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**APROXIMACIONES DE BORN-OPPENHEIMER
HARTREE-FOCK APLICADAS A CAMPOS CUÁNTICOS
RELATIVISTAS. VOLUMEN I**

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

Manuel Ignacio Albuja Bustamante
Investigador Independiente

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

Manuel Ignacio Albuja Bustamante¹

Ingaciomanuelalbujustamante@gmail.com

<https://orcid.org/0009-0005-0115-767X>

Investigador Independiente

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

¹ Autor principal

Correspondencia: Ingaciomanuelalbujustamante@gmail.com

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

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 multideterminantes de Slater.

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

RESULTADOS Y DISCUSIÓN.

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

$$H^{\text{el}} = T^{\text{el}} + V^{\text{nuc-el}} + V^{\text{el-el}} + V^{\text{NN}}$$

$$H^{\text{el}}(\mathbf{R})\Psi_i^{\text{el}}(\mathbf{r}; \mathbf{R}) = E_i^{\text{el}}\Psi_i^{\text{el}}(\mathbf{r}; \mathbf{R})$$

$$i\partial_t\Psi^{\text{el}}(\mathbf{r}; \mathbf{R}) = H^{\text{el}}\Psi^{\text{el}}(\mathbf{r}; \mathbf{R})$$

$$(T^{\text{nuc}} + E_i^{\text{el}})\Phi_{i,\alpha}^{\text{nuc}}(\mathbf{R}) = E_{i,\alpha}^{\text{tot}}\Phi_{i,\alpha}^{\text{nuc}}(\mathbf{R})$$

$$i\partial_t\Phi^{\text{nuc}}(\mathbf{R}) = (T^{\text{nuc}} + E_i^{\text{el}})\Phi^{\text{nuc}}(\mathbf{R})$$



$$\lambda=\sqrt{\frac{2\pi}{mkT}}$$

$$H=\sum_i\left(-\frac{1}{2}\nabla_i^2+v_{\rm ext}(\mathbf{r}_i)\right)+\sum_{i>j}\frac{1}{r_{ij}}+E_{NN}$$

$$\chi(\mathbf{r})=(x-A_x)^i(y-A_y)^j(z-A_z)^ke^{-\alpha(\mathbf{r}-\mathbf{A})^2}$$

$$\chi_{\mathbf{G}}(\mathbf{r})=\frac{1}{\sqrt{V}}e^{-i\mathbf{G}\cdot\mathbf{r}}$$

$$H=\sum_{ij}t_{ij}a_i^\dagger a_j+\frac{1}{2}\sum_{ijkl}v_{ijkl}a_i^\dagger a_j^\dagger a_la_k$$

$$|\Phi\rangle=\prod_{m=1}^Nc_m^\dagger|0\rangle$$

$$c_m^\dagger=\sum_iC_{mi}a_i^\dagger$$

$$\mathbf{F}(\mathbf{C})\mathbf{C}=\mathbf{C}\varepsilon$$

$$\gamma_{ij}=\langle\Phi|a_i^\dagger a_j|\Phi\rangle$$

$$\rho(\mathbf{r})=\sum_{ij}\gamma_{ij}\phi_i(\mathbf{r})\phi_j(\mathbf{r}); E\equiv E[\rho]$$

$$E[\rho]=T_s[\rho]+V_{ne}[\rho]+J[\rho]+E_{xc}[\rho]$$

$$|\Psi\rangle=\sum_Ic_I|\Phi_I\rangle$$

$$E=\frac{\langle\Phi_0|HTe^{-\int_0^\beta d\tau V_I(\tau)}|\Phi_0\rangle}{\langle\Phi_0|\mathcal{T}e^{-\int_0^\beta d\tau V_I(\tau)}|\Phi_0\rangle}=\langle\Phi_0|HTe^{-\int_0^\beta d\tau V_I(\tau)}|\Phi_0\rangle_c$$

$$|\Phi_{\rm HF}\rangle=e^{\sum_{pq}A_{pq}c_p^\dagger c_q}|\Phi_0\rangle$$

$$|\Psi\rangle=e^T|\Phi_0\rangle=e^{\sum_{pq}A_{pq}c_p^\dagger c_q+\sum_{pqrs}A_{pqrs}c_p^\dagger c_q^\dagger c_r c_s+\cdots}|\Phi_0\rangle$$

$$T=\sum_{ia}t_{ia}c_a^\dagger c_i+\sum_{ijab}t_{ijab}c_a^\dagger c_b^\dagger c_i c_j+\cdots$$

$$|\Psi\rangle=\sum_{\{n\}}\Psi^{n_1\dots n_K}|n_1n_2\dots n_K\rangle$$

$$\Psi^{n_1\dots n_K}=\sum_{\{i\}}A_{i_1}^{n_1}A_{i_1i_2}^{n_2}\dots A_{i_K}^{n_K}$$

$$E=\langle \Psi | H | \Psi \rangle = \sum_{nn'} |\Psi(n)|^2 \langle n | H | n' \rangle \frac{\Psi(n')}{\Psi(n)}$$

$$e^{-\beta H}|\Phi_0\rangle=e^{-\varepsilon H}e^{-\varepsilon H}\ldots e^{-\varepsilon H}|\Phi_0\rangle=\sum_{\mu_1\ldots\mu_T}(p_{\mu_1}o_{\mu_1})(p_{\mu_2}o_{\mu_2})\ldots(p_{\mu_T}o_{\mu_T})|\Phi_0\rangle$$

$$|\Psi\rangle=\sum_{\vec{\mu}}w_{\mu}|\Phi_{\vec{\mu}}\rangle$$

$$C = R_{\text{state prep}} \times C_{\text{refinement}}$$

$$E=\min_{\theta}\langle 0|U^{\dagger}(\theta)HU(\theta)|0\rangle$$

$$C = R_{\text{init}} \times C_{\text{refinement}}$$

$$C = R_{\text{state prep}} \times C_{\text{phase estimation}}$$

$$\mathcal{C} \sim \text{poly}(1/S) \times \text{poly}(L) \times \text{poly}(1/\varepsilon)$$

$$S=\langle \Phi \mid \Psi_0 \rangle$$

$$|0\rangle=\begin{pmatrix}1\\0\end{pmatrix},|1\rangle=\begin{pmatrix}0\\1\end{pmatrix}$$

$$\begin{aligned} |\varphi\rangle &= \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \\ \alpha, \beta &\in \mathbb{C}, \\ |\alpha|^2 + |\beta|^2 &= 1. \end{aligned}$$

$$\frac{1}{\sqrt{2}}(|00\rangle+|01\rangle)=|0\rangle\otimes\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$$

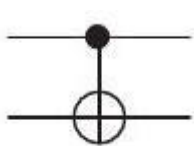
$$\frac{1}{\sqrt{2}}(|00\rangle+|11\rangle)$$

$$|\overline{0}\rangle=|0\rangle^{\otimes n}=|0\rangle\otimes|0\rangle\otimes\cdots\otimes|0\rangle$$

$$X=\begin{pmatrix}0&1\\1&0\end{pmatrix},Y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},Z=\begin{pmatrix}1&0\\0&-1\end{pmatrix},$$

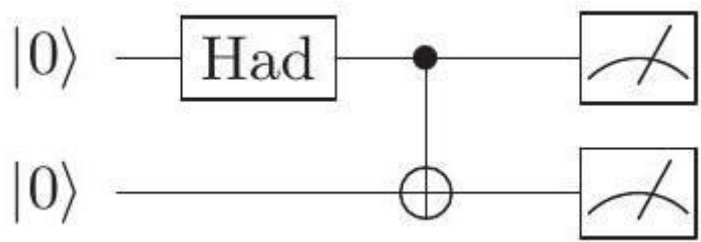
$$R_x(\theta)=e^{\left(\frac{-i\theta X}{2}\right)},R_y(\theta)=e^{\left(\frac{-i\theta Y}{2}\right)},R_z(\theta)=e^{\left(\frac{-i\theta Z}{2}\right)}$$

$$\text{Had}=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix},\text{T}=\begin{pmatrix}1&0\\0&e^{i\pi/4}\end{pmatrix}$$



$$|0\rangle\langle 0|_c\otimes I_T+|1\rangle\langle 1|_c\otimes X_T,$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



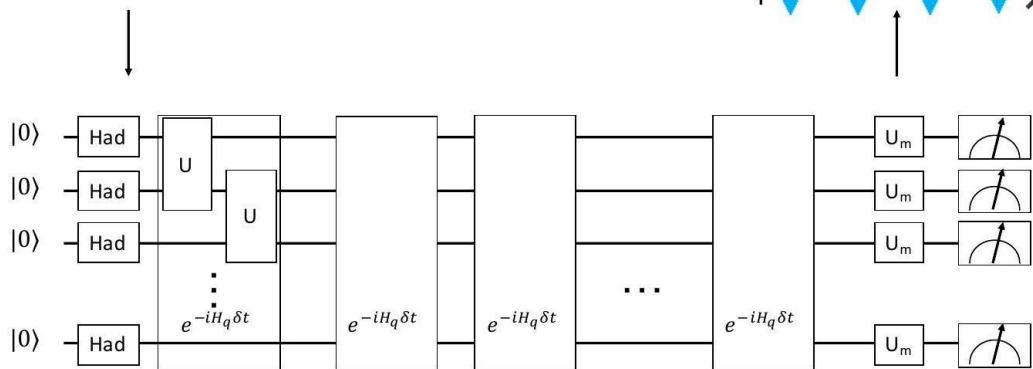
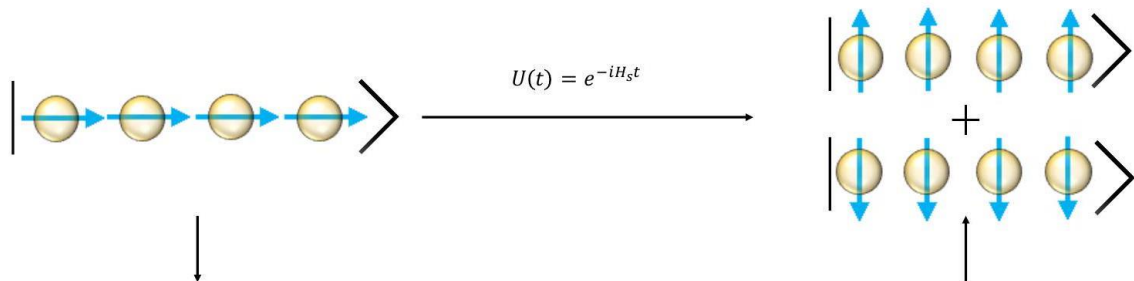
$$|\varphi\rangle = \prod_k U_k^{i_k,j_k}(\vec{\theta}_k)|\bar{0}\rangle$$

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \text{CNOT}^{0,1}\text{Had}^0|00\rangle$$

$$\bar{O} = \langle \varphi | O | \varphi \rangle$$

$$H_s = \sum_j h_j$$

$$e^{-iH_s\delta t} = e^{-i\sum_j h_j\delta t} \approx \prod_j e^{-ih_j\delta t} + \mathcal{O}(\delta t^2)$$



$$H = \sum_{\langle i,j \rangle} J_{ij} Z_i Z_j + \sum_i B_i X_i$$

$$U_{ij} = \text{CNOT}^{i,j} R_z^j(2J_{ij}) \text{CNOT}^{i,j} R_x^i(2B_i)$$

$$H = - \sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 - \sum_{i,I} \frac{e^2}{4\pi\epsilon_0} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} \\ + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2} \sum_{I \neq J} \frac{e^2}{4\pi\epsilon_0} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|}$$

$$H = - \sum_i \frac{\nabla_i^2}{2} - \sum_I \frac{\nabla_I^2}{2M'_I} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} \\ + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2} \sum_{I \neq J} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|}.$$

$$H_e = - \sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

$$\text{Rate} \propto e^{-\Delta E/k_BT}$$

$$|\Psi\rangle = \int_{\mathbf{x}_1, \dots, \mathbf{x}_N} \psi(\mathbf{x}_1, \dots, \mathbf{x}_N) \mathcal{A}(|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle) d\mathbf{x}_1, \dots, d\mathbf{x}_N$$

$$|\Psi\rangle = \sum_{\mathbf{x}_1, \dots, \mathbf{x}_N} \psi(\mathbf{x}_1, \dots, \mathbf{x}_N) \mathcal{A}(|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle)$$

$$\psi(\mathbf{x}_0 \dots \mathbf{x}_{N-1}) = \\ \frac{1}{\sqrt{N!}} \left| \begin{array}{cccc} \phi_0(\mathbf{x}_0) & \phi_1(\mathbf{x}_0) & \dots & \phi_{M-1}(\mathbf{x}_0) \\ \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \dots & \phi_{M-1}(\mathbf{x}_1) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_{N-1}) & \phi_1(\mathbf{x}_{N-1}) & \dots & \phi_{M-1}(\mathbf{x}_{N-1}) \end{array} \right|$$

$$\psi(\mathbf{x}_0,\mathbf{x}_1)=\\ \frac{1}{\sqrt{2}}\left| \begin{array}{cc} A_{\uparrow}(\mathbf{x}_0) & A_{\downarrow}(\mathbf{x}_0) \\ A_{\uparrow}(\mathbf{x}_1) & A_{\downarrow}(\mathbf{x}_1) \end{array} \right|=\\ \frac{1}{\sqrt{2}}(A_{\uparrow}(\mathbf{x}_0)A_{\downarrow}(\mathbf{x}_1)-A_{\downarrow}(\mathbf{x}_0)A_{\uparrow}(\mathbf{x}_1)).$$

$$\psi(\mathbf{x}_0 \dots \mathbf{x}_{N-1}) = |f_{M-1}, \dots, f_p, \dots, f_0\rangle = |f\rangle$$

$$\{a_p,a_q^\dagger\}=a_pa_q^\dagger+a_q^\dagger a_p=\delta_{pq}\\ \{a_p,a_q\}=\{a_p^\dagger,a_q^\dagger\}=0$$

$$a_p|f_{M-1},f_{M-2},\ldots,f_0\rangle\\ =\delta_{f_p,1}(-1)^{\sum_{i=0}^{p-1}f_i}|f_{M-1},f_{M-2},\ldots,f_p\oplus 1,\ldots,f_0\rangle,\\ a_p^\dagger|f_{M-1},f_{M-2},\ldots,f_0\rangle\\ =\delta_{f_p,0}(-1)^{\sum_{i=0}^{p-1}f_i}|f_{M-1},f_{M-2},\ldots,f_p\oplus 1,\ldots,f_0\rangle,$$

$$\hat{n}_i = a_i^\dagger a_i \\ \hat{n}_i |f_{M-1}, \dots, f_i, \dots, f_0\rangle = f_i |f_{M-1}, \dots, f_i, \dots, f_0\rangle$$

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$$h_{pq} = \int d\mathbf{x} \phi_p^*(\mathbf{x}) \left(-\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|} \right) \phi_q(\mathbf{x}),$$

$$h_{pqrs} = \int d\mathbf{x}_1 d\mathbf{x}_2 \frac{\phi_p^*(\mathbf{x}_1) \phi_q^*(\mathbf{x}_2) \phi_r(\mathbf{x}_2) \phi_s(\mathbf{x}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$H = -t \sum_{\langle i,j \rangle, \sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

$$|\Psi\rangle = \sum_f \alpha_f |f\rangle,$$

$$\hat{f} = \sum_{i,j} (h_{ij} + V_{ij}) a_i^\dagger a_j$$

$$V_{ij} = \sum_{k \in occ} (h_{ik kj} - h_{ik jk})$$

$$|\Psi_{\text{FCI}}\rangle = \left(I + \sum_{i,\alpha} C_{i\alpha} a_i^\dagger a_\alpha + \sum_{i>j,\alpha>\beta} C_{ij\alpha\beta} a_i^\dagger a_j^\dagger a_\alpha a_\beta + \cdots \right) |\Psi_{\text{HF}}\rangle$$

$$|\Psi_{\text{CC}}\rangle = \prod_{i,\alpha} (I + C_{i\alpha} a_i^\dagger a_\alpha) \times \prod_{i>j,\alpha>\beta} (I + C_{ij\alpha\beta} a_i^\dagger a_j^\dagger a_\alpha a_\beta) \times \dots |\Psi_{\text{HF}}\rangle.$$

$$|\Psi_{\text{CC}}\rangle = e^T |\Psi_{\text{HF}}\rangle,$$

$$T_1 = \sum_{i \in virt, \alpha \in occ} t_{i\alpha} a_i^\dagger a_\alpha,$$

$$T_2 = \sum_{i,j \in virt, \alpha,\beta \in occ} t_{ij\alpha\beta} a_i^\dagger a_j^\dagger a_\alpha a_\beta,$$

$$\cdots,$$

$$R_n^{\text{STO}}(r) \propto (\zeta r)^{n-1} e^{-\zeta r}$$

$$R_{nl}^{\text{GTO}}(r) \propto (\sqrt{\alpha_{nl}} r)^l e^{-\alpha_{nl} r^2}$$

$$\phi_v = \sqrt{\frac{1}{V}} \exp\left(\frac{2\pi i v r}{L}\right),$$

$$\langle \Psi | O | \Psi \rangle = \sum_{i,j} O_{ij} \rho_{ij}^1 + \sum_{i,j,k,l} V_{ijkl} \rho_{ijkl}^2,$$

$$\rho_{ij}^1 = \langle \Psi | a_i^\dagger a_j | \Psi \rangle, \rho_{ijkl}^2 = \langle \Psi | a_i^\dagger a_k^\dagger a_l a_j | \Psi \rangle,$$

$$|\Psi\rangle = \sum_{\mathbf{x}_1, \dots, \mathbf{x}_N} \psi(\mathbf{x}_1, \dots, \mathbf{x}_N) \mathcal{A}(|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle),$$

$$|\mathbf{x}_i\rangle = |\mathbf{r}_i\rangle|\sigma_i\rangle$$

$$|\mathbf{r}_i\rangle = |x_i\rangle|y_i\rangle|z_i\rangle, \forall i \in \{1, 2, \dots, N\}, x_i, y_i, z_i \in \{0, 1, \dots, P-1\}$$

$$\begin{aligned} |\varphi\rangle &= \frac{1}{\sqrt{6}}|00\rangle + \frac{1}{\sqrt{3}}|01\rangle + \frac{1}{\sqrt{3}}|10\rangle + \frac{1}{\sqrt{6}}|11\rangle \\ &= \frac{1}{\sqrt{6}}|\mathbf{0}\rangle + \frac{1}{\sqrt{3}}|\mathbf{1}\rangle + \frac{1}{\sqrt{3}}|\mathbf{2}\rangle + \frac{1}{\sqrt{6}}|\mathbf{3}\rangle \end{aligned}$$

$$|\phi\rangle = \frac{1}{\sqrt{3}}|\mathbf{0}\rangle + \frac{1}{\sqrt{6}}|\mathbf{1}\rangle + \frac{1}{\sqrt{6}}|\mathbf{2}\rangle + \frac{1}{\sqrt{3}}|\mathbf{3}\rangle.$$

$$\begin{aligned} |\Phi\rangle &= \frac{1}{\sqrt{2}}(|\varphi\rangle_1|\phi\rangle_2 - |\phi\rangle_1|\varphi\rangle_2) \\ &= \frac{1}{6\sqrt{2}}(|\mathbf{1}\rangle_1|\mathbf{0}\rangle_2 - |\mathbf{0}\rangle_1|\mathbf{1}\rangle_2 + |\mathbf{1}\rangle_1|\mathbf{3}\rangle_2 - |\mathbf{3}\rangle_1|\mathbf{1}\rangle_2 \\ &\quad + |\mathbf{2}\rangle_1|\mathbf{0}\rangle_2 - |\mathbf{0}\rangle_1|\mathbf{2}\rangle_2 + |\mathbf{2}\rangle_1|\mathbf{3}\rangle_2 - |\mathbf{3}\rangle_1|\mathbf{2}\rangle_2) \end{aligned}$$

$$|\Psi\rangle = \sum_{i=0}^{P-1} \sum_{j=0}^{P-1} \psi_{ij} (|\mathbf{i}\rangle_1 |\mathbf{j}\rangle_2 - |\mathbf{j}\rangle_1 |\mathbf{i}\rangle_2),$$

$$|\Psi_{\text{HF}}\rangle = \frac{1}{\sqrt{2}}(|\mathbf{0}\rangle_1|\mathbf{1}\rangle_2 - |\mathbf{1}\rangle_1|\mathbf{0}\rangle_2)$$

$$\begin{aligned} |\Psi\rangle &= \frac{\alpha}{\sqrt{2}}(|\mathbf{0}\rangle_1|\mathbf{1}\rangle_2 - |\mathbf{1}\rangle_1|\mathbf{0}\rangle_2) \\ &\quad + \frac{\beta}{\sqrt{2}}(|\mathbf{2}\rangle_1|\mathbf{3}\rangle_2 - |\mathbf{3}\rangle_1|\mathbf{2}\rangle_2) \\ &\quad + \frac{\gamma}{\sqrt{2}}(|\mathbf{0}\rangle_1|\mathbf{3}\rangle_2 - |\mathbf{3}\rangle_1|\mathbf{0}\rangle_2) \\ &\quad + \frac{\delta}{\sqrt{2}}(|\mathbf{1}\rangle_1|\mathbf{2}\rangle_2 - |\mathbf{2}\rangle_1|\mathbf{1}\rangle_2) \end{aligned}$$

$$\begin{aligned} H &= \sum_{i=1}^N \sum_{\alpha,\beta=0}^{M-1} h_{\alpha\beta} |\phi_\beta\rangle_i \langle \phi_\alpha|_i \\ &\quad + \frac{1}{2} \sum_{i \neq j}^N \sum_{\alpha,\beta,\gamma,\delta}^{M-1} h_{\alpha\beta\gamma\delta} |\phi_\alpha\rangle_i |\phi_\beta\rangle_j \langle \phi_\gamma|_j \langle \phi_\delta|_i \end{aligned}$$

$$h_{\alpha\beta} = \int \mathrm{d}\mathbf{x} \phi_\beta^*(\mathbf{x}) \left(-\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|} \right) \phi_\alpha(\mathbf{x}),$$

$$h_{\alpha\beta\gamma\delta} = \int \mathrm{d}\mathbf{x}_1 \mathrm{d}\mathbf{x}_2 \frac{\phi_\alpha^*(\mathbf{x}_1) \phi_\beta^*(\mathbf{x}_2) \phi_\gamma(\mathbf{x}_2) \phi_\delta(\mathbf{x}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

$$\phi_\alpha = \{|A_\uparrow\rangle, |A_\downarrow\rangle, |B_\uparrow\rangle, |B_\downarrow\rangle\}$$

$$\begin{aligned}
h_{A\uparrow B\uparrow}|B\uparrow\rangle_{e_1}\langle A\uparrow|_{e_1} &= \\
h_{A\uparrow B\uparrow}|10\rangle_{e_1}\langle 00|_{e_1} &= \\
h_{A\uparrow B\uparrow}(|1\rangle_{q_3}\langle 0|_{q_3})\otimes(|0\rangle_{q_2}\langle 0|_{q_2}) &= \\
h_{A\uparrow B\uparrow}\left(\frac{1}{2}(X_{q_3}-iY_{q_3})\right)\otimes\left(\frac{1}{2}(I_{q_2}-Z_{q_2})\right) &= \\
\frac{h_{A\uparrow B\uparrow}}{4}(X_{q_3}I_{q_2}-iY_{q_3}I_{q_2}-X_{q_3}Z_{q_2}+iY_{q_3}Z_{q_2}), &
\end{aligned}$$

$$\begin{aligned}
|f_{M-1},f_{M-2},\ldots,f_0\rangle &\rightarrow |q_{M-1},q_{M-2},\ldots,q_0\rangle \\
q_p &= f_p \in \{0,1\}.
\end{aligned}$$

$$\begin{aligned}
a_p &= Q_p \otimes Z_{p-1} \otimes \cdots \otimes Z_0, \\
a_p^\dagger &= Q_p^\dagger \otimes Z_{p-1} \otimes \cdots \otimes Z_0,
\end{aligned}$$

$$Q=|0\rangle\langle 1|=\frac{1}{2}(X+iY) \text{ and } Q^\dagger=|1\rangle\langle 0|=\frac{1}{2}(X-iY)(\mathfrak{G})^{\sum_{i=0}^{p-1}f_i}.$$

$$H=\sum_j h_j P_j=\sum_j h_j \prod_i \sigma_i^j$$

$$|\Psi_{\rm HF}\rangle=|0011\rangle$$

$$|\Psi\rangle=\alpha|0011\rangle+\beta|1100\rangle+\gamma|1001\rangle+\delta|0110\rangle.$$

Fermion	Jordan-Wigner	Parity	Bravyi-Kitaev
$a\, 0001\rangle+b\, 0010\rangle$	$a\, 0001\rangle+b\, 0010\rangle$	$a\, 1111\rangle+b\, 1110\rangle$	$a\, 1011\rangle+b\, 1010\rangle$
$+c\, 0100\rangle+d\, 1000\rangle$	$+c\, 0100\rangle+d\, 1000\rangle$	$+c\, 1100\rangle+d\, 1000\rangle$	$+c\, 1100\rangle+d\, 1000\rangle$
a_0	Q_0	$X_3X_2X_1Q_0$	$X_3X_1Q_0$
a_1	Q_1Z_0	$X_3X_2\left(Q_1\, 0\rangle\langle 0 _0-Q_1^\dagger\, 1\rangle\langle 1 _0\right)$	$X_3\left(Q_1\, 0\rangle\langle 0 _0-Q_1^\dagger\, 1\rangle\langle 1 _0\right)$
a_2	$Q_2Z_1Z_0$	$X_3\left(Q_2\, 0\rangle\langle 0 _1-Q_2^\dagger\, 1\rangle\langle 1 _1\right)$	$X_3Q_2Z_1$
a_3	$Q_3Z_2Z_1Z_0$	$Q_3\, 0\rangle\langle 0 _2-Q_3^\dagger\, 1\rangle\langle 1 _2$	$\frac{1}{2}\left(Q_3(\mathbf{1}+Z_2Z_1)-Q_3^\dagger(\mathbf{1}-Z_2Z_1)\right)$
$\hat{n}_i=a_i^\dagger a_i$	$ 1\rangle\langle 1 _i$	$ 1\rangle\langle 1 _{i=0},\,\frac{1}{2}\left(\mathbf{1}-Z_iZ_{i-1}\right)_{i=1,2,3}$	$ 1\rangle\langle 1 _{i=0,2},\,\frac{1}{2}(\mathbf{1}-Z_1Z_0)_{i=1},\,\frac{1}{2}(\mathbf{1}-Z_3Z_2Z_1)_{i=3}$

$$|f_{M-1},f_{M-2},\ldots,f_0\rangle\rightarrow |q_{M-1},q_{M-2},\ldots,q_0\rangle$$

$$q_p=\left[\sum_{i=0}^pf_i\right](\mathrm{mod}2).$$

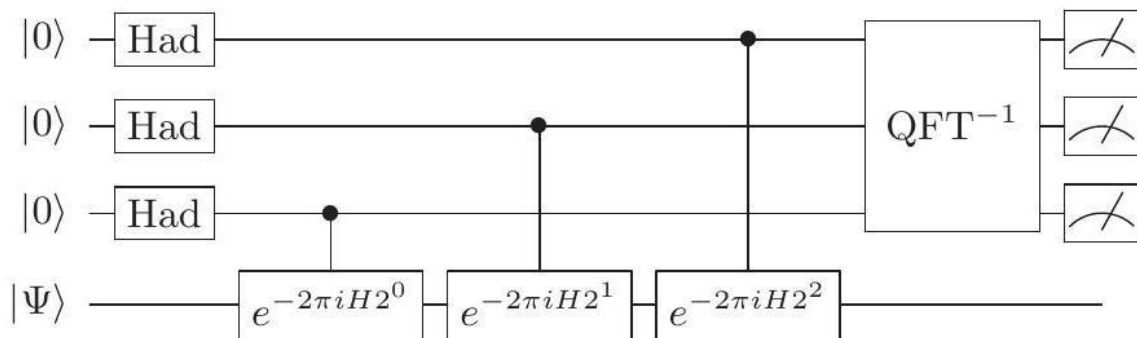
$$|f_{M-1},f_{M-2},\ldots,f_0\rangle\rightarrow |q_{M-1},q_{M-2},\ldots,q_0\rangle$$

$$q_p=\left[\sum_{q=0}^p\beta_{pq}f_q\right](\mathrm{mod}2)$$

$$\beta_1=[1]$$

$$\beta_{2^{x+1}}=\begin{pmatrix} \beta_{2^x} & \mathbf{0} \\ \mathbf{A} & \beta_{2^x} \end{pmatrix},$$

$$\beta_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$



$$\frac{1}{\sqrt{2^\omega}} \sum_i \sum_x |x\rangle c_i |E_i\rangle \rightarrow \frac{1}{\sqrt{2^\omega}} \sum_i \sum_x e^{-2\pi i E_i x} c_i |x\rangle |E_i\rangle.$$

