}'' [\epsilon_{\text{RPA}}^{-1}(\mathbf{r},\mathbf{r}'',\omega) - \delta(\mathbf{r},\mathbf{r}'')]V(\mathbf{r}'',\mathbf{r}')$$

$$\Sigma_c(\mathbf{r},\mathbf{r}',\omega) = \frac{i}{2\pi} \int d\nu e^{i\nu\delta^+} G_0(\mathbf{r},\mathbf{r}',\omega+\nu)W_{\text{RPA}}(\mathbf{r}',\mathbf{r},\nu)$$

$$\epsilon_{\mathbf{Q}\mathbf{Q}'}^{\text{RPA}}(\tilde{\mathbf{q}},\omega) = \delta_{\mathbf{Q}\mathbf{Q}'} - V(\tilde{\mathbf{q}}+\mathbf{Q})\chi_{\mathbf{Q}\mathbf{Q}'}^0(\tilde{\mathbf{q}},\omega),$$

$$W_{\mathbf{Q}\mathbf{Q}'}^{\text{RPA}}(\tilde{\mathbf{q}},\omega) = \left[\epsilon_{\mathbf{Q}\mathbf{Q}'}^{-1,\text{RPA}}(\tilde{\mathbf{q}},\omega) - \delta_{\mathbf{Q}\mathbf{Q}'} \right] V(\tilde{\mathbf{q}}+\mathbf{Q}')$$

$$\begin{aligned} \Sigma_c(\tilde{\mathbf{k}},\omega)_{n'n} = & \frac{i}{N_s\Omega_0} \sum_{m,\tilde{\mathbf{q}}} \sum_{\mathbf{G},\mathbf{G}'} \left[\sum_{\lambda,\mathbf{Q}} C_{\lambda\mathbf{G}+\mathbf{Q},m\tilde{\mathbf{k}}+\tilde{\mathbf{q}}}^* C_{\lambda\mathbf{Q},n'\tilde{\mathbf{k}}} \right]^* \left[\sum_{\lambda',\mathbf{Q}'} C_{\lambda'\mathbf{G}'+\mathbf{Q}',m\tilde{\mathbf{k}}+\tilde{\mathbf{q}}}^* C_{\lambda'\mathbf{Q}',n\tilde{\mathbf{k}}} \right] \\ & \times V(\tilde{\mathbf{q}}+\mathbf{G}) \int \frac{d\nu}{2\pi} e^{i\nu\eta} \frac{[\epsilon_{\mathbf{G}\mathbf{G}'}^{-1,\text{RPA}}(\tilde{\mathbf{q}},\nu) - \delta_{\mathbf{G}\mathbf{G}'}]}{\omega+\nu-\varepsilon_{m\tilde{\mathbf{k}}+\tilde{\mathbf{q}}} + i\delta \text{sgn}(\varepsilon_{m\tilde{\mathbf{k}}+\tilde{\mathbf{q}}} - \varepsilon_F)} \end{aligned}$$

$$\varepsilon_{n\mathbf{k}}^{\text{QP}} = \varepsilon_{n\mathbf{k}}^{\text{HF}} + Z_{n\tilde{\mathbf{k}}} \text{Re} \Sigma_c(\tilde{\mathbf{k}}, \varepsilon_{n\mathbf{k}}^{\text{HF}})_{nn},$$

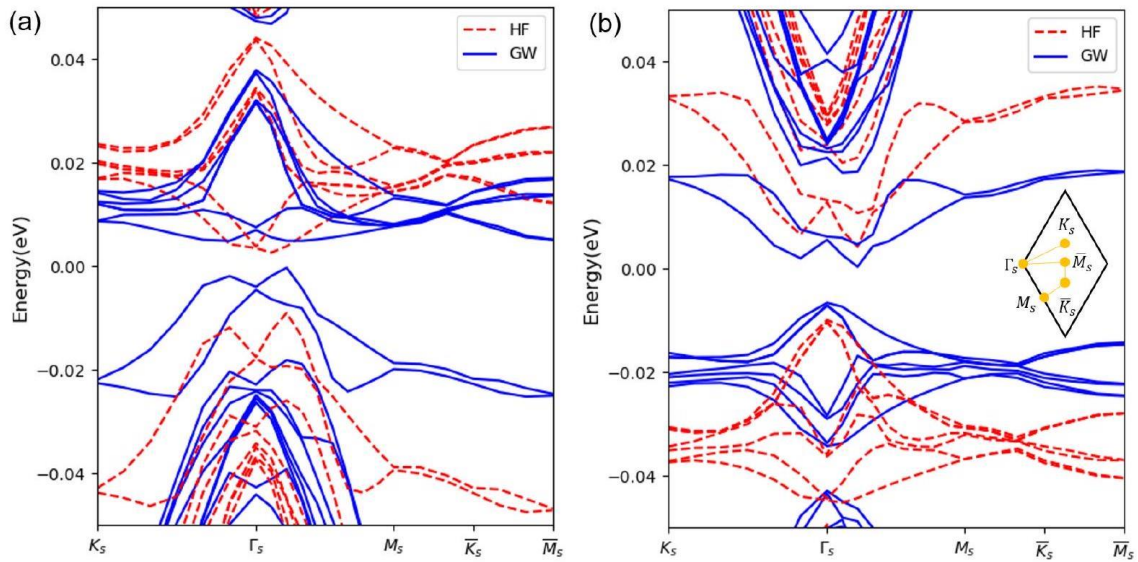


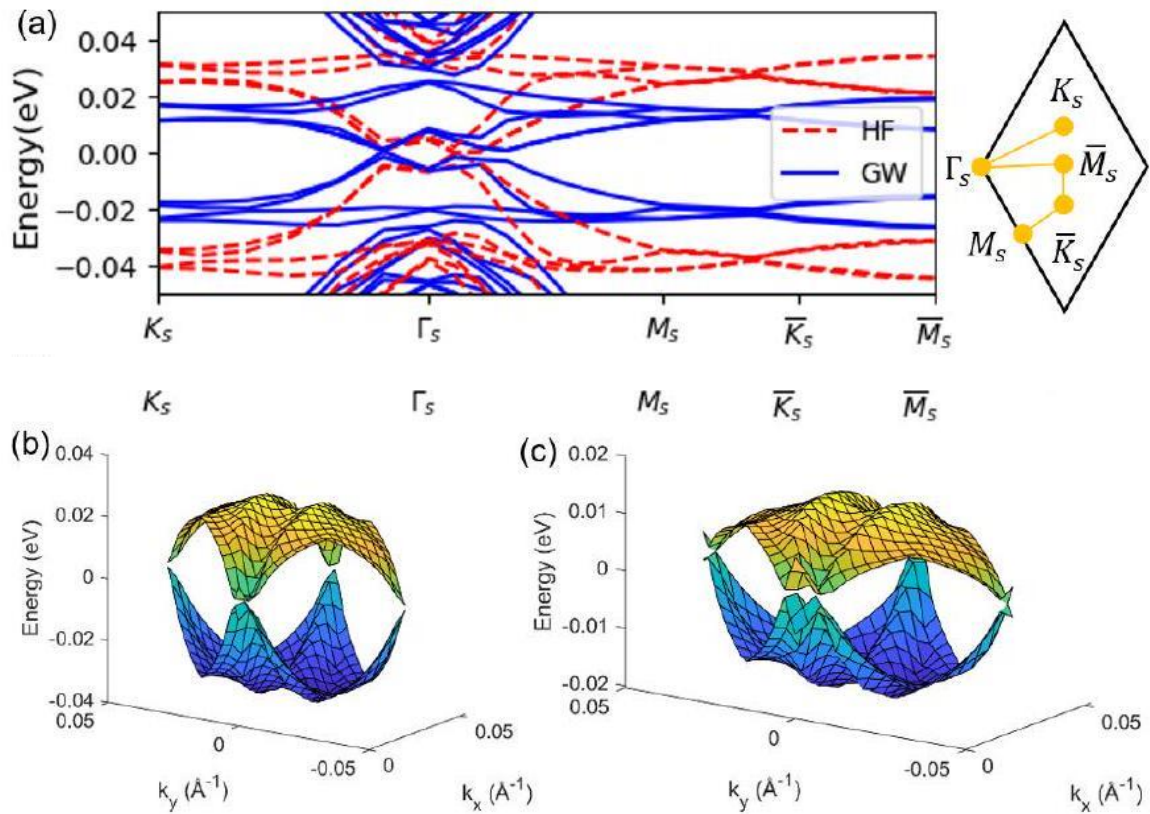
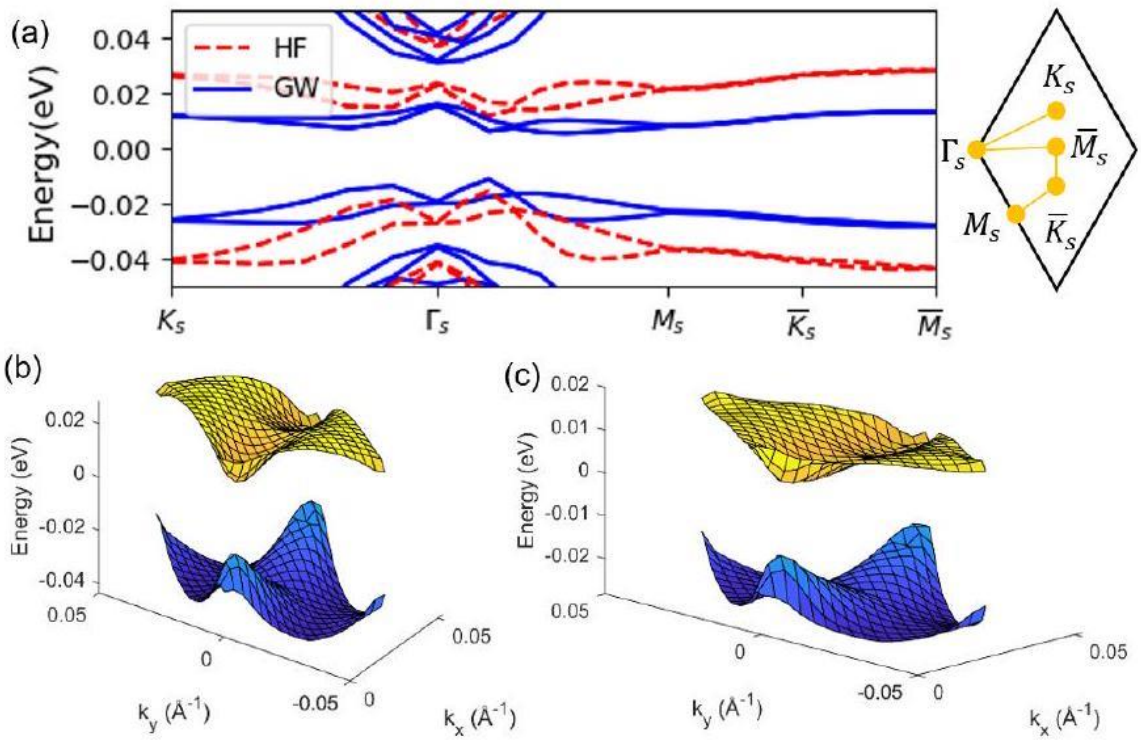
$$Z_{n\tilde{\mathbf{k}}} = \left[1 - \text{Re} \left(\frac{\partial \Sigma_c(\tilde{\mathbf{k}}, \omega)_{nn}}{\partial \omega} \right)_{\omega=\varepsilon_{n\tilde{\mathbf{k}}}^{\text{HF}}} \right]^{-1}.$$

$$\epsilon_{\mathbf{Q}\mathbf{Q}'}^{-1, \text{MPA}}(\tilde{\mathbf{q}}, \nu) - \delta_{\mathbf{Q}\mathbf{Q}'} = \sum_l^{N_p} \frac{2R_{l, \mathbf{Q}\mathbf{Q}'}(\tilde{\mathbf{q}})\Omega_{l, \mathbf{Q}\mathbf{Q}'}(\tilde{\mathbf{q}})}{\nu^2 - \Omega_{l, \mathbf{Q}\mathbf{Q}'}^2(\tilde{\mathbf{q}})},$$

$$\begin{aligned} \Sigma_c(\tilde{\mathbf{k}}, \omega)_{nn} = & \frac{1}{N_s \Omega_0} \sum_{m, \tilde{\mathbf{q}}} \sum_{\mathbf{G}, \mathbf{G}'} \left[\sum_{\lambda, \mathbf{Q}} C_{\lambda \mathbf{G} + \mathbf{Q}, m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}}^* C_{\lambda \mathbf{Q}, n\tilde{\mathbf{k}}} \right] \left[\sum_{\lambda', \mathbf{Q}'} C_{\lambda' \mathbf{G}' + \mathbf{Q}', m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}}^* C_{\lambda' \mathbf{Q}', n\tilde{\mathbf{k}}} \right] \\ & \times \sum_l^{N_p} \frac{V(\tilde{\mathbf{q}} + \mathbf{G}) R_{\mathbf{G}', \mathbf{G}, l}(\tilde{\mathbf{q}})}{\omega - \varepsilon_{m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}} + i\delta \text{sgn}(\varepsilon_{m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}} - \varepsilon_F) + \Omega_{\mathbf{G}', \mathbf{G}, l}(\tilde{\mathbf{q}})(2f_{m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}} - 1)} \end{aligned}$$

$$\begin{aligned} \frac{\partial \Sigma_c(\tilde{\mathbf{k}}, \omega)_{nn}}{\partial \omega} = & \frac{-1}{N_s \Omega_0} \sum_{m, \tilde{\mathbf{q}}} \sum_{\mathbf{G}, \mathbf{G}'} \left[\sum_{\lambda, \mathbf{Q}} C_{\lambda \mathbf{G} + \mathbf{Q}, m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}}^* C_{\lambda \mathbf{Q}, n\tilde{\mathbf{k}}} \right] \left[\sum_{\lambda', \mathbf{Q}'} C_{\lambda' \mathbf{G}' + \mathbf{Q}', m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}}^* C_{\lambda' \mathbf{Q}', n\tilde{\mathbf{k}}} \right] \\ & \times \sum_l^{N_p} \frac{V(\tilde{\mathbf{q}} + \mathbf{G}) R_{\mathbf{G}', \mathbf{G}, l}(\tilde{\mathbf{q}})}{[\omega - \varepsilon_{m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}} + i\delta \text{sgn}(\varepsilon_{m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}} - \varepsilon_F) + \Omega_{\mathbf{G}', \mathbf{G}, l}(\tilde{\mathbf{q}})(2f_{m\tilde{\mathbf{k}} + \tilde{\mathbf{q}}} - 1)]^2} \end{aligned}$$





$$E = \int d^3r \varepsilon(r)$$

$$\varepsilon = \varepsilon_{NN}[\tau_n, \tau_p, \rho_n, \rho_p, J_n, J_p] + \varepsilon_{N\Lambda}[\tau_\Lambda, \rho_\Lambda, \rho_N]$$

$$[\rho_q, \tau_q, \mathbf{J}_q] = \sum_{k=1}^{N_q} n_q^k \left[|\phi_q^k|^2, |\nabla \phi_q^k|^2, \phi_q^{k*} (\nabla \phi_q^k \times \sigma) / k \right].$$

$$V_q(\mathbf{r}_1, \mathbf{r}_2) = V_q' \left[1 - \frac{\rho_N((\mathbf{r}_1 + \mathbf{r}_2)/2)}{0.16 \text{fm}^{-3}} \right] \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

$$\varepsilon_{\Lambda} = \frac{\tau_{\Lambda}}{2m_{\Lambda}} + \varepsilon_{N\Lambda}(\rho_N, \rho_{\Lambda})$$

$$\rho_{\Lambda} \frac{B}{A}(0, \rho_{\Lambda}) + \varepsilon_{N\Lambda}(\rho_N, \rho_{\Lambda}) = (\rho_N + \rho_{\Lambda}) \frac{B}{A}(\rho_N + \rho_{\Lambda}) \\ - \rho_N \frac{B}{A}(\rho_N, 0)$$

$$\varepsilon_{N\Lambda}(\rho_N, \rho_{\Lambda}) = 2 \sum_{k < k_F^{(\Lambda)}} U_{\Lambda}(k) \\ + 2 \sum_{k < k_F^{(N)}} \left[U_N^{(N)}(k) \Big|_{\rho_{\Lambda}} - U_N^{(N)}(k) \Big|_{\rho_{\Lambda}=0} \right].$$

$$m_{\Lambda}^{\ast}=m_{\Lambda}+U_S^{\Lambda}$$

$$\varepsilon_{\Lambda} = \frac{1}{2m_{\Lambda}} \tau_{\Lambda} + \varepsilon_{N\Lambda}(\rho_N, \rho_{\Lambda}) \\ + \left(\frac{m_{\Lambda}}{m_{\Lambda}^*(\rho_N)} - 1 \right) \left(\frac{\tau_{\Lambda}}{2m_{\Lambda}} - \frac{3}{5} \frac{(3\pi^2)^{2/3}}{2m_{\Lambda}} \rho_{\Lambda}^{5/3} \right)$$

$$\left[-\nabla\cdot\frac{1}{2m_q^*(\boldsymbol{r})}\nabla+V_q(\boldsymbol{r})-i\boldsymbol{W}_q(\boldsymbol{r})\cdot(\nabla\times\boldsymbol{\sigma})\right]\phi_q^k(\boldsymbol{r})=e_q^k\phi_q^k(\boldsymbol{r}),$$

$$V_N = V_N^{\text{SHF}} + \frac{\partial \varepsilon_{N\Lambda}}{\partial \rho_N} \\ + \frac{\partial}{\partial \rho_N} \left(\frac{m_{\Lambda}}{m_{\Lambda}^*(\rho_N)} \right) \left(\frac{\tau_{\Lambda}}{2m_{\Lambda}} - \frac{3}{5} \frac{(3\pi^2)^{2/3}}{2m_{\Lambda}} \rho_{\Lambda}^{5/3} \right), \\ V_{\Lambda} = \frac{\partial \varepsilon_{N\Lambda}}{\partial \rho_{\Lambda}} - \left(\frac{m_{\Lambda}}{m_{\Lambda}^*(\rho_N)} - 1 \right) \frac{(3\pi^2)^{2/3}}{2m_{\Lambda}} \rho_{\Lambda}^{2/3}$$

$$\varepsilon_{N\Lambda} = -(\varepsilon_1 - \varepsilon_2 \rho_N + \varepsilon_3 \rho_N^2) \rho_N \rho_{\Lambda} \\ + (\varepsilon_4 - \varepsilon_5 \rho_N + \varepsilon_6 \rho_N^2) \rho_N \rho_{\Lambda}^{5/3} \\ - (\varepsilon_7 - \varepsilon_8 \rho_{\Lambda} + \varepsilon_9 \rho_{\Lambda}^2) \rho_{\Lambda}^2 \\ \frac{m_{\Lambda}^*}{m_{\Lambda}}(\rho_N) = -\mu_1 - \mu_2 \rho_N + \mu_3 \rho_N^2 - \mu_4 \rho_N^3.$$

$$\frac{1}{m_q} \rightarrow \frac{1}{m_q} - \frac{1}{M}$$

$$M=(N_n+N_p)m_N+N_\Lambda m_\Lambda$$

$$\beta_2^{(q)}\equiv\sqrt{\frac{\overline{\pi}}{5}}\frac{\langle 2z^2-r^2\rangle_q}{\langle r^2+z^2\rangle_q}$$

$$\Delta = \sqrt{\sum_{i=1}^N \left(B_{\Lambda,i}^{\text{Exp}} - B_{\Lambda,i}^{\text{SHF}}\right)^2/N}$$

$$\delta = \sqrt{\sum_{i=1}^N \left[(B_{\Lambda,i}^{\text{Exp}} - B_{\Lambda,i}^{\text{SHF}})/B_{\Lambda,i}^{\text{Exp}} \right]^2/N}$$

$$B_\Lambda = E\left(\begin{smallmatrix} A \\ \Lambda \end{smallmatrix} Z\right) - E\left(\begin{smallmatrix} A^{-1} \\ \Lambda \end{smallmatrix} Z\right).$$

$$H_{m,n}^{\lambda_N}(\boldsymbol{q})=\frac{|\boldsymbol{q}|^2}{2m}\delta_{m,n}+\Delta\langle m|\hat{L}(\boldsymbol{q})|n\rangle$$

$$\hat{L}(\boldsymbol{q})=\hat{\mathcal{D}}_{\boldsymbol{q}}^{\dagger}\hat{\mathcal{D}}_{\boldsymbol{q}},$$

$$\hat{\mathcal{D}}_{\boldsymbol{q}}=\hat{b}-\sqrt{B}q_{\bar{z}}\mathcal{P}_{N-1}^{\perp}$$

$$\hat{b}|n\rangle=\sqrt{n}|n-1\rangle$$

$$q_{\bar{z}}=(q_x-iq_y)/\sqrt{2}$$

$$\mathcal{P}_{N-1}^{\perp}=\sum_{n=0}^{N-2}|n\rangle\langle n|$$

$$\left|\psi_q^{(0)}\right\rangle=e^{i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}}\left|s_q^{(0)}\right\rangle$$

$$\hat{\mathcal{D}}_q\left|s_q^{(0)}\right\rangle=0$$

$$\left|s_q^{(0)}\right\rangle=\mathcal{N}_q\sum_{n=0}^{N-1}\frac{\left(\sqrt{B}q_{\bar{z}}\right)^n}{\sqrt{n!}}|n\rangle,$$

$$\mathcal{N}_q^{-2}=\left(\sum_{n=0}^{N-1}\frac{\left(\frac{B|\boldsymbol{q}|^2}{2}\right)^n}{n!}\right)=\frac{\exp\left(\frac{B|\boldsymbol{q}|^2}{2}\right)\Gamma\left(N,\frac{B}{2}|\boldsymbol{q}|^2\right)}{(N-1)!}$$

$$\Gamma(a,b)=\int_b^{\infty}dte^{-t}t^{a-1}$$

$$E^{(n)}(\boldsymbol{q})=\frac{|\boldsymbol{q}|^2}{2m}+\Delta\varepsilon^{(n)}(\boldsymbol{q})$$

$$\mathcal{F}_N(\boldsymbol{q},\boldsymbol{q}')=\left\langle\psi_{\boldsymbol{q}}^{(0)}\right|e^{i(\boldsymbol{q}-\boldsymbol{q}')\cdot\boldsymbol{r}}\left|\psi_{\boldsymbol{q}'}^{(0)}\right\rangle=\left\langle s_{\boldsymbol{q}}^{(0)}\mid s_{\boldsymbol{q}'}^{(0)}\right\rangle.$$

$$\mathcal{F}_N(\boldsymbol{q},\boldsymbol{q}')=\mathcal{N}_{\boldsymbol{q}}\mathcal{N}_{\boldsymbol{q}'}\sum_{n=0}^{N-1}\frac{(\mathcal{B}q_zq_z')^n}{n!}$$

$$\mathcal{F}_N(\boldsymbol{q},\boldsymbol{q}')=\mathcal{M}_N(\boldsymbol{q},\boldsymbol{q}')\mathcal{F}_{\text{LLL}}(\boldsymbol{q},\boldsymbol{q}')$$

$$\mathcal{M}_N(\boldsymbol{q},\boldsymbol{q}')=\frac{\Gamma(N,\mathcal{B}q_zq_z')}{\sqrt{\Gamma\left(N,\frac{\mathcal{B}}{2}|\boldsymbol{q}|^2\right)\Gamma\left(N,\frac{\mathcal{B}}{2}|\boldsymbol{q}'|^2\right)}},$$

$$\mathcal{F}_{\text{LLL}}(\boldsymbol{q},\boldsymbol{q}')=\exp\left(-\frac{\mathcal{B}}{4}(|\boldsymbol{q}-\boldsymbol{q}'|^2+2i\boldsymbol{q}\wedge\boldsymbol{q}')\right),$$

$$\lim_{N\rightarrow\infty}\mathcal{M}_N(\boldsymbol{q},\boldsymbol{q}')=1$$

$$\lim_{N\rightarrow\infty}\mathcal{F}_N(\boldsymbol{q},\boldsymbol{q}')=\mathcal{F}_{\text{LLL}}(\boldsymbol{q},\boldsymbol{q}'),$$

$$\begin{aligned}\mathcal{Q}_N^{ab}(\boldsymbol{q})&=\left\langle\partial_{q_a}u_{\boldsymbol{q}}^{(0)}\right|Q_{\boldsymbol{q}}\left|\partial_{q_b}u_{\boldsymbol{q}}^{(0)}\right\rangle\\&=g_N^{ab}(\boldsymbol{q})-\frac{i}{2}\epsilon^{ab}\Omega_N(\boldsymbol{q}),\end{aligned}$$

$$Q_{\boldsymbol{q}}=\mathbb{1}-\left|u_{\boldsymbol{q}}^{(0)}\right\rangle\left\langle u_{\boldsymbol{q}}^{(0)}\right|,a$$

$$\Omega_N(\boldsymbol{q})=\mathcal{B}+\mathcal{B}e^{-\frac{\mathcal{B}|\boldsymbol{q}|^2}{2}}\frac{E_{1-N}\left(\frac{\mathcal{B}}{2}|\boldsymbol{q}|^2\right)-E_{-N}\left(\frac{\mathcal{B}}{2}|\boldsymbol{q}|^2\right)}{\left(E_{1-N}\left(\frac{\mathcal{B}}{2}|\boldsymbol{q}|^2\right)\right)^2}$$

$$E_n(z)=z^{n-1}\Gamma(1-n,z)$$

$$\lim_{N\rightarrow\infty}\Omega_N(\boldsymbol{q})=\mathcal{B}$$

$$I_N(\kappa)=2\pi\int_0^\kappa d|\boldsymbol{q}||\boldsymbol{q}|\Omega_N(|\boldsymbol{q}|)=\pi\mathcal{B}\kappa^2-\frac{2\pi e^{-\frac{\mathcal{B}\kappa^2}{2}}}{E_{1-N}\left(\frac{\mathcal{B}\kappa^2}{2}\right)}$$

$$\lim_{\kappa\rightarrow\infty}I_N(\kappa)=2\pi(N-1)$$

$$g_N^{ab}(\boldsymbol{q})=\frac{1}{2}\Omega_N(\boldsymbol{q})\delta^{ab}$$

$$\text{Tr}(g_N^{ab}(\boldsymbol{q}))=|\Omega_N(\boldsymbol{q})|$$

$$\Omega_N(|\boldsymbol{q}|)=4(N-1)/(\mathcal{B}|\boldsymbol{q}|^4)+\mathcal{O}(1/|\boldsymbol{q}|^6)\text{ as }|\boldsymbol{q}|\rightarrow\infty)$$

$$\Omega_N(|\mathbf{q}|) = \mathcal{B} - \frac{N\mathcal{B}^N |\mathbf{q}|^{2(N-1)}}{2^{N-1}(N-1)!} + \mathcal{O}(|\mathbf{q}|^{2N}),$$

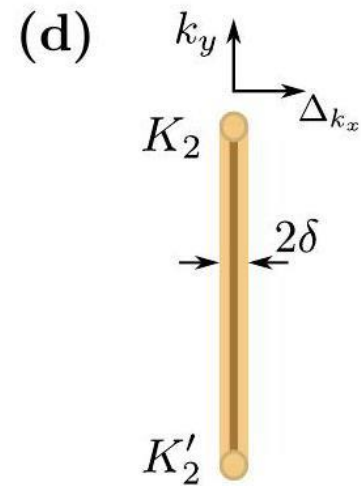
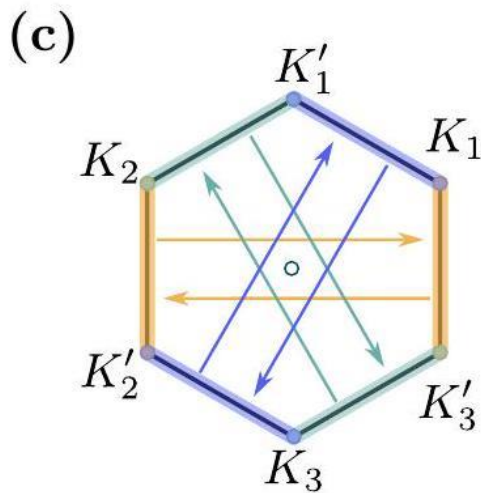
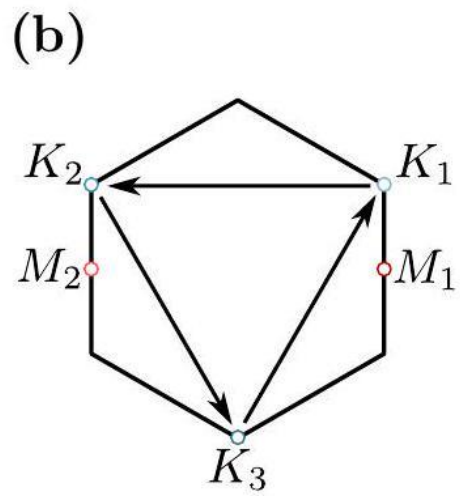
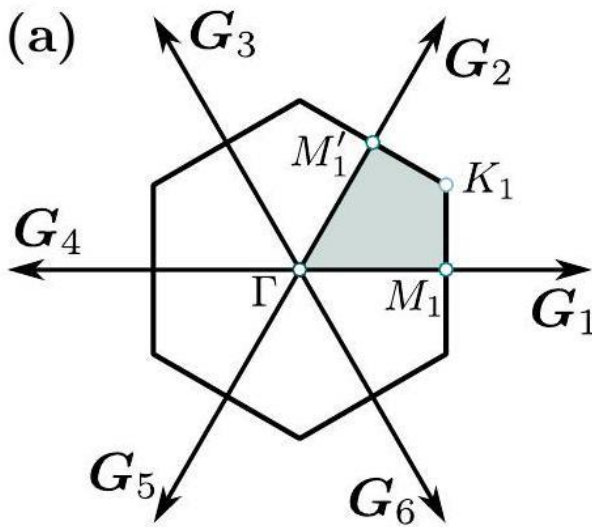
$$\mathcal{M}_N(\mathbf{0}, \mathbf{q}) = \sqrt{(N-1)!/\Gamma(N, \mathcal{B}|\mathbf{q}|^2/2)} = 1 + \mathcal{B}^N |\mathbf{q}|^{2N}/(2^{N+1}N!) + \mathcal{O}(|\mathbf{q}|^{2(N+1)})$$

$$U(\mathbf{r}) = -U_0 \sum_{\mathbf{G}_j} e^{i\mathbf{G}_j \cdot \mathbf{r}}$$

$$\mathbf{G}_j = g(\cos((j-1)\pi/3), \sin((j-1)\pi/3)) (j=1,2,3,4,5,6)$$

$$g=4\pi/(a_l\sqrt{3})$$

$$\hat{\mathcal{H}}=\hat{\mathcal{H}}_0+\hat{\mathcal{H}}_{\text{pot}},$$



$$\hat{\mathcal{H}}_0 = \sum_{\mathbf{k}, \mathbf{g}} c_{\mathbf{k}, \mathbf{g}}^\dagger \frac{|\mathbf{k} + \mathbf{g}|^2}{2m} c_{\mathbf{k}, \mathbf{g}} = \sum_{\mathbf{k}, \mathbf{g}} \varepsilon(\mathbf{k} + \mathbf{g}) c_{\mathbf{k}, \mathbf{g}}^\dagger c_{\mathbf{k}, \mathbf{g}}$$

$$\hat{\mathcal{H}}_{\text{pot}} = -U_0 \sum_{\mathbf{G}_i} \hat{\rho}_{\mathbf{G}_i},$$

$$\mathcal{E}(\boldsymbol{q}) = |\boldsymbol{q}|^2/2m$$

$$c_{\boldsymbol{k},\boldsymbol{g}}^\dagger \equiv c_{\boldsymbol{k}+\boldsymbol{g}}^\dagger \left| \psi_{\boldsymbol{k}+\boldsymbol{g}}^{(0)} \right\rangle, \tilde{\rho}_{\boldsymbol{q}}$$

$$\tilde{\rho}_{\boldsymbol{q}} = \sum_{\boldsymbol{k},\boldsymbol{g}} c_{\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{q}}^\dagger \mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{q},\boldsymbol{k}+\boldsymbol{g}) c_{\boldsymbol{k}+\boldsymbol{g}}$$

$$\boldsymbol{g} = n_1 \boldsymbol{G}_1 + n_2 \boldsymbol{G}_2 (n_1, n_2 \in \mathbb{Z})$$

$$U_0|\mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{G}_i,\boldsymbol{k}+\boldsymbol{g})|\arg\left[\mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{G}_i,\boldsymbol{k}+\boldsymbol{g})\right]$$