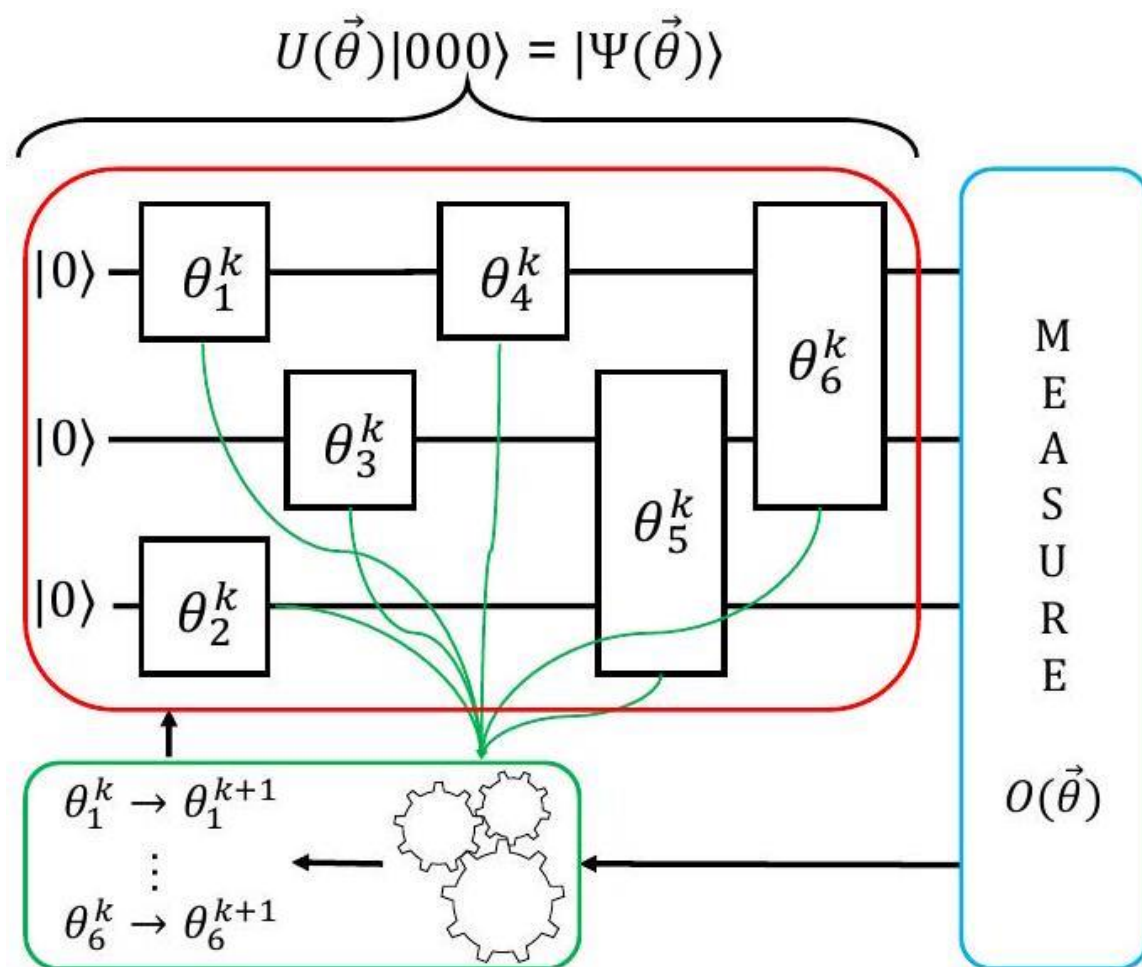
$$\frac{1}{\sqrt{2^\omega}} \sum_i \sum_x e^{-2\pi i E_i x} c_i |x\rangle |E_i\rangle \overset{\text{QFT}^{-1}}{\rightarrow} \sum_i c_i |\text{bin}(E_i)\rangle |E_i\rangle.$$

$$\omega = n + \left\lceil \log_2 \left(2 + \frac{1}{2p} \right) \right\rceil$$

$$T \approx \mathcal{O}\left(\frac{M^4}{\min_s \Delta(t)}\right)$$

$$\Delta(t) = E_1(t) - E_0(t)$$

$$e^{-iHt} = \left(\prod_i e^{-ih_it/s}\right)^S + \mathcal{O}(t^2/S)$$



$$\langle \Psi(\vec{\theta}) | H | \Psi(\vec{\theta}) \rangle \geq E_0,$$

$$|\Psi_{\text{ref}}\rangle = U_{\text{prep}}|\bar{0}\rangle.$$

$$U(\vec{\theta}) = U_N(\theta_N) \dots U_k(\theta_k) \dots U_1(\theta_1)$$

$$|\Psi(\vec{\theta})\rangle = U(\vec{\theta})|\Psi_{\text{ref}}\rangle$$

$$H = \sum_j h_j P_j = \sum_j h_j \prod_i \sigma_i^j,$$

$$E(\vec{\theta}_k) = \sum_j^N h_j \langle \Psi(\vec{\theta}_k) | \prod_i \sigma_i^j | \Psi(\vec{\theta}_k) \rangle.$$

$$U(\vec{\theta}) = e^{T-T^\dagger}$$

$$T = \sum_i T_i$$

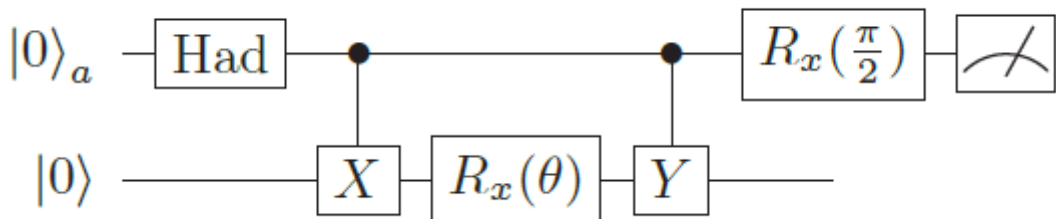
$$T_1=\sum_{i\in virt,\alpha\in occ}t_{i\alpha}a_i^\dagger a_\alpha$$

$$T_2=\sum_{i,j\in virt,\alpha,\beta\in occ}t_{ij\alpha\beta}a_i^\dagger a_j^\dagger a_\alpha a_\beta$$

$$\dots$$

$$U=\prod_s\prod_i\exp\left(\theta_i^sP_i\right)$$

$$N_m=\frac{(\sum_i|h_i|)^2}{\epsilon^2}$$



$$|\Psi\rangle=R_x(\theta)|0\rangle$$

$$E(\theta)=\langle\Psi(\theta)|H|\Psi(\theta)\rangle=\langle0|R_x^\dagger(\theta)YR_x(\theta)|0\rangle$$

$$\frac{\partial E}{\partial \theta}=\frac{i}{2}(\langle0|XR_x^\dagger(\theta)YR_x(\theta)|0\rangle-\langle0|R_x^\dagger(\theta)YR_x(\theta)X|0\rangle)$$

$$H^{\mathrm{QSE}}\mathcal{C}=S^{\mathrm{QSE}}\mathcal{C}E$$

$$H^{\mathrm{QSE}}_{ij,kl}=\langle E_0|a_ia_j^\dagger Ha_k^\dagger a_l|E_0\rangle$$

$$S^{\mathrm{QSE}}_{ij,kl}=\langle E_0|a_ia_j^\dagger a_k^\dagger a_l|E_0\rangle.$$

$$H^{ijkl}_{\alpha\beta\gamma\delta,\epsilon\zeta\eta\theta}=\langle E_0|a_\alpha a_\beta^\dagger a_\gamma a_\delta^\dagger(a_t^\dagger a_j^\dagger a_k a_l)a_\epsilon^\dagger a_\zeta a_\eta^\dagger a_\theta|E_0\rangle$$

$$H'=H+\alpha|E_0\rangle\langle E_0|,$$

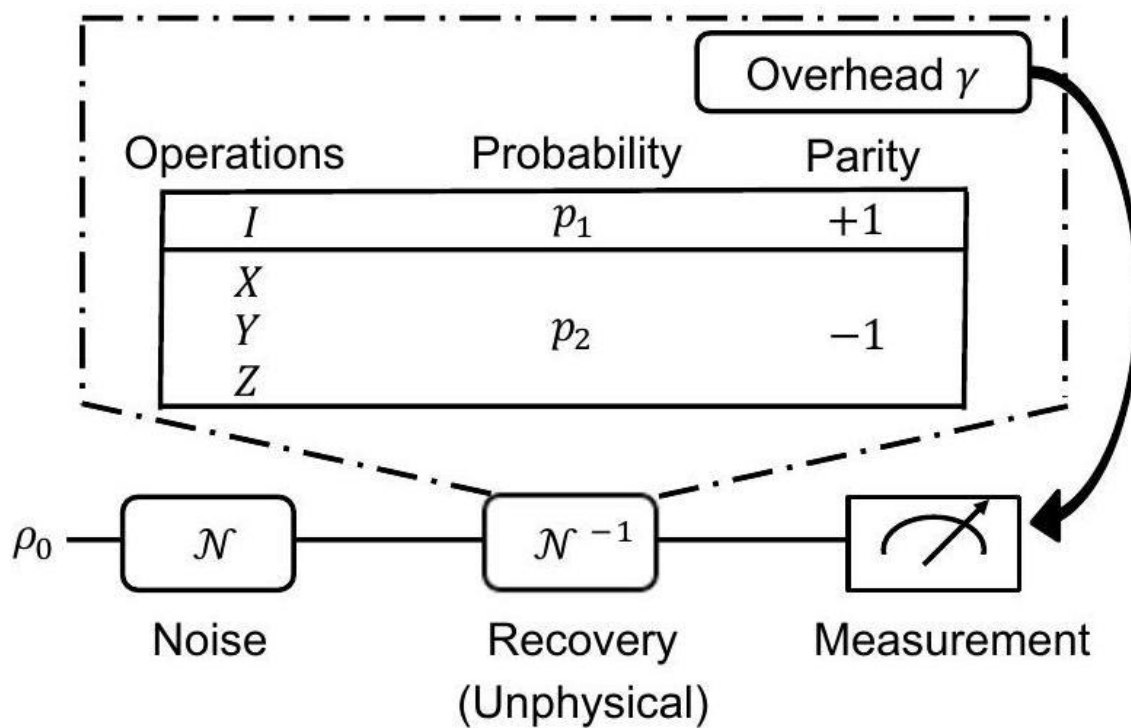
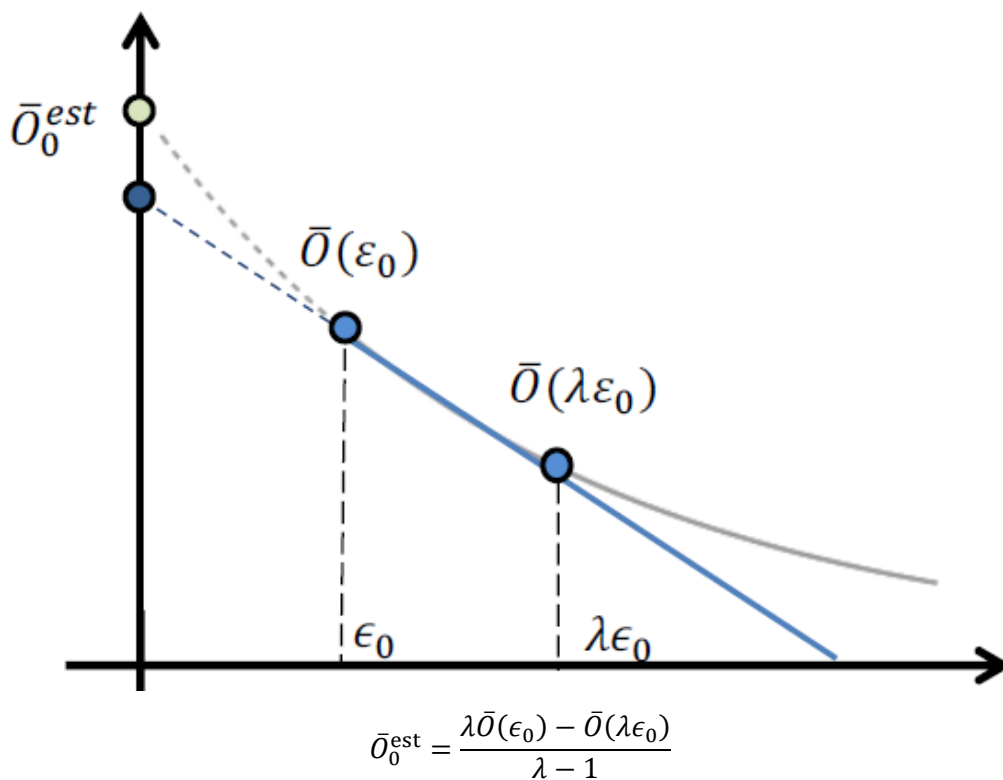
$$\mathcal{C}(\vec{\theta})=\sum_{j=0}^k\langle\phi_j|U^\dagger(\vec{\theta})HU(\vec{\theta})|\phi_j\rangle$$

$$\rho_0=\mathcal{U}_G\circ\cdots\circ\mathcal{U}_2\circ\mathcal{U}_1(|\overline{0}\rangle\langle\overline{0}|),$$

$$\rho,\mathcal{U}(\rho)=U\rho U^\dagger$$

$$\bar{O}_0=\mathrm{Tr}[\rho_0O]$$

$$\rho=\prod_i\mathcal{N}_i\circ\mathcal{U}_i(|\overline{0}\rangle\langle\overline{0}|),$$



$$\rho = \mathcal{D}(\rho_0) = \left(1 - \frac{3}{4}p\right)\rho_0 + \frac{p}{4}(X\rho_0X + Y\rho_0Y + Z\rho_0Z)$$

$$\rho_0 = \mathcal{D}^{-1}(\rho) = \gamma[p_1\rho - p_2(X\rho X + Y\rho Y + Z\rho Z)],$$

$$\gamma = (p + 2)/(2 - 2p) \geq 1, p_1 = (4 - p)/(2p + 4)$$

$$p_2 = p/(2p + 4)$$

$$\begin{aligned}\bar{O}_0 &= \text{Tr}[O\mathcal{D}^{-1}(\rho)] \\ &= \gamma[p_1\langle O \rangle_\rho - p_2(\langle O \rangle_{X\rho X} + \langle O \rangle_{Y\rho Y} + \langle O \rangle_{Z\rho Z})] \\ &= \gamma[p_1\langle O \rangle_\rho - p_2(\langle XOX \rangle_\rho + \langle YOY \rangle_\rho + \langle ZOZ \rangle_\rho)],\end{aligned}$$

$$\langle O \rangle_\rho = \text{Tr}[O\rho]$$

$$H_{ij}^{\text{QSE}} = \langle \tilde{E}_0 | P_i H P_j | \tilde{E}_0 \rangle.$$

$$S_{ij}^{\text{QSE}} = \langle \tilde{E}_0 | P_i P_j | \tilde{E}_0 \rangle$$

$$H^{\text{QSE}}C = S^{\text{QSE}}CE,$$

$$H_{\text{H}_2} = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,l} \frac{Z_l}{|\mathbf{r}_i - \mathbf{R}_l|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

$$H=\sum_{p,q}h_{pq}a_p^\dagger a_q+\frac{1}{2}\sum_{p,q,r,s}h_{pqrs}a_p^\dagger a_q^\dagger a_r a_s,$$

$$h_{pq}=\int \mathrm{d}\mathbf{x}\phi_p^*(\mathbf{x})\left(-\frac{\nabla^2}{2}-\sum_l\frac{Z_l}{|\mathbf{r}-\mathbf{R}_l|}\right)\phi_q(\mathbf{x}),$$

$$h_{pqrs}=\int \mathrm{d}\mathbf{x}_1\,\mathrm{d}\mathbf{x}_2\frac{\phi_p^*(\mathbf{x}_1)\phi_q^*(\mathbf{x}_2)\phi_r(\mathbf{x}_2)\phi_s(\mathbf{x}_1)}{|\mathbf{x}_1-\mathbf{x}_2|}$$

$$|1s_{A\uparrow}\rangle, |1s_{A\downarrow}\rangle, |1s_{B\uparrow}\rangle, |1s_{B\downarrow}\rangle,$$

$$|\sigma_{g\uparrow}\rangle=\frac{1}{\sqrt{N_g}}(|1s_{A\uparrow}\rangle+|1s_{B\uparrow}\rangle),$$

$$|\sigma_{g\downarrow}\rangle=\frac{1}{\sqrt{N_g}}(|1s_{A\downarrow}\rangle+|1s_{B\downarrow}\rangle),$$

$$|\sigma_{u\uparrow}\rangle=\frac{1}{\sqrt{N_u}}(|1s_{A\uparrow}\rangle-|1s_{B\uparrow}\rangle),$$

$$|\sigma_{u\downarrow}\rangle=\frac{1}{\sqrt{N_u}}(|1s_{A\downarrow}\rangle-|1s_{B\downarrow}\rangle),$$

$$N_g=2(1+\langle 1s_A\mid 1s_B\rangle), N_u=2(1-\langle 1s_A\mid 1s_B\rangle)$$

$$|\psi\rangle=\left|f_{\sigma_{u\downarrow}},f_{\sigma_{u\uparrow}},f_{\sigma_{g\downarrow}},f_{\sigma_{g\uparrow}}\right\rangle,$$

$$\begin{aligned}H=&h_0I+h_1Z_0+h_2Z_1+h_3Z_2+h_4Z_3\\&+h_5Z_0Z_1+h_6Z_0Z_2+h_7Z_1Z_2+h_8Z_0Z_3+h_9Z_1Z_3\\&+h_{10}Z_2Z_3+h_{11}Y_0Y_1X_2X_3+h_{12}X_0Y_1Y_2X_3\\&+h_{13}Y_0X_1X_2Y_3+h_{14}X_0X_1Y_2Y_3\end{aligned}$$

$$|\Psi_{\text{HF}}^{\text{H}_2}\rangle=|0011\rangle.$$

$$\Psi_{\text{HF}}^{\text{H}_2}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}\Big(\sigma_{g\uparrow}(\mathbf{r}_1)\sigma_{g\downarrow}(\mathbf{r}_2)-\sigma_{g\uparrow}(\mathbf{r}_2)\sigma_{g\downarrow}(\mathbf{r}_1)\Big),$$

$$|\Psi^{\text{H}_2}\rangle=\alpha|0011\rangle+\beta|1100\rangle+\gamma|1001\rangle+\delta|0110\rangle,$$

$$|\Psi_g^{H_2}\rangle = 0.9939|0011\rangle - 0.1106|1100\rangle.$$

$$U = e^{(T_1 - T_1^\dagger) + (T_2 - T_2^\dagger)}$$

$$T_1 = \sum_{i \in virt, \alpha \in occ} t_{i\alpha} a_i^\dagger a_\alpha$$

$$T_2 = \sum_{i,j \in virt, \alpha, \beta \in occ} t_{ij\alpha\beta} a_i^\dagger a_j^\dagger a_\alpha a_\beta$$

$$U = e^{t_{02}(a_2^\dagger a_0 - a_0^\dagger a_2) + t_{13}(a_3^\dagger a_1 - a_1^\dagger a_3) + t_{0123}(a_3^\dagger a_2^\dagger a_1 a_0 - a_0^\dagger a_1^\dagger a_2 a_3)}.$$

$$U = e^{t_{02}(a_2^\dagger a_0 - a_0^\dagger a_2)} \times e^{t_{13}(a_3^\dagger a_1 - a_1^\dagger a_3)} \\ \times e^{t_{0123}(a_3^\dagger a_2^\dagger a_1 a_0 - a_0^\dagger a_1^\dagger a_2 a_3)}$$

$$(a_2^\dagger a_0 - a_0^\dagger a_2) = \frac{i}{2} (X_2 Z_1 Y_0 - Y_2 Z_1 X_0)$$

$$(a_3^\dagger a_1 - a_1^\dagger a_3) = \frac{i}{2} (X_3 Z_2 Y_1 - Y_3 Z_2 X_1)$$

$$(a_3^\dagger a_2^\dagger a_1 a_0 - a_0^\dagger a_1^\dagger a_2 a_3) =$$

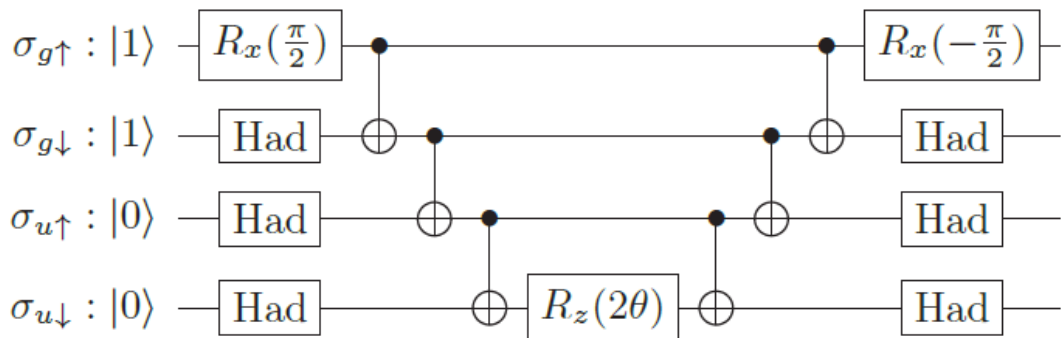
$$\frac{i}{8} (X_3 Y_2 X_1 X_0 + Y_3 X_2 X_1 X_0 + Y_3 Y_2 Y_1 X_0 + Y_3 Y_2 X_1 Y_0$$

$$- X_3 X_2 Y_1 X_0 - X_3 X_2 X_1 Y_0 - Y_3 X_2 Y_1 Y_0 - X_3 Y_2 Y_1 Y_0)$$

$$e^{t_{02}(a_2^\dagger a_0 - a_0^\dagger a_2)} = e^{\frac{it_{02}}{2} X_2 Z_1 Y_0} \times e^{\frac{-it_{02}}{2} Y_2 Z_1 X_0}.$$

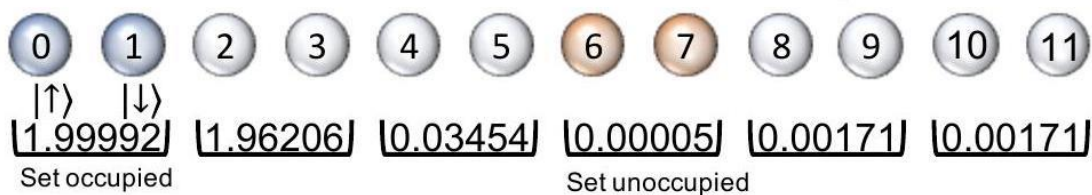
$$U = e^{-i\theta X_3 X_2 X_1 Y_0}$$

$$U|0011\rangle = (\cos(\theta)I - i\sin(\theta)X_3X_2X_1Y_0)|0011\rangle \\ = \cos(\theta)|0011\rangle - \sin(\theta)|1100\rangle$$

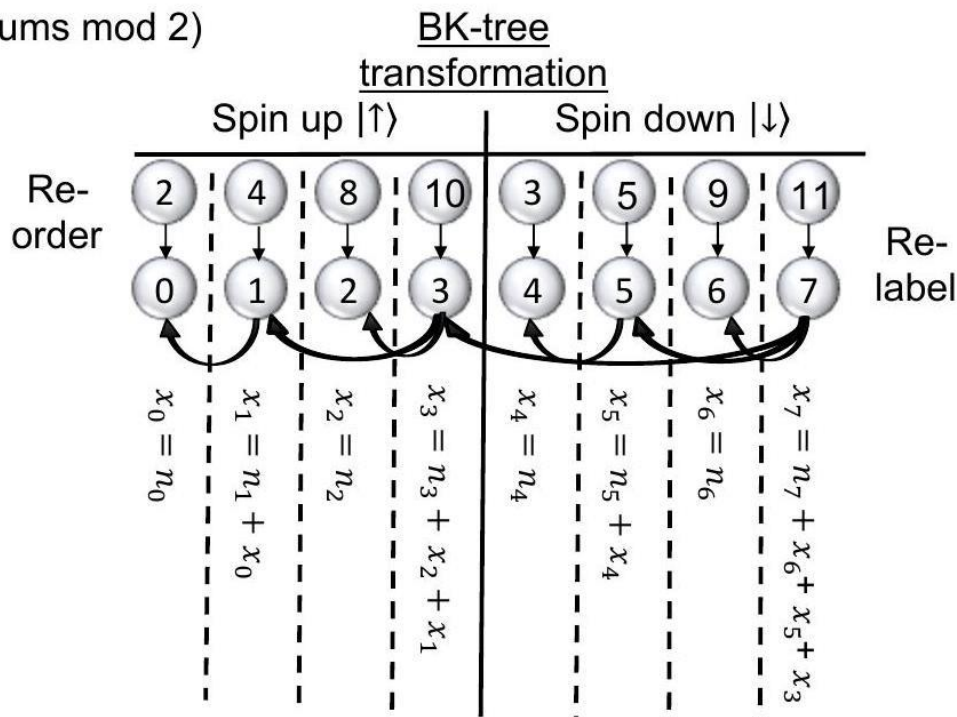


$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

Fermionic orbitals: STO-3G LiH



(All sums mod 2)



$$\begin{pmatrix} 1.9999 & -0.0005 & 0.0006 & 0.0000 & 0.0000 & -0.0010 \\ -0.0005 & 1.9598 & 0.0668 & 0.0000 & 0.0000 & 0.0084 \\ 0.0006 & 0.0668 & 0.0097 & 0.0000 & 0.0000 & -0.0138 \\ 0.0000 & 0.0000 & 0.0000 & 0.0017 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0017 & 0.0000 \\ -0.0010 & 0.0084 & -0.0138 & 0.0000 & 0.0000 & 0.0273 \end{pmatrix}$$

$$\begin{pmatrix} 1.99992 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 1.96206 & 0.00000 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.03454 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00005 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00171 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00171 & 0.00171 \end{pmatrix}$$

$$|\Psi\rangle = \sum_{i=1}^{2^n} c_i |b_i\rangle$$

$$\sum_{i=1}^L \|c_i\|^2 \geq \alpha_L \text{ and } \|c_i\|^2 \geq \beta_L \forall i \leq L$$

$$|\psi_k\rangle = e^{-ikHt} |\psi_0\rangle,$$

$$\mathbf{H}v = \tilde{E} \mathbf{S} v.$$

$$\mathbf{H}_{ij} = \langle \psi_i | H | \psi_j \rangle, \mathbf{S}_{ij} = \langle \psi_i | \psi_j \rangle$$

$$|\phi\rangle = \sum_k v_k |\psi_k\rangle \in \mathcal{K}_d$$

$$U_k(t) = \mathrm{e}^{-\mathrm{i}kHt} \langle \psi_i | H | \psi_j \rangle$$

$$|\Psi_k\rangle = \left(\prod_{j=1}^k \mathrm{e}^{-\mathrm{i}Ht}\right) |\Psi_{\mathrm{init}}\rangle = \mathrm{e}^{-\mathrm{i}Hkt} |\Psi_{\mathrm{init}}\rangle,$$

$$H=\sum_{i=1}^{\mathcal{N}}c_ih_i$$

$$V_{\boldsymbol{k}} = \prod_{j=1}^N \mathrm{e}^{-\mathrm{i}h_{k_j}t\lambda/N}$$

$$\mathcal{E}_{\text{qDRIFT}}[\rho] = \sum_k p_k V_k \rho V_k^\dagger$$

$$p_{\boldsymbol{k}} = \lambda^{-N} \prod_{i=1}^N c_{k_i}$$

$$\mathcal{U}_t[\cdot] = \mathrm{e}^{\mathrm{i}Ht}(\cdot)\mathrm{e}^{-\mathrm{i}Ht}$$

$$\{|\psi_k\rangle\} \, N_r 1 - p_{\text{fail}}\left(L,N_r,\delta\right) p_{\text{fail}}\left(L,N_r,\delta\right) > L$$

$$\tilde{E}-E_0\leq \xi$$

$$\xi = \frac{\chi}{|\gamma_0'|^2} + \frac{6||H||}{|\gamma_0'|^2} \bigg(\frac{2\chi}{\Delta'} + \zeta + 8 \bigg(1 + \frac{\pi \Delta'}{4||H||} \bigg)^{-2d+1} \bigg)$$

$$\begin{aligned}\chi &\leq 2\epsilon_Q\|H\|,\\ \zeta &\leq 2d(\epsilon_R+\epsilon_Q),\\ |\gamma_0'|^2 &\geq |\gamma_0|^2-2\epsilon_R-2\epsilon_Q,\end{aligned}$$

$$\epsilon_Q = d(d-1)t\lambda \left(\frac{t(d-1)\lambda}{N} + \sqrt{\frac{11\ln{(2^{n+1}/\delta)}}{NN_r}} \right)$$

$$|\gamma_0|^2|\psi_0\rangle\Delta'=\Delta-\chi/|\gamma_0'|^2$$

$$\Delta = E_1 - E_0$$

$$t=\pi/(E_{2^n-1}-E_0)$$

$$H=\sum_ic_ih_i$$

$$\lambda = \sum_i |c_i|$$

$$|\phi_0\rangle \text{ is } (\alpha_L^{(0)}, \beta_L^{(0)})\text{-concentrated}$$

$$\langle \tilde{\phi} | H | \tilde{\phi} \rangle - \langle \phi_0 | H | \phi_0 \rangle \leq \sqrt{8} \|H\| \left(1 - \sqrt{\alpha_L^{(0)}}\right)^{1/2}$$

$$p_{fail} \leq L((1-\delta)(1-p)^S + \delta)^{N_r}$$

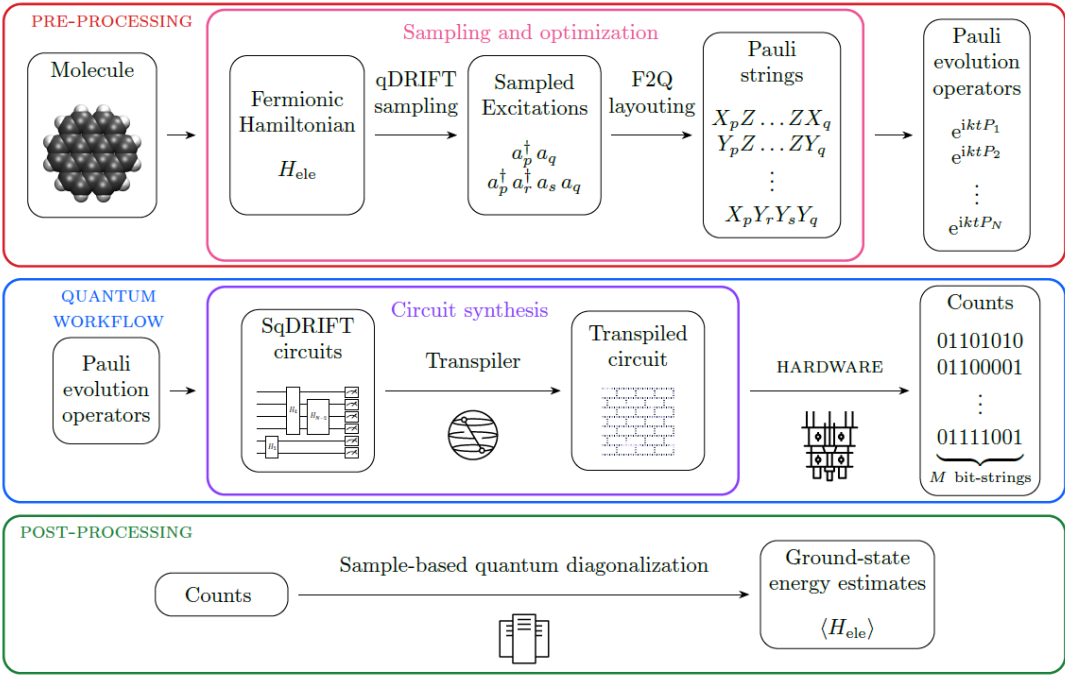
$$p=\left(\frac{|\gamma_0|\sqrt{\beta_L}}{d}-\epsilon\right)^2,$$

$$\epsilon = \frac{t^2 \lambda^2}{N} + t \lambda \sqrt{\frac{11 \ln{(2^{n+1}/\delta)}}{N}}$$

$$\beta_L = \beta_L^{(0)} - 2\sqrt{2}\sqrt{1-\sqrt{1-\xi/\Delta}}$$

$$\Delta = E_1 - E_0$$

$$t = \pi/(E_{2^{n-1}} - E_0)$$



$$\| |\psi\rangle - |\phi_0\rangle \|^2 \leq \tilde{\xi} = O\left(\frac{\xi}{\Delta E_1}\right).$$

$$|\phi_0\rangle \, (\, \alpha_L^{(0)}, \beta_L^{(0)} \, |\psi\rangle \text{ is } (\, \alpha_L, \beta_L \,)\text{-sparse}$$

$$\alpha_L = \alpha_L^{(0)} - 2\sqrt{\xi} \text{ and } \beta_L = \beta_L^{(0)} - 2\sqrt{\xi}.$$



$$|\psi^k\rangle = \sum_{j=1}^N \sqrt{p^k(b_j)} |b_j\rangle$$

$$|p^k(b_i)| \geq \frac{|\gamma_0|^2 \beta_L}{d^2}.$$

$$1-\delta, \left| \sqrt{p(b_i)} - \sqrt{\tilde{p}_{\mathbf{k}}(b_i)} \right| \leq \epsilon$$

$$\langle \left| \sqrt{p(b_i)} \sqrt{p^k(b_i)} \right| \rangle \langle \left| \sqrt{\tilde{p}_{\mathbf{k}}(b_i)} \sqrt{p(b_i)} \right| \rangle$$

$$\mathbf{k}=(k_1,\ldots,k_N)$$

$$1-\delta, \left| \sqrt{\tilde{p}_{\mathbf{k}}(b_i)} \right| \geq \frac{|\gamma_0| \sqrt{\beta_L}}{d} - \epsilon$$