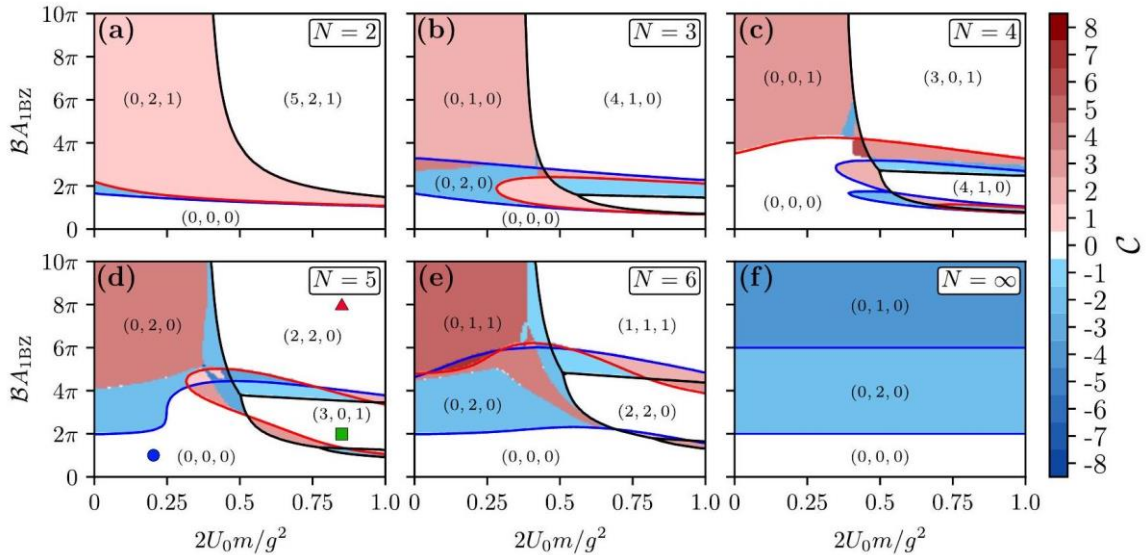
$$|\varphi_{\boldsymbol{k}}\rangle = \sum_{\boldsymbol{g}} v_{\boldsymbol{g}}(\boldsymbol{k}) \left| \psi_{\boldsymbol{k}+\boldsymbol{g}}^{(0)} \right\rangle$$

$$\langle \varphi_{\boldsymbol{k}} | \hat{\mathcal{H}} | \varphi_{\boldsymbol{k}} \rangle = E_{\text{kin}}(\boldsymbol{k}) + E_{\text{pot}}(\boldsymbol{k}),$$

$$E_{\text{kin}}(\boldsymbol{k}) = \sum_{\boldsymbol{g}} \left| v_{\boldsymbol{g}}(\boldsymbol{k}) \right|^2 \frac{|\boldsymbol{k}+\boldsymbol{g}|^2}{2m}$$

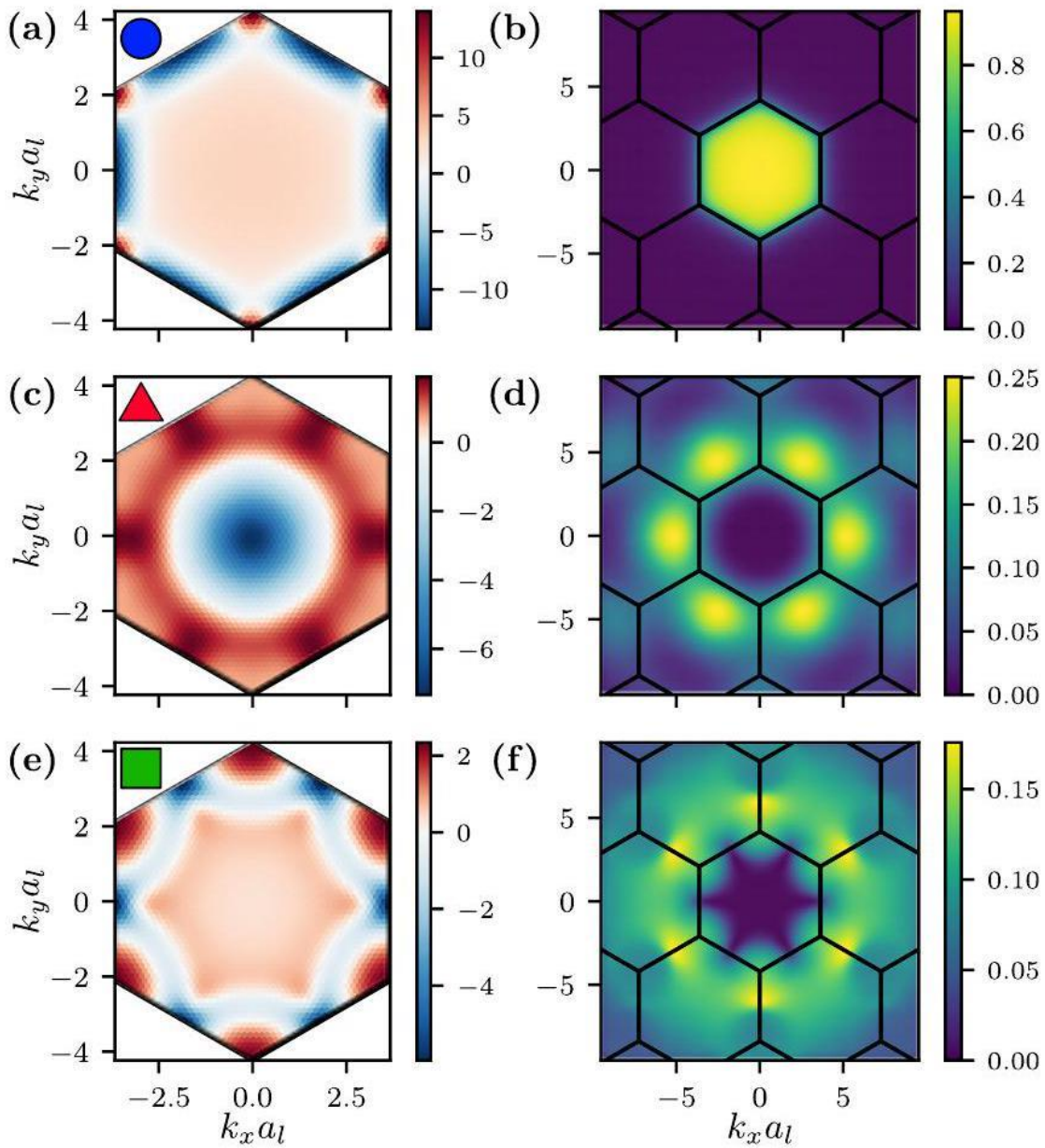
$$E_{\text{pot}}(\boldsymbol{k}) = -U_0 \sum_{\boldsymbol{g}, \boldsymbol{G}_i} v_{\boldsymbol{g}+\boldsymbol{G}_i}^*(\boldsymbol{k}) v_{\boldsymbol{g}}(\boldsymbol{k}) \\ \times \mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{G}_i,\boldsymbol{k}+\boldsymbol{g})$$

$$E_{\text{hop}}^{\boldsymbol{g},\boldsymbol{g}+\boldsymbol{G}_i}(\boldsymbol{k}) = -U_0 v_{\boldsymbol{g}+\boldsymbol{G}_i}^*(\boldsymbol{k}) v_{\boldsymbol{g}}(\boldsymbol{k}) \mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{G}_i,\boldsymbol{k}+\boldsymbol{g}) - U_0 v_{\boldsymbol{g}+\boldsymbol{G}_i}(\boldsymbol{k}) v_{\boldsymbol{g}}^*(\boldsymbol{k}) \mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g},\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{G}_i) \\ = -2U_0 |v_{\boldsymbol{g}+\boldsymbol{G}_i}(\boldsymbol{k})| |v_{\boldsymbol{g}}(\boldsymbol{k})| |\mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{G}_i,\boldsymbol{k}+\boldsymbol{g})| \\ \times \cos\left(\arg\left[\mathcal{F}_N(\boldsymbol{k}+\boldsymbol{g}+\boldsymbol{G}_i,\boldsymbol{k}+\boldsymbol{g})\right] + \arg\left[v_{\boldsymbol{g}}(\boldsymbol{k})\right] - \arg\left[v_{\boldsymbol{g}+\boldsymbol{G}_i}(\boldsymbol{k})\right]\right)$$



$$\hat{R}_{2\pi m/n_{\boldsymbol{\kappa}}}|\varphi_{\boldsymbol{\kappa}}\rangle = \sum_{\boldsymbol{g}} v_{\boldsymbol{g}}(\boldsymbol{\kappa}) \left| \psi_{R_{2\pi m/n_{\boldsymbol{\kappa}}}(\boldsymbol{\kappa}+\boldsymbol{g})}^{(0)} \right\rangle \\ = \exp\left[\frac{i2\pi m\ell_{\boldsymbol{\kappa}}}{n_{\boldsymbol{\kappa}}}\right]|\varphi_{\boldsymbol{\kappa}}\rangle$$

$$\mathcal{C} = \ell_{\Gamma} + 2\ell_K + 3\ell_M \pmod{6}$$



$$\left\langle c_{\mathbf{k},\mathbf{g}}^{\dagger} c_{\mathbf{k},\mathbf{g}} \right\rangle |v_{\mathbf{g}}(\mathbf{k})|^2$$

$$\mathcal{E}(\mathbf{k}+\mathbf{g})=\mathcal{E}(\mathbf{k}+\mathbf{g}+\mathbf{G}_i)$$

$$|\varphi_{\Gamma}\rangle=|\psi_0^{(0)}\rangle$$

$$\left| \varphi_K^{(\ell_K)} \right\rangle = \frac{1}{\sqrt{3}} \Big(\left| \psi_{K_1}^{(0)} \right\rangle + \bar{\omega}^{\ell_K} \left| \psi_{K_2}^{(0)} \right\rangle + \bar{\omega}^{2\ell_K} \left| \psi_{K_3}^{(0)} \right\rangle \Big)$$

$$\left| \varphi_M^{(\ell_M)} \right\rangle = \frac{1}{\sqrt{2}} \Big(\left| \psi_{M_1}^{(0)} \right\rangle + e^{i\pi \ell_M} \left| \psi_{M_2}^{(0)} \right\rangle \Big)$$

$$\left| \varphi_K^{(\ell_K)} \right\rangle \left| \varphi_M^{(\ell_M)} \right\rangle E_{\text{pot}}^{(\ell_K)} = \left\langle \varphi_K^{(\ell_K)} \right| \hat{\mathcal{H}}_{\text{pot}} \left| \varphi_K^{(\ell_K)} \right\rangle$$

$$E_{\text{pot}}^{(\ell_M)} = \left\langle \varphi_M^{(\ell_M)} \left| \hat{\mathcal{H}}_{\text{pot}} \right| \varphi_M^{(\ell_M)} \right\rangle$$

$$E_{\text{pot}}^{(\ell_M)} = (-1)^{\ell_M+1} U_0 \frac{e^{-\frac{\mathcal{B}A_{1\text{BZ}}}{2\sqrt{3}}} \Gamma\left(N, -\frac{\mathcal{B}A_{1\text{BZ}}}{4\sqrt{3}}\right)}{\Gamma\left(N, \frac{\mathcal{B}A_{1\text{BZ}}}{4\sqrt{3}}\right)}.$$

$$E_{\text{pot}}^{(\ell_M)} = (-1)^{\ell_M+1} U_0 \exp\left(-\frac{\mathcal{B}A_{1\text{BZ}}}{2\sqrt{3}}\right)$$

$$E_{\text{pot}}^{(\ell_K)} = -\frac{2U_0 e^{-\frac{\mathcal{B}A_{1\text{BZ}}}{2\sqrt{3}}}}{\Gamma\left(N, \frac{\mathcal{B}A_{1\text{BZ}}}{3\sqrt{3}}\right)} \text{Re}\left(\exp\left(i\left(\frac{2\pi\ell_K}{3} + \frac{\mathcal{B}A_{1\text{BZ}}}{6}\right)\right) \Gamma\left(N, \frac{\mathcal{B}A_{1\text{BZ}}}{18}(3i - \sqrt{3})\right)\right)$$

$$\min_{\ell_K} \left[-\cos\left(\frac{2\pi\ell_K}{3} + \frac{\mathcal{B}A_{1\text{BZ}}}{6} + \phi(N, \mathcal{B}A_{1\text{BZ}})\right) \right]$$

$$\phi(N, \mathcal{B}A_{1\text{BZ}}) = \arg\left[\Gamma(N, (3i - \sqrt{3})\mathcal{B}A_{1\text{BZ}}/18)\right]$$

$$E_{\text{pot}}^{(\ell_K)} = -2U_0 e^{-\frac{\mathcal{B}A_{1\text{BZ}}}{2\sqrt{3}}} \cos\left(\frac{1}{6}(\mathcal{B}A_{1\text{BZ}} + 4\pi\ell_K)\right)$$

$$\Omega(\mathbf{k}) = i \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) \left(\partial_{k_x} + iA_x^{\text{P}}(\mathbf{k} + \mathbf{g}_3) - iA_x^{\text{P}}(\mathbf{k} + \mathbf{g}_2) \right) \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2}(\mathbf{k}) \left(\partial_{k_y} + iA_y^{\text{P}}(\mathbf{k} + \mathbf{g}_1) - iA_y^{\text{P}}(\mathbf{k} + \mathbf{g}_3) \right) \mathcal{P}_{\mathbf{g}_1 \mathbf{g}_3}(\mathbf{k}) - (x \leftrightarrow y) \\ + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^{\text{P}}(\mathbf{k} + \mathbf{g})$$

$$\mathcal{P}_{\mathbf{g}_1 \mathbf{g}_2}(\mathbf{k}) = \left\langle c_{\mathbf{k} \mathbf{g}_1}^\dagger c_{\mathbf{k} \mathbf{g}_2} \right\rangle$$

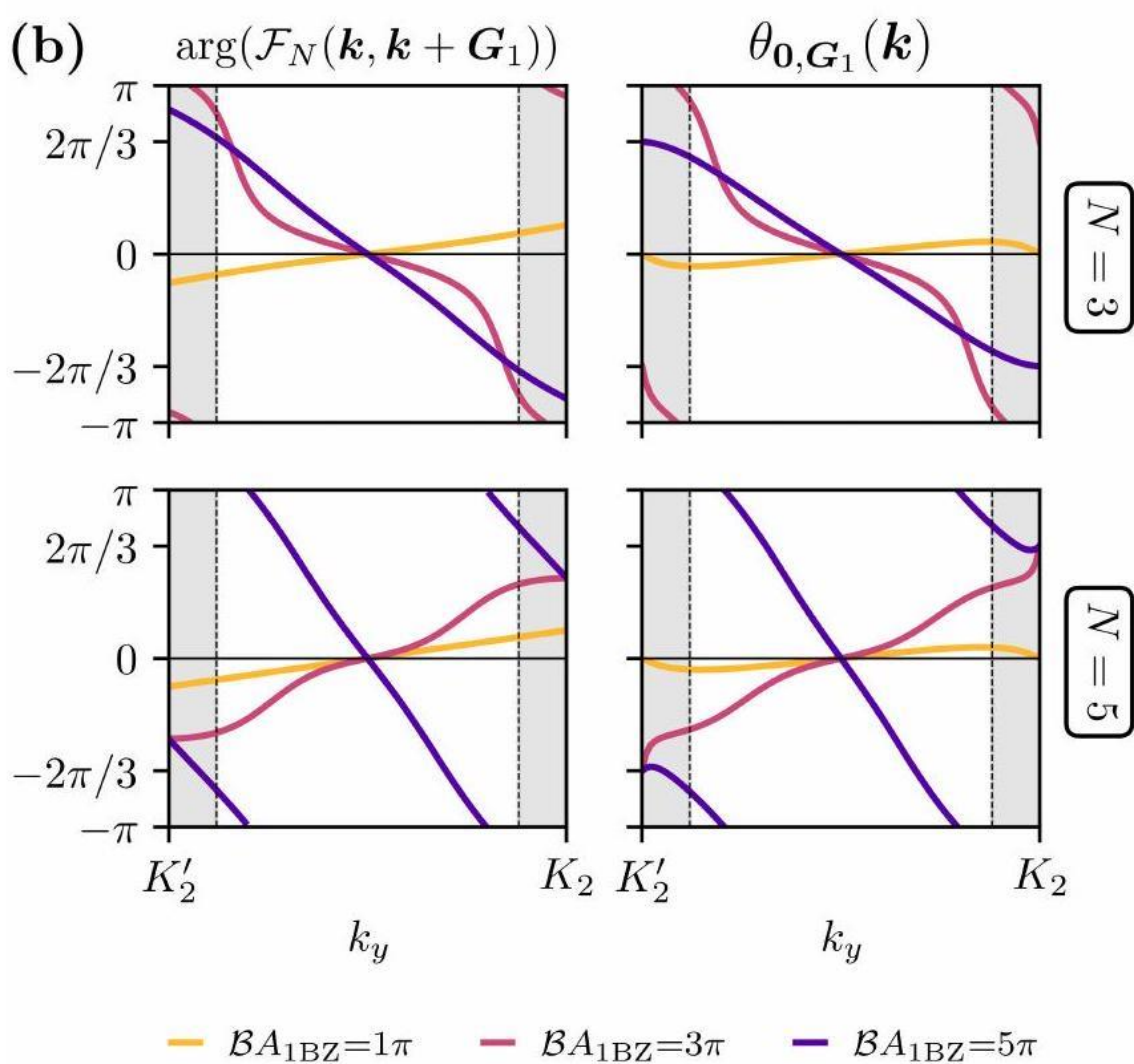
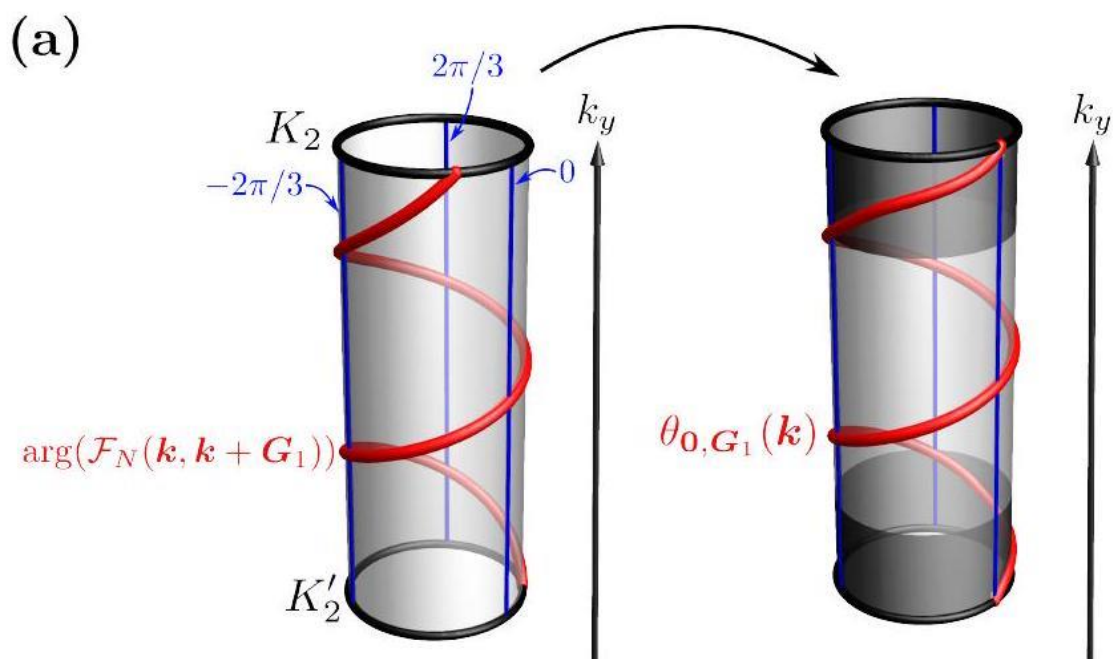
$$\begin{aligned} \mathcal{P}_{\mathbf{g} \mathbf{g}'}(\mathbf{k}) &= v_{\mathbf{g}}^*(\mathbf{k}) v_{\mathbf{g}'}(\mathbf{k}) \\ &= \sqrt{n(\mathbf{k} + \mathbf{g}) n(\mathbf{k} + \mathbf{g}')} e^{i\theta_{\mathbf{g}' \mathbf{g}}(\mathbf{k})} \end{aligned}$$

$$\begin{aligned} \Omega(\mathbf{k}) = & - \sum_{\mathbf{g}_2, \mathbf{g}_3} n(\mathbf{k} + \mathbf{g}_2) \left[\left(\partial_{k_x} \theta_{\mathbf{g}_2 \mathbf{g}_3}(\mathbf{k}) + A_x^{\text{P}}(\mathbf{k} + \mathbf{g}_3) - A_x^{\text{P}}(\mathbf{k} + \mathbf{g}_2) \right) \partial_{k_y} n(\mathbf{k} + \mathbf{g}_3) \right. \\ & \left. - \left(\partial_{k_y} \theta_{\mathbf{g}_2 \mathbf{g}_3}(\mathbf{k}) + A_y^{\text{P}}(\mathbf{k} + \mathbf{g}_3) - A_y^{\text{P}}(\mathbf{k} + \mathbf{g}_2) \right) \partial_{k_x} n(\mathbf{k} + \mathbf{g}_3) \right] \\ & + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^{\text{P}}(\mathbf{k} + \mathbf{g}) \end{aligned}$$

$$\Omega^{\text{bulk}}(\mathbf{k}) \approx \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^{\text{P}}(\mathbf{k} + \mathbf{g}) \approx \Omega^{\text{P}}(\mathbf{k})$$

$$\begin{aligned} & \int_{-\delta}^{\delta} d\Delta_{k_x} \Omega^{W_1}(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \\ &= - \left(\partial_{k_y} \theta_{\mathbf{0} \mathbf{G}_1}(\mathbf{k}^{\text{LW}}) + A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) \right) \end{aligned}$$

$$\begin{aligned}
\Phi_{W_1} &= - \int_{\text{LW}} dk_y \left(\partial_{k_y} \theta_{0\mathbf{G}_1}(\mathbf{k}) + A_y^{\text{P}}(\mathbf{k} + \mathbf{G}_1) - A_y^{\text{P}}(\mathbf{k}) \right) \\
&\quad - \left[\int_{W_1} dk_y \left(A_y^{\text{P}}(\mathbf{k}) - A_y^{\text{P}}(\mathbf{k} + \mathbf{G}_1) \right) \right] \\
\int dk_y \left(A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) \right) &= - \frac{1}{3} \int_{\text{1BZ}} d^2k \Omega^P(\mathbf{k}) = - \frac{1}{3} \Phi_{\text{1BZ}}^{\text{parent}} \\
\Phi &= 3\Phi_{W_1} + \int d^2k \Omega_{\text{bulk}} \\
&= -3 \int_{K'_2}^{K_2} dk_y \partial_{k_y} \theta_{0\mathbf{G}_1}(\mathbf{k})
\end{aligned}$$



$$\arg\left(\mathcal{F}_N(\mathbf{k}, \mathbf{k} + \mathbf{G}_1)\right) \arg\left(\mathcal{F}_N(K_2, K_2 + \mathbf{G}_1)\right) \arg\left(\mathcal{F}_N(K'_2, K'_2 + \mathbf{G}_1)\right)$$

$$\theta_{\mathbf{0G}_1}(\mathbf{k}) = \arg\left(\mathcal{F}_N(\mathbf{k}, \mathbf{k} + \mathbf{G}_1)\right)$$

$$\int_{K'_2}^{K_2} dk_y \partial_{k_y} \theta_{\mathbf{0G}_1} = \int_{K'_2}^{K_2} \partial_{k_y} \arg\left(\mathcal{F}_N(\mathbf{k}, \mathbf{k} + \mathbf{G}_1)\right) dk_y + \arg\left(\mathcal{F}_N(K'_2, K'_2)\right) - \left[\arg\left(\mathcal{F}_N(K'_2, K'_2)\right)\right]_{2\pi/3} \\ - \arg\left(\mathcal{F}_N(K_2, K_1)\right) + \left[\arg\left(\mathcal{F}_N(K_2, K_1)\right)\right]_{2\pi/3}$$

$$\mathcal{C} = \frac{\Phi}{2\pi} = -\frac{3}{2\pi} \left[\int_{K'_2}^{K_2} \partial_{k_y} \arg\left(\mathcal{F}_N(\mathbf{k}, \mathbf{k} + \mathbf{G}_1)\right) dk_y + \arg\left(\mathcal{F}_N(K'_2, K'_2)\right) - \arg\left(\mathcal{F}_N(K_2, K_1)\right) \right] \\ - \left[\frac{3}{2\pi} \arg\left(\mathcal{F}_N(K_2, K_1)\right) \right] + \left[\frac{3}{2\pi} \arg\left(\mathcal{F}_N(K'_2, K'_2)\right) \right]$$

$$C = -2 \left[\frac{\mathcal{B}A_{1BZ}}{4\pi} \right]$$

$$(\ell_\Gamma, \ell_K, \ell_M) = (0, (-N+1) \bmod 3, (-N+1) \bmod 2)$$

$$(\ell_\Gamma, \ell_K, \ell_M) = ((-N+1) \bmod 6, (-N+1) \bmod 3, (-N+1) \bmod 2)$$

$$\mathcal{F}_N(\mathbf{q}, \mathbf{q}') \approx \frac{(q_z q'_z)^{N-1}}{(|q_z| |q'_z|)^{N-1}} = e^{i(N-1)(\phi_q - \phi_{q'})}$$

$$\phi_F(\mathbf{q}, \mathbf{q}') = (N-1)(\phi_q - \phi_{q'})$$

$$E_{\text{hopp}}^{\mathbf{g}, \mathbf{g} + \mathbf{G}_i}(\mathbf{k}) \approx -2U_0 |v_{\mathbf{g} + \mathbf{G}_i}(\mathbf{k})| |v_{\mathbf{g}}(\mathbf{k})| \cos\left((N-1)(\phi_{\mathbf{k} + \mathbf{g} + \mathbf{G}_i} - \phi_{\mathbf{k} + \mathbf{g}}) + \arg[v_{\mathbf{g}}(\mathbf{k})] - \arg[v_{\mathbf{g} + \mathbf{G}_i}(\mathbf{k})]\right),$$

$$\arg\left[v_{\mathbf{g}}(\mathbf{k})\right] = (N-1)\phi_{\mathbf{k} + \mathbf{g}}.$$

$$\hat{R}_{2\pi m/n_{\kappa}}|\varphi_{\kappa}\rangle = \sum_{\mathbf{g}} |v_{\mathbf{g}}(\kappa)| e^{i\phi_{\kappa+\mathbf{g}}} \left| \psi_{R_{2\pi m/n_{\kappa}}}^{(0)}(\kappa + \mathbf{g}) \right\rangle \\ = \exp\left[-i(N-1)\frac{2\pi m}{n_{\kappa}}\right] |\varphi_{\kappa}\rangle$$

$$\ell_K = -(N-1) \bmod 3, \ell_M = -(N-1) \bmod 2$$

$$\begin{aligned} \mathcal{C} \bmod 6 = & \left[-(N-1) - 2[(N-1) \bmod 3] \right. \\ & \left. - 3[(N-1) \bmod 2] \right] \bmod 6 \\ = & 0 \quad (52) \end{aligned}$$

$$\theta_{gg'} = (N-1)(\arg(\mathbf{k} + \mathbf{g}) - \arg(\mathbf{k} + \mathbf{g}'))$$

$$\nabla \theta_{gg'} = \frac{N-1}{|\mathbf{k} + \mathbf{g}|} \hat{\phi}(\mathbf{k} + \mathbf{g}) - \frac{N-1}{|\mathbf{k} + \mathbf{g}'|} \hat{\phi}(\mathbf{k} + \mathbf{g}')$$

$$A^{\text{P}}(\mathbf{k} + \mathbf{g}) = \frac{(N-1)}{|\mathbf{k} + \mathbf{g}|} \hat{\phi}(\mathbf{k} + \mathbf{g})$$

$$\oint_{k \gg \sqrt{N/B}} \mathbf{A}^{\text{P}} \cdot d\mathbf{k} = \Phi = 2\pi(N-1)$$

$$\partial_{k_x}\theta_{g g'}-A_x^{\text{P}}(\mathbf{k}+\mathbf{g})+A_x^{\text{P}}(\mathbf{k}+\mathbf{g}')=0$$

$$\Omega(\mathbf{k})=\sum_{\mathbf{g}}n(\mathbf{k}+\mathbf{g})\Omega^{\text{P}}(\mathbf{k}+\mathbf{g})$$

$$\hat{\mathcal{H}}=\hat{\mathcal{H}}_0+\hat{\mathcal{H}}_{\text{int}},$$

$$\hat{\mathcal{H}}_0=\sum_q\frac{|q|^2}{r_s^2}c_q^\dagger c_q$$

$$\begin{aligned}\hat{\mathcal{H}}_{\text{int}}&=\frac{1}{2A}\sum_qV(\mathbf{q})\colon\tilde{\rho}_q\tilde{\rho}_{-q}\colon\\&=\frac{1}{2A}\sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_4}\tilde{V}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3\mathbf{q}_4}c_{\mathbf{q}_1}^\dagger c_{\mathbf{q}_2}^\dagger c_{\mathbf{q}_3}c_{\mathbf{q}_4}.\end{aligned}$$