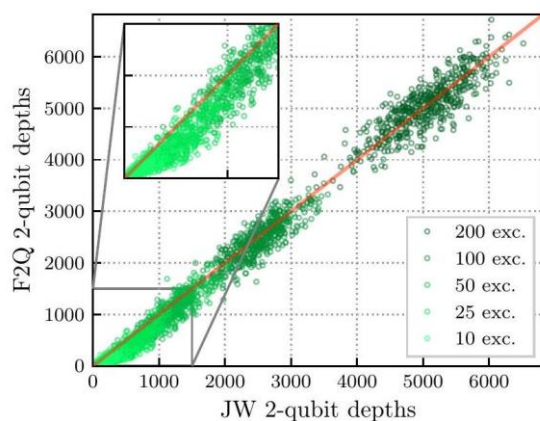
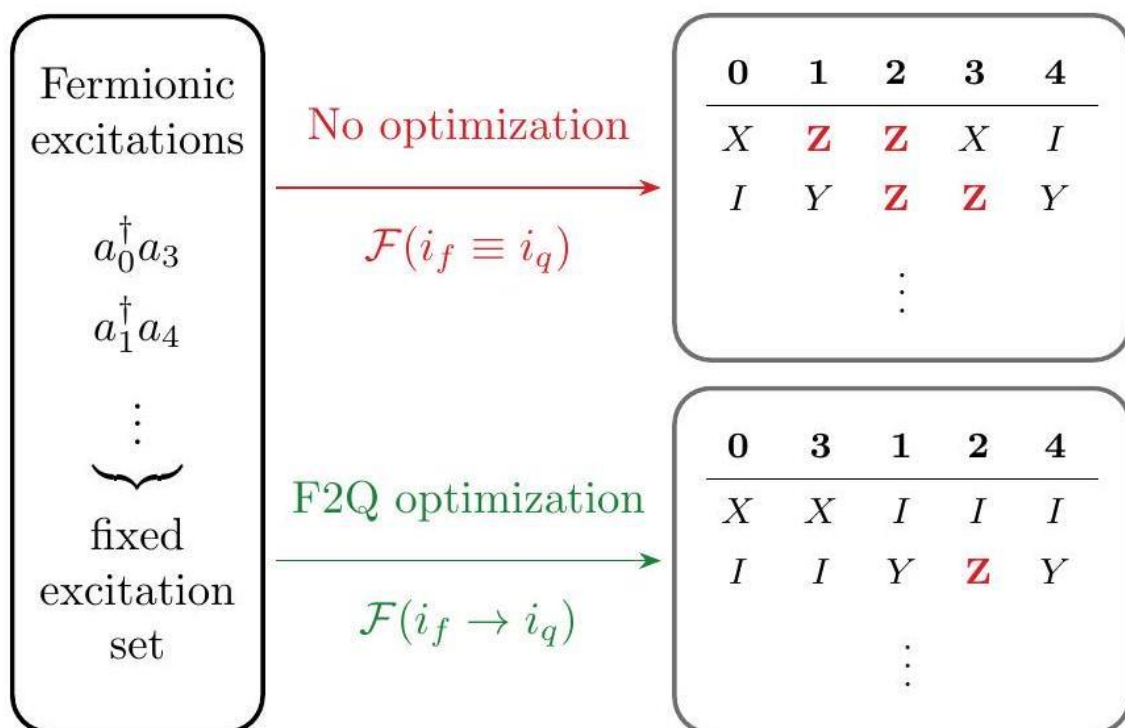
$$1-\tilde{p}_{\mathbf{k}}(b_i) \leq 1-\left(\frac{|\gamma_0| \sqrt{\beta_L}}{d} - \epsilon\right)^2 =: 1-p$$

$$p_{\text{fail}}\left(b_i\right) \leq ((1-\delta)(1-p)^S+\delta)^{N_r}.$$

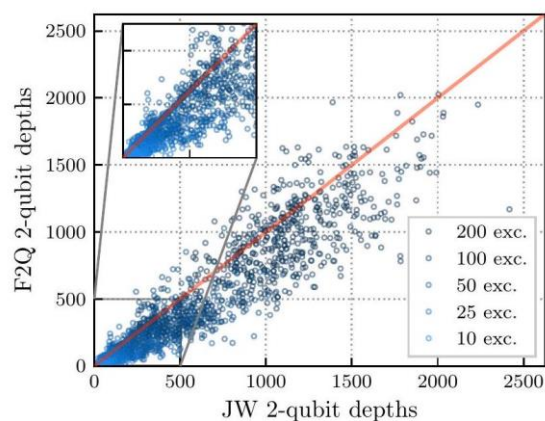
$$|\tilde{\phi}\rangle = (1/C) \sum_{j=0}^{L-1} a_j |b_j\rangle$$

$$C=\sqrt{\sum_{j=0}^{L-1}|a_j|^2}$$

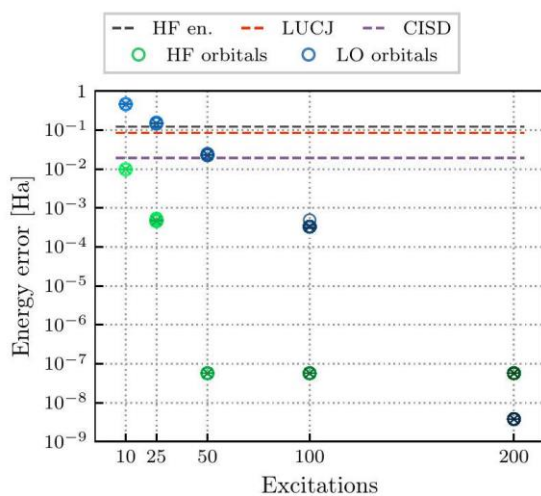
$$\begin{aligned} H_{\text{ele}} = & \sum_{pq}^{N_{\text{MO}}} \sum_{\sigma \in \{\alpha, \beta\}} h_{pq} a_{p\sigma}^{\dagger} a_{q\sigma} \\ & + \frac{1}{2} \sum_{pqrs}^{N_{\text{MO}}} \sum_{\sigma, \sigma' \in \{\alpha, \beta\}} (pq \mid rs) a_{p\sigma}^{\dagger} a_{r\sigma'}^{\dagger} a_{s\sigma'} a_{q\sigma} \end{aligned}$$



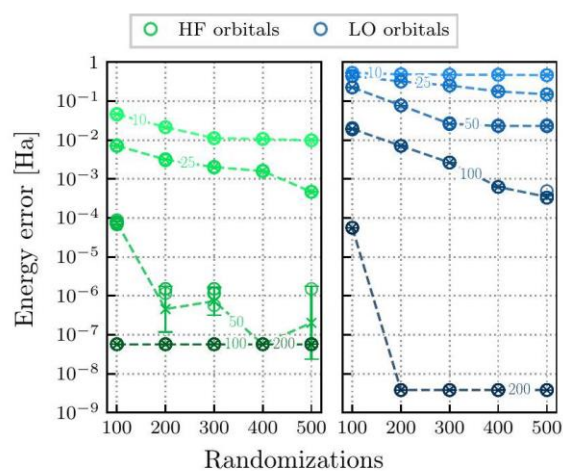
(a)



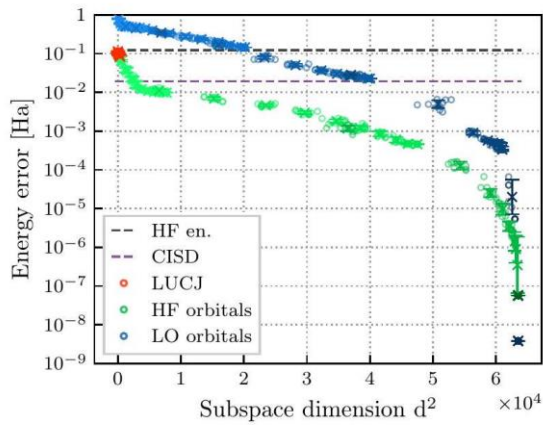
(b)



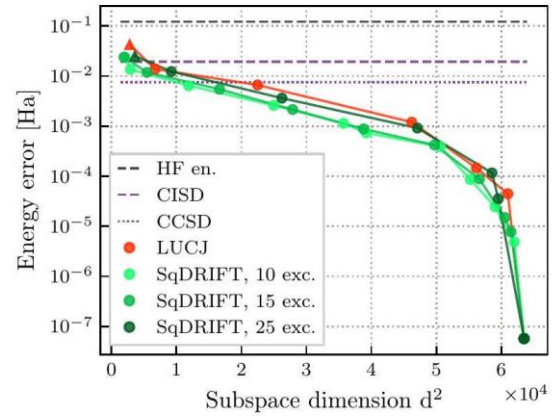
(a)



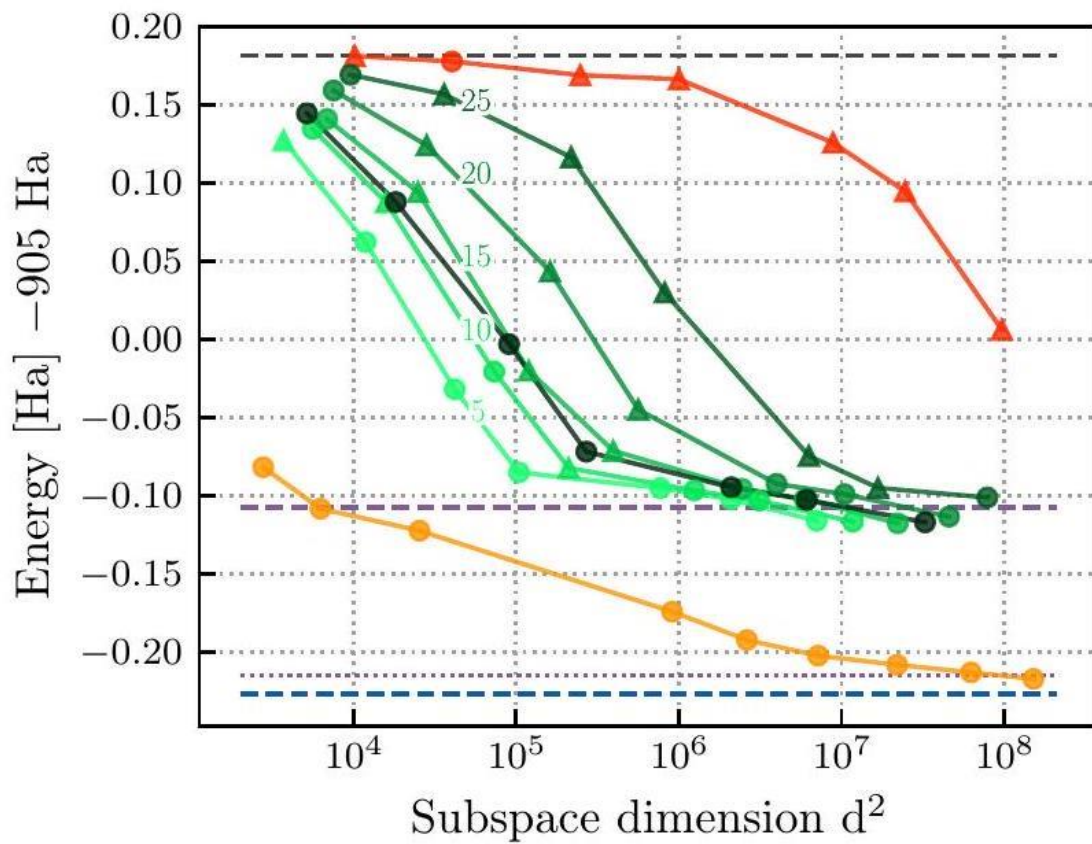
(b)



(a) Simulated results



(b) Hardware experiments



$$U^j := e^{ijHt} :: |\psi^j\rangle := U^j|\psi_0\rangle$$

$$V_{\mathbf{k}}^j: \mathbf{k} = (k_1, \dots, k_N) \blacksquare |\tilde{\psi}_{\mathbf{k}}^j\rangle := V_{\mathbf{k}}^j|\psi_0\rangle$$

$$V^j := \frac{1}{N_r} \sum_{m=1}^{N_r} V_{\mathbf{k}_m}^j: |\tilde{\psi}^j\rangle := V^j|\psi_0\rangle$$

$$\mathbb{E}[V^j] := \sum_{\mathbf{k}} p_{\mathbf{k}}^j V_{\mathbf{k}}^j: \mathbb{E}[|\tilde{\psi}^j\rangle] := \mathbb{E}[V^j]|\psi_0\rangle$$

$$|\psi_k\rangle = e^{-ikHt}|\psi_0\rangle$$

$$\tilde{E}-E_0\leq \xi$$

$$\xi=\frac{\chi}{|\gamma_0'|^2}+\frac{6\|H\|}{|\gamma_0'|^2}\left(\frac{2\chi}{\Delta'}+\zeta+8\left(1+\frac{\pi\Delta'}{4\|H\|}\right)^{-2d+1}\right)$$

$$\chi \leq 2\epsilon_Q\|H\|$$

$$\zeta \leq 2d(\epsilon_R+\epsilon_Q)$$

$$|\gamma_0'|^2\geq |\gamma_0|^2-2\epsilon_R-2\epsilon_Q$$

$$\epsilon_Q = d(d-1)t\lambda\left(\frac{2t\lambda}{N} + \sqrt{\frac{11\ln{(2^{n+1}/\delta)}}{NN_r}}\right)$$

$$\Delta'=\Delta-\chi/|\gamma_0'|^2$$

$$\Delta=E_1-E_0$$

$$t=\pi/(E_{2^n-1}-E_0)$$

$$\mathbf{v}=\left[e^{-i\frac{(d-1)}{2}Ht}|\psi_0\rangle,e^{-i\frac{(d-3)}{2}Ht}|\psi_0\rangle,\ldots,e^{i\frac{d-1}{2}Ht}|\psi_0\rangle\right]$$

$$(\mathbf{H},\mathbf{S})=(\mathbf{V}^\dagger H \mathbf{V},\mathbf{V}^\dagger \mathbf{V})$$

$$\mathbf{H}_{ij}=\langle\psi_0|U^iH U^j|\psi_0\rangle=\langle\psi_0|U^{j-i}H|\psi_0\rangle$$

$$\mathbf{S}_{ij}=\langle\psi_0|U^{j-i}|\psi_0\rangle$$

$$U^iH-\frac{(d-1)}{2}\leq i,j\leq \frac{d-1}{2}$$

$$\mathbf{H}_{ij}'=\sum_{\mathbf{k}}p_{\mathbf{k}}^{j-i}\langle\psi_0|V_{\mathbf{k}}^{j-i}H|\psi_0\rangle=\langle\psi_0|\mathbb{E}[V^{j-i}]H|\psi_0\rangle$$

$$\mathbf{S}_{ij}'=\sum_{\mathbf{k}}p_{\mathbf{k}}^{j-i}\langle\psi_0|V_{\mathbf{k}}^{j-i}|\psi_0\rangle=\langle\psi_0|\mathbb{E}[V^{j-i}]|\psi_0\rangle$$

$$\|\mathbf{H}-\mathbf{H}'\| \text{ and } \|\mathbf{S}-\mathbf{S}'\|.$$

$$\begin{aligned}\|\mathbf{S}-\mathbf{S}'\| &\leq d\|\mathbf{S}-\mathbf{S}'\|_{\max}=d\max_{i,j}|\mathbf{S}_{ij}-\mathbf{S}_{ij}'|\\ &\leq d\max_{i,j}\|U^{j-i}-\mathbb{E}[V^{j-i}]\| \end{aligned}$$

$$\|\mathbf{S}-\mathbf{S}'\|\leq d\max_{-\frac{(d-1)}{2}\leq i,j\leq \frac{d-1}{2}}\frac{((j-i)t)^2\lambda^2}{N}=d\frac{(d-1)^2t^2\lambda^2}{N}$$

$$\|V^{j-i}-\mathbb{E}[V^{j-i}]\|< t(j-i)\lambda\sqrt{\frac{11\ln{(2^{n+1}/\delta)}}{NN_r}}.$$

$$\|\mathbf{S}-\mathbf{S}''\|\leq d(d-1)t\lambda\left(\frac{t(d-1)\lambda}{N}+\sqrt{\frac{11\ln{(2^{n+1}/\delta)}}{NN_r}}\right)=:\epsilon_Q$$

$$\|\mathbf{H}-\mathbf{H}'\|\mid \langle \psi_0\mid (U^j-\mathbb{E}[V^j])H\mid \psi_0\rangle\mid \leq \|U^j-\mathbb{E}[V^j]\|\cdot\|H\|$$

$$\|\mathbf{H}-\mathbf{H}''\|\leq \epsilon_Q\|H\|$$

$$\chi:=\|\mathbf{H}-\mathbf{H}'\|+\|\mathbf{S}-\mathbf{S}'\|\cdot\|H\|\leq 2\epsilon_Q\|H\|,$$

$$\zeta:=2d(\epsilon_R+\|\mathbf{S}-\mathbf{S}'\|)\leq 2d(\epsilon_R+\epsilon_Q),$$

$$|\gamma_0'|^2:=|\gamma_0|^2-2\epsilon_R-2\|\mathbf{S}-\mathbf{S}'\|\geq |\gamma_0|^2-2\epsilon_R-2\epsilon_Q,$$

$$|\gamma_0|^2\geq 2\|\mathbf{S}-\mathbf{S}'\|$$

$$\| |\psi\rangle-|\phi_0\rangle\|^2\leq \tilde{\xi}=o\left(\frac{\xi}{\Delta E_1}\right)$$

$$|\phi_0\rangle\,(\,\alpha_L^{(0)},\beta_L^{(0)}\,)|\psi\rangle\,(\,\alpha_L,\beta_L\,)\text{-sparse}$$

$$\alpha_L=\alpha_L^{(0)}-2\sqrt{\tilde{\xi}}\text{ and }\beta_L=\beta_L^{(0)}-2\sqrt{\tilde{\xi}}$$

$$|\psi^k\rangle=\sum_{j=1}^N\sqrt{p^k(b_j)}|b_j\rangle$$

$$|p^k(b_i)|\geq \frac{|\gamma_0|^2\beta_L}{d^2}$$

$$V_{\mathbf{k}}^k\rightarrow V_{\mathbf{k}}, V^k\rightarrow V\text{ and }p_{\mathbf{k}}^k\rightarrow p_{\mathbf{k}}$$

$$1-\delta,\left|\sqrt{p(b_i)}-\sqrt{\tilde{p}_{\mathbf{k}}(b_i)}\right|\leq \epsilon$$

$$\epsilon=\frac{t^2\lambda^2}{N}+t\lambda\sqrt{\frac{11\ln{(2^{n+1}/\delta)}}{N}}$$

$$\sqrt{\tilde{p}_{\mathbf{k}}(b_i)}\sqrt{p(b_i)}\left|\sqrt{p(b_i)}-\sqrt{\tilde{p}_{\mathbf{k}}(b_i)}\right|$$

$$\left|\sqrt{p(b_i)}-\sqrt{\tilde{p}_{\mathbf{k}}(b_i)}\right|\leq \| |\psi\rangle-|\tilde{\psi}_{\mathbf{k}}\rangle\|\leq \|U-V_{\mathbf{k}}\|$$

$$\|U-V_{\mathbf{k}}\|\leq \|U-\mathbb{E}[V]\|+\|\mathbb{E}[V]-V_{\mathbf{k}}\|$$

$$\|U-\mathbb{E}[V]\|\leq \frac{t^2\lambda^2}{N}$$

$$\|V_{\mathbf{k}}-\mathbb{E}[V]\|< t\lambda\sqrt{\frac{11\ln{(2^{n+1}/\delta)}}{N}}$$

$$\left|\sqrt{p(b_i)}-\sqrt{\tilde{p}_{\mathbf{k}}(b_i)}\right|1-\delta$$

$$\left| \sqrt{p(b_i)} - \sqrt{\tilde{p}_{\mathbf{k}}(b_i)} \right| \leq \frac{t^2 \lambda^2}{N} + t \lambda \sqrt{\frac{11 \ln(2^{n+1}/\delta)}{N}}$$

$$1-\delta, \left| \sqrt{\tilde{p}_{\mathbf{k}}(b_i)} \right| \geq \frac{|\gamma_0| \sqrt{\beta_L}}{d} - \epsilon$$

$$1-\tilde{p}_{\mathbf{k}}(b_i) \leq 1-\left(\frac{|\gamma_0| \sqrt{\beta_L}}{d}-\epsilon\right)^2 =: 1-p$$

$$\frac{1}{N_r S} \sum_{l=1}^{N_r} \sum_{s=1}^S \left[V_{\mathbf{k}_l} \rho V_{\mathbf{k}_l}^\dagger\right] = \frac{1}{N_r} \sum_{l=1}^{N_r} \left[V_{\mathbf{k}_l} \rho V_{\mathbf{k}_l}^\dagger\right] = \mathcal{E}(t;N,N_r)$$

$$\mathbb{P}[X(b_i)=1]=\sum_{\mathbf{k}}p_{\mathbf{k}}\tilde{p}_{\mathbf{k}}(b_i)$$

$$p_{\text{fail}}(b_i) \mathop{:}= \mathbb{P}[X(b_i)=0] = \left(\sum_{\mathbf{k}} p_{\mathbf{k}} (1-\tilde{p}_{\mathbf{k}}(b_i))^S\right)^{N_r}$$

$$\sum_{\mathbf{k}} p_{\mathbf{k}} = 1$$

$$p_{\text{fail}}(b_i) \leq ((1-\delta)(1-p)^S + \delta)^{N_r}$$

$$|\tilde{\phi}\rangle=(1/C)\sum_{j=0}^{L-1}a_j|b_j\rangle$$

$$C=\sqrt{\sum_{j=0}^{L-1}|a_j|^2}$$

$$\langle \tilde{\phi} | H | \tilde{\phi} \rangle - \langle \phi_0 | H | \phi_0 \rangle \leq \sqrt{8} \| H \| \left(1 - \sqrt{\alpha_L^{(0)}} \right)^{1/2}$$

# exc.	mean	std. dev.	min	25%	median	75%	max	# exc.	mean	std. dev.	min	25%	median	75%	max
10	69.40	68.74	2.00	23.00	45.50	96.25	450.00	10	112.85	116.37	4.00	35.00	72.00	152.00	855.00
15	140.22	117.45	4.00	51.75	104.00	199.25	684.00	15	246.46	217.23	12.00	91.75	174.00	349.25	1420.00
25	354.71	221.90	19.00	186.00	315.50	490.00	1200.00	25	691.73	467.31	49.00	341.00	591.00	928.25	2499.00

(a) Two-qubit gate depths

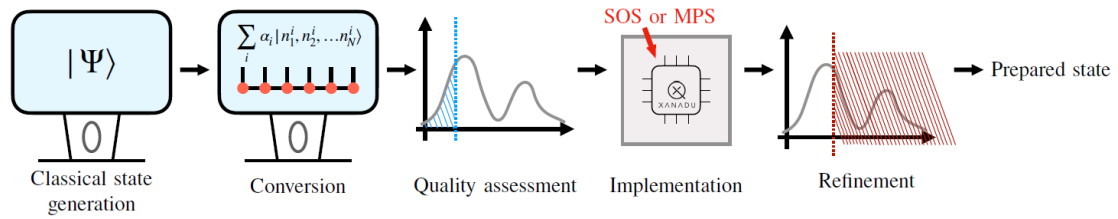
(b) Two-qubit gate counts

# exc.	mean	std. dev.	min	25%	median	75%	max	# exc.	mean	std. dev.	min	25%	median	75%	max
5	39.95	37.61	0.00	15.00	26.00	56.00	303.00	5	68.26	61.13	0.00	28.00	49.00	92.25	481.00
10	114.50	96.23	2.00	48.00	84.50	151.00	560.00	10	231.10	196.34	7.00	99.75	175.00	293.00	1332.00
15	253.50	193.00	6.00	108.00	200.00	349.00	1456.00	15	570.42	455.03	20.00	247.75	438.50	757.75	3165.00
20	499.83	328.37	13.00	237.00	441.00	701.00	2029.00	20	1257.57	921.03	39.00	553.50	1007.00	1720.25	5492.00
25	891.80	557.08	57.00	472.00	786.50	1194.25	3259.00	25	2450.08	1698.26	123.00	1151.50	2059.50	3246.25	9485.00

(a) Two-qubit gate depths

(b) Two-qubit gate counts





$$|\psi_{\text{Slater}}\rangle = |n_1, n_2, \dots, n_N\rangle \text{ or } |n_1, n_2, \dots, n_{2N}\rangle.$$

$$|\psi_{\text{CISD}}\rangle = |\text{HF}\rangle + \sum_i c_i |S_i\rangle + \sum_i d_i |D_i\rangle,$$

$$|\psi_{\text{CCSD}}\rangle = e^{\hat{T}_1 + \hat{T}_2} |\text{HF}\rangle,$$

$$|\psi_{\text{CASCI}}\rangle = \sum_{n_l, n_{l+1}, \dots, n_L} c_{n_l, n_{l+1}, \dots, n_L} |2, \dots, 2, n_l, n_{l+1}, \dots, n_L, 0, \dots, 0\rangle$$

$$|\psi_{\text{SCI}}\rangle = \sum_{n_1, n_2, \dots, n_N} c_{n_1, n_2, \dots, n_N} |n_1, n_2, \dots, n_N\rangle,$$

$$|\psi_{\text{MPS}}\rangle = \sum_{\substack{\alpha_1, \dots, \alpha_{N-1} \\ n_1, \dots, n_N}} A_{1; \alpha_1}^{n_1} A_{2; \alpha_1 \alpha_2}^{n_2} \dots A_{N; \alpha_{N-1}}^{n_N} |n_1, n_2, \dots, n_N\rangle$$

$$n_i \in \{0, \alpha, \beta, 2\}, \alpha_i \leq \chi$$

$$|\psi\rangle = \sum_{i=1}^D \alpha_i |v_i\rangle,$$

$$|v_i\rangle = |n_{i,1} n_{i,2} \cdots n_{i,2N}\rangle$$

$$b_i := (u_1 \cdot \tilde{v}_i, \dots, u_{2\log D-1} \cdot \tilde{v}_i)$$

$$\begin{pmatrix} u_1^T \\ \vdots \\ u_{2\log D-1}^T \end{pmatrix} (\tilde{v}_1 \quad \cdots \quad \tilde{v}_D) = (b_1 \quad \cdots \quad b_D),$$

$$\sum_{i=1}^D \alpha_i |0\rangle |i\rangle |0\rangle,$$

$$O|0\rangle|i\rangle|0\rangle = |v_i\rangle|i\rangle|0\rangle.$$

$$\sum_{i=1}^D \alpha_i |v_i\rangle |i\rangle |0\rangle.$$

$$\begin{aligned} & \sum_{i=1}^D \alpha_i |v_i\rangle |i\rangle (|u_1 \cdot \tilde{v}_i\rangle |0\rangle) \\ &= \sum_{i=1}^D \alpha_i |v_i\rangle |i\rangle (|b_{i,1}\rangle |0\rangle) \end{aligned}$$

$$\sum_{i=1}^D \alpha_i |v_i\rangle |i\rangle |b_i\rangle,$$

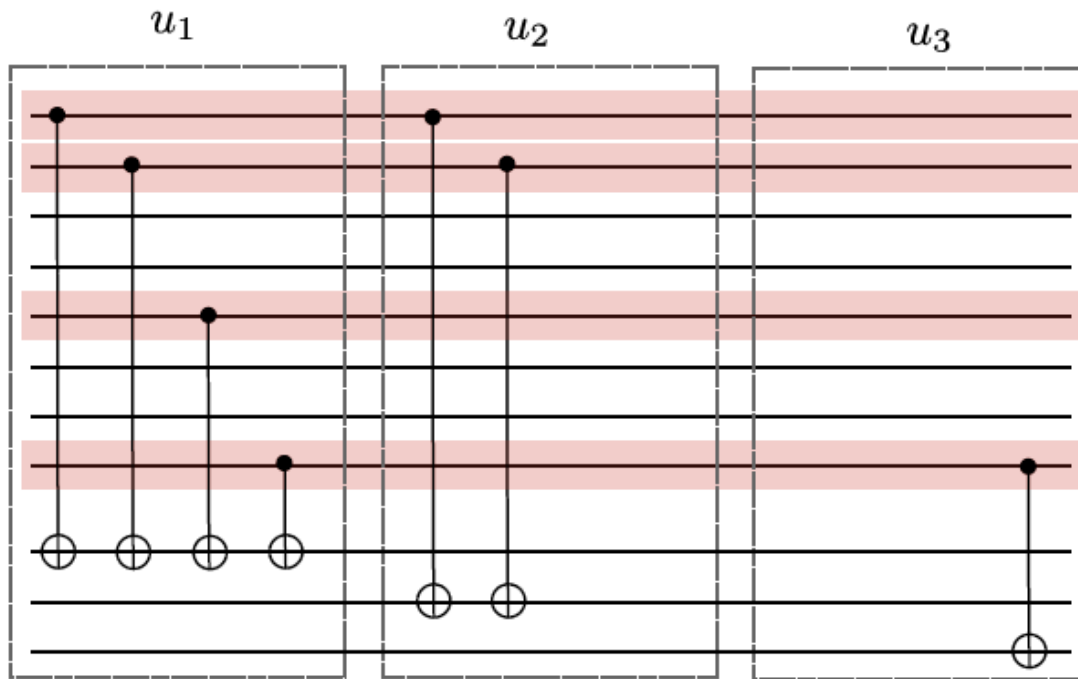
$$\sum_{i=1}^D \alpha_i |v_i\rangle |0\rangle |b_i\rangle.$$

$$\sum_{i=1}^D \alpha_i |v_i\rangle |0\rangle |0\rangle,$$

$$(2\log D - 2)D + 2^{\log D+1} + D < (2\log D + 3)D = O(D\log D)$$

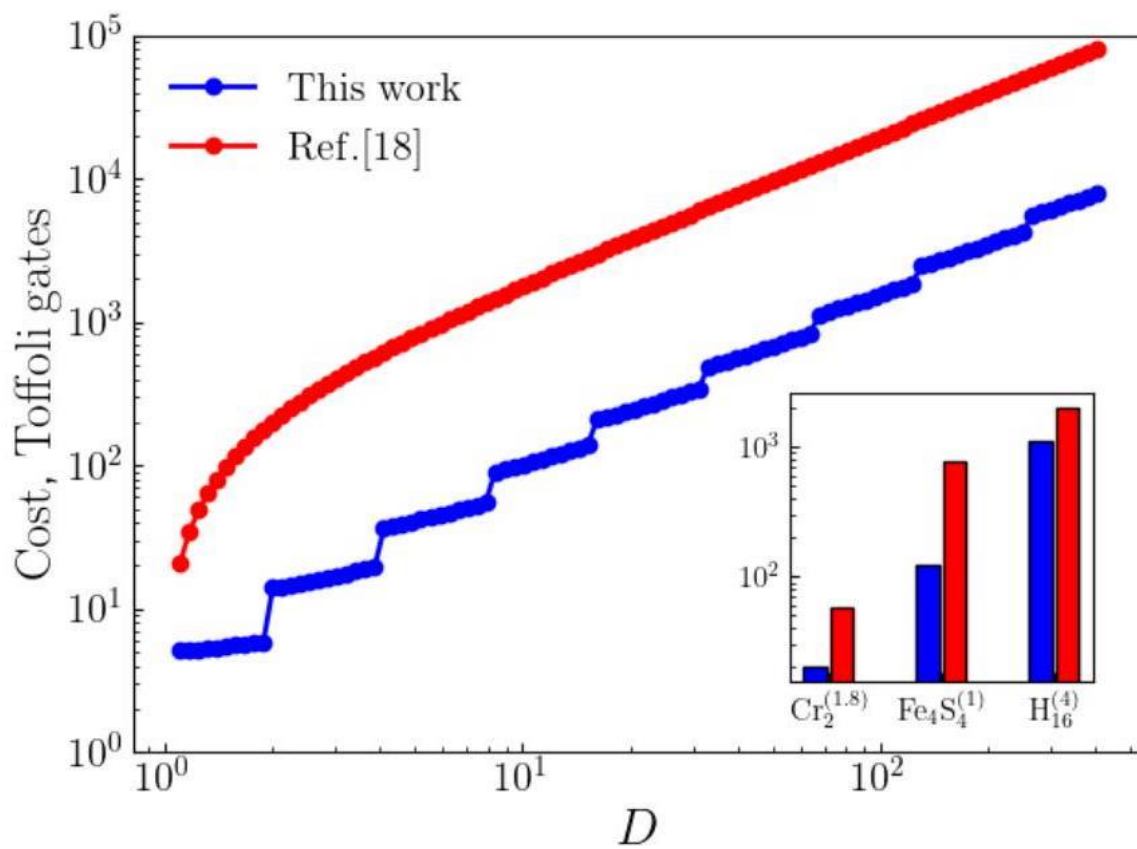
$$\begin{array}{c} \nu_1 \ \nu_2 \ \nu_3 \ \nu_4 \\ \left(\begin{array}{cccc} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array} \right) \end{array} \longrightarrow \begin{array}{c} \tilde{\nu}_1 \ \tilde{\nu}_2 \ \tilde{\nu}_3 \ \tilde{\nu}_4 \\ \left(\begin{array}{cccc} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right) \end{array}$$

$$\begin{array}{c} u_1 \\ u_2 \\ u_3 \end{array} \left(\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right) \begin{array}{c} \tilde{\nu}_1 \ \tilde{\nu}_2 \ \tilde{\nu}_3 \ \tilde{\nu}_4 \\ \left(\begin{array}{cccc} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{array} \right) \end{array} = \begin{array}{c} b_1 \ b_2 \ b_3 \ b_4 \\ \left(\begin{array}{cccc} 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array} \right) \end{array}$$