$$\begin{aligned}\tilde{V}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3\mathbf{q}_4}&=V(\mathbf{q}_1-\mathbf{q}_4)\mathcal{F}_N(\mathbf{q}_1,\mathbf{q}_4)\mathcal{F}_N(\mathbf{q}_2,\mathbf{q}_3)\\&\quad\times\delta(\mathbf{q}_1+\mathbf{q}_4-\mathbf{q}_2-\mathbf{q}_3)\end{aligned}$$

$$\hat{\mathcal{H}}_{\text{HF}}=\hat{\mathcal{H}}_0+\hat{\mathcal{H}}_{\text{H}}+\hat{\mathcal{H}}_{\text{F}}$$

$$\begin{aligned}\hat{\mathcal{H}}_0&=\sum_{\mathbf{k},\mathbf{g}_1}\frac{|\mathbf{k}+\mathbf{g}_1|^2}{r_s^2}c_{\mathbf{k}\mathbf{g}_1}^\dagger c_{\mathbf{k}\mathbf{g}_1}\\\mathcal{H}_{\text{H}}&=\frac{1}{A}\sum_{\substack{\mathbf{k}_1\mathbf{k}_2\\ \mathbf{g}_1\mathbf{g}_2\mathbf{g}_3\mathbf{g}_4}}\tilde{V}_{\mathbf{k}_1+\mathbf{g}_1,\mathbf{k}_2+\mathbf{g}_2,\mathbf{k}_2+\mathbf{g}_3,\mathbf{k}_1+\mathbf{g}_4}\\&\quad\times\mathcal{P}_{\mathbf{g}_1\mathbf{g}_4}(\mathbf{k}_1)c_{\mathbf{k}_2\mathbf{g}_2}^\dagger c_{\mathbf{k}_2\mathbf{g}_3}\\\mathcal{H}_{\text{F}}&=-\frac{1}{A}\sum_{\substack{\mathbf{k}_1\mathbf{k}_2\\ \mathbf{g}_1\mathbf{g}_3\mathbf{g}_4}}\tilde{V}_{\mathbf{k}_1+\mathbf{g}_1,\mathbf{k}_2+\mathbf{g}_2,\mathbf{k}_1+\mathbf{g}_3,\mathbf{k}_2+\mathbf{g}_4}\\&\quad\times\mathcal{P}_{\mathbf{g}_1\mathbf{g}_3}(\mathbf{k}_1)c_{\mathbf{k}_2\mathbf{g}_2}^\dagger c_{\mathbf{k}_2\mathbf{g}_4}\end{aligned}$$

$$a_l=\sqrt{2/(\sqrt{3}\pi)}$$

$$\mathcal{C}=\left|\int_{\text{1BZ}}d^2k\Omega_N(\mathbf{k})/(2\pi)\right|,$$

$$\int_{\text{1BZ}}d^2k\Omega_N(\mathbf{k})=\pi(2a+1)$$

$$\begin{aligned}\mathcal{H}_F = & -\frac{1}{A} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \mathbf{g}_1 \mathbf{g}_2 \mathbf{g}_3}} V(\mathbf{k}_1 + \mathbf{g}_1 - \mathbf{k}_2 - \mathbf{g}_4) \\ & \times e^{i(N-1)(\phi_{\mathbf{k}_1 + \mathbf{g}_1} - \phi_{\mathbf{k}_2 + \mathbf{g}_4})} e^{i(N-1)(\phi_{\mathbf{k}_2 + \mathbf{g}_2} - \phi_{\mathbf{k}_1 + \mathbf{g}_3})} \\ & \times \mathcal{P}_{\mathbf{g}_1 \mathbf{g}_3}(\mathbf{k}_1) c_{\mathbf{k}_2 \mathbf{g}_2}^\dagger c_{\mathbf{k}_2 \mathbf{g}_4} \delta(\mathbf{g}_1 + \mathbf{g}_2 - \mathbf{g}_3 - \mathbf{g}_4).\end{aligned}$$

$$\arg [v_{\mathbf{g}}(\mathbf{k})] = (N-1)\phi_{\mathbf{k}+\mathbf{g}},$$

$$\begin{aligned}\mathcal{P}_{\mathbf{g}_1 \mathbf{g}_2}(\mathbf{k}) &= v_{\mathbf{g}_1}(\mathbf{k})^* v_{\mathbf{g}_2}(\mathbf{k}) \\ &= |v_{\mathbf{g}_1}(\mathbf{k}) v_{\mathbf{g}_2}(\mathbf{k})| e^{i(N-1)(\phi_{\mathbf{k}+\mathbf{g}_2} - \phi_{\mathbf{k}+\mathbf{g}_1})}\end{aligned}$$

$$E_F^{\text{small}q} = -\frac{1}{A} \sum_{\mathbf{k}} \sum_{q \ll g} \sum_{\mathbf{g}_1, \mathbf{g}_2} V(q) \mathcal{F}_N(\mathbf{k} + \mathbf{q} + \mathbf{g}_1, \mathbf{k} + \mathbf{g}_1) \mathcal{F}_N(\mathbf{k} + \mathbf{g}_2, \mathbf{k} + \mathbf{q} + \mathbf{g}_2) \mathcal{P}_{\mathbf{g}_1 \mathbf{g}_2}(\mathbf{k} + \mathbf{q}) \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}).$$

$$\mathcal{F}_N(\mathbf{k} + \mathbf{q} + \mathbf{g}_1, \mathbf{k} + \mathbf{g}_1) \approx e^{-\frac{1}{2}g_{ij}(\mathbf{k}+\mathbf{g}_1)q_iq_j} e^{i\int_{\mathbf{k}+\mathbf{g}_1}^{\mathbf{k}+\mathbf{q}+\mathbf{g}_1} \mathbf{A}(\mathbf{k}') \cdot d\mathbf{k}'}$$

$$\begin{aligned}E_F^{\text{small}q} = & -\frac{1}{A} \sum_{\mathbf{k}} \sum_{q \ll g} \sum_{\mathbf{g}_1, \mathbf{g}_2} V(q) e^{-\frac{1}{2}(g_{ij}(\mathbf{k}+\mathbf{g}_1)+g_{ij}(\mathbf{k}+\mathbf{g}_2))q_iq_j} e^{i\int_{\mathbf{k}}^{\mathbf{k}+\mathbf{q}} [\mathbf{A}(\mathbf{k}'+\mathbf{g}_1)-\mathbf{A}(\mathbf{k}'+\mathbf{g}_2)] \cdot d\mathbf{k}'} \\ & \times \mathcal{F}_N(\mathbf{k} + \mathbf{g}_2, \mathbf{k} + \mathbf{q} + \mathbf{g}_2) \mathcal{P}_{\mathbf{g}_1 \mathbf{g}_2}(\mathbf{k} + \mathbf{q}) \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k})\end{aligned}$$

$$\begin{aligned}& \left| \sum_{\mathbf{g}} \int_{\text{1BZ}} d^2k \Omega_N(\mathbf{k} + \mathbf{g}) \mathcal{P}_{\mathbf{g}\mathbf{g}}(\mathbf{k}) / (2\pi) \right| \\ h_{\text{RNG}}(\mathbf{q}) = & \begin{pmatrix} u_d & -v_F\sqrt{2}q_z & & & & & & \\ -v_F\sqrt{2}q_{\bar{z}} & u_d & t_1 & & & & & \\ & t_1 & 2u_d & -v_F\sqrt{2}q_z & & & & \\ & & -v_F\sqrt{2}q_{\bar{z}} & 2u_d & t_1 & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & t_1 & Nu_d & -v_F\sqrt{2}q_z & \\ & & & & & -v_F\sqrt{2}q_{\bar{z}} & Nu_d & \end{pmatrix},\end{aligned}$$

$$\psi_{(Al)}^{(e)}(\mathbf{q}) \approx \mathcal{N}_q^{(e)} (\sqrt{2}q_{\bar{z}}/q_0)^{l-1}$$

$$\psi_{(Bl)}^{(e)}(\mathbf{q}) \approx -\mathcal{N}_q^{(e)} \mathcal{N}_q^{(e)} l \frac{u_d}{t_1} (\sqrt{2}q_{\bar{z}}/q_0)^l$$

$$\psi_{(Bl)}^{(h)}(\mathbf{q}) \approx \mathcal{N}_q^{(h)} (\sqrt{2}q_z/q_0)^{N-l}$$

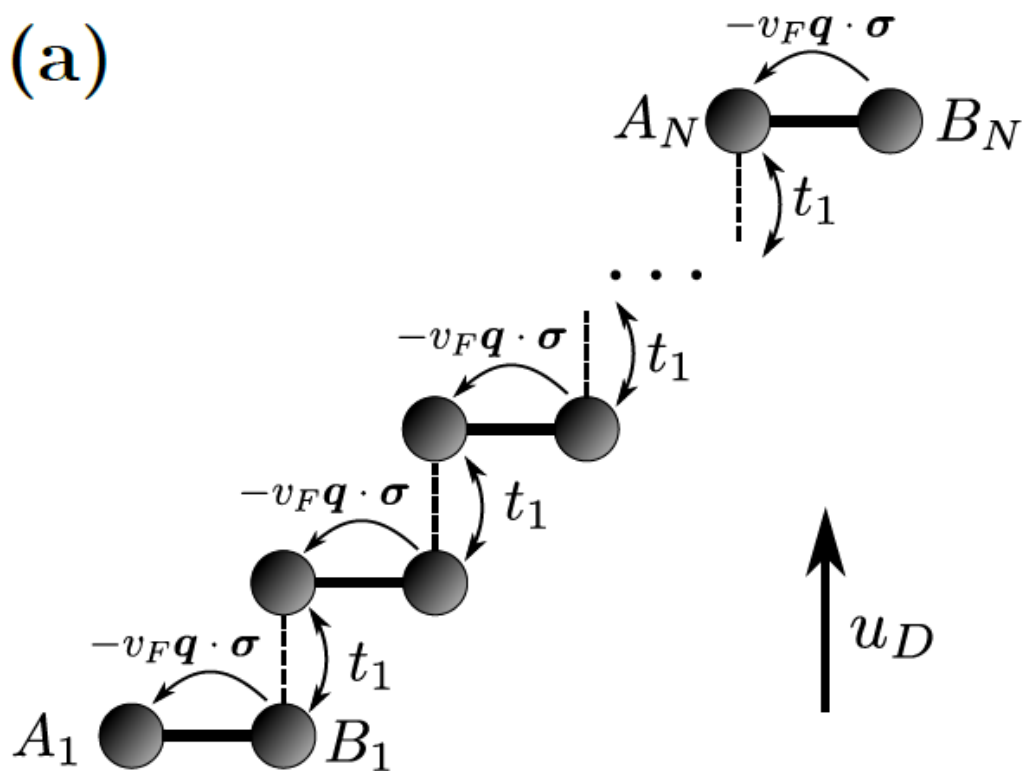
$$\psi_{(AN)}^{(h)}(\mathbf{q}) \approx -\mathcal{N}_q^{(h)} (N-l+1) \frac{u_d}{t_1} (\sqrt{2}q_z/q_0)^{N-l+1}$$

$$h_{\text{Schur}}^{(e)}(\mathbf{q}) = h_{AA}(\mathbf{q}) - h_{AB}(\mathbf{q}) h_{BB}^{-1}(\mathbf{q}) h_{BA}(\mathbf{q}),$$

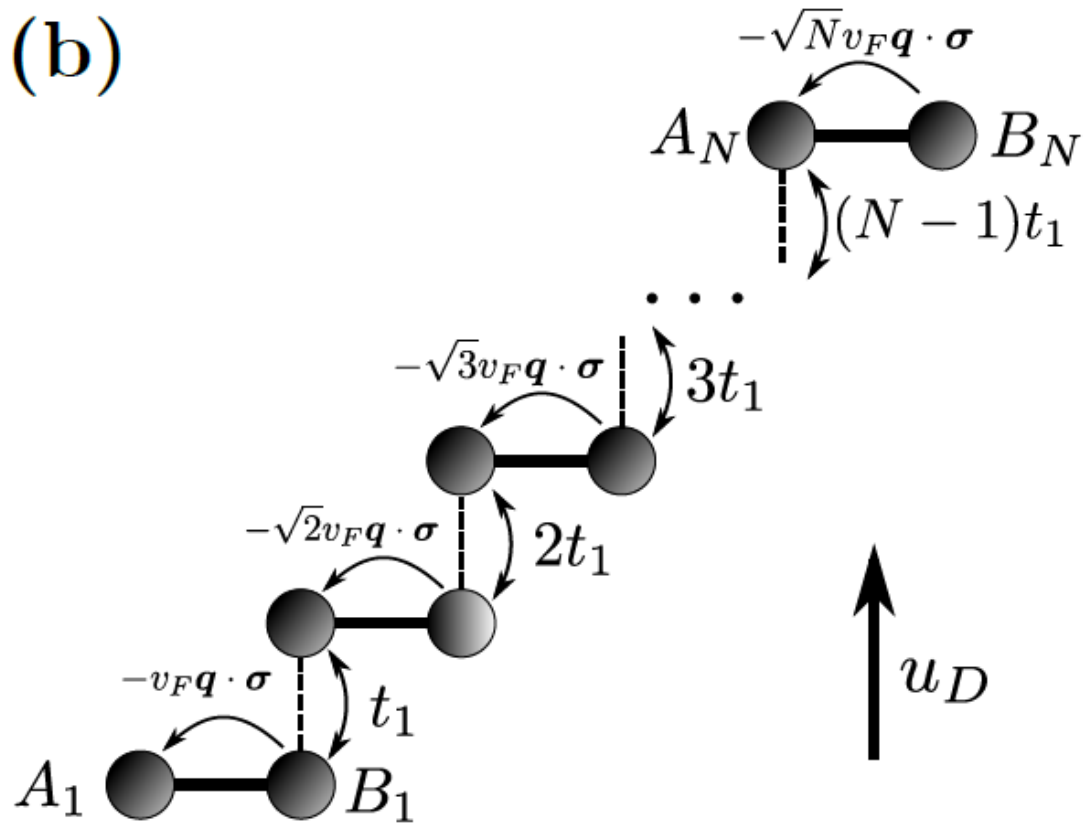
$$h_{\text{Schur}}^{(h)}(\mathbf{q}) = h_{BB}(\mathbf{q}) - h_{BA}(\mathbf{q}) h_{AA}^{-1}(\mathbf{q}) h_{AB}(\mathbf{q}),$$

$$\begin{aligned}
 h_{AA}(\mathbf{q}) &= h_{BB}(\mathbf{q}) = \begin{pmatrix} u_d & & & \\ & 2u_d & & \\ & & \ddots & \\ & & & Nu_d \end{pmatrix} \\
 h_{AB}(\mathbf{q}) &= \begin{pmatrix} -v_F\sqrt{2}q_z & & & \\ t_1 & -v_F\sqrt{2}q_z & & \\ & \ddots & \ddots & \\ & & t_1 & -v_F\sqrt{2}q_z \end{pmatrix} \\
 h_{BA}(\mathbf{q}) &= \begin{pmatrix} -v_F\sqrt{2}q_{\bar{z}} & t_1 & & \\ & -v_F\sqrt{2}q_{\bar{z}} & \ddots & \\ & & \ddots & t_1 \\ & & & -v_F\sqrt{2}q_{\bar{z}} \end{pmatrix} \\
 h_{\text{Schur}}^{(e)}(\mathbf{q}) &= u_d \begin{pmatrix} 1 & & & \\ & 2 & & \\ & & 3 & \\ & & & \ddots \\ & & & & N \end{pmatrix}
 \end{aligned}$$