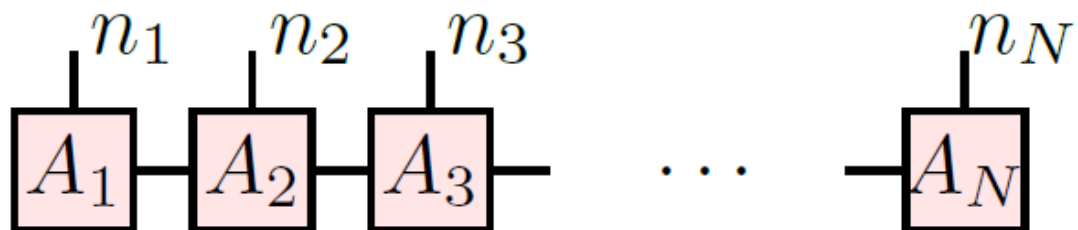


$$4\log D - 3 + \log D = 5\log D - 3 = O(\log D).$$

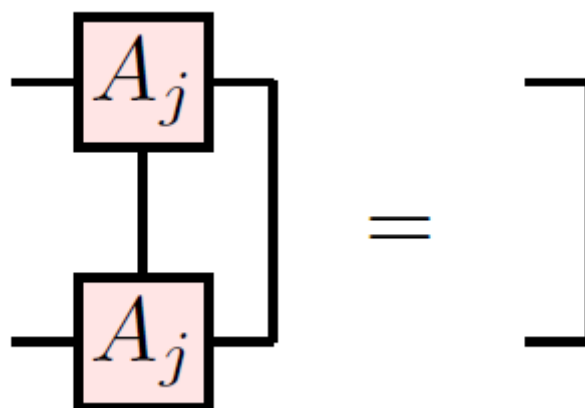
$$\min(2\sqrt{32ND}, D) + (7\log D + 2\sqrt{32\log D})\sqrt{D}$$



$$A_{j; \alpha_{j-1} \alpha_j}^{n_j} = \alpha_{j-1} - \boxed{A_j} - \alpha_j \quad \begin{array}{c} | \\ n_j \end{array}$$

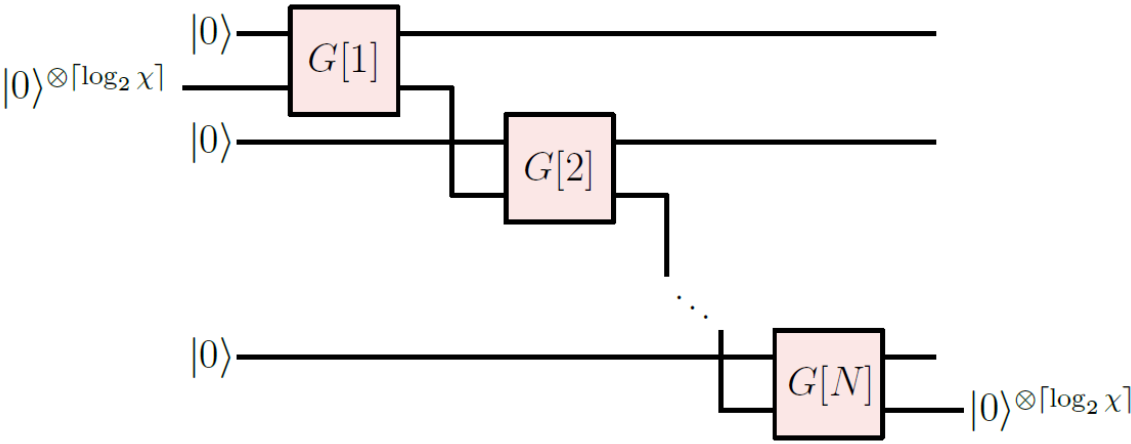


$$\sum_{\alpha_j, n_j} A_{j; \alpha_{j-1} \alpha_j}^{n_j} \left(A_{j; \alpha'_{j-1} \alpha_j}^{n_j} \right)^* = \delta_{\alpha_{j-1} \alpha'_{j-1}},$$



$$G[j]_{\alpha_j n_j, \alpha_{j-1} 0} = A_{j; \alpha_{j-1} \alpha_j}^{n_j},$$

$$\alpha_{j-1} - \boxed{A_j} - \alpha_j \quad \begin{array}{c} | \\ n_j \end{array} \quad \rightarrow \quad \begin{array}{c} 0 \\ \alpha_{j-1} \end{array} - \boxed{G[j]} - \begin{array}{c} n_j \\ \alpha_j \end{array}.$$

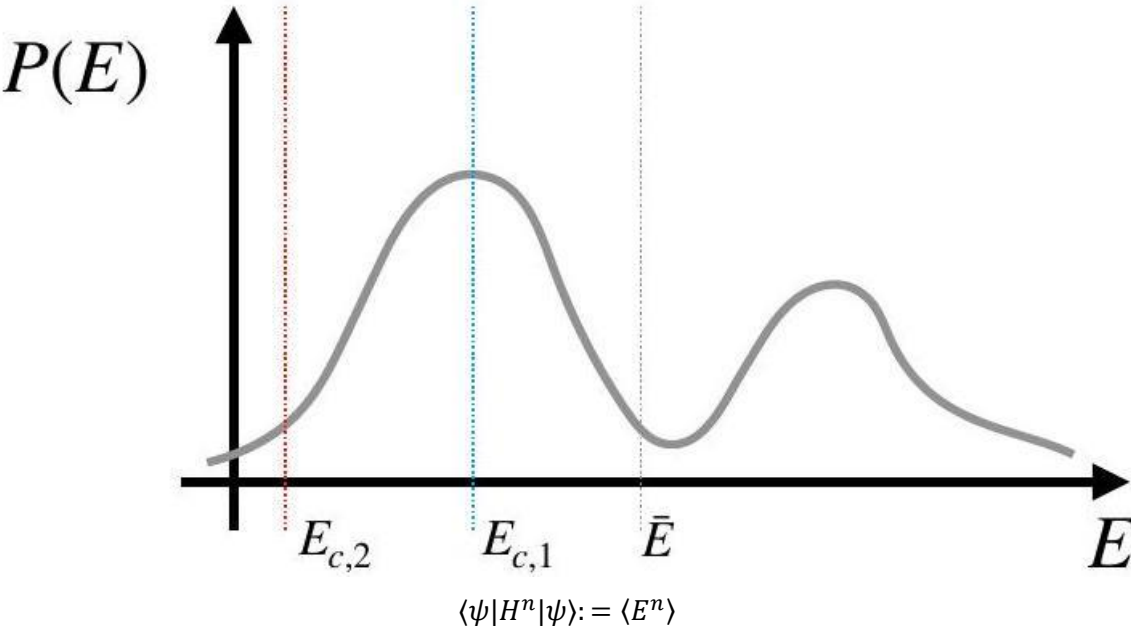


$$\chi_{j-1}[8\chi_j d + (b+1)\log(\chi_j d)]$$

$$P(E)=\sum_n|\langle E_n|\psi\rangle|^2f_{\eta}(E_n-E),$$

$$\sum_n|\langle E_n|\psi\rangle|^2\frac{1}{2^{2k}}\bigg(\frac{\sin^2\left(\pi2^kE_n\right)}{\sin^2\left(\pi\left[E_n-x_m/2^k\right]\right)}\bigg).$$

$$\frac{1}{2^{2k}}\bigg(\frac{\sin^2\left(\pi2^kE_n\right)}{\sin^2\left(\pi\left[E_n-x_m/2^k\right]\right)}\bigg)$$



order	Gram-Charlier coefficient
3	$-\frac{1}{3!}\mu_3$
4	$\frac{1}{4!}[\mu_4 - 3]$
5	$\frac{1}{5!}[-\mu_5 + 10\mu_3]$
6	$\frac{1}{6!}[\mu_6 - 15\mu_4 + 30]$
7	$\frac{1}{7!}[-\mu_7 + 21\mu_5 - 105\mu_3]$
8	$\frac{1}{8!}[\mu_8 - 28\mu_6 + 210\mu_4 - 315]$

$$\tilde{P}(E) = \frac{\exp(-E^2/2)}{\sqrt{2\pi}} \left[1 + \sum_{n=3}^{\infty} (-1)^n c_n He_n(E) \right],$$

$$He_n(E) = (-1)^n \exp(E^2/2) \frac{d^n}{dE^n} \exp(-E^2/2)$$

$$c_n = \frac{(-1)^n}{n!} \int dE P(E) He_n(E)$$

$$\mu_n = \int dE P(E) E^n = \langle E^n \rangle$$

$$\begin{aligned} \tilde{P}(E) = & \frac{\exp(-x^2/2)}{\sqrt{2\pi}} \left[1 + \frac{\kappa_3}{6} He_3(E) \right. \\ & \left. + \left(\frac{\kappa_4}{24} He_4(E) + \frac{\kappa_3^2}{72} He_6(E) \right) + \dots \right] \end{aligned}$$

$$P(E, \eta) = -\text{Im} G(E, \eta)$$

$$G(E, \eta) = \frac{1}{\pi} \langle \psi | \frac{1}{H - E + i\eta} | \psi \rangle$$

$$P(E, \eta) = -\frac{1}{\pi} \sum_n |\langle E_n | \psi \rangle|^2 \text{Im} \left(\frac{1}{E_n - E + i\eta} \right),$$

$$\text{Im} \frac{1}{E_n - E + i\eta} = \frac{-\eta}{(E_n - E)^2 + \eta^2}$$

$$\begin{aligned} |\varphi\rangle &= \frac{1}{\pi} \frac{1}{(H - E + i\eta)} |\psi\rangle, \\ \Rightarrow \pi(H - E + i\eta)|\varphi\rangle &= |\psi\rangle. \end{aligned}$$

$$[(H-E)^2+\eta^2]|Y\rangle=-\frac{\eta}{\pi}|\psi\rangle.$$

$$\mathrm{Im}G=\langle\psi\mid Y\rangle$$

$$\langle Y|[(H-E)^2+\eta^2]|Y\rangle+\frac{\eta}{\pi}\langle Y\mid\psi\rangle.$$

$$f(E)=\frac{1}{2^{2k}}\frac{\sin^2\left(\pi 2^kE\right)}{\sin^2\left(\pi E\right)}$$

$$\begin{array}{l} |\psi_0\rangle\!=\!0.86|2,2,2,0,0,0\rangle\\ \qquad\!-0.36(|\beta,2,\alpha,\alpha,0,\beta\rangle+|\alpha,2,\beta,\beta,0,\alpha\rangle) \end{array}$$

$$\tilde{P}(x_m)=\int\,dEP(E)\frac{1}{2^{2k}}\Bigg(\frac{\sin^2\left(\pi 2^kE\right)}{\sin^2\left(\pi [E-x_m/2^k]\right)}\Bigg)$$

$$P(E_o)=\tilde{P}(x_m)/2^{-k}$$

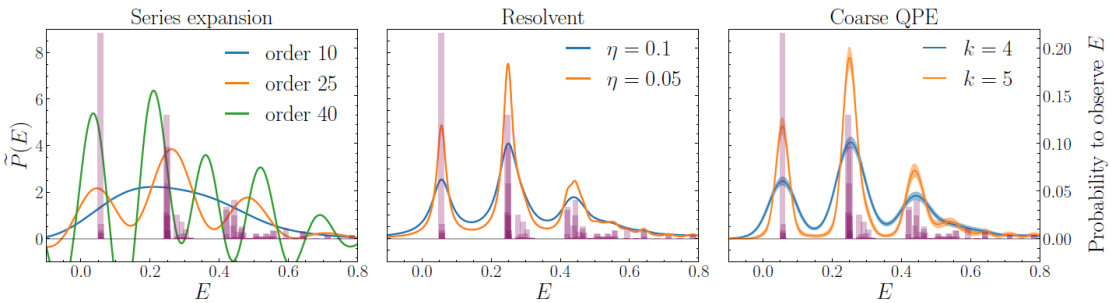
$$E_{\min,K}=\min\big(E^{(1)},\ldots,E^{(K)}\big)$$

$$C_{\min,N}(E)=1-(1-p_{<}(E))^K.$$

$$p_{<}(E)=\int_{-\infty}^E dE' P(E')$$

$$P_K(E)=KP(E)(1-p_{<}(E))^{K-1}$$

$$\int\,dEP_K(E)E$$



$$|\psi\rangle=\sum_n c_n|E_n\rangle$$

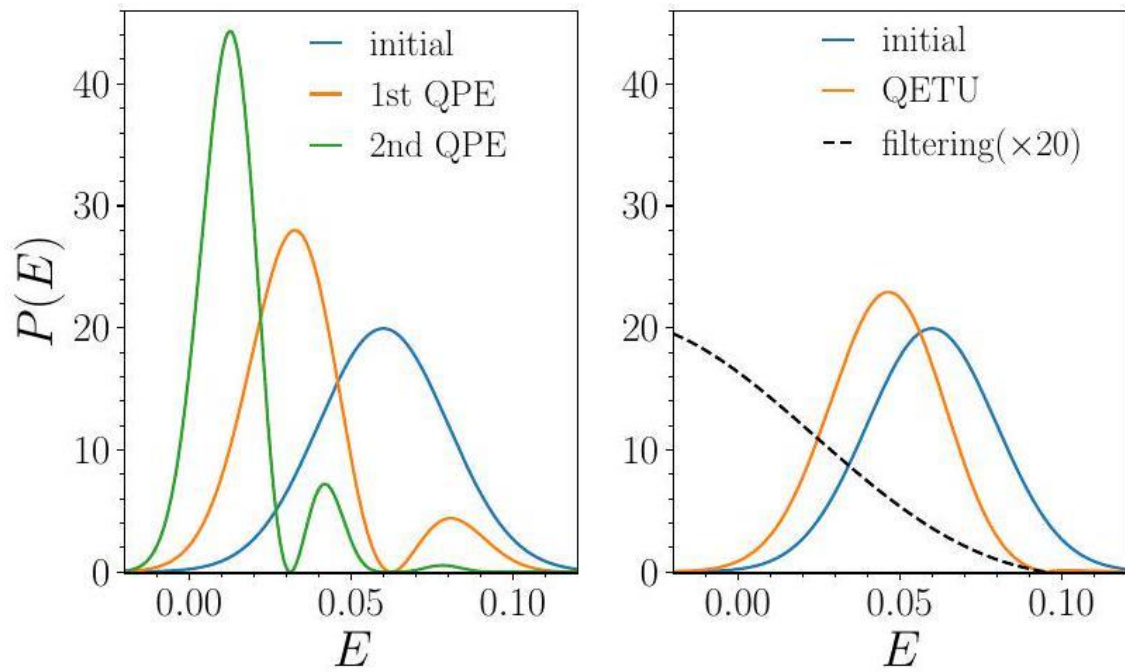
$$P(n)=|c_n|^2\frac{1}{2^{2k}}\Bigg(\frac{\sin^2\left(\pi 2^kE_n\right)}{\sin^2\left(\pi [E_n-x_m/2^k]\right)}\Bigg).$$

$$\sim \left|2^kE-x_m\right|^{-2}$$

$$f(H)=P(\cos\left(H/2\right))$$

$$U=e^{-iH}$$

$$O(\Gamma^{-1}\log\epsilon^{-1})$$



$$|\psi\rangle = \sum_n c_n |E_n\rangle$$

$$p_{\text{leak}} = \sum_{n \neq 0} \sum_{x_j < x_{\text{upper}}} \frac{1}{2^{2k}} \left(\frac{\sin^2(\pi \delta_n)}{\sin^2\left(\frac{\pi}{2^k} [x_n + \delta_n - x_j]\right)} \right),$$

$$x_{\text{upper}} = \lceil 2^k (E_0 - \epsilon) \rceil, 2^k E_n = x_n + \delta_n$$

$$O\left(\max\left[2^{-2k}, (x_n - x_{\text{upper}})^{-2}\right]\right)$$

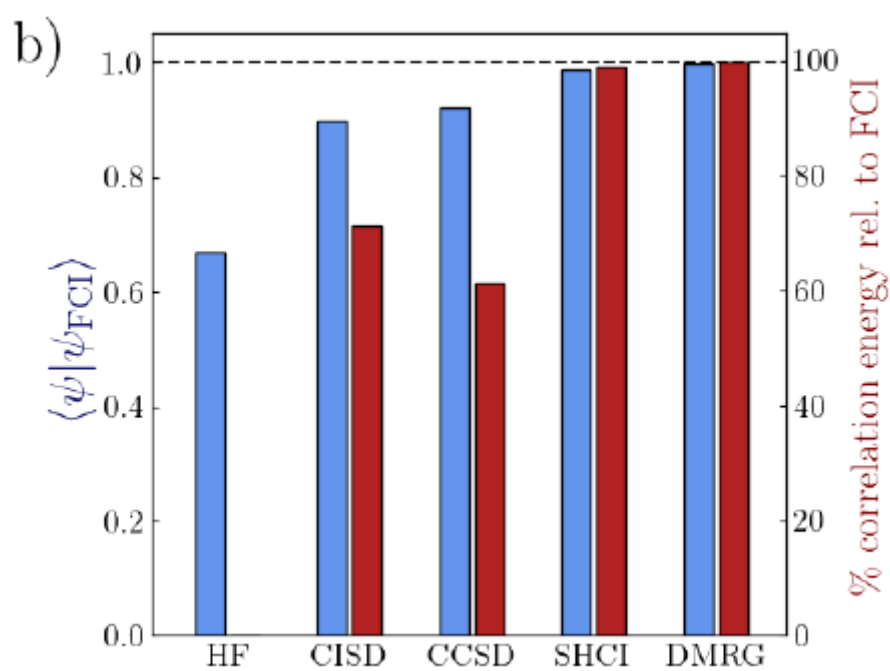
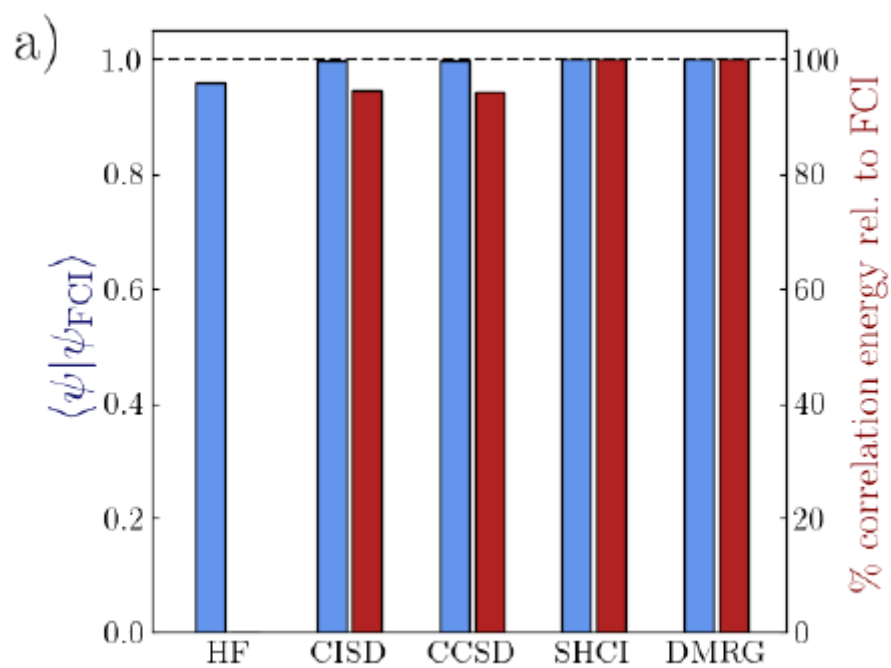
$$p_{\text{leak}}(E_n) = \frac{\sin^2(\pi \delta_n)}{\pi^2} \frac{1}{x_n - x_{\text{upper}} + \delta_n}.$$

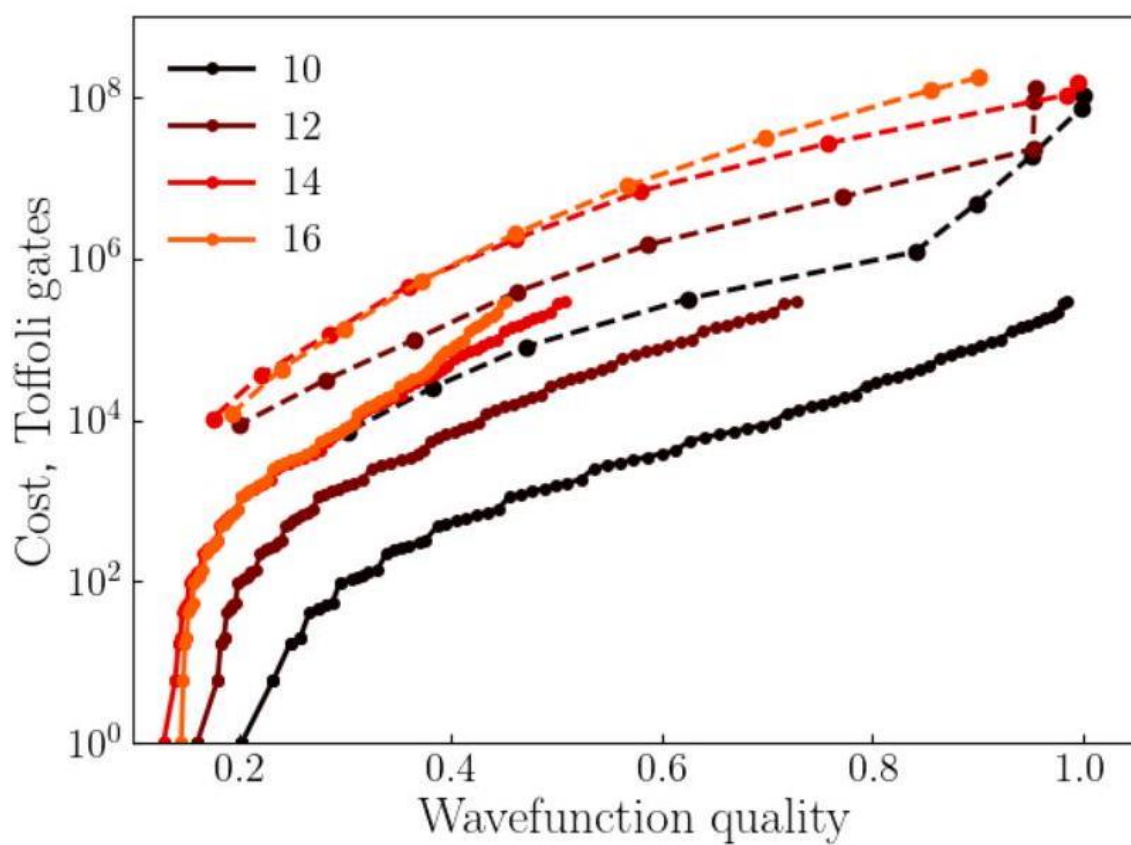
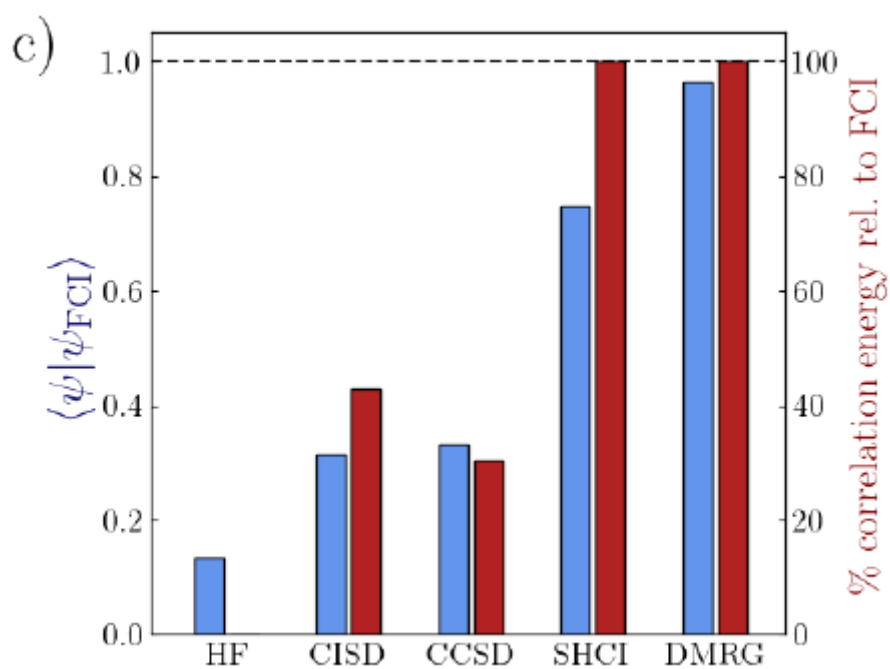
$$p_{\text{leak}} = \frac{1}{\pi^2 2^k} \int_{E_0 + \epsilon} dE P(E) \frac{\sin^2(\pi 2^k E)}{E - \frac{x_{\text{upper}}}{2^k}}$$

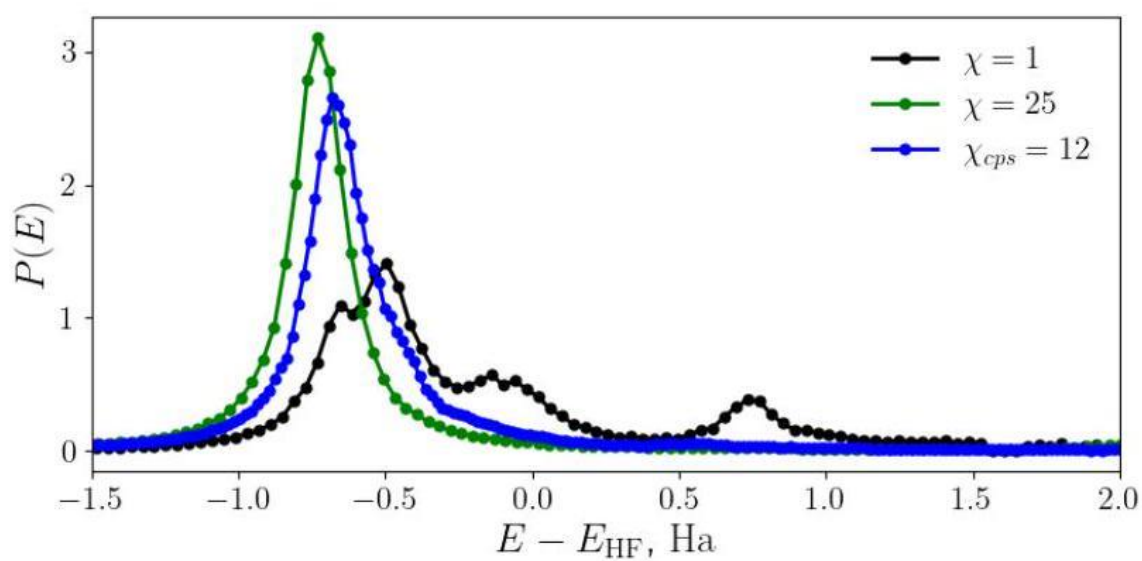
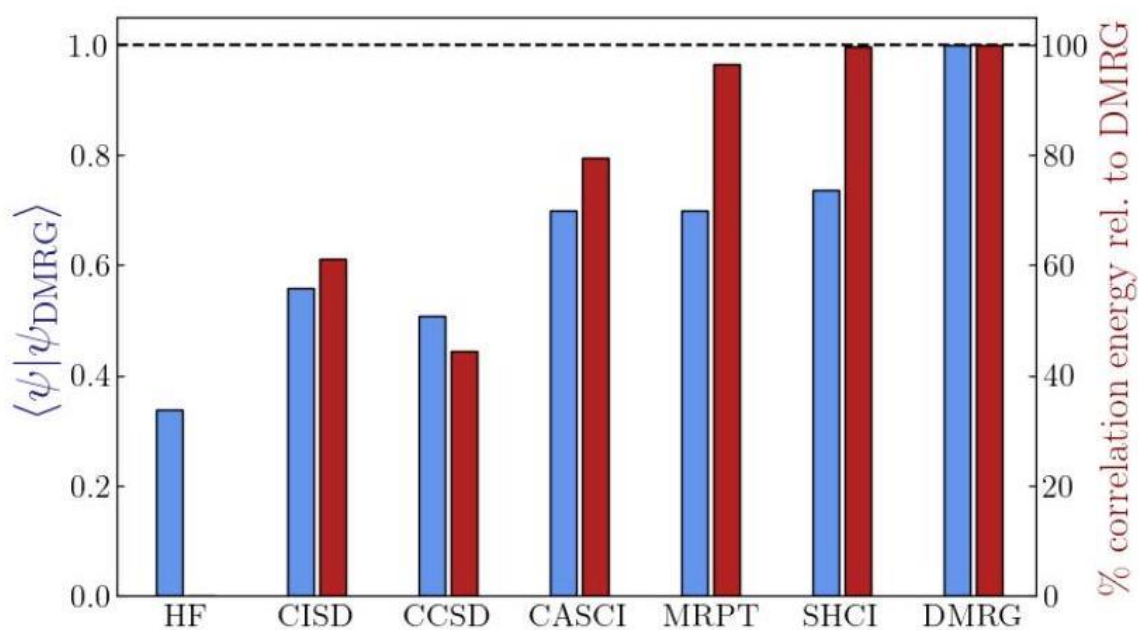
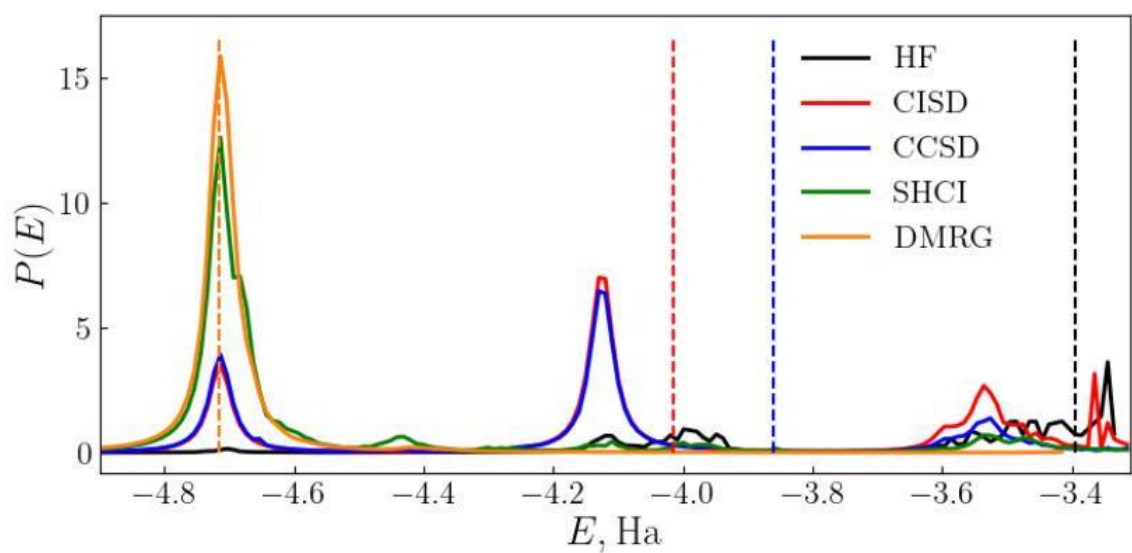
$$\frac{1}{2\pi^2 2^k} \frac{1}{E_p - E_0}$$

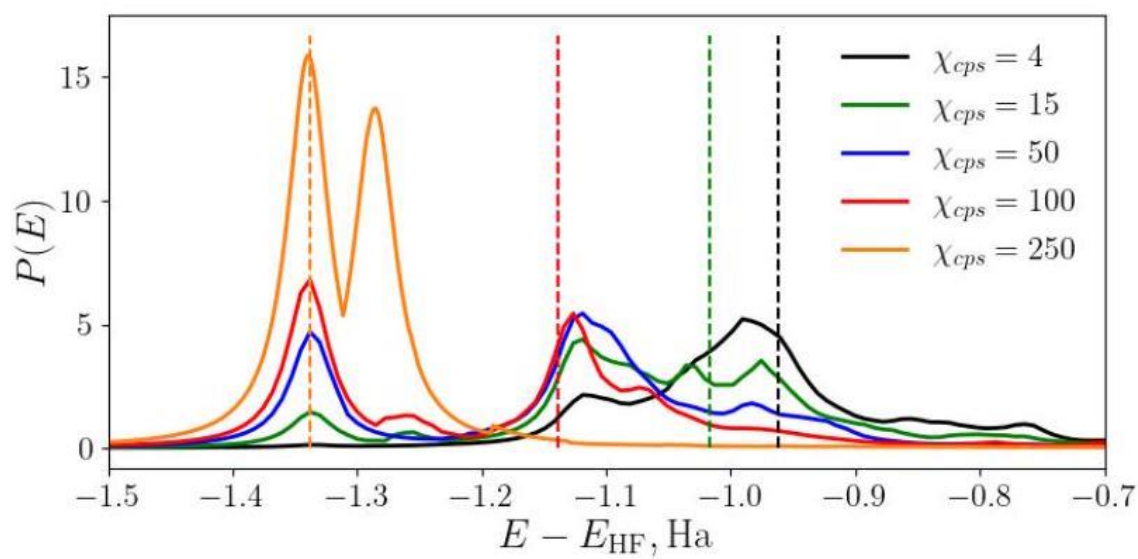
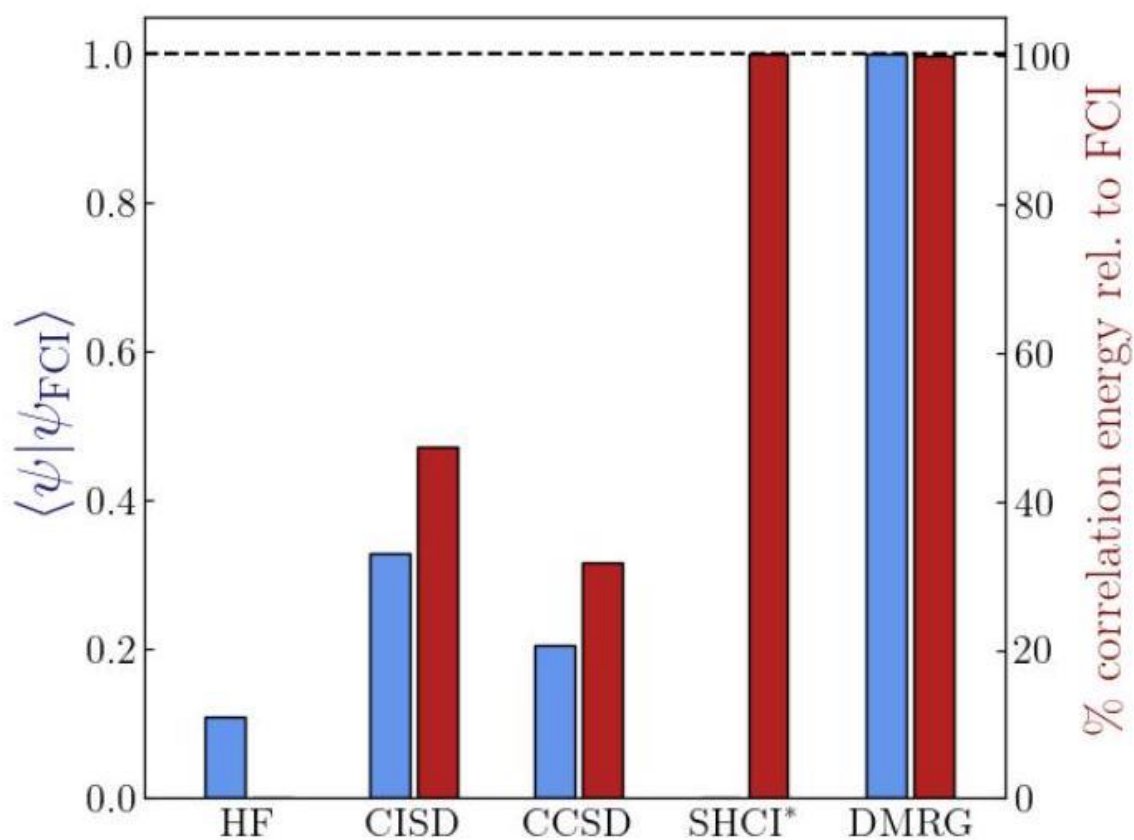
$$2^k = O\left([p_0(E_p - E_0)]^{-1}\right)$$

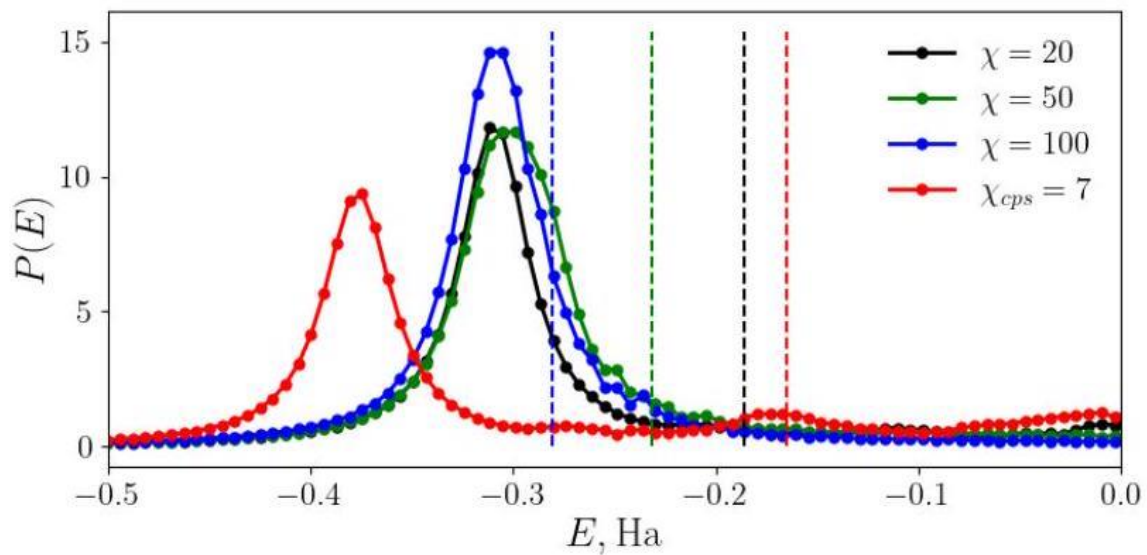
$$2^k = O\left(\max\left([p_0(E_p - E_0)]^{-1}, \epsilon^{-1}\right)\right).$$











$$c(n_1,\ldots,n_N)=\sum_{\alpha_1\ldots\alpha_{N-1}}A_{1;\alpha_1}^{n_1}\ldots A_{N;\alpha_{N-1}}^{n_N}$$

$$c_{\alpha_p}^{(p)}(n_1,\ldots,n_p)=\sum_{\alpha_1\ldots\alpha_{p-1}}A_{1;\alpha_1}^{n_1}\ldots A_{p;\alpha_{p-1}\alpha_p}^{n_p}$$

$$\sum_{\alpha_p} \left| c_{\alpha_p}^{(p)}(n_1,\ldots,n_p) \right|^2 \left| n_1,\ldots,n_{a_p},\ldots \right\rangle$$

$$U\colon \mathbb{F}_2^r \rightarrow \mathbb{F}_2^{2\log D-1}$$

$$U(v_i)\neq U(v_j)\leftrightarrow v_i-v_j\notin\ker U,\forall i\neq j$$

$$v_i-v_j\notin\ker U,\forall i\neq j, v_i\notin\ker U,\forall i, \text{ unless } v_i=\mathbf{0}.$$

$$\log D-1<\log(D)\Rightarrow \dim \mathbb{F}_2^{\log D-1}=2^{\log D-1}<D$$

$$\log D \leq r \leq 2\log D-1$$

$$r \leq 2\log D-1$$

$$r=2\log D-1+t$$

$$\dim \mathrm{Im} U + \dim \ker U = \dim \mathbb{F}_2^r = r = 2\log D-1+t$$

$$w_1,\ldots,w_t\in\mathcal{V}_r:=\mathrm{span}\langle v_1,\ldots,v_r\rangle$$

$$2\log D-1, \text{ so } \dim \mathrm{Im} U = 2\log D-1 \Rightarrow \dim \ker U = t$$

$$\forall i: w_i \in \ker U$$

$$\dim \ker U = \dim \mathcal{W}$$

$$\ker U = \mathcal{W}$$

$$v_i-v_j=v_i+v_j$$

$$t = 1 \Rightarrow r = 2 \log D$$

$$\{v_i, v_i - v_j\}_{i,j}$$

$$D + \binom{D}{2} = (D^2 + D)/2 \leq 2^{2 \log D-1} + 2^{\log D-1} < |\mathbb{F}_2^r| = 2^r = 2^{2 \log D}$$

$$w \in \mathbb{F}_2^r - \{v_i, v_i - v_j\}_{i,j}$$

$$(D^2+D)/2+1$$

$$v_1, \ldots, v_{2 \log D-1+t}$$

$$w_1, \ldots, w_{r-1} \in \mathcal{V}_{r-1} = \text{span}\langle v_1, \ldots, v_{r-1} \rangle$$

$$\mathcal{V}_{r-1} \subset \mathcal{V}_r = \text{span}\langle v_1, \ldots, v_r \rangle$$

$$\mathcal{M}:=\{v_i \mid v_i \in \mathcal{V}_{r-1}\}$$

$$\mathcal{N}:=\{v_i \mid v_i \in \mathcal{V}_r - \mathcal{V}_{r-1}\}$$

$$|\mathcal{M}|+1+|\mathcal{N}|=D$$

$$v_i=m'_i+v_r\in\mathcal{N}$$

$$l\neq\mathbf{0}, m'_i+l\neq\mathbf{0}$$

$$l\neq m_j, m'_i+l\neq m_j$$

$$l\notin\{\mathbf{0}, m'_i, m_j, m_j+m'_i\}$$

$$1+|\mathcal{N}|+|\mathcal{M}|+|\mathcal{M}|\cdot|\mathcal{N}|$$

$$1+|\mathcal{N}|+|\mathcal{M}|=D\leq D+(D-1-|\mathcal{N}|)|\mathcal{N}|\leq D+D^2/4\leq 2^{\log D}+2^{2\log D-2}<2^{r-1}=2^{2\log D-t-2}\text{ as }t>1$$

$$r-1=2\log D-1+t-1$$

$$\mathcal{W}=\text{span}\langle w_1,\ldots,w_{t-1}\rangle\subset\mathcal{V}_{r-1}$$

$$v_i, v_i + v_j \notin \mathcal{W}$$

$$(\{v_r\}\cup\mathcal{N})\subset\mathcal{V}_r-\mathcal{V}_{r-1}\Rightarrow(\{v_r\}\cup\mathcal{N})\cap\mathcal{V}_{r-1}=\emptyset\text{ while }\mathcal{W}\subset\mathcal{V}_{r-1}$$

$$v_i+v_j\notin\mathcal{W}(\{v_r\}\cup\mathcal{N})$$

$$v_i\in(\{v_r\}\cup\mathcal{N})v_j=m_j\in\mathcal{M}. \text{ If } v_i=v_r+m_j\notin\mathcal{W}v_i\in\mathcal{N}m'_i+v_r+m_j\notin\mathcal{W}$$

$$\mathcal{W}\subset\mathcal{V}_{r-1}$$

$$v_i, v_j \in (\{v_r\} \cup \mathcal{N})$$

$$v_r+m'_j+v_r=m'_j\notin\mathcal{W}$$

$$m'_i+v_r+m'_j+v_r=m'_i+m'_j\notin\mathcal{W}$$

$$l+m'_j+l=m'_j\notin\mathcal{W}$$

$$l+m'_i+l+m'_j=m'_i+m'_j\notin\mathcal{W}$$



$$w_t = v_r + l$$

$$\mathcal{W}' = \mathcal{W} \oplus w_t \subset \mathcal{V}_r = \mathcal{V}_{r-1} \oplus v_r$$

$$v_i \notin \mathcal{W}' - \mathcal{W} \text{ or } v_i - v_j \notin \mathcal{W}' - \mathcal{W}$$

$$v_i \in \mathcal{W}' - \mathcal{W} \text{ or } v_i - v_j \in \mathcal{W}' - \mathcal{W}$$

$$v_i \in \mathcal{W}' - \mathcal{W}, v_i = w_t + w = v_r + l + w$$

$$v_i - l = v_r + w$$

$$v_i \in \mathcal{V}_r - \mathcal{V}_{r-1}$$

$$v_i \in (\{v_r\} \cup N)$$

$$v_i = m'_i + v_r \in N$$

$$m'_i + l = w \in \mathcal{W}$$

$$v_i - v_j = v_r + l + w$$

$$v_i = v_r \text{ or } v_i = m'_i + v_r$$

$$l - v_j = w \in \mathcal{W} \text{ or } m'_i + l - v_j = w \in \mathcal{W}$$

$$O(D^2/2 + D)$$

$$O(tD^2) \; t \leq \min(2N,D) - 2\log D + 1$$

$$O(D^2(\min(2N,D) - 2\log D + 1))$$

$$O(L/\lambda + \lambda c)$$

$$\lambda = \sqrt{L/c} \; (O(\sqrt{Lc}))$$

$$2D/\lambda + 8(2N)\lambda \text{ with } \lambda = \sqrt{2D/16N} \boxtimes 2\sqrt{32ND}$$

$$\sum_{i=1}^D \alpha_i |i\rangle |v_i\rangle_v |b_i\rangle_b$$

$$O|b_i\rangle_b|0\rangle^{\otimes \log D} = |b_i\rangle_b|i\rangle$$

$$2\log D - 1$$

$$O\left(\sqrt{D^2 \cdot \log D}\right) = O(D\sqrt{\log D})$$

$$D \sim 2^{\log D}$$

$$\lambda = \lceil \sqrt{D} \rceil$$

$$b_{l_1} < \cdots < b_{l_D}$$

$$|b_j\rangle|0\rangle^{\otimes \lceil \log D/2 \rceil} \rightarrow |b_j\rangle|f(j)\rangle$$

$$b_{l_{\lambda(f(j)-1)}} < b_j < b_{l_{\lambda f(j)}}$$

$$\lambda f(j) > D$$

$$i_{\lambda f(j)} = D(2\log D - 1 + 2\log D - 1) \left\lceil \frac{D}{\lambda} \right\rceil b_j > b_{q\lambda} \lceil \log D/2 \rceil + 1$$

$$q \in \left\{1, \dots, \left\lceil \frac{D}{\lambda} \right\rceil\right\} \lceil \log D/2 \rceil \cdot \left\lceil \frac{D}{\lambda} \right\rceil$$

$$(4\log D - 2 + \lceil \log D/2 \rceil) \left\lceil \frac{D}{\lambda} \right\rceil \sim \frac{9\log D\sqrt{D}}{2}$$

$$\sum_{i=1}^D \alpha_i |i\rangle |v_i\rangle_v |b_i\rangle_b |f(i)\rangle$$

$$2^{\log D/2} \left| b_{l_{\lambda(f(j)-1)+1}}, \dots, b_{l_{\lambda f(j)}} \right\rangle$$

$$\sum_{i=1}^D \alpha_i |i\rangle |v_i\rangle_v |b_i\rangle_b |f(i)\rangle \left| b_{l_{\lambda(f(i)-1)+1}}, \dots, b_{l_{\lambda f(i)}} \right\rangle$$

$$(2\log D - 1)\lambda \sim (2\log D - 1)\sqrt{D}$$

$$\sum_{i=1}^D \alpha_i |i\rangle |v_i\rangle_v |b_i\rangle_b |f(i)\rangle \otimes$$

$$\left| b_{l_{\lambda(f(i)-1)+1}} \oplus b_i, \dots, b_{l_{\lambda f(i)}} \oplus b_i \right\rangle$$

$$(2\log D + \lceil \log D/2 \rceil - 1)\lambda \sim \frac{5\log D\sqrt{D}}{2}$$

$$\sum_{i=1}^D \alpha_i |i\rangle |v_i\rangle_v |b_i\rangle_b |f(i)\rangle \otimes$$

$$\left| b_{l_{\lambda(f(i)-1)+1}} \oplus b_i, \dots, b_{l_{\lambda f(i)}} \oplus b_i \right\rangle |g(i)\rangle$$

$$|f(i), g(i)\rangle \text{ has } 2^{\left\lceil \frac{\log D}{2} \right\rceil} \sim \log D$$

$$O(|f(i), g(i)\rangle |0\rangle^{\otimes \log D} = |f(i), g(i)\rangle |i\rangle$$

$$2\sqrt{16\log(D)2^{\log D}} < 2\sqrt{32\log(D)D} < \sqrt{32\log(D)D}$$

$$(2\log D - 1)\sqrt{D}$$

$$\min(2\sqrt{32ND}, D) + \frac{9\log D\sqrt{D}}{2} + \frac{5\log D\sqrt{D}}{2} + 2^{\log D/2} + 2\sqrt{32\log(D)D}$$

$$\sim \min(2\sqrt{32ND}, D) + (7\log D + 2\sqrt{32\log D})\sqrt{D}$$

$$\sum_{i=1}^{\lceil \log D \rceil - 2} (2i - 1)(2^i - 1) + (2\lceil \log D \rceil - 1)(D - 2^{\lceil \log D \rceil - 1})$$

$$\sum_{i=1}^{\lceil \log D \rceil - 2} (2i - 1)(2^i - 1) + (2\lceil \log D \rceil - 1)(D - 2^{\lceil \log D \rceil - 1}) + (\log(D\pi/\epsilon) - 3)D$$

$$G[j] = \sum_{\alpha_{j-1}} \left(|u_{\alpha_{j-1}}\rangle \langle \alpha_{j-1}, 0| \right) + \dots$$



$$|u_{\alpha_{j-1}}\rangle = \sum_{\alpha_j, n_j} A_{j; \alpha_{j-1} \alpha_j}^{n_j} |\alpha_j, n_j\rangle.$$

$$|0\rangle\langle 1| \otimes G[j] + |1\rangle\langle 0| \otimes G[j]^\dagger = \prod_{\alpha_{j-1}=1}^{\chi_{j-1}} \left(1 - 2P_{\alpha_{j-1}}\right)$$

$$P_{\alpha_{j-1}} = \left|w_{\alpha_{j-1}}\right\rangle\left\langle w_{\alpha_{j-1}}\right|$$

$$\begin{aligned} \left|w_{\alpha_{j-1}}\right\rangle &= |1\rangle \otimes |\alpha_{j-1},0\rangle - |0\rangle \otimes |u_{\alpha_{j-1}}\rangle \\ &= W_{\alpha_{j-1}}|0\rangle \otimes |0,0\rangle \end{aligned}$$

$$\left|w_{\alpha_{j-1}}\right\rangle|0\rangle\otimes|0,0\rangle$$

$$1-2P_{\alpha_{j-1}}=W_{\alpha_{j-1}}[1-2|0,0,0\rangle\langle 0,0,0|]W_{\alpha_{j-1}}^\dagger$$

$$\left|u_{\alpha_{j-1}}\right\rangle = V_{\alpha_{j-1}}|0,0\rangle$$

$$W_{\alpha_{j-1}} = \left(\bar{C}V_{\alpha_{j-1}}\right)\left(C_{\alpha_{j-1}}\right)((ZH)\otimes \mathbb{I})$$

$$\frac{1}{\sqrt{2}}\big[|0,0,0\rangle-|1,\alpha_j,0\rangle\big]$$

$$[1-2|0\rangle^{\otimes v}\langle 0|^{\otimes v}]$$

$$\left|u_{\alpha_{j-1}}\right\rangle = V_{\alpha_{j-1}}|0,0\rangle$$

$$|u_{\alpha_{j-1}}\rangle = \sum_{\alpha_j, n_j} A_{j; \alpha_{j-1} \alpha_j}^{n_j} |\alpha_j, n_j\rangle$$

$$2^{-b/2}\sum_{k=0}^{2^b-1}e^{-2\pi ik/2^b}|k\rangle$$

$$b=\log\left(1/\delta_r\right)$$

$$2^{\nu+2}+\nu b$$

$$\chi_{j-1}[8\chi_jd+b\log\left(\chi_jd\right)+\log\left(\chi_jd\right)]$$

$$2\frac{2^{\nu+2}}{\lambda}+4\cdot 2\lambda \nu b+\nu b$$

$$\lambda = O(\sqrt{2^\nu})$$

$$\chi_{j-1}\left[8\frac{\chi_jd}{\lambda}+8\lambda b\log\left(\chi_jd\right)+b\log\left(\chi_jd\right)+\log\left(\chi_jd\right)\right]$$

s	Edgeworth term
1	$(\kappa_3/6) \text{He}_3(x)$
2	$(\kappa_4/24)\text{He}_4(x) + (\kappa_3^2/72)\text{He}_6(x)$
3	$(\kappa_5/120)\text{He}_5(x) + (\kappa_4\kappa_3/144)\text{He}_7(x) + (\kappa_3^3/1296)\text{He}_9(x)$
4	$(\kappa_6/720)\text{He}_6(x) + (\kappa_5\kappa_3/720 + \kappa_4^2/1152)\text{He}_8(x) + (\kappa_4\kappa_3^2/1728)\text{He}_{10}(x) + (\kappa_3^4/31104)\text{He}_{12}(x)$
5	$(\kappa_7/5040)\text{He}_7(x) + (\kappa_6\kappa_3/4320 + \kappa_5\kappa_4/2880)\text{He}_9(x) + (\kappa_5\kappa_3^2/8640 + \kappa_4^2\kappa_3/6912)\text{He}_{11}(x) + (\kappa_4\kappa_3^3/31104)\text{He}_{13}(x)$

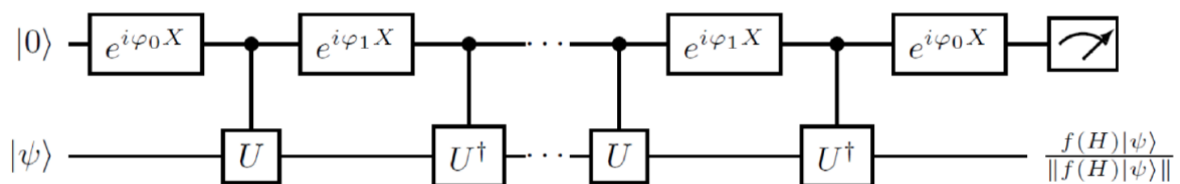
$$p_E(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}} \left[1 + \sum_{s=1}^{\infty} \sum_{\{k_m\}} He_{s+2r}(x) \prod_{m=1}^s \frac{1}{k_m!} \left(\frac{\kappa_{m+2}}{(m+2)!} \right)^{k_m} \right]$$

$$k_1+2k_2+\cdots +sk_s=s,$$

$$r=\sum k_m$$

$$\hat{p}(x) = \frac{1}{Mh} \sum_{i=1}^M K\left(\frac{x-X_i}{h}\right),$$

$$\text{MISE} = \mathbb{E} \left(\int dx (\hat{p}(x) - p(x))^2 \right)$$



$$f(H)=P(\cos{(H/2)})\|P(\cos{(H/2)})|\psi\rangle\|U=e^{-iH}\odot\varphi_0,\varphi_1,\ldots,\varphi_{d/2}$$

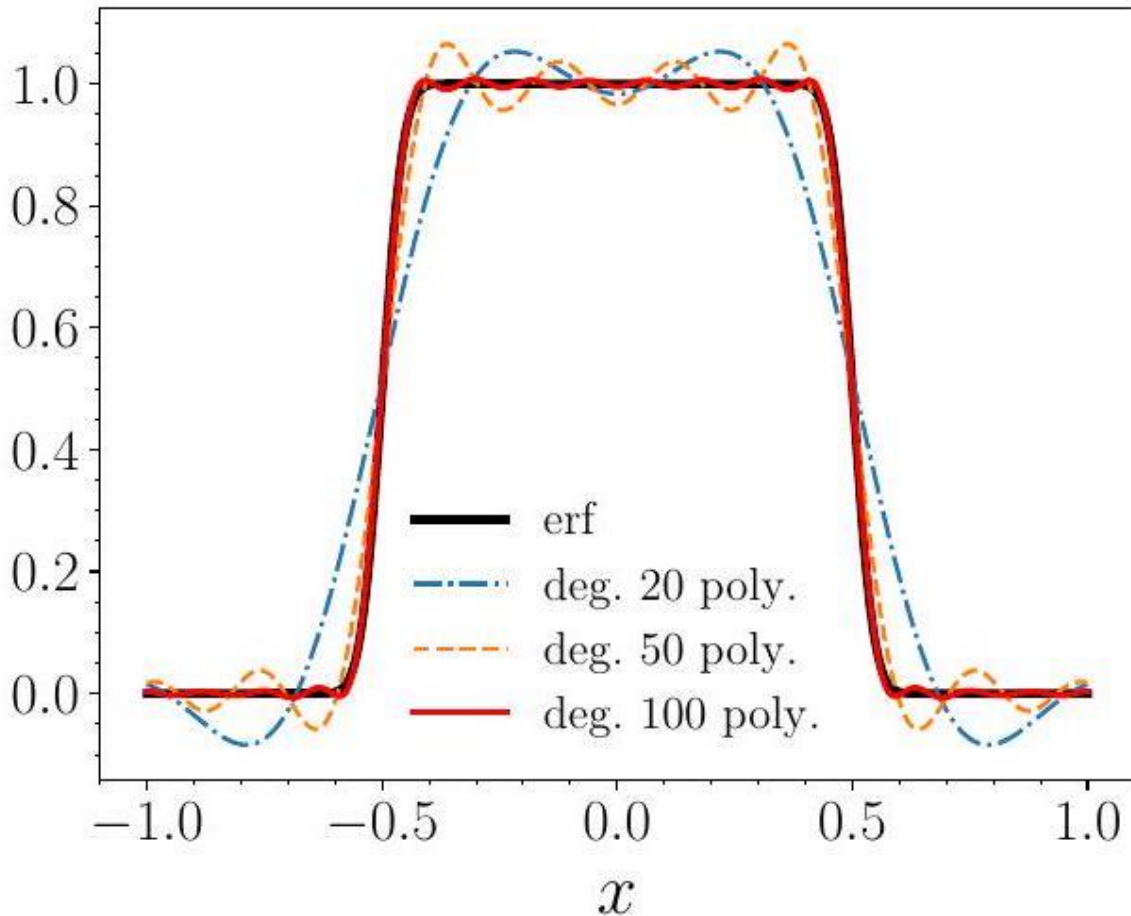
$$\xi_{k,\mu}(x)=\frac{1}{2}[\mathrm{erf}(-k(x-\mu))+\mathrm{erf}(k(x+\mu))],$$

$$p_{\mathrm{perf},k,n}=\frac{2ke^{-k^2/2}}{\sqrt{\pi}}(I_0(k^2/2)+\sum_{j=1}^{(n-1)/2}(-1)^jI_j(k^2/2)\left[\frac{T_{2j+1}(x)}{2j+1}-\frac{T_{2j-1}(x)}{2j-1}\right]\Bigg),$$

$$|\psi\rangle=\sum_E\varphi_E|E\rangle$$

$$\sum_E \varphi_E P(\cos(E/2)) |E\rangle |0\rangle$$

$$\mu = \frac{\cos(E_u/2) + \cos(E_l/2)}{2} \text{ and } \frac{1}{k} = \zeta \frac{\cos(E_u/2) - \cos(E_l/2)}{2}$$



$$A(E)=\frac{1}{\sqrt{2\pi}\sigma_E}e^{-\frac{(E-\bar{E})^2}{2\sigma_E^2}},$$

$$p_{\text{leak}}(E_n)=\sum_{x_j<x_{\text{upper}}}\frac{1}{2^{2k}}\left(\frac{\sin^2(\pi\delta_n)}{\sin^2\left(\frac{\pi}{2^k}[x_n+\delta_n-x_j]\right)}\right),$$

$$\begin{aligned} I(x_0) &= \frac{\sin^2(\pi\delta_n)}{2^{2k}} \int_{-2^{k-1}}^{x_0} \frac{dx}{\sin^2\left(\frac{\pi}{2^k}(x_n+\delta_n-x)\right)} \\ &= \frac{\sin^2(\pi\delta_n)}{2^{2k}} \left[\frac{2^k}{\pi} \cot\left(\frac{\pi}{2^k}(x_n+\delta_n-x)\right) \right]_{-2^{k-1}}^{x_0} \end{aligned}$$

$$I(x_{\text{upper}}-1)\leq p_{\text{leak}}(E_n)\leq I(x_{\text{upper}}).$$

$$O\left(\max\left[2^{-2k},(x_n-x_{\text{upper}})^{-2}\right]\right)$$

$$I(x_{\text{upper}})-I(x_{\text{upper}}-1)$$

$$\hat{H}_e = \sum_{p,q=1}^N h_{pq} \hat{a}_p^\dagger \hat{a}_q + \sum_{p,q,r,s=1}^N g_{pqrs} \hat{a}_p^\dagger \hat{a}_q \hat{a}_r^\dagger \hat{a}_s$$

$$|\psi\rangle=c_0|0\rangle+c_1|1\rangle,$$

$$c_0,c_1\in\mathbb{C},|c_0|^2+|c_1|^2=1$$

$$\hat{z}|z\rangle=(-1)^z|z\rangle, z\in\mathbb{F}_2$$

$$|\vec{z}\rangle:=|z_1z_2\ldots z_N\rangle, z_i\in\mathbb{F}_2.$$

$$|\psi\rangle=\sum_{\vec{z}\in\mathbb{F}_2^N}c_{\vec{z}}|\vec{z}\rangle,$$

$$\sum_{\vec{z}\in\mathbb{F}_2^N}|c_{\vec{z}}|^2=1$$

$$\hat{z}_k|\vec{z}\rangle=(-1)^{z_k}|\vec{z}\rangle$$

$$\begin{aligned}\hat{H}_{\text{ising}} &= d_0 + \sum_{k=1}^N d_k \hat{z}_k + \sum_{k>l}^N d_{kl} \hat{z}_k \hat{z}_l + \cdots \\ &= p(\hat{z}_1, \ldots, \hat{z}_N)\end{aligned}$$

$$\begin{aligned}\hat{H}_{\text{ising}} &= \sum_{\vec{z}\in\mathbb{F}_2^N} E_{\vec{z}} |\vec{z}\rangle\langle\vec{z}| \\ E_{\vec{z}} &= p((-1)^{z_1},\ldots,(-1)^{z_N}).\end{aligned}$$

$$\bar{H}_{\text{ising}}=\sum_{\vec{z}\in\mathbb{F}_2^N}\frac{M_{\vec{z}}}{M}E_{\vec{z}}.$$