(a)



(b)



$$-\frac{t_1^2}{u_d} \begin{pmatrix} (|\mathbf{q}|/q_0)^2 & -\sqrt{2}q_z/q_0 & & & \\ -\sqrt{2}q_z/k_0 & (|\mathbf{q}|/q_0)^2 + 1 & -\sqrt{2}q_z/(2q_0) & & \\ & -\sqrt{2}q_z/(2q_0) & (|\mathbf{q}|/q_0)^2 + 1/2 & \ddots & \\ & \ddots & \ddots & \ddots & -\sqrt{2}q_z/((N-1)q_0) \\ & & -\sqrt{2}q_z/((N-1)q_0) & & (|\mathbf{q}|/q_0)^2 + 1/N \end{pmatrix}.$$

$$\langle m | \hat{L}(\mathbf{q}) | n \rangle = \begin{pmatrix} \frac{|\mathbf{q}|^2}{2} \mathcal{B} & -k_z \sqrt{\mathcal{B}} & & & \\ -q_z \sqrt{\mathcal{B}} & \frac{|\mathbf{q}|^2}{2} \mathcal{B} + 1 & \sqrt{2\mathcal{B}} q_z & & \\ & \sqrt{2\mathcal{B}} q_z & \frac{|\mathbf{q}|^2}{2} \mathcal{B} + 2 & \ddots & \\ & & \ddots & \ddots & \sqrt{(N-1)\mathcal{B}} q_z \\ & & & \sqrt{(N-1)\mathcal{B}} q_z & (N-1) \end{pmatrix}_{mn}$$

$$\tilde{h}_{\text{RNG}}(\mathbf{q}) = \begin{pmatrix} u_d & -\sqrt{2}v_F q_z & & & \\ -v_F \sqrt{2}q_z & u_d & t_1 & & \\ & t_1 & 2u_d & -2v_F q_z & \\ & & -2v_F q_z & 2u_d & 2t_1 \\ & & & \ddots & \ddots \\ & & & & (N-1)t_1 & (N-1)u_d & -\sqrt{2N}v_F q_z \\ & & & & & -\sqrt{2N}v_F q_z & Nu_d \end{pmatrix}$$

$$\tilde{h}_{AA}(\mathbf{q}) = \tilde{h}_{BB}(\mathbf{q}) = \begin{pmatrix} u_d & & & \\ & 2u_d & & \\ & & \ddots & \\ & & & Nu_d \end{pmatrix}$$

$$\tilde{h}_{AB}(\mathbf{q}) = \begin{pmatrix} -v_F\sqrt{2}q_z & & & \\ t_1 & -v_F2q_z & & \\ & \ddots & & \ddots \\ & & (N-1)t_1 - v_F\sqrt{2N}q_z & \end{pmatrix}$$

$$\tilde{h}_{BA}(\mathbf{q}) = \begin{pmatrix} -v_F\sqrt{2}q_{\bar{z}} & t_1 & & \\ & -v_F2q_{\bar{z}} & \ddots & \\ & & \ddots & (N-1)t_1 \\ & & & -v_F\sqrt{2N}q_{\bar{z}} \end{pmatrix}.$$

$$\tilde{h}_{\text{Schur}}(\mathbf{q}) = \tilde{h}_{AA}(\mathbf{q}) - \tilde{h}_{AB}(\mathbf{q})\tilde{h}_{BB}^{-1}(\mathbf{q})\tilde{h}_{BA}(\mathbf{q})$$

$$= u_d \begin{pmatrix} 1 & & & \\ 2 & & & \\ 3 & & & \\ & \ddots & & \\ & & N & \end{pmatrix} - \frac{t_1^2}{u_d} \begin{pmatrix} (|\mathbf{q}|/q_0)^2 & -\sqrt{2}q_z/q_0 & & & \\ -\sqrt{2}q_{\bar{z}}/q_0 & (|\mathbf{q}|/q_0)^2 + 1 & -2q_z/q_0 & & \\ & -2q_{\bar{z}}/q_0 & (|\mathbf{q}|/q_0)^2 + 2 & \ddots & \\ & & \ddots & \ddots & -\sqrt{2(N-1)}q_z/q_0 \\ & & & -\sqrt{2(N-1)}q_{\bar{z}}/q_0 & (|\mathbf{q}|/q_0)^2 + (N-1) \end{pmatrix}$$

$$\approx -\frac{t_1^2}{u_d} \begin{pmatrix} (|\mathbf{q}|/q_0)^2 & -\sqrt{2}q_z/q_0 & & & \\ -\sqrt{2}q_{\bar{z}}/q_0 & (|\mathbf{q}|/q_0)^2 + 1 & -2q_z/q_0 & & \\ & -2q_{\bar{z}}/q_0 & (|\mathbf{q}|/q_0)^2 + 2 & \ddots & \\ & & \ddots & \ddots & -\sqrt{2(N-1)}q_z/q_0 \\ & & & -\sqrt{2(N-1)}q_{\bar{z}}/q_0 & (N-1) \end{pmatrix},$$

$$\Omega(\mathbf{k}) = i\text{Tr}\left(P(\mathbf{k})\partial_{k_x}P(\mathbf{k})\partial_{k_y}P(\mathbf{k})\right) - i\text{Tr}\left(P(\mathbf{k})\partial_{k_y}P(\mathbf{k})\partial_{k_x}P(\mathbf{k})\right)$$

$$P = |u_{\mathbf{k}}\rangle\langle u_{\mathbf{k}}| = \sum_{\mathbf{g}_1, \mathbf{g}_2} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) |u_{\mathbf{k}}, \mathbf{g}_1\rangle\langle u_{\mathbf{k}}, \mathbf{g}_2|,$$

$$\mathcal{P}_{\mathbf{g}\mathbf{g}'}(\mathbf{k}) = \left\langle c_{\mathbf{k}\mathbf{g}}^\dagger c_{\mathbf{k}\mathbf{g}'} \right\rangle$$

$$|u_{\mathbf{k}}, \mathbf{g}_1\rangle = e^{-i\mathbf{k}\cdot\mathbf{r}}|\mathbf{k} + \mathbf{g}_1\rangle = e^{i\mathbf{g}_1\cdot\mathbf{r}}|s_{\mathbf{k}+\mathbf{g}_1}\rangle$$

$$\partial_{k_x}P = \sum_{\mathbf{g}_3, \mathbf{g}_4} \partial_{k_x}\mathcal{P}_{\mathbf{g}_4\mathbf{g}_3}|u_{\mathbf{k}}, \mathbf{g}_3\rangle\langle u_{\mathbf{k}}, \mathbf{g}_4| + \sum_{\mathbf{g}_3, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_4\mathbf{g}_3}\partial_{k_x}(|u_{\mathbf{k}}, \mathbf{g}_3\rangle\langle u_{\mathbf{k}}, \mathbf{g}_4|)$$

$$P\partial_{k_x}P = \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2\mathbf{g}_1}(\mathbf{k}) |u_{\mathbf{k}}, \mathbf{g}_1\rangle\langle u_{\mathbf{k}}, \mathbf{g}_2| \left(\partial_{k_x}\mathcal{P}_{\mathbf{g}_4\mathbf{g}_3}|u_{\mathbf{k}}, \mathbf{g}_3\rangle\langle u_{\mathbf{k}}, \mathbf{g}_4| + \mathcal{P}_{\mathbf{g}_4\mathbf{g}_3}\partial_{k_x}(|u_{\mathbf{k}}, \mathbf{g}_3\rangle\langle u_{\mathbf{k}}, \mathbf{g}_4|) \right)$$



$$\begin{aligned}\langle u_k, \mathbf{g}_2 | u_k, \mathbf{g}_3 \rangle &= \delta_{\mathbf{g}_2, \mathbf{g}_3} \\ \langle u_k, \mathbf{g}_2 | \partial_k | u_k, \mathbf{g}_3 \rangle &= -iA^P(\mathbf{k} + \mathbf{g}_2) \delta_{\mathbf{g}_2, \mathbf{g}_3},\end{aligned}$$

$$\begin{aligned}\langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_3\rangle \langle u_k, \mathbf{g}_4|) &= -iA^P(\mathbf{k} + \mathbf{g}_2) \delta_{\mathbf{g}_2, \mathbf{g}_3} \langle u_k, \mathbf{g}_4| + \delta_{\mathbf{g}_2, \mathbf{g}_3} \partial_{k_x} \langle u_k, \mathbf{g}_4| \\ &= \delta_{\mathbf{g}_2, \mathbf{g}_3} \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|)\end{aligned}$$

$$P \partial_{k_x} P = \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) |u_k, \mathbf{g}_1\rangle \left(\partial_{k_x} \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \langle u_k, \mathbf{g}_4| + \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|) \right)$$

$$\begin{aligned}\partial_{k_x} P \partial_{k_y} P &= \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_5, \mathbf{g}_6} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) |u_k, \mathbf{g}_1\rangle \left(\partial_{k_x} \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \langle u_k, \mathbf{g}_4| + \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|) \right) P \\ &\quad \times \left[\partial_{k_y} \mathcal{P}_{\mathbf{g}_6 \mathbf{g}_5} |u_k, \mathbf{g}_5\rangle \langle u_k, \mathbf{g}_6| + \mathcal{P}_{\mathbf{g}_6 \mathbf{g}_5} \partial_{k_y} (|u_k, \mathbf{g}_5\rangle \langle u_k, \mathbf{g}_6|) \right]\end{aligned}$$

$$\begin{aligned}&= \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_6} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) \partial_{k_x} \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \partial_{k_y} \mathcal{P}_{\mathbf{g}_6 \mathbf{g}_4} |u_k, \mathbf{g}_1\rangle \langle u_k, \mathbf{g}_6| \\ &+ \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_6} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) \partial_{k_x} \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \mathcal{P}_{\mathbf{g}_6 \mathbf{g}_4} |u_k, \mathbf{g}_1\rangle \langle u_k, \mathbf{g}_4 | \partial_{k_y} (|u_k, \mathbf{g}_4\rangle \langle u_k, \mathbf{g}_6|) \\ &+ \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_6} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \partial_{k_y} \mathcal{P}_{\mathbf{g}_6 \mathbf{g}_4} |u_k, \mathbf{g}_1\rangle \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|) |u_k, \mathbf{g}_4\rangle \langle u_k, \mathbf{g}_6| \\ &+ \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_5, \mathbf{g}_6} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \mathcal{P}_{\mathbf{g}_6 \mathbf{g}_5} |u_k, \mathbf{g}_1\rangle \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|) \partial_{k_y} (|u_k, \mathbf{g}_5\rangle \langle u_k, \mathbf{g}_6|)\end{aligned}$$

$$\begin{aligned}\text{Tr} \left(P \partial_{k_x} P \partial_{k_y} P \right) &= \sum_{\mathbf{g}} \langle u_k, \mathbf{g} | P \partial_{k_x} P \partial_{k_y} P | u_k, \mathbf{g} \rangle \\ &= \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}}(\mathbf{k}) \partial_{k_x} \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \partial_{k_y} \mathcal{P}_{\mathbf{g} \mathbf{g}_4} + \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}}(\mathbf{k}) \partial_{k_x} \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \mathcal{P}_{\mathbf{g} \mathbf{g}_4} \langle u_k, \mathbf{g}_4 | \partial_{k_y} (|u_k, \mathbf{g}_4\rangle \langle u_k, \mathbf{g}|) | u_k, \mathbf{g} \rangle \\ &+ \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \partial_{k_y} \mathcal{P}_{\mathbf{g} \mathbf{g}_4} \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|) | u_k, \mathbf{g}_4 \rangle \\ &+ \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_5} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \mathcal{P}_{\mathbf{g} \mathbf{g}_5} \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|) \partial_{k_y} (|u_k, \mathbf{g}_5\rangle \langle u_k, \mathbf{g}|) | u_k, \mathbf{g} \rangle\end{aligned}$$

$$\begin{aligned}\langle u_k, \mathbf{g}_4 | \partial_{k_y} (|u_k, \mathbf{g}_4\rangle \langle u_k, \mathbf{g}|) | u_k, \mathbf{g} \rangle &= \langle u_k, \mathbf{g}_4 | \partial_{k_y} | u_k, \mathbf{g}_4 \rangle + \partial_{k_y} (\langle u_k, \mathbf{g}|) | u_k, \mathbf{g} \rangle \\ &= -iA_y^P(\mathbf{k} + \mathbf{g}_4) + iA_y^P(\mathbf{k} + \mathbf{g})\end{aligned}$$

$$\begin{aligned}\text{Tr} \left(P \partial_{k_x} P \partial_{k_y} P \right) &= \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}}(\mathbf{k}) \partial_{k_x} \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \left(\partial_{k_y} + iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \mathcal{P}_{\mathbf{g}_4} \\ &+ \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \partial_{k_y} \mathcal{P}_{\mathbf{g}_4} \left(iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \\ &+ \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_5} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4 \mathbf{g}_2} \mathcal{P}_{\mathbf{g}_5} \langle u_k, \mathbf{g}_2 | \partial_{k_x} (|u_k, \mathbf{g}_2\rangle \langle u_k, \mathbf{g}_4|) \partial_{k_y} (|u_k, \mathbf{g}_5\rangle \langle u_k, \mathbf{g}|) | u_k, \mathbf{g} \rangle\end{aligned}$$

$$\begin{aligned} \text{Tr}(P\partial_{k_x}P\partial_{k_y}P) &= \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \left(\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \left(\partial_{k_y} + iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \\ &\quad - \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \mathcal{P}_{\mathbf{g}\mathbf{g}_4} \left(iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \left(iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \\ &\quad + \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_5} \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \mathcal{P}_{\mathbf{g}\mathbf{g}_5} \langle u_{\mathbf{k}}, \mathbf{g}_2 | \partial_{k_x} (|u_{\mathbf{k}}, \mathbf{g}_2\rangle \langle u_{\mathbf{k}}, \mathbf{g}_4|) \partial_{k_y} (|u_{\mathbf{k}}, \mathbf{g}_5\rangle \langle u_{\mathbf{k}}, \mathbf{g}|) | u_{\mathbf{k}}, \mathbf{g} \rangle \end{aligned}$$