Classical:
Pre-process the Hamiltonian

1. Obtain partitioning

$$\hat{H} = \sum_{\alpha} \hat{H}_{\alpha}$$

2. Solve fragments

$$\hat{H}_{\alpha} = \hat{U}_{\alpha}^{\dagger} p_{\alpha}(\hat{z}_1, \dots, \hat{z}_N) \hat{U}_{\alpha}$$

3. Allocate measurements

$$M = \sum_{\alpha} M_{\alpha}$$

Quantum:
Measure Hamiltonian fragments

Measure fragments based on
measurement allocations

$$|\psi\rangle \rightarrow \hat{U}_1 \rightarrow \text{meter} \rightarrow \vec{z}_i^{(1)}$$

M_1 repetitions

$$|\psi\rangle \rightarrow \hat{U}_2 \rightarrow \text{meter} \rightarrow \vec{z}_i^{(2)}$$

M_2 repetitions

⋮

Classical: Post-process the measurements

1. Average measurement results

$$\bar{H}_\alpha = \frac{1}{M_\alpha} \sum_{i=1}^{M_\alpha} p_\alpha(\vec{v}_i^{(\alpha)})$$

$$\vec{v}_i^{(\alpha)} = ((-1)^{z_{i,1}^{(\alpha)}}, \dots, (-1)^{z_{i,N}^{(\alpha)}})$$

2. Sum fragment estimates

$$\bar{H} = \sum_{\alpha} \bar{H}_\alpha$$

$$\hat{H} = \sum_{\alpha} \hat{H}_\alpha p_\alpha(\hat{z}_1, \dots, \hat{z}_N) \langle \psi | \hat{H} | \psi \rangle$$

$$\hat{H} = \hat{U}^\dagger p(\hat{z}_1, \dots, \hat{z}_N) \hat{U},$$

$$\text{PVM} \equiv \{ \hat{U} | \vec{z} \rangle \langle \vec{z} | \hat{U}^\dagger \}$$

$$\langle \psi | \hat{H} | \psi \rangle = \langle \hat{U} \psi | p(\hat{z}_1, \dots, \hat{z}_N) | \hat{U} \psi \rangle,$$

$$\hat{H} = \sum_{\alpha} \hat{H}_\alpha,$$

$$\langle \psi | \hat{H} | \psi \rangle = \sum_{\alpha} \langle \psi | \hat{H}_\alpha | \psi \rangle.$$

$$\bar{H} = \sum_{\alpha} \bar{H}_\alpha$$

$$\bar{H}_\alpha = \frac{1}{M_\alpha} \sum_{i=1}^{M_\alpha} H_{\alpha,i}$$

$$\langle \psi | \hat{H}_\alpha | \psi \rangle, \bar{H}_\alpha$$

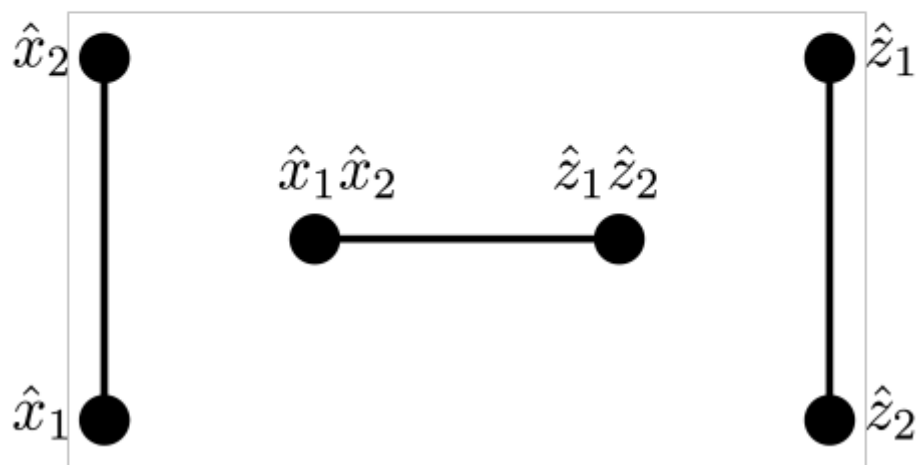
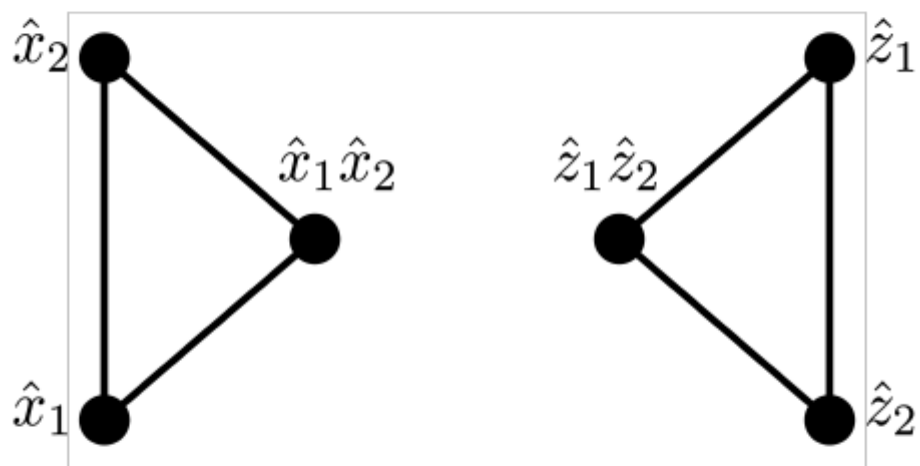
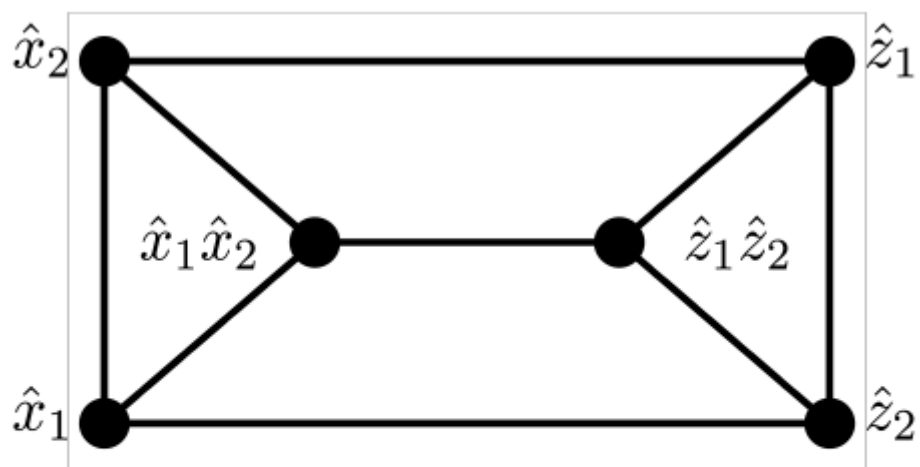
$$\hat{H}_{\text{ising}} = p(\hat{z}_1, \dots, \hat{z}_N)$$

$$\hat{H}_{\text{fc}} = p(\hat{C}_1, \dots, \hat{C}_K)$$



$$\hat{U}_c \hat{H}_{\text{fc}} \hat{U}_c^\dagger = p(\hat{z}_1, \dots, \hat{z}_K)$$

$$\hat{P} = \bigotimes_{i=1}^N \hat{\sigma}_i, \hat{Q} = \bigotimes_{i=1}^N \hat{\tau}_i [\hat{\sigma}_i, \hat{\tau}_i] = i$$



$$\hat{E}_{pq} = \hat{a}_p^\dagger \hat{a}_q$$

$$\hat{n}_p = \hat{E}_{pp} (1 - \hat{z}_p)/2$$

$$\hat{E}_{pq}+\hat{E}_{qp},\hat{E}_{pq}\hat{E}_{rs}+\hat{E}_{sr}\hat{E}_{qp}$$

$$\hat{H}_{1e}=\sum_{p\geq q}^N h_{pq}\hat{E}_{pq}$$

$$\hat{U}\hat{H}_{1e}\hat{U}^\dagger=\sum_{p=1}^N\epsilon_p\hat{n}_p$$

$$\hat{U}=\exp\left(\sum_{p>q}^N\theta_{pq}(\hat{E}_{pq}-\hat{E}_{qp})\right),$$

$$\theta_{pq}=[\log{(u)}]_{pq}$$

$$\hat{H}_{1e}=\sum_{p=1}^N\epsilon_p\hat{C}_p$$

$$\hat{C}_p=\hat{U}^\dagger\hat{n}_p\hat{U}$$

$$\hat{G}_{pq}(\phi_{pq})=\exp\left(\phi_{pq}(\hat{E}_{pq}-\hat{E}_{qp})\right)$$

$$\hat{U}=\prod_{p>q}^N\hat{G}_{pq}(\phi_{pq})$$

$$\hat{H}_{2e}=\sum_{p\geq q}^N\lambda_{pq}\hat{C}_p\hat{C}_q,\hat{C}_p=\hat{U}^\dagger\hat{n}_p\hat{U}$$

$$\hat{U}\hat{H}_{2e}\hat{U}^\dagger=\sum_{p\geq q}\lambda_{pq}\hat{n}_p\hat{n}_q$$

$$f\left(\lambda_{pq}^{(\alpha)},\hat{U}^{(\alpha)}\right)=\left\|\hat{H}_e-\sum_{\alpha}U_{\alpha}^{\dagger}\left(\sum_{p\geq q}\lambda_{pq}^{(\alpha)}\hat{n}_p\hat{n}_q\right)\hat{U}_{\alpha}\right\|$$

$$\lambda_{pq}^{(\alpha)}=\epsilon_p^{(\alpha)}\epsilon_q^{(\alpha)}\left(\sum_{p=1}^N\epsilon_p^{(\alpha)}\hat{C}_p\right)^2$$

$$\{\hat{X}_i\}_{i=1}^d\left\{c_{ij}^{(k)}\right\}$$

$$[\hat{X}_i,\hat{X}_j]=\mathrm{i}\sum_kc_{ij}^{(k)}\hat{X}_k\{\hat{C}_k\}_{k=1}^r$$

$$\hat{H}=\sum_{i=1}^dc_i\hat{X}_i=\sum_{k=1}^r\epsilon_k\hat{U}^\dagger\hat{C}_k\hat{U}$$

$$\hat{H}=c_0+\sum_{i=1}^dc_i\hat{X}_i+\sum_{i\geq j}^dc_{ij}\hat{X}_i\hat{X}_j+\cdots$$

$$\mathcal{E}_{\mathcal{A}}=\mathbb{F}\oplus\mathcal{A}\oplus\mathcal{A}^2\oplus\mathcal{A}^3\oplus\cdots$$

$$\{\hat{E}_{pq}+\hat{E}_{qp}\}\cup\{\mathrm{i}(\hat{E}_{pq}-\hat{E}_{qp})\}$$

$$\{\mathrm{i}(\hat{E}_{pq}-\hat{E}_{qp})\}\{\hat{n}_p\}\{\hat{U}^\dagger\hat{n}_p\hat{U}\}$$

$$\hat{H}_{\mathrm{QMF}}=p(\hat{S}_1,\ldots,\hat{S}_N)$$

$$\hat{S}_k=\alpha_k\hat{x}_k+\beta_k\hat{y}_k+\gamma_k\hat{z}_k+\delta_k\hat{1}_k$$

$$\hat{S}_k=e^{-\mathrm{i}\theta_k\hat{\eta}_k}(\epsilon_k\hat{z}_k+\delta_k\hat{1}_k)e^{\mathrm{i}\theta_k\hat{\eta}_k}$$

$$\hat{\eta}_k=\tau_x^{(k)}\hat{x}_k+\tau_y^{(k)}\hat{y}_k+\tau_z^{(k)}\hat{z}_k$$

$$\epsilon_k=\sqrt{\alpha_k^2+\beta_k^2+\gamma_k^2}$$

$$\text{sum}\oplus_{k=1}^Nu\{\hat{x}_k,\hat{y}_k,\hat{z}_k,\hat{1}_k\}$$

$$\hat{\gamma}_{2p}\!=\!\hat{a}_p^\dagger+\hat{a}_p$$

$$\hat{\gamma}_{2p+1}=\mathrm{i}(\hat{a}_p^\dagger-\hat{a}_p),$$

$$\hat{H}=2\mathrm{i}\sum_{ij=1}^{2N}\tilde{h}_{ij}\hat{\gamma}_i\hat{\gamma}_j+\sum_{ijkl=1}^{2N}\tilde{g}_{ijkl}\hat{\gamma}_i\hat{\gamma}_j\hat{\gamma}_k\hat{\gamma}_l$$

$$\hat{H}_{1m}=2\mathrm{i}\sum_{i>j}^{2N}h_{ij}\hat{\gamma}_i\hat{\gamma}_j$$

$$\{\hat{\gamma}_i,\hat{\gamma}_j\}=2\delta_{ij}$$

$$\{\hat{A},\hat{B}\}=\hat{A}\hat{B}+\hat{B}\hat{A}$$

$$\{\hat{\gamma}_i\}_{i=1}^{2N}\cup\{\mathrm{i}\hat{\gamma}_i\hat{\gamma}_j\}_{i>j}^{2N}$$

$$\{\mathrm{i}\hat{\gamma}_{2k-1}\hat{\gamma}_{2k}\}_{k=1}^N$$

$$\hat{U}_g=\exp\left(-\sum_{i>j}^N\theta_{ij}\hat{\gamma}_i\hat{\gamma}_j\right)$$

$$\hat{U}_g\hat{H}_{1m}\hat{U}_g^\dagger=2\mathrm{i}\sum_{k=1}^N\epsilon_k\hat{\gamma}_{2k-1}\hat{\gamma}_{2k}$$

$$\mathrm{i}\hat{\gamma}_{2k-1}\hat{\gamma}_{2k}=1-2\hat{n}_k$$

$$\{\hat{A}_i\}_{i=1}^K \hat{H}_{\text{ac}} = \sum_{i=1}^K c_i \hat{A}_i \{A_i\}_{i=1}^K$$

$$\hat{H}_{\text{twc-ac}} = \sum_i \hat{H}_{\text{ac}}^{(i)}$$

$$\hat{H}_{k-\text{local}} = \sum_r \hat{W}_r$$

$$\hat{W}_r = A_{r,1}^{(S_{r,1})} \otimes A_{r,2}^{(S_{r,2})} \otimes \cdots,$$

$$\hat{A}_{r,i}^{(S_{r,i})}|S_{r,i}| \leq k$$

$$[\hat{W}_r,\hat{W}_s]=0$$

$$\hat{H}_{so} = \sum_{i=1}^K c_i \hat{A}_i + \mathrm{i} \sum_{j>k}^K d_{jk} \hat{A}_j \hat{A}_k$$

$$\hat{H}_{\text{twc-so}} = \sum_{i=1}^L \hat{H}_{so}^{(i)}$$

$$\oplus_{i=1}^L so(K_i+1)$$

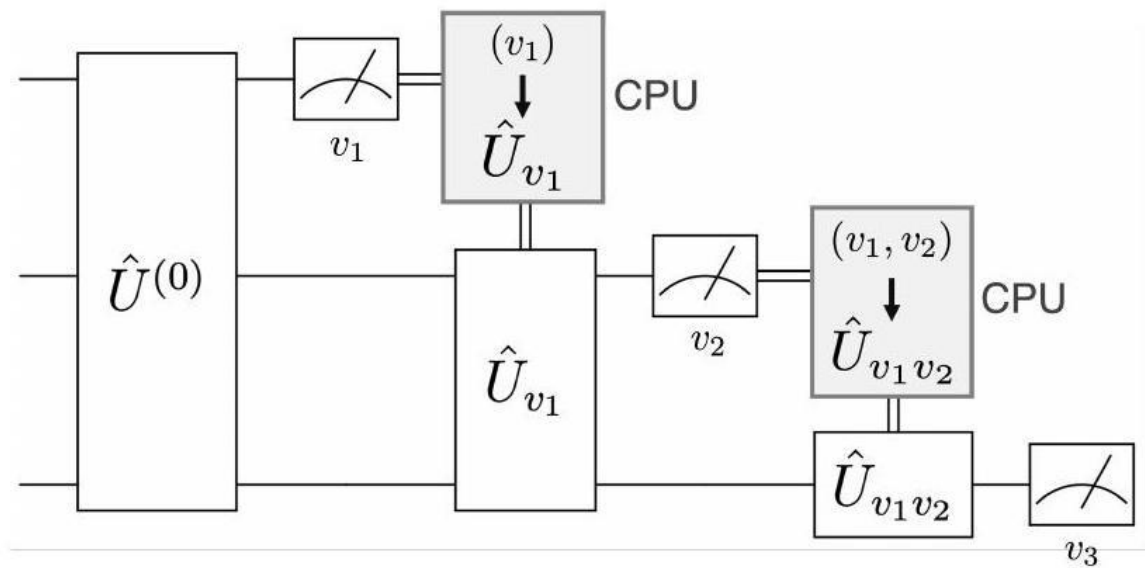
$$[\hat{\mathcal{C}}_k,\hat{\mathcal{C}}_l]=[\hat{\mathcal{C}}_k,\hat{X}_a]=0$$

$$\hat{H} = \sum_{a=1}^d \hat{c}_a \hat{X}_a$$

$$\hat{c}_a = p_a(\hat{C}_1, \ldots, \hat{C}_K)$$

$$\hat{H}\hat{\mathcal{P}}_{\vec{v}}=\hat{H}_{\vec{v}}\hat{\mathcal{P}}_{\vec{v}}$$

$$\hat{H}_{\vec{v}} = \sum_{a=1}^d p_a(v_1, \ldots, v_K) \hat{X}_a$$



$$\hat{H} = \hat{U}^\dagger \left[\sum_{pq \in S_1} \left(\sum_{k \in S_2} h_{pq}^{(k)} \hat{n}_k \right) \hat{E}_{pq} + \sum_{kl \in S_2} \lambda_{kl} \hat{n}_k \hat{n}_l \right] \hat{U}$$

$$\hat{O}_1^{(k_1)} v_1 \in \{-1,1\}$$

$$\hat{H}(v_1)=\hat{H}\hat{\mathcal{P}}_1(v_1)$$

$$\hat{O}_1^{(k_1)}=v_1\int\hat{O}_2^{(k_2)}(v_2)v_2$$

$$\hat{H}(v_1,v_2)=\hat{H}\hat{\mathcal{P}}_1(v_1)\hat{\mathcal{P}}_2(v_2)$$

$$\langle \psi | \hat{O} | \psi \rangle = \text{Tr}[\hat{\rho} \hat{O}]$$

$$\mathcal{M}(\hat{\rho}) = \sum_{\vec{z} \in \mathbb{F}_2^N} |\vec{z}\rangle \langle \vec{z}| \hat{\rho} |\vec{z}\rangle \langle \vec{z}|$$

$$\vec{z} = (z_1, \ldots, z_N)$$

$$\hat{\rho} = \mathcal{M}^{-1}(\mathcal{M}(\hat{\rho}))$$

$$\mathcal{M}_{\mathcal{G}}(\hat{\rho}) \, = \, \mathbb{E}_{u \in \mathcal{G}}[u^\dagger \circ \mathcal{M} \circ u(\hat{\rho})]$$

$$= \mathbb{E}_{u \in \mathcal{G}} \left[\sum_{\vec{z}} u^\dagger (|\vec{z}\rangle \langle \vec{z}|) \langle \vec{z}| u(\hat{\rho}) |\vec{z}\rangle \right]$$

$$\mathcal{U}(\rho)=\hat{U}\hat{\rho}\hat{U}^\dagger$$

$$\text{Tr}(\hat{H}\hat{\rho})\!=\!\text{Tr}[\hat{H}\cdot\mathcal{M}_{\mathcal{G}}^{-1}\circ\mathcal{M}_{\mathcal{G}}(\hat{\rho})]$$

$$= \mathbb{E}_{u \in \mathcal{G}} \left[\sum_{\vec{z}} \text{Tr}(\hat{H} \cdot \mathcal{M}_{\mathcal{G}}^{-1} \circ u^\dagger (|\vec{z}\rangle \langle \vec{z}|)) \right. \\ \left. \times \langle \vec{z}| u(\hat{\rho}) |\vec{z}\rangle \right]$$

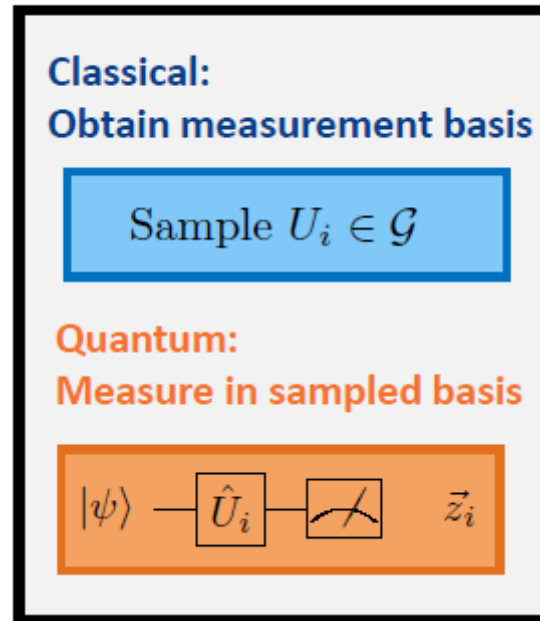
$$\text{Tr}(\hat{H} \cdot \mathcal{M}_{\mathcal{G}}^{-1} \circ u^\dagger (|\vec{z}\rangle \langle \vec{z}|)) \langle \vec{z}| u(\hat{\rho}) |\vec{z}\rangle$$

$$\bar{H} = \frac{1}{M} \sum_{i=1}^M \bar{H}^{(i)}$$

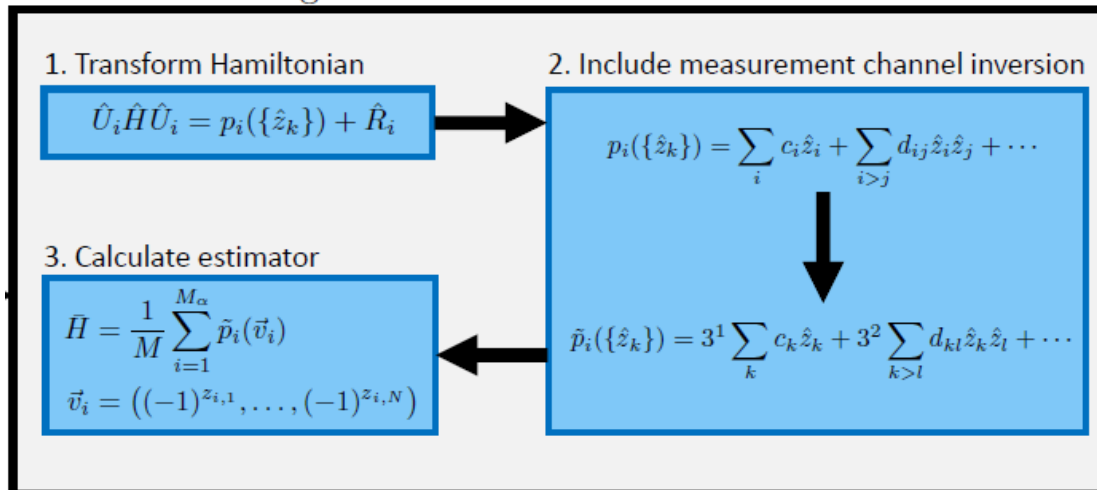
$$\bar{H}^{(i)} = \sum_P \alpha_P f(\hat{B}^{(i)}, \hat{P}) \mu(\hat{B}^{(i)}, \text{supp}(\hat{P}))$$

$$\hat{P} = \bigotimes_{i=1}^N \hat{\sigma}_i, f(\hat{B}^{(i)}, \hat{P})$$

1. Sampling Phase



2. Post-Processing Phase



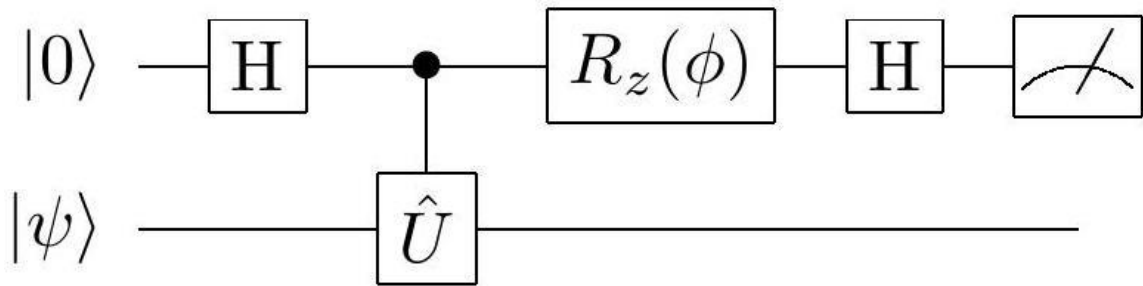
$$f(\hat{B}, \hat{P}) = \prod_{j=1}^K f_j(\hat{B}_j, \hat{\sigma}_j)$$

$$f_j(\hat{B}_j, \hat{\sigma}_j) = \begin{cases} 1 & \text{if } \hat{\sigma}_j = \hat{1} \\ 3 & \text{if } \hat{B}_j = \hat{\sigma}_j \neq \hat{1} \\ 0 & \text{otherwise.} \end{cases}$$

$$\bar{H} = \sum_P \sum_{i=1}^M \alpha_P \frac{f(\hat{B}^{(i)}, \hat{P})}{M} \mu(\hat{B}^{(i)}, \text{supp}(\hat{P})).$$

$$\mu(\hat{B}^{(i)}, \text{supp}(\hat{P}))$$

$$M/f(\hat{B}^{(i)}, \hat{P})$$



$$\hat{O}=\sum_j\alpha_j\hat{U}_j,\hat{U}_j\hat{U}_j^\dagger=\hat{1}$$

$$\langle\psi|\hat{O}|\psi\rangle=\sum_j\alpha_j\langle\psi|\hat{U}_j|\psi\rangle,$$

$$\hat{r}_p=1-2\hat{n}_p$$

$$\hat{H}_{2e}=\sum_{\mu\nu=1}^M\xi_{\mu\nu}\hat{U}_\mu^\dagger(\hat{n}_{1\downarrow}+\hat{n}_{1\uparrow})\hat{U}_\mu\hat{U}_\nu^\dagger(\hat{n}_{1\downarrow}+\hat{n}_{1\uparrow})\hat{U}_\nu,$$

$$\hat{H}=\sum_k c_k \hat{P}_k$$

$$\{\hat{P}_k\}_{k=1}^{4^N}\{\hat{P}_k\otimes\hat{P}_k\}_{k=1}^{4^N}\langle\Psi|\hat{P}_k\otimes\hat{P}_k|\Psi\rangle$$

$$|\Psi\rangle=|\psi\rangle\otimes|\psi\rangle$$

$$\langle\Psi|\hat{P}_k\otimes\hat{P}_k|\Psi\rangle=)|\langle\psi|\hat{P}_k|\psi|^2$$

$$\sum_k c_k |\langle \hat{P}_k \rangle|$$

$$\sum_m \hat{M}_m^\dagger \hat{M}_m = \hat{1}$$

$$\Pr(m)=\langle\psi|\hat{M}_m^\dagger\hat{M}_m|\psi\rangle$$

$$\hat{\Pi}_m=\hat{M}_m^\dagger\hat{M}_m$$

$$\{\hat{\Pi}_m\}\langle\psi|\hat{\Pi}_m|\psi\rangle\geq|\psi\rangle$$

$$\sum_m \hat{\Pi}_m = \hat{1}$$

$$\hat{H} = \sum_{\alpha} \hat{H}_{\alpha}$$

$$\hat{H}_{\alpha} = \sum_{\vec{z} \in \mathbb{F}_2^N} e_{\vec{z}, \alpha} \hat{U}_{\alpha} |\vec{z}\rangle \langle \vec{z}| \hat{U}_{\alpha}^{\dagger}$$

$$\mathcal{P}_{\alpha} = \{ \hat{U}_{\alpha} |\vec{z}\rangle \langle \vec{z}| \hat{U}_{\alpha}^{\dagger} \}$$

$$\hat{H} = \sum_{\alpha} \sum_{\vec{z} \in \mathbb{F}_2^N} \left(\frac{e_{\vec{z}, \alpha}}{w_{\alpha}} \right) w_{\alpha} \hat{U}_{\alpha} |\vec{z}\rangle \langle \vec{z}| \hat{U}_{\alpha}^{\dagger}$$

$$\bigcup_{\hat{U} \in \mathcal{G}} \{1/|\mathcal{G}| \hat{U} |\vec{z}\rangle \langle \vec{z}| \hat{U}^{\dagger}\} \{\hat{\Pi}_m\}$$

$$\hat{H} = \sum_m \omega_m \hat{\Pi}_m$$

$$\Pr(m) = \langle \hat{\Pi}_m \rangle$$

$$\langle \hat{H} \rangle = \sum_m \omega_m \langle \hat{\Pi}_m \rangle$$

$$\bar{H} = \frac{1}{S} \sum_{s=1}^S \omega_{m_s}$$

$$\{\hat{\Pi}_m\}_{m=1}^{4^N} \{\hat{U}|m\rangle\langle m|\hat{U}^\dagger\}$$

$$\langle \psi | \hat{\Pi}_m | \psi \rangle = \langle \psi | \langle \phi_0 | \hat{U} | m \rangle \langle m | \hat{U}^\dagger | \psi \rangle | \phi_0 \rangle,$$

$$\{\hat{\Pi}_{i\alpha}, i, \alpha \in \{0,1\}\}$$

$$\text{PVM}\left\{\hat{U}|i\alpha\rangle\langle i\alpha|\hat{U}^\dagger\right\}$$

$$\hat{U} = \sum_{ij\alpha\beta} u_{j\beta}^{i\alpha} |i\alpha\rangle\langle j\beta|.$$

$$\hat{\Pi}_{i\alpha} = |\pi_{i\alpha}\rangle\langle\pi_{i\alpha}|$$

$$|\pi_{i\alpha}\rangle = \sum_j \left(u_{j0}^{i\alpha}\right)^* |j\rangle.$$

$$\bigcup_{\mu} \left\{ \hat{P}_0^{(\mu)}, \hat{P}_1^{(\mu)} \right\} \left\{ \hat{P}_0^{(\mu)}, \hat{P}_1^{(\mu)} \right\}$$

$$\mathcal{M}_k = \left\{ \hat{\Pi}_{m_k}^{(k)} \colon 1 \leq m_k \leq 4 \right\}$$

$$\hat{\Pi}_{\mathbf{m}} = \hat{\Pi}_{m_1}^{(1)} \otimes \cdots \otimes \hat{\Pi}_{m_N}^{(N)}.$$

$$\hat{P}_k = \otimes_i \hat{\sigma}_i^{(k)}$$

$$\omega_{\mathbf{m}} = \sum_k c_k d_{k,\mathbf{m}}$$

$$H = \sum_{\alpha} \hat{H}_{\alpha}$$

$$\langle \hat{H}_{\alpha} \rangle = \langle \psi | \hat{H}_{\alpha} | \psi \rangle$$

$$\mathrm{Var}(\hat{H}_{\alpha}) = \langle \psi | \hat{H}_{\alpha}^2 | \psi \rangle - \langle \psi | \hat{H}_{\alpha} | \psi \rangle^2$$