$$\begin{aligned} &\langle u_{\mathbf{k}}, \mathbf{g}_2 | \partial_{k_x} (|u_{\mathbf{k}}, \mathbf{g}_2\rangle \langle u_{\mathbf{k}}, \mathbf{g}_4|) \partial_{k_y} (|u_{\mathbf{k}}, \mathbf{g}_5\rangle \langle u_{\mathbf{k}}, \mathbf{g}|) | u_{\mathbf{k}}, \mathbf{g} \rangle \\ &= (-iA_x^P(\mathbf{k} + \mathbf{g}_2) \langle u_{\mathbf{k}}, \mathbf{g}_4 | + \partial_{k_x} \langle u_{\mathbf{k}}, \mathbf{g}_4 |) \left(\partial_{k_y} |u_{\mathbf{k}}, \mathbf{g}_5\rangle + iA_y^P(\mathbf{k} + \mathbf{g}) |u_{\mathbf{k}}, \mathbf{g}_5\rangle \right) \\ &= (-iA_x^P(\mathbf{k} + \mathbf{g}_2)) \left(-i\delta_{\mathbf{g}_4, \mathbf{g}_5} A_y^P(\mathbf{k} + \mathbf{g}_4) + i\delta_{\mathbf{g}_4, \mathbf{g}_5} A_y^P(\mathbf{k} + \mathbf{g}) \right) \\ &\quad + \left(i\delta_{\mathbf{g}_4, \mathbf{g}_5} A_x^P(\mathbf{k} + \mathbf{g}_4) \right) \left(iA_y^P(\mathbf{k} + \mathbf{g}) \right) + (\partial_{k_x} \langle u_{\mathbf{k}}, \mathbf{g}_4 |) \partial_{k_y} |u_{\mathbf{k}}, \mathbf{g}_5\rangle \\ &= \delta_{\mathbf{g}_4, \mathbf{g}_5} \left(iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \left(+iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \\ &\quad + \partial_{k_x} \left(\langle u_{\mathbf{k}}, \mathbf{g}_4 | \partial_{k_y} |u_{\mathbf{k}}, \mathbf{g}_5\rangle \right) - \langle u_{\mathbf{k}}, \mathbf{g}_4 | \partial_{k_x} \partial_{k_y} |u_{\mathbf{k}}, \mathbf{g}_5\rangle \\ &= \delta_{\mathbf{g}_4, \mathbf{g}_5} \left(iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \left(+iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \\ &\quad - i\delta_{\mathbf{g}_4, \mathbf{g}_5} \partial_{k_x} A_y^P(\mathbf{k} + \mathbf{g}_4) - \langle u_{\mathbf{k}}, \mathbf{g}_4 | \partial_{k_x} \partial_{k_y} |u_{\mathbf{k}}, \mathbf{g}_5\rangle. \end{aligned}$$

$$\begin{aligned} \text{Tr}(P\partial_{k_x}P\partial_{k_y}P) &= \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \left(\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \left(\partial_{k_y} + iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \mathcal{P}_{\mathbf{g}_4} \\ &\quad - i \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \partial_{k_x} A_y^P(\mathbf{k} + \mathbf{g}_4) \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \mathcal{P}_{\mathbf{g}_4} - \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4, \mathbf{g}_5} \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \mathcal{P}_{\mathbf{g}_5} \langle u_{\mathbf{k}}, \mathbf{g}_4 | \partial_{k_x} \partial_{k_y} |u_{\mathbf{k}}, \mathbf{g}_5\rangle \end{aligned}$$

$$\begin{aligned} \text{Tr}(P\partial_{k_x}P\partial_{k_y}P) &= \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \left(\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \left(\partial_{k_y} + iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \mathcal{P}_{\mathbf{g}\mathbf{g}_4} \\ &\quad - i \sum_{\mathbf{g}_4} \partial_{k_x} A_y^P(\mathbf{k} + \mathbf{g}_4) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_4}(\mathbf{k}) - \sum_{\mathbf{g}_4, \mathbf{g}_5} \mathcal{P}_{\mathbf{g}_4\mathbf{g}_5} \langle u_{\mathbf{k}}, \mathbf{g}_4 | \partial_{k_x} \partial_{k_y} |u_{\mathbf{k}}, \mathbf{g}_5\rangle \end{aligned}$$

$$\begin{aligned} \Omega(\mathbf{k}) &= i\text{Tr}(P\partial_{k_x}P\partial_{k_y}P) - i\text{Tr}(P\partial_{k_y}P\partial_{k_x}P) \\ &= i \sum_{\mathbf{g}, \mathbf{g}_2, \mathbf{g}_4} \mathcal{P}_{\mathbf{g}_2\mathbf{g}}(\mathbf{k}) \left(\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_4) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \mathcal{P}_{\mathbf{g}_4\mathbf{g}_2} \left(\partial_{k_y} + iA_y^P(\mathbf{k} + \mathbf{g}) - iA_y^P(\mathbf{k} + \mathbf{g}_4) \right) \mathcal{P}_{\mathbf{g}_4} - x \leftrightarrow y \\ &\quad + \sum_{\mathbf{g}} \mathcal{P}_{\mathbf{g}\mathbf{g}} \left(\partial_{k_x} A_y^P(\mathbf{k} + \mathbf{g}) - \partial_{k_y} A_x^P(\mathbf{k} + \mathbf{g}) \right) - i \sum_{\mathbf{g}_4, \mathbf{g}_5} \mathcal{P}_{\mathbf{g}_4\mathbf{g}_5} \langle u_{\mathbf{k}}, \mathbf{g}_4 | \left(\partial_{k_x} \partial_{k_y} - \partial_{k_y} \partial_{k_x} \right) | u_{\mathbf{k}}, \mathbf{g}_5 \rangle \end{aligned}$$

$$\begin{aligned} \Omega(\mathbf{k}) &= i\text{Tr}(P\partial_{k_x}P\partial_{k_y}P) - i\text{Tr}(P\partial_{k_y}P\partial_{k_x}P) \\ &= i \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3} \mathcal{P}_{\mathbf{g}_2\mathbf{g}_1}(\mathbf{k}) \left(\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \mathcal{P}_{\mathbf{g}_3\mathbf{g}_2} \left(\partial_{k_y} + iA_y^P(\mathbf{k} + \mathbf{g}_1) - iA_y^P(\mathbf{k} + \mathbf{g}_3) \right) \mathcal{P}_{\mathbf{g}_1\mathbf{g}_3} - (x \leftrightarrow y) \\ &\quad + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g}). \end{aligned}$$

$$\left(\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - iA_x^P(\mathbf{k} + \mathbf{g}_2) \right) \mathcal{P}_{\mathbf{g}_3\mathbf{g}_2}$$

$$|\mathbf{k} + \mathbf{g}\rangle \rightarrow e^{i\alpha_{\mathbf{k}+\mathbf{g}}} |\mathbf{k} + \mathbf{g}\rangle \text{ and } A^p(\mathbf{k} + \mathbf{g}) \rightarrow A^p(\mathbf{k} + \mathbf{g}) - \nabla\alpha_{\mathbf{k}+\mathbf{g}}$$

$$\mathcal{P}_{\mathbf{g}_3\mathbf{g}_2} \rightarrow e^{-i\alpha_{\mathbf{k}+\mathbf{g}_2} + i\alpha_{\mathbf{k}+\mathbf{g}_3}} \mathcal{P}_{\mathbf{g}_3\mathbf{g}_2}$$



$$\begin{aligned}
& (\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - iA_x^P(\mathbf{k} + \mathbf{g}_2)) \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2} \\
& \rightarrow (\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - i\partial_{k_x} \alpha_{\mathbf{k} + \mathbf{g}_3} - iA_x^P(\mathbf{k} + \mathbf{g}_2) + i\partial_{k_x} \alpha_{\mathbf{k} + \mathbf{g}_2}) e^{-i\alpha_{\mathbf{k} + \mathbf{g}_2} + i\alpha_{\mathbf{k} + \mathbf{g}_3}} \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2} \\
& = e^{-i\alpha_{\mathbf{k} + \mathbf{g}_2} + i\alpha_{\mathbf{k} + \mathbf{g}_3}} (\partial_{k_x} - i\partial_{k_x} \alpha_{\mathbf{k} + \mathbf{g}_2} + i\partial_{k_x} \alpha_{\mathbf{k} + \mathbf{g}_3} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - i\partial_{k_x} \alpha_{\mathbf{k} + \mathbf{g}_3} - iA_x^P(\mathbf{k} + \mathbf{g}_2) + i\partial_{k_x} \alpha_{\mathbf{k} + \mathbf{g}_2}) \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2} \\
& = e^{-i\alpha_{\mathbf{k} + \mathbf{g}_2} + i\alpha_{\mathbf{k} + \mathbf{g}_3}} (\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - iA_x^P(\mathbf{k} + \mathbf{g}_2)) \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2}
\end{aligned}$$

$$\mathcal{P}_{\mathbf{g}_{g'}} = \sqrt{n(\mathbf{k} + \mathbf{g})n(\mathbf{k} + \mathbf{g}')} e^{i\theta_{g'g}}$$

$$\begin{aligned}
& (\partial_{k_x} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - iA_x^P(\mathbf{k} + \mathbf{g}_2)) \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2} \\
& = \left(i\partial_{k_x} \theta_{\mathbf{g}_2 \mathbf{g}_3} + iA_x^P(\mathbf{k} + \mathbf{g}_3) - iA_x^P(\mathbf{k} + \mathbf{g}_2) + \frac{1}{2} \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3)) \right) \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2}
\end{aligned}$$

$$\begin{aligned}
\Omega(\mathbf{k}) = & -i \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3} \mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1} \mathcal{P}_{\mathbf{g}_1 \mathbf{g}_3} \left(\partial_{k_x} \theta_{\mathbf{g}_2 \mathbf{g}_3} + A_x^P(\mathbf{k} + \mathbf{g}_3) - A_x^P(\mathbf{k} + \mathbf{g}_2) - \frac{i}{2} \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3)) \right) \\
& \left(\partial_{k_y} \theta_{\mathbf{g}_3 \mathbf{g}_1} + A_y^P(\mathbf{k} + \mathbf{g}_1) - A_y^P(\mathbf{k} + \mathbf{g}_3) - \frac{i}{2} \partial_{k_y} \ln(n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_3)) \right) - x \leftrightarrow y \\
& + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g})
\end{aligned}$$

$$\mathcal{P}_{\mathbf{g}_3 \mathbf{g}_2} \mathcal{P}_{\mathbf{g}_2 \mathbf{g}_1} \mathcal{P}_{\mathbf{g}_1 \mathbf{g}_3} = n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3)$$

$$\begin{aligned}
\Omega(\mathbf{k}) = & -i \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3} n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3) [\\
& \left(\partial_{k_x} \theta_{\mathbf{g}_2 \mathbf{g}_3} + A_x^P(\mathbf{k} + \mathbf{g}_3) - A_x^P(\mathbf{k} + \mathbf{g}_2) \right) \left(\partial_{k_y} \theta_{\mathbf{g}_3 \mathbf{g}_1} + A_y^P(\mathbf{k} + \mathbf{g}_1) - A_y^P(\mathbf{k} + \mathbf{g}_3) \right) \\
& - \frac{1}{4} \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3)) \partial_{k_y} \ln(n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_3)) \\
& - \frac{i}{2} \left(\partial_{k_x} \theta_{\mathbf{g}_2 \mathbf{g}_3} + A_x^P(\mathbf{k} + \mathbf{g}_3) - A_x^P(\mathbf{k} + \mathbf{g}_2) \right) \partial_{k_y} \ln(n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_3)) \\
& - \frac{i}{2} \left(\partial_{k_y} \theta_{\mathbf{g}_3 \mathbf{g}_1} + A_y^P(\mathbf{k} + \mathbf{g}_1) - A_y^P(\mathbf{k} + \mathbf{g}_3) \right) \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3))] \\
& - x \leftrightarrow y + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g})
\end{aligned}$$

$$\begin{aligned}
\Omega(\mathbf{k}) = & - \sum_{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3} n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3) \left[\left(\partial_{k_x} \theta_{\mathbf{g}_2 \mathbf{g}_3} + A_x^P(\mathbf{k} + \mathbf{g}_3) - A_x^P(\mathbf{k} + \mathbf{g}_2) \right) \partial_{k_y} \ln(n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_3)) \right. \\
& \left. - \left(\partial_{k_y} \theta_{\mathbf{g}_3 \mathbf{g}_1} + A_y^P(\mathbf{k} + \mathbf{g}_1) - A_y^P(\mathbf{k} + \mathbf{g}_3) \right) \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_2)n(\mathbf{k} + \mathbf{g}_3)) \right] \\
& + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g}).
\end{aligned}$$

$$\begin{aligned}
\sum_{\mathbf{g}_1} n(\mathbf{k} + \mathbf{g}_1) \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_1)n(\mathbf{k} + \mathbf{g}_3)) & = \partial_{k_x} \sum_{\mathbf{g}_1} n(\mathbf{k} + \mathbf{g}_1) + \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_3)) \sum_{\mathbf{g}_1} n(\mathbf{k} + \mathbf{g}_1) \\
& = \partial_{k_x} \ln(n(\mathbf{k} + \mathbf{g}_3))
\end{aligned}$$



$$\begin{aligned}\Omega(\mathbf{k}) = & - \sum_{\mathbf{g}_2, \mathbf{g}_3} n(\mathbf{k} + \mathbf{g}_2) \left[\left(\partial_{k_x} \theta_{\mathbf{g}_2 \mathbf{g}_3} + A_x^P(\mathbf{k} + \mathbf{g}_3) - A_x^P(\mathbf{k} + \mathbf{g}_2) \right) \partial_{k_y} n(\mathbf{k} + \mathbf{g}_3) \right. \\ & \left. - \left(\partial_{k_y} \theta_{\mathbf{g}_2 \mathbf{g}_3} + A_y^P(\mathbf{k} + \mathbf{g}_3) - A_y^P(\mathbf{k} + \mathbf{g}_2) \right) \partial_{k_x} n(\mathbf{k} + \mathbf{g}_3) \right] \\ & + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g})\end{aligned}$$

$$\Omega^{\text{bulk}}(\mathbf{k}) \approx \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g}) \approx \Omega^P(\mathbf{k}).$$

$$\begin{aligned}\Omega^{\text{LW}}(\mathbf{k}) = & -n(\mathbf{k}) \left[\left(\partial_{k_x} \theta_{\mathbf{0} \mathbf{G}_1} + A_x^P(\mathbf{k} + \mathbf{G}_1) - A_x^P(\mathbf{k}) \right) \partial_{k_y} n(\mathbf{k} + \mathbf{G}_1) - \left(\partial_{k_y} \theta_{\mathbf{0} \mathbf{G}_1} + A_y^P(\mathbf{k} + \mathbf{G}_1) - A_y^P(\mathbf{k}) \right) \partial_{k_x} n(\mathbf{k} + \mathbf{G}_1) \right] \\ & -n(\mathbf{k} + \mathbf{G}_1) \left[\left(\partial_{k_x} \theta_{\mathbf{G}_1 \mathbf{0}} + A_x^P(\mathbf{k}) - A_x^P(\mathbf{k} + \mathbf{G}_1) \right) \partial_{k_y} n(\mathbf{k}) - \left(\partial_{k_y} \theta_{\mathbf{G}_1 \mathbf{0}} + A_y^P(\mathbf{k}) - A_y^P(\mathbf{k} + \mathbf{G}_1) \right) \partial_{k_x} n(\mathbf{k}) \right] \\ & + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g}) \\ = & - \left(\partial_{k_x} \theta_{\mathbf{0} \mathbf{G}_1} + A_x^P(\mathbf{k} + \mathbf{G}_1) - A_x^P(\mathbf{k}) \right) \left(n(\mathbf{k}) \partial_{k_y} n(\mathbf{k} + \mathbf{G}_1) - n(\mathbf{k} + \mathbf{G}_1) \partial_{k_y} n(\mathbf{k}) \right) \\ & + \left(\partial_{k_y} \theta_{\mathbf{0} \mathbf{G}_1} + A_y^P(\mathbf{k} + \mathbf{G}_1) - A_y^P(\mathbf{k}) \right) \left(n(\mathbf{k}) \partial_{k_x} n(\mathbf{k} + \mathbf{G}_1) - n(\mathbf{k} + \mathbf{G}_1) \partial_{k_x} n(\mathbf{k}) \right) + \sum_{\mathbf{g}} n(\mathbf{k} + \mathbf{g}) \Omega^P(\mathbf{k} + \mathbf{g})\end{aligned}$$