$$\mathrm{Var}(\hat{H}_{\alpha})/M_{\alpha}$$

$$\langle \psi | \hat{H} | \psi \rangle = \sum_{\alpha} \mu_{\alpha}$$

$$\mathrm{Var}[\bar{H}] = \sum_{\alpha} \mathrm{Var}[\bar{H}_{\alpha}] = \sum_{\alpha} \frac{\mathrm{Var}(\hat{H}_{\alpha})}{M_{\alpha}}.$$

$$\Pr(|\bar{H}_{\alpha} - \langle \hat{H}_{\alpha} \rangle| \geq k \mathrm{Var}^{1/2}[\bar{H}_{\alpha}]) \leq \frac{1}{k^2}$$

$$\Pr(|\bar{H}_{\alpha} - \langle \hat{H}_{\alpha} \rangle| \geq t) \leq 2e^{-2M_{\alpha}t^2/(\Delta E_{\alpha})^2}$$

$$\Delta E_{\alpha} = E_{\max}^{(\alpha)} - E_{\min}^{(\alpha)}, \text{ and } E_{\min/\max}^{(\alpha)}$$

$$\Pr(|\bar{H}_{\alpha} - \langle \hat{H}_{\alpha} \rangle| \geq k \mathrm{Var}^{1/2}[\bar{H}_{\alpha}]) \\ \leq 2 \exp \left[- \frac{k^2 \mathrm{Var}(\hat{H}_{\alpha})}{2 \mathrm{Var}(\hat{H}_{\alpha})_{\max}} \right],$$

$$\mathrm{Var}(\hat{H}_{\alpha})_{\max} = (\Delta E_{\alpha})^2/4$$

$$\Pr(|\bar{H}_{\alpha} - \mu_{\alpha}| \geq k \mathrm{Var}^{1/2}[\bar{H}_{\alpha}]) \leq \frac{\sqrt{2}}{k\pi} e^{-k^2/2}$$

$$O(e^{-k^2/2}/k)$$

$$\hat{H} = \sum_{\alpha} \hat{H}_{\alpha} \mathrm{Var}(\hat{H}_{\alpha})$$

$$M = \sum_{\alpha} M_{\alpha}$$

$$\mathrm{Var}(\hat{H}_{\alpha}) \left(\sum_{\alpha} \sqrt{\mathrm{Var}(\hat{H}_{\alpha})} \right)^2$$

$$\mathrm{Var}(\hat{H}_{\alpha})^{1/2} \leq \frac{(E_{\max}^{(\alpha)} - E_{\min}^{(\alpha)})}{2} \leq \sum_n |c_n^{(\alpha)}|$$

$$\begin{aligned}\hat{H} &= \hat{H}_1 + \hat{H}_2 \\ \hat{H}_1 &= \hat{P}_1 + a\hat{P}_2, \hat{H}_2 = (1-a)\hat{P}_2 + \hat{P}_3 \\ a \in \mathbb{R}, [\hat{P}_1, \hat{P}_2] &= [\hat{P}_2, \hat{P}_3] = 0, \text{ but } [\hat{P}_1, \hat{P}_3] \neq 0\end{aligned}$$

$$\begin{aligned}\text{Var}[\bar{H}] &= \frac{\text{Var}(\hat{H}_1)}{M_1} + \frac{\text{Var}(H_2)}{M_2} \\ &= [\text{Var}(\hat{P}_1) + a^2\text{Var}(\hat{P}_2) + 2a\text{Cov}_{1,2}]/M_1 \\ &\quad + [\text{Var}(\hat{P}_3) + (1-a)^2\text{Var}(\hat{P}_2) \\ &\quad + 2(1-a)\text{Cov}_{2,3}]/M_2\end{aligned}$$

$$\text{Var}(\hat{P}_i) = 1 - \langle \psi | \hat{P}_i | \psi \rangle^2$$

$$\text{Cov}_{i,j} = \langle \psi | \hat{P}_i \hat{P}_j | \psi \rangle - \langle \psi | \hat{P}_i | \psi \rangle \langle \psi | \hat{P}_j | \psi \rangle$$

$$\hat{H} = \sum_i w_i \hat{P}_i$$

$$\begin{aligned}\hat{H} &= \sum_{\alpha} \hat{H}_{\alpha} \\ \hat{H}_{\alpha} &= \sum_i w_{i,\alpha} \hat{P}_i\end{aligned}$$

$$\sum_{\alpha} w_{i,\alpha} = w_i \forall i \text{ and } w_{i,\alpha} = 0 \text{ for all } \hat{P}_i$$

$$\begin{aligned}\text{Var}[\bar{H}] &= \sum_{\alpha} \frac{1}{M_{\alpha}} \left(\sum_i w_{i,\alpha}^2 \text{Var}(\hat{P}_i) \right. \\ &\quad \left. + \sum_{ij} 2w_{i,\alpha} w_{j,\alpha} \text{Cov}_{i,j} \right)\end{aligned}$$

$$M = \sum_{\alpha} M_{\alpha} \text{ and } w_i = \sum_{\alpha} w_{i,\alpha} \forall i$$

$$w_{i,1} = M_1 w / (M_1 + M_2) \text{ and } w_{i,2} = M_2 w / (M_1 + M_2)$$

$$\hat{U}_{\alpha}^{\dagger} \hat{n}_p \hat{U}_{\alpha} = \hat{C}_p^{(\alpha)} = \left[\hat{C}_p^{(\alpha)} \right]^2.$$

$$\begin{aligned}\left[\hat{H}_{2e}^{(\alpha)}\right]' &= \hat{H}_{2e}^{(\alpha)} - \sum_p \epsilon_p^{(\alpha)} \hat{C}_p^{(\alpha)} \\ &= \sum_{\alpha,\beta} \left(\lambda_{pq}^{(\alpha)} - \epsilon_p^{(\alpha)} \delta_{pq}\right) \hat{C}_p^{(\alpha)} \hat{C}_q^{(\alpha)}\end{aligned}$$

$$\epsilon_p^{(\alpha)} \in \mathbb{R} \left[\hat{H}_{2e}^{(\alpha)} \right]'$$

$$\hat{H}_{1e} = \sum_p \lambda_p \hat{U}_0^{\dagger} \hat{n}_p \hat{U}_0$$



$$\hat{H}_{1e} + \sum_{\alpha} \sum_p \epsilon_p^{(\alpha)} \hat{C}_p^{(\alpha)} = \hat{U}'_0 \left[\sum_p \lambda'_p \hat{n}_p \right] \hat{U}'_0{}^\dagger.$$

$$\hat{O} = \sum_P \alpha_P \hat{P}$$

$$\|\hat{O}\|_{sh}^2 = \max_{\mu} \mathbb{E}_{\hat{B}} \mathbb{E}_{\mu(\hat{B})} \left[\sum_{P,Q} \alpha_P \alpha_Q f(\hat{B}, \hat{P}) f(\hat{B}, \hat{Q}) \right. \\ \left. \cdot \mu(\hat{B}, \text{supp}(\hat{P})) \mu(\hat{B}, \text{supp}(\hat{Q})) \right]$$

$$\|\hat{P}\|_{sh} = 3^l, \, l = |\text{supp}(\hat{P})|$$

$$\|\hat{O}\|_{sh} = 4^l \|\hat{O}\|_{\infty}$$

$$\bar{H} = \sum_P \alpha_P \sum_{i=1}^M \frac{f(\hat{B}^{(i)}, \hat{P}, \beta)}{M} \mu(\hat{B}^{(i)}, \text{supp}(\hat{P}))$$

$$f(\hat{B},\hat{P},\beta) \, = \prod_{j=1}^K f_j(\hat{B}_j,\hat{\sigma}_j,\beta_j)$$

$$f_j(\hat{B}_j,\hat{\sigma}_j) \, = \begin{cases} 1 & \text{if } \hat{\sigma}_j = \hat{1} \\ \beta_j(\hat{B}_j)^{-1} & \text{if } \hat{B}_j = \hat{\sigma}_j \neq \hat{1} \\ 0 & \text{otherwise} \end{cases}$$

$$\hat{P} = \otimes_{j=1}^N \hat{\sigma}_j$$

$$\hat{H} = \sum_j \alpha_j \hat{U}_j$$

$$\lambda = \sum_j |\alpha_j|$$

$$\Delta E = E_{\max} - E_{\min} \{\hat{S}_k = s_k\}_{k=1}^K$$

$$\hat{N}_e = \sum_p \hat{n}_p$$

$$\hat{K}(\vec{\xi}) = \left(\xi_0 + \sum_{pq} \xi_{pq} \hat{E}_{pq} \right) (\hat{N}_e - N_e)$$

$$M_{\rho}(\epsilon) = \frac{1}{\epsilon^2} \sum_{\alpha} \frac{\text{Tr}(\hat{H}_{\alpha}^2 \hat{\rho}) - \text{Tr}(\hat{H}_{\alpha} \hat{\rho})^2}{m_{\alpha}}$$

$$\hat{\rho} = \frac{1}{N_s} \sum_{k=1}^{N_s} |C_k\rangle\langle C_k|$$

$$D_{q_1\cdots q_k}^{p_1\cdots p_k}=\mathrm{Tr}(\hat{a}_{p_1}^\dagger\cdots \hat{a}_{p_k}^\dagger \hat{a}_{q_k}\cdots \hat{a}_{q_1}\hat{\rho})$$

$$O\left[\binom{N}{k}k^{3/2}\log N/\epsilon^2\right]$$

$$O[N^k\log N/\epsilon^2]$$

$$\begin{aligned} S_{pq} &= \mathrm{Tr}(\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_q \hat{a}_p \hat{U} \hat{\rho} \hat{U}^\dagger) \\ &= \sum_{ijkl} u_{pi} u_{qj} u_{ql} u_{pk} D_{ij}^{kl} \end{aligned}$$

$$|\psi(\vec{\theta})\rangle=\prod_j e^{\mathrm{i}\theta_j\hat{G}_{k_j}}|\psi_0\rangle=\hat{U}(\vec{\theta})|\psi_0\rangle.$$

$$E(\vec{\theta})=\langle\psi|\hat{U}^\dagger(\vec{\theta})\hat{H}\hat{U}(\vec{\theta})|\psi\rangle.$$

$$\frac{\partial E}{\partial \theta} = \sum_{l=1}^{N_t} c_l \langle \psi | U_2^\dagger e^{\mathrm{i}(\theta + s_l)\hat{G}} \hat{U}_1^\dagger \hat{H} \hat{U}_1 e^{-\mathrm{i}(\theta + s_l)\hat{G}} \hat{U}_2 | \psi \rangle$$

$$\left.\frac{\partial}{\partial \theta} \langle \psi | e^{-\mathrm{i} \theta \hat{G}_k} \hat{H} e^{\mathrm{i} \theta \hat{G}_k} | \psi \rangle \right|_{\theta=0} = \mathrm{i} \langle \psi | [\hat{G}_k, \hat{H}] | \psi \rangle.$$

$$\boldsymbol{H}\vec{c}=\boldsymbol{S}\boldsymbol{E}\vec{c}$$

$$\boldsymbol{H}_{\mu\nu}=\langle\phi_{\mu}|\hat{H}|\phi_{\nu}\rangle,$$

$$\boldsymbol{S}_{\mu\nu}=\langle\phi_{\mu}\mid\phi_{\nu}\rangle$$

$$\sum_{\mu}c_{\mu}|\phi_{\mu}\rangle$$

$$|\phi_{\mu}\rangle=\hat{O}_{\mu}|\psi_0\rangle$$

$$\hat{O}_{\mu}\in\{\hat{E}_{pq}\}$$

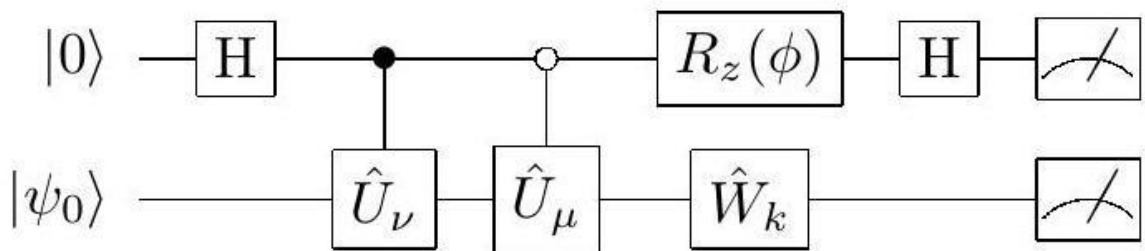
$$\boldsymbol{H}_{\mu\nu}=\langle\psi_0|\hat{O}_{\mu}^{\dagger}\hat{H}\hat{O}_{\nu}|\psi_0\rangle$$

$$\boldsymbol{S}_{\mu\nu}=\langle\psi_0|\hat{O}_{\mu}^{\dagger}\hat{O}_{\nu}|\psi_0\rangle$$

$$\hat{A}_n\in\{\hat{O}_{\mu}^{\dagger}\hat{H}\hat{O}_{\nu}\}\cup\{\hat{O}_{\mu}^{\dagger}\hat{O}_{\nu}\}$$

$$\hat{A}_n=\sum_{\alpha}\hat{U}_{\alpha}^{\dagger}p_n^{(\alpha)}(\hat{z}_1,\ldots,\hat{z}_N)\hat{U}_{\alpha}.$$

$$|\phi_{\mu}\rangle=\hat{U}_{\mu}|\psi_0\rangle$$



$$\mathrm{Re}\langle\psi|\hat{H}_k|\psi\rangle(\phi=0)$$

$$\mathrm{Im}\langle\psi|\hat{H}_k|\psi\rangle(\phi=\pi/2)$$

$$R_z(\phi)=e^{-\mathrm{i}\phi\hat{Z}/2}$$

$$\hat{H}=\sum_k c_k \hat{V}_k.$$

$$\boldsymbol{H}_{\mu\nu}=\sum_k c_k\langle\psi_0|\hat{U}_\mu^\dagger\hat{V}_k\hat{U}_\nu|\psi_0\rangle$$

$$\boldsymbol{S}_{\mu\nu}=\langle\psi_0|\hat{U}_\mu^\dagger\hat{U}_\nu|\psi_0\rangle$$

$$\hat{N}_e=\sum_p \hat{n}_p$$

$$\tilde{H}=(\hat{x}+\mathrm{i}\hat{y})\otimes\hat{H}$$

$$\hat{H}=\sum_k\hat{H}_k=\sum_k\hat{W}_k^\dagger\hat{D}_k\hat{W}_k,$$

$$|\varphi_{\mu\nu}\rangle=\frac{1}{\sqrt{2}}(|0\rangle\hat{U}_\mu|\psi_0\rangle+|1\rangle\hat{U}_\nu|\psi_0\rangle)$$

$$\boldsymbol{H}_{\mu\nu}=\sum_k\langle\varphi_{\mu\nu}|(\hat{x}+\mathrm{i}\hat{y})\otimes\hat{H}_k|\varphi_{\mu\nu}\rangle$$

$$\boldsymbol{S}_{\mu\nu}=\langle\varphi_{\mu\nu}|(\hat{x}+\mathrm{i}\hat{y})\otimes\hat{1}|\varphi_{\mu\nu}\rangle$$

$$\{\hat{x}\otimes\hat{H}_k\}\{\mathrm{i}\hat{y}\otimes\hat{H}_k\}\tilde{H}$$

$$\hat{G}_{pq}(\phi_{pq})(\,q=p\pm1\,)i(\hat{x}_p\hat{y}_q-\hat{y}_p\hat{x}_q)/2$$

$$U(1)=\{\exp\left(i\theta\hat{N}_e\right)\,|\,\theta\in[0,2\pi)\}$$

$$\hat{p}=(-1)^{\hat{N}_e}$$

$$\hat{p}^2=\hat{1}$$

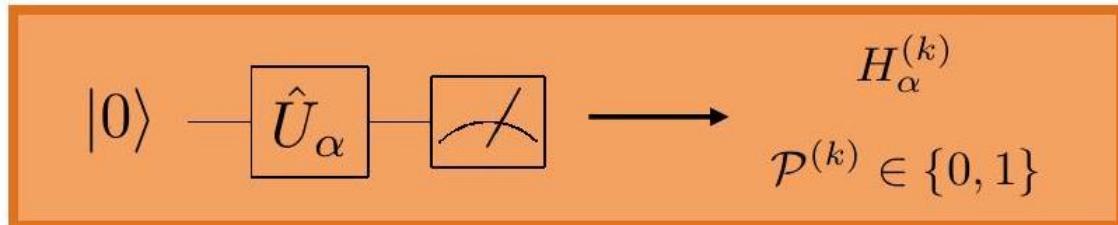
$$\hat{\mathcal{P}}\hat{\rho}'\hat{\mathcal{P}}/\mathrm{Tr}(\hat{\rho}'\hat{\mathcal{P}})$$

$$\langle\hat{H}\rangle_{\mathrm{sv}}=\frac{\mathrm{Tr}(\hat{\rho}'\hat{\mathcal{P}}\hat{H})}{\mathrm{Tr}(\hat{\rho}'\hat{\mathcal{P}})}.$$

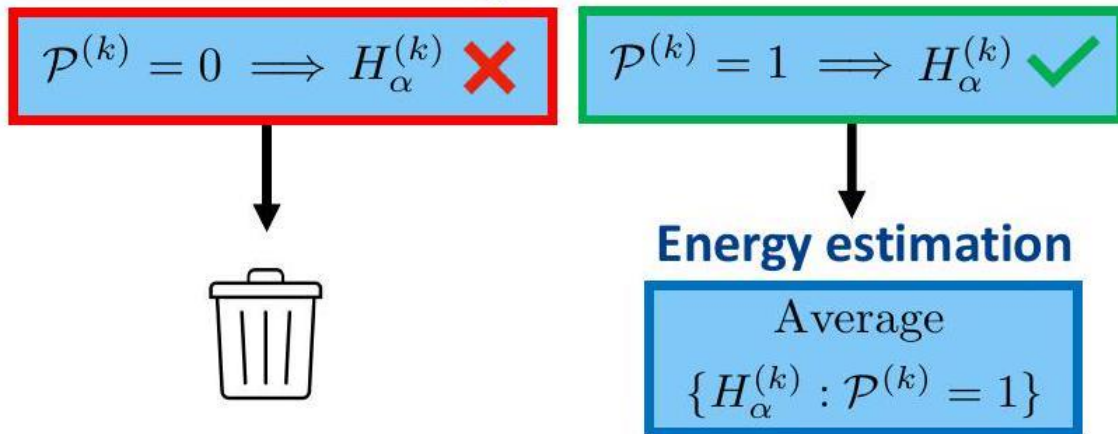
$$\hat{H}=\sum_{\alpha}\hat{H}_{\alpha}$$

$$\bar{H}_{\alpha, \mathcal{P}} = \frac{\sum_{k=1}^{M_\alpha} H_\alpha^{(k)} \mathcal{P}^{(k)}}{\sum_{k=1}^{M_\alpha} \mathcal{P}^{(k)}}$$

Quantum measurement

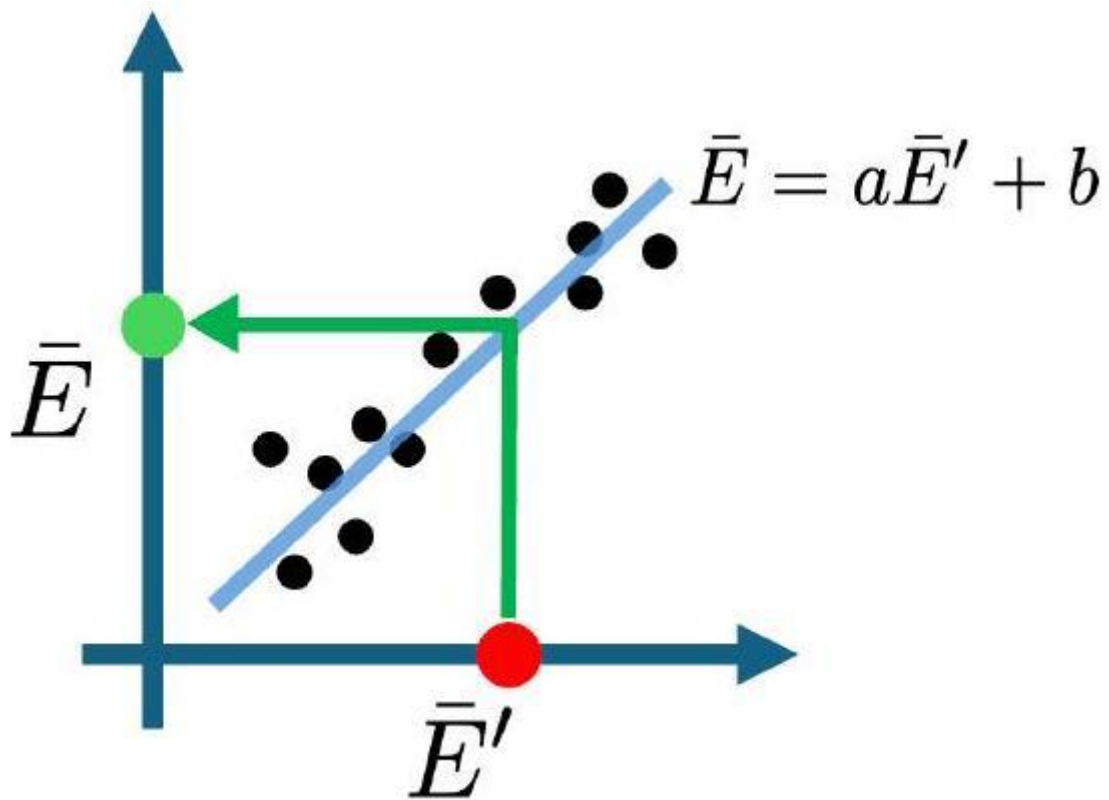


Classical post-selection



$$\bar{H}_{\alpha, \mathcal{P}} = \frac{1}{N_1} \sum_{k: \mathcal{P}^{(k)}=1} H_\alpha^{(k)},$$

$$\prod_{i=1}^N \hat{z}_i \{\hat{U}_\alpha\} \hat{N}_e \rightarrow \sum_{i=1}^N (1 - \hat{z}_i)/2$$



$$\langle \psi | \hat{H}_\alpha | \psi \rangle \hat{H}_\alpha = \hat{U}_\alpha^\dagger p(\hat{z}_1, \dots, \hat{z}_N) \hat{U}_\alpha$$

$$\{|\phi_i\rangle\}|\hat{U}_\alpha\psi\rangle\{\langle\phi_i|p(\hat{z}_1,\dots,\hat{z}_N)|\phi_i\rangle\}$$

$$\hat{h}=\sum_{ij}h_{ij}\hat{a}_i^\dagger\hat{a}_j+\mu_{ij}\hat{a}_i^\dagger\hat{a}_j^\dagger-\mu_{ij}^*\hat{a}_i\hat{a}_j\{h_{ij},\mu_{ij}\}$$

$$\mathcal{V}' = \Lambda \circ \mathcal{V}$$

$$\mathcal{V}'(\hat{\rho}) \rightarrow \mathbb{E}_{\mathcal{U} \in \mathcal{G}} \big[\mathcal{U}^\dagger \circ \Lambda \circ \mathcal{U} \circ \mathcal{V}(\hat{\rho}) \big] = \Lambda_{\mathcal{G}} \circ \mathcal{V}(\hat{\rho})$$

$$\Lambda_{\mathcal{G}}(\hat{\rho}) = \sum_{\lambda} c_{\lambda} \mathcal{P}_{\mathcal{G}}^{\lambda}(\hat{\rho}).$$

$$\mathcal{V}' = \Lambda^{(1)} \circ \mathcal{V}^{(1)} \circ \Lambda^{(2)} \circ \mathcal{V}^{(2)} \circ \ldots$$

$$\mathcal{V}' \equiv \Lambda_{\mathrm{eff}} \circ \mathcal{V}^{(1)} \circ \mathcal{V}^{(2)} \circ \ldots$$

$$\mathcal{M}' = \mathcal{M} \circ \Lambda_{\mathrm{eff}}$$

$$\hat{H} \text{ as } \text{Tr}\left(\hat{H}\cdot\left[\mathcal{M}'_{\mathcal{G}}\right]^{-1}\circ\mathcal{U}^\dagger(|\vec{z}\rangle\langle\vec{z}|)\right)$$

$$|q_0\rangle|\Phi\rangle=|q_0\rangle\sum_n c_n|\Psi_n\rangle,$$

$$\hat{H}|\Psi_n\rangle=E_n|\Psi_n\rangle$$

$$\hat{U} = \exp\left[it \hat{p} \otimes \hat{H} \right]$$

$$\exp [i\Delta\hat{p}]|q_0\rangle = |q_0 + \Delta\rangle$$

$$\hat{U}|q_0\rangle|\Phi\rangle = \sum_n c_n|q_0 + tE_n\rangle|\Psi_n\rangle,$$

$$\langle q_0 + tE_m | q_0 + tE_n \rangle = \delta_{nm} |q_0 + tE_n\rangle |\Psi_n\rangle |c_n|^2$$

$$\begin{aligned} e^{i\Delta\hat{p}}f(x) &= \hat{U}_{FT}^\dagger [\hat{U}_{FT} e^{i\Delta\hat{p}} \hat{U}_{FT}^\dagger] \hat{U}_{FT} f(x) \\ \hat{U}_{FT} e^{i\Delta\hat{p}} \hat{U}_{FT}^\dagger &= e^{2\pi i y \Delta} \\ \hat{U}_{FT} f(x) &= \int dx e^{2\pi i y x} f(x) = F(y) \end{aligned}$$

$$|\Psi\rangle = a|\phi\rangle + \sqrt{1-a^2}|\phi^\perp\rangle,$$

$$\hat{W} = -\hat{R}_\Psi \hat{R}_\phi, \hat{R}_\Psi = 1 - 2|\Psi\rangle\langle\Psi|$$

$$\hat{R}_\phi = 1 - 2|\phi\rangle\langle\phi| \{|\phi\rangle, |\phi^\perp\rangle\}$$

$$\begin{aligned} \mathbf{W} &= \begin{pmatrix} \langle\phi|W|\phi\rangle & \langle\phi|W|\phi^\perp\rangle \\ \langle\phi^\perp|W|\phi\rangle & \langle\phi^\perp|W|\phi^\perp\rangle \end{pmatrix} \\ &= \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \end{aligned}$$

$$|\Psi\rangle = \sin{(\theta/2)}|\phi\rangle + \cos{(\theta/2)}|\phi^\perp\rangle$$

$$a=\sin{(\theta/2)}$$

$$\hat{W}^k|\Psi\rangle = \sin{[\theta(2k+1)/2]}|\phi\rangle + \cos{[\theta(2k+1)/2]}|\phi^\perp\rangle$$

$$\begin{aligned} \hat{P} &= \hat{\mathcal{P}}_+ - \hat{\mathcal{P}}_- \\ \hat{\mathcal{P}}_{\pm} &= \sum_i |i_{\pm}\rangle\langle i_{\pm}| \end{aligned}$$

$$|\Psi\rangle = \sin{(\theta/2)}|\Psi_{-}\rangle + \cos{(\theta/2)}|\Psi_{+}\rangle,$$

$$|\Psi_{\pm}\rangle = \hat{\mathcal{P}}|\Psi\rangle/\|\hat{\mathcal{P}}|\Psi\rangle\|$$

$$\theta, \langle\Psi|\hat{P}|\Psi\rangle = \cos^2{(\theta/2)} - \sin^2{(\theta/2)} = \cos{(\theta)}$$

$$\{|\Psi_{\pm}\rangle\} \text{or } \{|\Psi\rangle, \hat{P}|\Psi\rangle\} \{|\Psi_{\pm}\rangle\} \hat{W}$$

$$|\Psi^\perp\rangle = \frac{1}{\sqrt{1-|\langle\hat{U}\rangle|^2}}[\hat{U}|\Psi\rangle - \langle\hat{U}\rangle|\Psi\rangle]$$

$$\mathbf{W} = \begin{pmatrix} 2|\bar{U}|^2-1 & 2\bar{U}\sqrt{1-|\bar{U}|^2} \\ -2\bar{U}^*\sqrt{1-|\bar{U}|^2} & 2|\bar{U}|^2-1 \end{pmatrix}$$

$$\bar{U} = \langle\Psi|\hat{U}|\Psi\rangle$$

$$e^{\pm i\theta}\cos{(\theta)} = 2|\bar{U}|^2-1$$

$$\hat{U}_1 = c - \hat{U}$$

$$\hat{U}_2 = e^{i\hat{Z}_a\pi/4}\hat{U}_1$$

$$\begin{aligned} |\langle \Psi, +_a | \hat{U}_1 | \Psi, +_a \rangle| &= |1 + \bar{U}|/2 \\ |\langle \Psi, +_a | \hat{U}_2 | \Psi, +_a \rangle| &= |1 - i\bar{U}|/2 \end{aligned}$$

$$\hat{U}_L = \begin{pmatrix} \hat{\partial}/c & \hat{U}_{01} \\ \hat{U}_{10} & \hat{U}_{11} \end{pmatrix}$$

$$R_\Psi = 1 - 2|\Psi,0\rangle\langle\Psi,0|$$

$$R_{U\Psi} = 1 - 2\hat{U}_L|\Psi,0\rangle\langle\Psi,0|\hat{U}_L^\dagger$$

$$\Pr(d \mid k, \phi) = \frac{1}{2}[1 + d\cos(k\theta + \phi)]$$

$$\bar{P} = \langle \Psi | \hat{P} | \Psi \rangle$$

$$\hat{W} = \hat{R}_\Psi \hat{P}$$

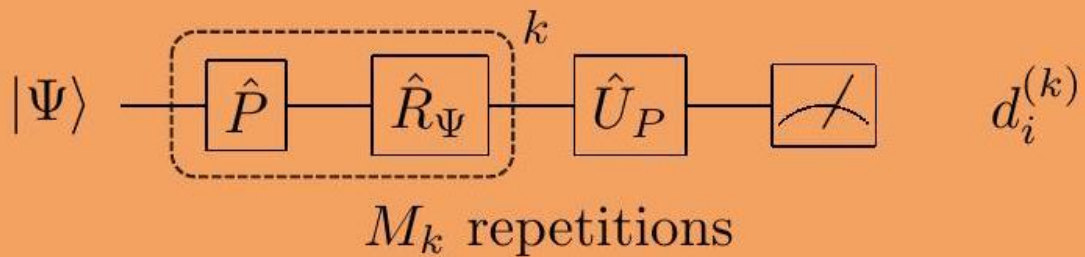
$$\hat{R}_\Psi = 1 - 2|\Psi\rangle\langle\Psi|$$

$$|k\rangle = \hat{W}^k|\Psi\rangle$$

$$\langle k|\hat{P}|k\rangle = T_{2k+1}(\bar{P})$$

$$\begin{aligned} |k=1\rangle &= (\hat{P} - 2\bar{P})|\Psi\rangle \\ \langle k=1|\hat{P}|k=1\rangle &= 4\bar{P}^3 - 3\bar{P} \\ &= T_3(\bar{P}) \end{aligned}$$

$$\begin{array}{ccc} \hat{W} = \hat{R}_\Psi \hat{P} & \longrightarrow & M_k \text{ samples of} \\ \bar{P} = \langle \Psi | \hat{P} | \Psi \rangle & & T_{2k+1}(\bar{P}) \end{array}$$