$$\Omega^{\text{LW}}(\mathbf{k}) \approx \left(\partial_{k_y} \theta_{\mathbf{0} \mathbf{G}_1} + A_y^P(\mathbf{k} + \mathbf{G}_1) - A_y^P(\mathbf{k}) \right) \left(n(\mathbf{k}) \partial_{k_x} n(\mathbf{k} + \mathbf{G}_1) - n(\mathbf{k} + \mathbf{G}_1) \partial_{k_x} n(\mathbf{k}) \right)$$

$$\begin{aligned}& \int_0^\delta d\Delta_{k_x} \Omega^{\text{LW}}(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \\ & \approx \int_0^\delta d\Delta_{k_x} \left(\partial_{k_y} \theta_{\mathbf{0} \mathbf{G}_1} + A_y^P(\mathbf{k}^{\text{LW}} + \Delta_{k_x} + \mathbf{G}_1) - A_y^P(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right) \\ & \times \left(n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x} + \mathbf{G}_1) - n(\mathbf{k}^{\text{LW}} + \Delta_{k_x} + \mathbf{G}_1) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right)\end{aligned}$$

$$\begin{aligned}& \int_0^\delta d\Delta_{k_x} \Omega^{\text{LW}}(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \\ & \approx \left(\partial_{k_y} \theta_{\mathbf{0} \mathbf{G}_1} + A_y^P(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) - A_y^P(\mathbf{k}^{\text{LW}}) \right) \\ & \times \int_0^\delta d\Delta_{k_x} \left(n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x} + \mathbf{G}_1) - n(\mathbf{k}^{\text{LW}} + \Delta_{k_x} + \mathbf{G}_1) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right)\end{aligned}$$

$$\Omega^{\text{RW}}(\mathbf{k}) \approx \left(\partial_{k_y} \theta_{-\mathbf{G}_1 \mathbf{0}} + A_y^P(\mathbf{k}) - A_y^P(\mathbf{k} - \mathbf{G}_1) \right) \left(n(\mathbf{k} - \mathbf{G}_1) \partial_{k_x} n(\mathbf{k}) - n(\mathbf{k}) \partial_{k_x} n(\mathbf{k} - \mathbf{G}_1) \right),$$

$$\begin{aligned}& \int_{-\delta}^0 d\Delta_{k_x} \Omega^{\text{RW}}(\mathbf{k}^{\text{RW}} + \Delta_{k_x}) \\ & \approx \left(\partial_{k_y} \theta_{-\mathbf{G}_1 \mathbf{0}} + A_y^P(\mathbf{k}^{\text{RW}}) - A_y^P(\mathbf{k}^{\text{RW}} - \mathbf{G}_1) \right) \\ & \times \int_0^\delta d\Delta_{k_x} \left(n(\mathbf{k}^{\text{RW}} - \mathbf{G}_1 + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{RW}} + \Delta_{k_x}) - n(\mathbf{k}^{\text{RW}} + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{RW}} - \mathbf{G}_1 + \Delta_{k_x}) \right)\end{aligned}$$



$$\begin{aligned}
& \int_{-\delta}^0 d\Delta_{k_x} \Omega^{\text{RW}}(\mathbf{k}^{\text{RW}} + \Delta_{k_x}) \\
& \approx \left(\partial_{k_y} \theta_{0\mathbf{G}_1} + A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) \right) \\
& \times \int_0^\delta d\Delta_{k_x} \left(n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \mathbf{G}_1 + \Delta_{k_x}) - n(\mathbf{k}^{\text{LW}} + \mathbf{G}_1 + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right) \\
& \int_{-\delta}^\delta d\Delta_{k_x} \Omega^{W_1}(\mathbf{k} + \Delta_{k_x}) \\
& \approx \left(\partial_{k_y} \theta_{0\mathbf{G}_1} + A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) \right) \\
& \times \int_{-\delta}^\delta d\Delta_{k_x} \left(n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \mathbf{G}_1 + \Delta_{k_x}) - n(\mathbf{k}^{\text{LW}} + \mathbf{G}_1 + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right) \\
& \left(n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \mathbf{G}_1 + \Delta_{k_x}) - n(\mathbf{k}^{\text{LW}} + \mathbf{G}_1 + \Delta_{k_x}) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right) \\
& = n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \left(-\partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right) - \left(1 - n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right) \partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \\
& = -\partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \\
& \int_{-\delta}^\delta d\Delta_{k_x} \left(-\partial_{k_x} n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right) = \left[-n(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) \right]_{-\delta}^\delta \\
& = -1
\end{aligned}$$

$$\int_{-\delta}^\delta \Omega^{W_1}(\mathbf{k}^{\text{LW}} + \Delta_{k_x}) d\Delta_{k_x} = - \left(\partial_{k_y} \theta_{0\mathbf{G}_1} + A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) \right)$$

$$\begin{aligned}
\Phi_{W_1} &= - \int_{W_1} dk_y \left(\partial_{k_y} \theta_{0\mathbf{G}_1} + A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) \right) \\
&= - \int_{W_1} dk_y \partial_{k_y} \theta_{0\mathbf{G}_1} + \int_{W_1} dk_y \left(A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) \right)
\end{aligned}$$

$$\int dk_y \left(A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) \right)$$

$$\int dk_y \left(A_y^{\text{P}}(\mathbf{k}^{\text{LW}}) - A_y^{\text{P}}(\mathbf{k}^{\text{LW}} + \mathbf{G}_1) \right) = -\frac{1}{3} \Phi_{\text{BZ}}^{\text{parent}}$$

$$\begin{aligned}
\Phi &= 3\Phi_{W_1} + \int d^2k \Omega_{\text{bulk}} \\
&= -3 \int_{W_1} dk_y \partial_{k_y} \theta_{0\mathbf{G}_1}
\end{aligned}$$

$$\begin{aligned}
W_{\text{capped}} &= \int_{W_1} \partial_{k_y} \arg(\mathcal{F}(\mathbf{k}, \mathbf{k} + \mathbf{G}_1)) + \arg(\mathcal{F}(\mathbf{K}'_2, \mathbf{K}'_2 + \mathbf{G}_1)) - \left[\arg(\mathcal{F}(\mathbf{K}'_2, \mathbf{K}'_2 + \mathbf{G}_1)) \right]_{2\pi/3} \\
&\quad - \arg(\mathcal{F}(\mathbf{K}_2, \mathbf{K}_2 + \mathbf{G}_1)) + \left[\arg(\mathcal{F}(\mathbf{K}_2, \mathbf{K}_2 + \mathbf{G}_1)) \right]_{2\pi/3} \\
&= \int_{W_1} \partial_{k_y} \arg(\mathcal{F}(\mathbf{k}, \mathbf{k} + \mathbf{G}_1)) + \arg(\mathcal{F}(\mathbf{K}'_2, \mathbf{K}'_3)) - \arg(\mathcal{F}(\mathbf{K}_2, \mathbf{K}_1)) \\
&\quad + \left[\arg(\mathcal{F}(\mathbf{K}_2, \mathbf{K}_1)) \right]_{2\pi/3} - \left[\arg(\mathcal{F}(\mathbf{K}'_2, \mathbf{K}'_3)) \right]_{2\pi/3}
\end{aligned}$$



$$\begin{aligned}\mathcal{C} &= -\frac{3}{2\pi}W_{\text{capped}} \\ &= -\frac{3}{2\pi}\left[\int_{W_1}\partial_{k_y}\arg(\mathcal{F}(\mathbf{k},\mathbf{k}+\mathbf{G}_1))dk_y + \arg(\mathcal{F}(\mathbf{K}'_2,\mathbf{K}'_3)) - \arg(\mathcal{F}(\mathbf{K}_2,\mathbf{K}_1))\right] \\ &\quad -\left[\frac{3}{2\pi}\arg(\mathcal{F}(\mathbf{K}_2,\mathbf{K}_1))\right]_1 + \left[\frac{3}{2\pi}\arg(\mathcal{F}(\mathbf{K}'_2,\mathbf{K}'_3))\right]_1 \\ &\quad \left[\int_{W_1}\partial_{k_y}\arg(\mathcal{F}(\mathbf{k},\mathbf{k}+\mathbf{G}_1)) + \arg(\mathcal{F}(\mathbf{K}'_2,\mathbf{K}'_3)) - \arg(\mathcal{F}(\mathbf{K}_2,\mathbf{K}_1))\right]\end{aligned}$$

$$\mathcal{F}_N(\mathbf{k},\mathbf{k}') = \mathcal{N}_{\mathbf{k}}\mathcal{N}_{\mathbf{k}'}\sum_{n=0}^{N-1}\frac{(\mathcal{B}k_zk'_z)^n}{n!}$$

$$k_z=\frac{1}{\sqrt{2}}(k_x+ik_y)$$

$$k_z=\frac{1}{\sqrt{2}}\Big(-\frac{g}{2}+ik_y\Big)$$

$$(k+G)_z=\frac{1}{\sqrt{2}}\Big(+\frac{g}{2}+ik_y\Big)$$

$$\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G})=\sum_{n=0}^{N-1}\frac{\mathcal{B}^n}{n!\times 2^n}(-1)^n\Big(-\frac{g}{2}+ik_y\Big)^{2n}$$

$$\frac{1}{\mathcal{F}_N}\partial_{k_y}|\mathcal{F}_N|e^{i\theta}=i\partial_{k_y}\theta+\frac{\partial_{k_y}|\mathcal{F}_N|}{|\mathcal{F}_N|}$$

$$\partial_{k_y}\arg(\mathcal{F}_N(\mathbf{k},\mathbf{k}+\mathbf{G}))=\frac{1}{i\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G})}\partial_{k_y}\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G})-\frac{1}{2i|\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G})|^2}\partial_{k_y}|\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G})|^2$$

$$\begin{aligned}\partial_{k_y}\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G}) &= i\sum_{n=1}^{N-1}\frac{\mathcal{B}^n}{(n-1)!\times 2^{n-1}}(-1)^n\Big(-\frac{g}{2}+ik_y\Big)^{2n-1} \\ &= -i\mathcal{B}\Big(-\frac{g}{2}+ik_y\Big)\sum_{n=1}^{N-1}\frac{\mathcal{B}^{n-1}}{(n-1)!\times 2^{n-1}}(-1)^{n-1}\Big(-\frac{g}{2}+ik_y\Big)^{2n-2} \\ &= -i\mathcal{B}\Big(-\frac{g}{2}+ik_y\Big)\sum_{n=0}^{N-2}\frac{\mathcal{B}^n}{n!\times 2^n}\Big(-\frac{g}{2}+ik_y\Big)^{2n} \\ &= -i\mathcal{B}\Big(-\frac{g}{2}+ik_y\Big)\tilde{\mathcal{F}}_{N-1}(\mathbf{k},\mathbf{k}+\mathbf{G})\end{aligned}$$

$$\int_{W_1}\partial_{k_y}\arg(\mathcal{F}_N(\mathbf{k},\mathbf{k}+\mathbf{G}))=\int_{K'_2}^{K_2}dk_y\mathcal{B}\Big(\frac{g}{2}-ik_y\Big)\frac{\tilde{\mathcal{F}}_{N-1}(\mathbf{k},\mathbf{k}+\mathbf{G})}{\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G})}$$

$$\tilde{\mathcal{F}}_N(\mathbf{k},\mathbf{k}+\mathbf{G})=1-\frac{\mathcal{B}}{2}\Big(\frac{g}{2}-ik_y\Big)^2=1-\frac{\mathcal{B}}{2}(g^2/4-k_y^2)+i\frac{\mathcal{B}}{2}k_yg$$

$$\frac{\tilde{\mathcal{F}}_{N-1}(\mathbf{k}, \mathbf{k} + \mathbf{G})}{\tilde{\mathcal{F}}_N(\mathbf{k}, \mathbf{k} + \mathbf{G})} = \frac{1 - \frac{\mathcal{B}}{2}(g^2/4 - k_y^2) - i\frac{\mathcal{B}}{2}k_y g}{\left(1 - \frac{\mathcal{B}}{2}(g^2/4 - k_y^2)\right)^2 + \frac{\mathcal{B}^2 g^2 k_y^2}{4}}$$

$$\begin{aligned} \int_{\text{wire 1}} \partial_{k_y} \arg(\mathcal{F}_N(\mathbf{k}, \mathbf{k} + \mathbf{G})) &= \int dk_y \frac{\mathcal{B}g}{2} \frac{1 - \frac{\mathcal{B}}{2}(g^2/4 - k_y^2)}{\left(1 - \frac{\mathcal{B}}{2}(g^2/4 - k_y^2)\right)^2 + \frac{\mathcal{B}^2 g^2 k_y^2}{4}} - \frac{\mathcal{B}k_y}{2} \frac{\frac{\mathcal{B}}{2}k_y g}{\left(1 - \frac{\mathcal{B}}{2}(g^2/4 - k_y^2)\right)^2 + \frac{\mathcal{B}^2 g^2 k_y^2}{4}} \\ &= \int dk_y \frac{\mathcal{B}g}{2} \frac{1 - \frac{\mathcal{B}}{2}(g^2/4)}{\left(1 - \frac{\mathcal{B}}{2}(g^2/4 - k_y^2)\right)^2 + \frac{\mathcal{B}^2 g^2 k_y^2}{4}} \end{aligned}$$

$$-3 \int_{W_1} dk_y \partial_{k_y} \arg(\mathcal{F}_\infty(\mathbf{k}, \mathbf{k} + \mathbf{G})) = -3 \int dk_y \mathcal{B}(g/2 - ik_y) = -3 \int dk_y \mathcal{B}g/2 = -3\mathcal{B}g/2 \cdot L$$

$$= -\frac{\sqrt{3}}{2} \mathcal{B}g^2 = -\mathcal{B}A_{1BZ}$$

$$\begin{aligned} \arg(\mathcal{F}_\infty(\mathbf{K}'_2, \mathbf{K}'_2 + \mathbf{G})) &= \arg\left(\mathcal{F}_\infty\left(-\frac{g}{2}\hat{x} - \frac{g}{2\sqrt{3}}\hat{y}, \frac{g}{2}\hat{x} - \frac{g}{2\sqrt{3}}\hat{y}\right)\right) \\ &= \arg\left(e^{-i\frac{\mathcal{B}}{2}\left(-\frac{g}{2}\hat{x} - \frac{g}{2\sqrt{3}}\hat{y}\right) \times \left(\frac{g}{2}\hat{x} - \frac{g}{2\sqrt{3}}\hat{y}\right)}\right) \\ &= -\frac{\mathcal{B}}{2} \frac{g^2}{2\sqrt{3}} \\ &= -\frac{\mathcal{B}A}{6} \end{aligned}$$

$$\begin{aligned} W_{\text{capped}} &= \mathcal{B}A_{1BZ}/3 + (-\mathcal{B}A_{1BZ}/6 + [\mathcal{B}A_{1BZ}/6]_{2\pi/3}) - (\mathcal{B}A_{1BZ}/6 - [\mathcal{B}A_{1BZ}/6]_{2\pi/3}) \\ &= 2[\mathcal{B}A_{1BZ}/6]_{2\pi/3} \end{aligned}$$

$$\begin{aligned} C &= -\frac{3}{2\pi} W_{\text{capped}} \\ &= -\frac{6}{2\pi} [\mathcal{B}A_{1BZ}/6]_{2\pi/3} \\ &= -\left[\frac{\mathcal{B}A_{1BZ}}{2\pi}\right]_{\frac{2\pi}{3}} \frac{6}{2\pi} \\ &= -\left[\frac{\mathcal{B}A_{1BZ}}{2\pi}\right]_2 \end{aligned}$$

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 diseñado planos divergentes de curvatura además de establecer modelos matriciales y superoperadores para describir, la acción gravitacional de la partícula oscura o estrella en un momento específico 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.



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