Classical: Maximum Likelihood Estimation

$$\bar{\theta} = \arg \max_{\theta} \prod_k \prod_{i=1}^{M_k} \Pr(d_i^{(k)} | \theta, k)$$

$$\bar{P} = \cos(\bar{\theta})$$

$$T_{2k+1}(\bar{P}) = \langle \Psi | (\hat{W}^k)^\dagger \hat{P} \hat{W}^k | \Psi \rangle$$

$$\hat{W} = \hat{R}_\Psi \hat{P}$$

$$d_i^{(k)} \in \{-1,1\}$$

$$\Pr\left(d_i^{(k)} \mid \theta, k\right)$$

$$\mathrm{Var}(x) = \mathrm{Var}(y)[df^{-1}(y)/dy]^2$$

$$\mathrm{Var}_k(\bar{P}) = \frac{\mathrm{Var}_0(\bar{P})}{(2k+1)^2}$$

$$\mathrm{Var}_0(\bar{P}) = 1 - \bar{P}^2$$

$$I_F = \sum_d \frac{1}{\Pr(d \mid \bar{P})} \left(\frac{\partial}{\partial \bar{P}} \Pr(d \mid \bar{P}) \right)^2,$$

$$\Pr(d \mid \theta, k) = \frac{1}{2} (1 + d \cos [(2k+1)\theta]).$$

$$|\vec{\sigma}\rangle\rangle = |\hat{\sigma}_1 \otimes \cdots \otimes \hat{\sigma}_N\rangle\rangle, \hat{\sigma}_i \in \{\hat{\sigma}_0, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\}$$

$$\hat{\sigma}_0 = \hat{1}/\sqrt{2}, \hat{\sigma}_x = \hat{x}/\sqrt{2}, \hat{\sigma}_y = \hat{y}/\sqrt{2}, \hat{\sigma}_z = \hat{z}/\sqrt{2}$$

$$\langle\langle \vec{\sigma}_a \mid \vec{\sigma}_b \rangle\rangle = \mathrm{Tr}(\vec{\sigma}_a^\dagger \vec{\sigma}_b)$$

$$[|\hat{\rho}\rangle\rangle]_a = \langle\langle \vec{\sigma}_a \mid \hat{\rho} \rangle\rangle = \mathrm{Tr}(\vec{\sigma}_a^\dagger \hat{\rho})$$

$$[M]_{ab} = \langle\langle \vec{\sigma}_a \mid \mathcal{M}(\vec{\sigma}_b) \rangle\rangle = \mathrm{Tr}\left(\vec{\sigma}_a^\dagger \mathcal{M}(\vec{\sigma}_b)\right).$$

$$\Gamma_{\vec{\mu}} = \prod_{i=1}^k \hat{\gamma}_{\mu_i}$$

$$\mathbf{M} = \mathrm{diag}[1,0,0,1]^{\otimes N}$$

$$\mathcal{D}(\hat{\rho}) = (1-p)\hat{\rho} + p\hat{\sigma}_0^{\otimes N}$$

$$\mathcal{D}^{-1}(\hat{\rho}) = (1-2p)^{-1}[(1-p)\hat{\rho} - p\hat{\sigma}_0^{\otimes N}]$$



$$|0\rangle\langle 0|=(\hat{1}+\hat{z})/\sqrt{2} \text{ and } |1\rangle\langle 1|=(\hat{1}-\hat{z})/\sqrt{2}$$

$$\mathsf{M} = \left(\left| \hat{\sigma}_0 \right\rangle \right) \left\langle \left\langle \hat{\sigma}_0 \right| + \left| \hat{\sigma}_z \right\rangle \right\rangle \left\langle \left\langle \hat{\sigma}_z \right| \right\rangle^{\otimes N}$$

$$\mathbb{E}_{U\in\mathcal{G}}[\mathsf{U}^\dagger\mathsf{M}\mathsf{U}]|\hat{\rho}\rangle\rangle=\mathsf{M}_{\mathcal{G}}|\hat{\rho}\rangle\rangle$$

$$\mathsf{M}_{\mathcal{G}} = \sum_{\lambda} \frac{\mathrm{Tr}(\mathsf{M}_{\mathcal{G}} \Pi_{\mathcal{G}}^{\lambda})}{d_{\lambda}} \Pi_{\mathcal{G}}^{\lambda}$$

$$\mathcal{H}_{\lambda},\,\Pi_{\mathcal{G}}^{\lambda}\Pi_{\mathcal{G}}^{\lambda'}=\delta_{\lambda\lambda'}\Pi_{\mathcal{G}}^{\lambda}$$

$$d_{\lambda}=\mathrm{Tr}(\Pi_{\mathcal{G}}^{\lambda})$$

$$\mathcal{H}_{\lambda} \cdot \mathsf{M}_{\mathcal{G}}$$

$$\mathrm{Tr}(\mathsf{M}_{\mathcal{G}}\Pi_{\mathcal{G}}^{\lambda})\neq 0, \forall \lambda$$

$$\mathsf{M}_{\mathcal{G}}^{-1} = \sum_{\lambda} \frac{d_{\lambda}}{\mathrm{Tr}(\mathsf{M}_{\mathcal{G}}\Pi_{\mathcal{G}}^{\lambda})} \Pi_{\mathcal{G}}^{\lambda}$$

$$\begin{aligned} \mathrm{Tr}(\hat{O}\hat{\rho}) &\equiv \left\langle \left\langle \hat{O}^\dagger \mid \hat{\rho} \right\rangle \right\rangle \\ &= \mathbb{E}_{u\in\mathcal{G}} \left[\left\langle \left\langle \hat{O}^\dagger \mid \mathsf{M}_{\mathcal{G}}^{-1} \mathsf{U}^\dagger \mathsf{M} \mathsf{U} \mid \hat{\rho} \right\rangle \right\rangle \right] \\ &\equiv \mathbb{E}_{u\in\mathcal{G}} \left[\sum_{\vec{z}\in\{1,-1\}^N} \mathrm{Tr}(\hat{O} \cdot \mathcal{M}_{\mathcal{G}}^{-1} \circ \mathcal{U}^\dagger(|\vec{z}\rangle\langle\vec{z}|)) \right. \\ &\quad \left. \times \langle \vec{z} | \mathcal{U}(\hat{\rho}) | \vec{z} \rangle \right] \end{aligned}$$

$$\mathrm{Tr}(\hat{O} \cdot \mathcal{M}_{\mathcal{G}}^{-1} \circ \mathcal{U}^\dagger(|\vec{z}\rangle\langle\vec{z}|)) \langle \vec{z} | \hat{U} \hat{\rho} \hat{U}^\dagger | \vec{z} \rangle$$

$$\mathrm{Tr}(\hat{O} \cdot \mathcal{M}_{\mathcal{G}}^{-1} \circ \mathcal{U}^\dagger(|\vec{z}\rangle\langle\vec{z}|))$$

$$\mathsf{M}_{\mathcal{C}l(N)} = \frac{1}{|\mathcal{C}l(N)|} \sum_{U \in \mathcal{C}l(N)} \mathsf{U}^\dagger \mathsf{M} \mathsf{U}$$

$$\mathcal{H}\colon=\mathrm{span}\{\left|\vec{\sigma}_0\right\rangle\}$$

$$\mathcal{H}^{(1)}=\mathcal{H}_{d^2}\setminus\mathcal{H}^{(0)}$$

$$\Pi_0=|\vec{\sigma}_0\rangle\langle\vec{\sigma}_0|,\Pi_1=\mathsf{I}-\Pi_0$$

$$c_0=\frac{\mathrm{Tr}(\mathsf{M}\Pi_0)}{d_0}=1$$

$$c_1=\frac{\mathrm{Tr}(\mathsf{M}\Pi_1)}{d_1}=\frac{d-1}{d^2-1}=\frac{1}{d+1}$$

$$\mathsf{M}_{\mathcal{C}l(N)}^{-1}=\Pi_0+(d+1)\Pi_1=(d+1)\mathsf{I}-d\Pi_0$$

$$\mathbf{M}_{\text{Cl}(N)}^{-1}\mathbb{E}_u[\mathbf{U}^\dagger\mathbf{M}\mathbf{U}]|\hat{\rho}\rangle\rangle=(d+1)\mathbb{E}_u[\mathbf{U}^\dagger\mathbf{M}\mathbf{U}]|\hat{\rho}\rangle\rangle\\-d\mathbb{E}_u[\Pi_0\mathbf{U}^\dagger\mathbf{M}\mathbf{U}]|\hat{\rho}\rangle\rangle$$

$$\Pi_0\mathbf{U}^\dagger\mathbf{M}\mathbf{U}|\hat{\rho}\rangle\rangle=|\vec{\sigma}_0\rangle\rangle\left\langle\left\langle\vec{\sigma}_0|\mathbf{U}^\dagger\mathbf{M}\mathbf{U}|\hat{\rho}\right\rangle\right\rangle\\ \equiv\frac{1}{d}\hat{1}^{\otimes N}\text{Tr}(\hat{1}^{\otimes N}\cdot\mathcal{U}^\dagger\circ M\circ\mathcal{U}(\hat{\rho}))\\ =\frac{1}{d}\hat{1}^{\otimes N}$$

$$\hat{\rho}=(d+1)\mathbb{E}_u\left[\sum_{\vec{z}\in\{1,-1\}^N}\mathcal{U}^\dagger(|\vec{z}\rangle\langle\vec{z}|)\langle\vec{z}|\mathcal{U}(\hat{\rho})|\vec{z}\rangle\right]-\hat{1}^{\otimes N}.$$

$$p=d/(d+1)$$

$$|\text{Cl}(N)|=2^{N^2+2N}\prod_{j=1}^N(4^j-1)$$

$$\text{Cl}(1)\otimes\text{Cl}(1)$$

$$\mathcal{H}^{(0)}\otimes\mathcal{H}^{(0)},\mathcal{H}^{(0)}\otimes\mathcal{H}^{(1)},\mathcal{H}^{(1)}\otimes\mathcal{H}^{(0)}$$

$$\mathcal{H}^{(1)}\otimes\mathcal{H}^{(1)}$$

$$\mathcal{H}^{(1)}\otimes\mathcal{H}^{(1)}$$

$$\vec{h}=(h_1,\ldots,h_N)\in\{0,1\}^N$$

$$\mathcal{H}^{(\vec{h})}=\otimes_{i=1}^N\mathcal{H}^{(h_i)}$$

$$\mathcal{H}^{(0)}=\text{span}\{|\hat{\sigma}_0\rangle\rangle\}$$

$$\mathcal{H}^{(1)}=\mathcal{H}_{2^2}\setminus\mathcal{H}^{(0)}$$

$$\Pi^{(\vec{h})}=\otimes_{i=1}^N\Pi^{(h_i)}\text{Cl}(1)^{\otimes N}$$

$$\mathbf{M}_{\text{Cl}(1)^{\otimes N}}^{-1}=\bigotimes_{j=1}^N\left(\Pi^{(0)}+3\Pi^{(1)}\right)=\sum_{\vec{h}\in\{0,1\}^N}3^{|\vec{h}|}\Pi^{(\vec{h})}$$

$$\hat{\rho}=\mathbb{E}_u\left[\sum_{\vec{z}\in\{1,-1\}^N}\bigotimes_{j=1}^N\left(3\mathcal{U}_j^\dagger(|z_j\rangle\langle z_j|)-\hat{1}\right)\langle\vec{z}|\mathcal{U}(\hat{\rho})|\vec{z}\rangle\right]$$

$$\mathcal{U}=\bigotimes_{j=1}^N\mathcal{U}_j$$

$$\mathcal{U}_i\in\text{Cl}(1)\text{ and }|\vec{z}\rangle=|z_1z_2\ldots z_N\rangle$$

$$\hat{P}=\otimes_{j=1}^N\hat{\sigma}_j$$

$$\mathrm{Tr}(\hat{\rho}\hat{P}) = \mathbb{E}_u[\sum_z \prod_{i=1}^N (3\langle z_j|\mathcal{U}_j(\hat{\sigma}_j)|z_j\rangle - \mathrm{Tr}(\hat{\sigma}_j)) \langle z|\mathcal{U}(\hat{\rho})|z\rangle]$$

$$\left(3\langle z_j|\mathcal{U}_j(\hat{\sigma}_j)|z_j\rangle - \mathrm{Tr}(\hat{\sigma}_j)\right)f_j(\hat{B}_j,\hat{\sigma}_j)$$

$$\hat{U}(e^A)=\exp\left(-\frac{1}{4}\sum_{\mu,\nu=0}^{2N-1}A_{\mu\nu}\hat{\gamma}_{\mu}\hat{\gamma}_{\nu}\right),$$

$$\hat{U}(e^A)^\dagger(\hat{\gamma}_\mu)=\sum_{\nu=0}^{2N-1}(e^A)_{\mu\nu}\hat{\gamma}_\nu$$

$$\mathcal{H}^{(k)} = \text{span}(\{\Gamma_{\vec{\mu}}\colon |\vec{\mu}| = k\}), k = 1, \dots, 2N.$$

$$U(e^A)\in \mathrm{FGU}(N)\cap \mathrm{Cl}(N)\colon=\mathrm{cFGU}(N),e^A$$

$$\mathcal{H}^{(\text{even})}=\bigoplus_{k=0}^N\mathcal{H}^{(2k)}$$

$$\mathsf{M}_{\text{cFGU}}=\sum_{k=0}^N\lambda_{2k}\Pi_{2k},\lambda_{2k}=\binom{N}{k}/\binom{2N}{2k}$$

$$|\psi(\vec{\theta})\rangle\langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle$$

$$H(s) = (1-s)H_0 + sH_1, s \in [0,1]$$

$$\hat{H}_{mol}(\vec{r})\psi(\vec{r},t)=E\psi(\vec{r},t)$$

$$\hat{H}_{mol}=-\sum_i\frac{\nabla_{\vec{R}_i}^2}{2M_i}-\sum_i\frac{\nabla_{\vec{r}_i}^2}{2}-\sum_{i,j}\frac{Z_i}{|\vec{R}_i-\vec{r}_j|}+\sum_{i,j>i}\frac{Z_iZ_j}{|\vec{R}_i-\vec{R}_j|}+\sum_{i,j>i}\frac{1}{|\vec{r}_i-\vec{r}_j|},$$

$$\hat{H}_{\rm mol}=\hat{H}_{\rm nucl}\left(\vec{R}\right)+\hat{H}_{\rm elec}\left(\vec{R},\vec{r}\right).$$

$$\psi(\vec{R},\vec{r})=\phi_{\rm nucl}\left(\vec{R}\right)\chi_{\rm elec}\left(\vec{R},\vec{r}\right),$$

$$\hat{H}_{\rm elec}\chi_{\rm elec}\left(\vec{R},\vec{r}\right)=E_{\rm elec}\left(\vec{R}\right)\chi_{\rm elec}\left(\vec{R},\vec{r}\right)$$

$$\hat{H}_{\rm elec}=-\sum_i\frac{\nabla_{\vec{r}_i}^2}{2}-\sum_{i,j}\frac{Z_i}{|\vec{R}_i-\vec{r}_j|}+\sum_{i,j>i}\frac{1}{|\vec{r}_i-\vec{r}_j|}.$$

$$(\hat{H}_{nucl}+E_{\rm elec}\left(\vec{R}\right))\phi_{\rm nucl}\left(\vec{R}\right)=E\phi_{\rm nucl}\left(\vec{R}\right),$$

$$E_T=\frac{\int\,\mathrm{d}\vec{r}^{3N}\Psi_T(\vec{r})H(\vec{r})\Psi_T^*(\vec{r})}{\int\,\mathrm{d}\vec{r}^{3N}\Psi_T(\vec{r})\Psi_T^*(\vec{r})}$$

$$|\Psi_{\text{MPS}}\rangle=\sum_{\{\alpha\}}\mathbf{A}^{\alpha_1}\mathbf{A}^{\alpha_2}\dots\dots\mathbf{A}^{\alpha_n}|\alpha_1\alpha_2\cdots\alpha_n\rangle$$

$$i\frac{\partial}{\partial t}\Psi(\vec{r},t)=H\Psi(\vec{r},t)$$

$$\Psi(\vec{r},t)=\exp{(-iHt)}\Psi(\vec{r},0)$$

$$\Psi(\vec{r},t)=\sum_j c_j \exp{(-iE_jt)}\psi_j(\vec{r})$$

$$|\psi\rangle=\sum_{i_1,i_2,\cdots,i_n\in\{0,1\}}a_{i_1i_2\cdots i_n}|i_1\rangle\otimes|i_2\rangle\otimes\cdots\otimes|i_n\rangle.$$

$$\sum_i \psi_i |i\rangle$$

$$H_{2q}=\sum_{p,q}h_{pq}a_p^\dagger a_q+\sum_{p,q,r,s}h_{pqrs}a_p^\dagger a_q^\dagger a_r a_s$$

$$\{a_i,a_j^\dagger\}=a_ia_j^\dagger+a_j^\dagger a_i=\delta_{ij} \text{ and } \{a_i,a_j\}=\{a_i^\dagger,a_j^\dagger\}=0$$

$$X=\begin{pmatrix}0&1\\1&0\end{pmatrix},Y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},Z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

$$H_{k-local}=\sum_i c_i \sigma_{i,1} \sigma_{i,2} \cdots \sigma_{i,k}$$

$$|\psi_j\rangle|0\rangle\mapsto|\psi_j\rangle|\tilde{\varphi}_j\rangle,$$

$$|\phi\rangle=\sum_j\beta_j|\psi_j\rangle$$

$$\sum_j \beta_j |\psi_j\rangle |\tilde{\varphi}_j\rangle$$

$$|\psi(t)\rangle=e^{-iHt}|\psi_0\rangle$$

$$\vec{q}'=U_{Dus}\vec{q}+\vec{d}$$

$$a'^{\dagger}=\hat{U}_{Dok}^{\dagger}a^{\dagger}\hat{U}_{Dok},$$

$$\hat{U}_{Dok}=\hat{S}_{\Omega}^{\dagger}\hat{R}_U\hat{S}_{\Omega}\hat{D}_{\delta}$$

$$FCP(\omega)=\sum_{\mathbf{m}}\left|\left\langle\mathbf{m}|U_{Dok}|0\right\rangle\right|^2\delta\left(\omega_{\text{vib}}-\sum_k^N\omega'_km_k\right)$$

$$\mathrm{perm}(M)=\sum_{\sigma\in S_n}\prod_{i=1}^nm_{i,\sigma(i)}$$

$$U(t)=e^{-iHt}$$

$$H=\sum_{j=1}^{\ell}H_j e^{-iH_j\Delta t}$$

$$U(t) \approx \left(e^{-iH_1 t/n} \dots e^{-iH_\ell t/n} \right)^n O(\ell \tau^2/\epsilon) \tau = \|H\| t$$

$$\begin{aligned} O_{loc} |k,r,z\rangle &= |k,r,z \oplus l\rangle \\ O_{val} |l,r,z\rangle &= |l,r,z \oplus H_{l,r}\rangle \end{aligned}$$

$$H=\sum_{j=0}^{L-1}\alpha_jV_j$$

$$\text{select}(V)|j\rangle|\psi\rangle=|j\rangle V_j|\psi\rangle$$

$$|G\rangle, H = \langle G|U_{\text{signal}}|G\rangle$$

$$O\big(\text{poly}(N,d)(\tau^2/\epsilon)\big)e^{(A+B)\Delta t}\approx e^{A\Delta t/2}e^{B\Delta t}e^{A\Delta t/2}$$

$$\tau_{\max} = t \|H\|_{\max}$$

$$H=\sum_j\alpha_jU_j$$

$$e^{-iH\Delta t}\approx\sum_{k=0}^K\frac{(-i\Delta t)^k}{k!}\left(\sum_j\alpha_jU_j\right)^k$$

$$O\left(d^2\tau\frac{\log\left(d^2\tau_{\max}/\epsilon\right)}{\log\log\left(d^2\tau_{\max}/\epsilon\right)}\right)$$

$$O\left(T\frac{L(n+\log L)\log(T/\epsilon)}{\log\log(T/\epsilon)}\right)$$

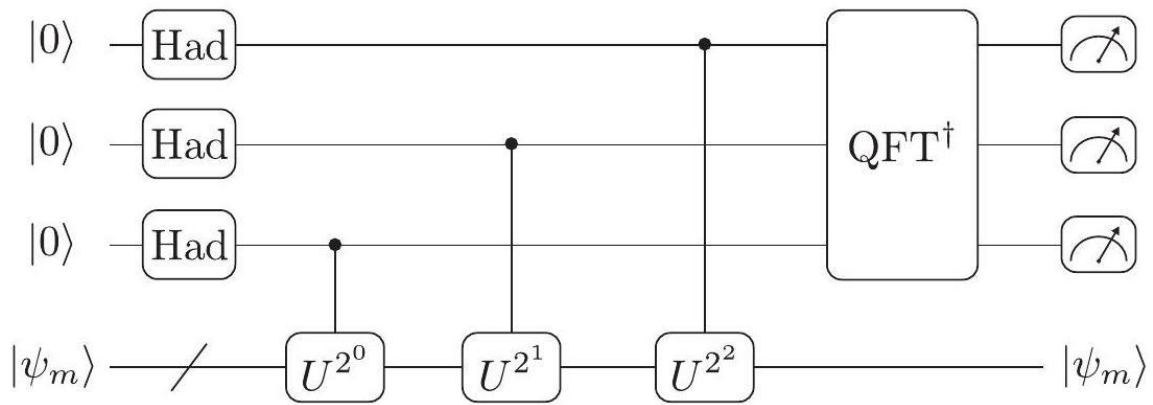
$$T=\sum_{j=0}^{L-1}\alpha_j$$

$$O\left(d\tau_{\max}+\frac{\log\left(1/\epsilon\right)}{\log\log\left(1/\epsilon\right)}\right)$$

$$W=\sum_{\lambda}e^{i\theta_{\lambda}}|u_{\lambda}\rangle\langle u_{\lambda}|$$

$$W \rightarrow V_{\text{ideal}} = \sum_{\lambda} e^{i h(\theta_{\lambda})} |u_{\lambda}\rangle \langle u_{\lambda}|$$

$$h(\theta)=-\tau\sin\left(\theta\right)$$



$$\frac{1}{\sqrt{2^T}} \sum_x |x\rangle (e^{-i\lambda_m t})^{2^k}$$

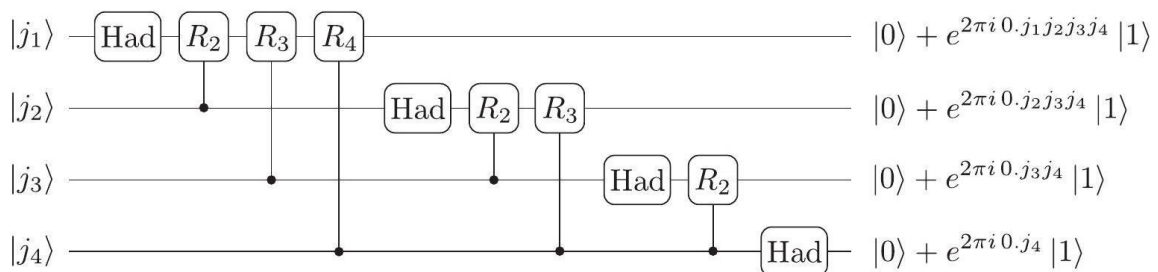
$$(|0\rangle + |1\rangle)|\psi_m\rangle \rightarrow \left(|0\rangle + e^{-2^k i \lambda_m t} |1\rangle\right)|\psi_m\rangle.$$

$$|x_1x_2\ldots x_T\rangle\lambda_mt/2\pi\approx 0.x_1x_2\ldots x_T$$

$$\left(T-\left\lceil\log\left(2+\frac{1}{2\epsilon}\right)\right\rceil\right)$$

$$\sum_m a_m |\psi\rangle$$

$$\sum_m a_m |\tilde{\lambda}_m t/2\pi\rangle |\psi_m\rangle |a_m|^2$$

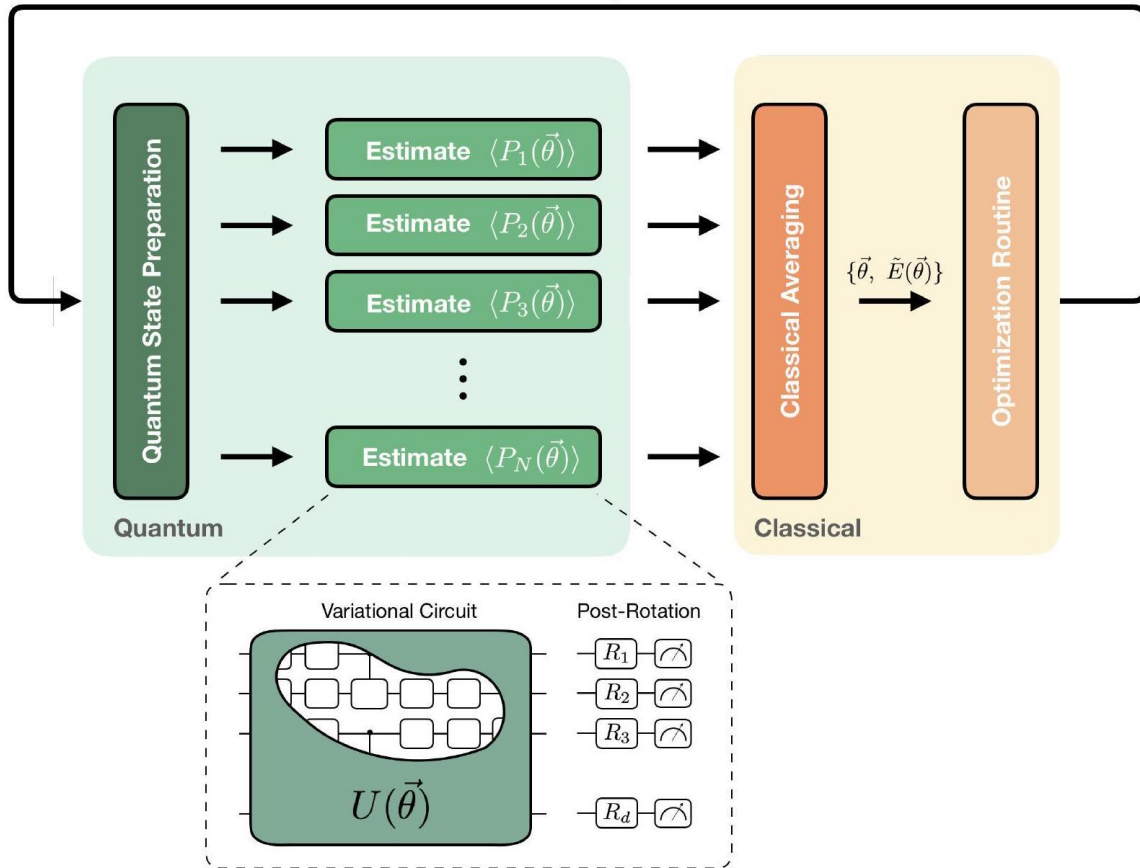


$$\text{QFT}|j\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i jk/N} |k\rangle.$$

$$j=j_12^{n-1}+j_22^{n-2}+\cdots+j_n2^0=:j_1j_2\ldots j_n$$

$$\text{QFT}|j_1,j_2,\ldots,j_n\rangle = \frac{(|0\rangle + e^{2\pi i 0.j_n} |1\rangle)(|0\rangle + e^{2\pi i 0.j_{n-1}j_n} |1\rangle) \ldots (|0\rangle + e^{2\pi i 0.j_1j_2\ldots j_n} |1\rangle)}{2^{n/2}}$$

$$O(N^3/\epsilon + N^2\log\,1/\epsilon)$$



$$R_i \in \{I, R_X(-\pi/2), R_Y(\pi/2)\}$$

$$U(\vec{\theta})|\Psi_0\rangle = |\Psi(\vec{\theta})\rangle$$

$$|\Psi_{CC}\rangle = e^T|\Phi_0\rangle$$

$$T = \sum_{i=1}^{\eta} T_i$$

$$T_1 = \sum_{\substack{i \in \text{occ} \\ a \in \text{virt}}} t_a^i a_a^\dagger a_i$$

$$T_2 = \sum_{\substack{i > j \in \text{occ} \\ a > b \in \text{virt} \\ \dots}} t_{ab}^{ij} a_a^\dagger a_b^\dagger a_i a_j$$

$$e^{-T} H e^T |\Phi_0\rangle = E_{CC} |\Phi_0\rangle$$

$$|\Psi_{UCC}\rangle = e^{T-T^\dagger} |\Phi_0\rangle e^{-(T-T^\dagger)} H e^{T-T^\dagger}$$

$$O(N^2\eta^2) < O(N^4)$$

$$f \in O(\log(N))$$

$$H = \sum_i h_i O_i$$

$$H=\sum_j H_j$$

$$|\Psi(\theta)\rangle=\left(\prod_{b=1}^S\left[U_{H_j}(\theta_j^b)\dots U_{H_1}(\theta_1^b)\right]\right)|\Psi_0\rangle,$$

$$U_{H_k}(\theta_k^b)=\exp\left(\theta_k^bH_j\right),\theta[\theta_1^1,\cdots,\theta_k^b,\cdots,\theta_j^S]U_{H_k}(\theta_k^b)$$

$$H(t)=A(t)H_0+B(t)H_1$$

$$\Delta t = \frac{t}{S}$$

$$H_i=\sum_j h_j^i O_j$$

$$H=-t\sum_{\langle i,j\rangle,\sigma}a_{i,\sigma}^\dagger a_{j,\sigma}+U\sum_i a_{i,\uparrow}^\dagger a_{i,\uparrow}a_{i,\downarrow}^\dagger a_{i,\downarrow}$$

$$H=h_h+h_v+h_U$$

$$|\Psi(\theta)\rangle=\prod_{b=1}^S\left[U_U^\dagger\left(-\frac{\sigma_U^b}{2}\right)U_h(\theta_h^b)U_v(\theta_v^b)U_U\left(\frac{\theta_U^b}{2}\right)\right]|\Psi_0\rangle,$$

$$\begin{aligned} H_{\text{diag}} &= \sum_p \sum_p \epsilon_p a_p^\dagger a_p + \sum_{p,q} h_{pqqp} a_p^\dagger a_p a_q^\dagger a_q \\ H_{\text{hop}} &= \sum_{p,q} h_{pq} a_p^\dagger a_q + \sum_{p,q,r} h_{prrq} a_p^\dagger a_q a_r^\dagger a_r \\ H_{\text{ex}} &= \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_s a_r \end{aligned}$$

$$|\Psi(\theta)\rangle=\prod_{b=1}^S\left[U_{ex}^\dagger\left(-\frac{\sigma_{ex}^b}{2}\right)U_{hop}^\dagger\left(-\frac{\theta_{hop}^b}{2}\right)U_{diag}(\theta_{diag}^b)U_{hop}\left(\frac{\theta_{hop}^b}{2}\right)U_{ex}\left(\frac{\theta_{ex}^b}{2}\right)\right]|\Psi_0\rangle,$$

$$\begin{aligned} H=&\frac{1}{2N}\sum_{\nu,p',q',\sigma}k_\nu^2\cos\left[k_\nu\cdot r_{q'-p'}\right]a_{p',\sigma}^\dagger a_{q',\sigma}-\frac{4\pi}{\Omega}\sum_{\substack{p',\sigma\\j,v\neq 0}}\frac{\zeta_j\cos\left[k_\nu\cdot\left(R_j-r_{p'}\right)\right]}{k_\nu^2}n_{p',\sigma}\\&+\frac{2\pi}{\Omega}\sum_{\substack{(p',q')\neq(q',\sigma')\\v\neq 0}}\frac{\cos\left[k_\nu\cdot r_{p'-q'}\right]}{k_\nu^2}n_{p',\sigma}n_{q',\sigma'}\\&=\sum_{pq}T_{pq}a_p^\dagger a_q+\sum_pU_pn_p+\sum_{p\neq q}V_{pq}n_pn_q \end{aligned}$$

$$H = \sum_p \left(\frac{T_{pq} + U_p}{2} + \sum_q \frac{V_{pq}}{2} \right) Z_p + \sum_{p \neq q} V_{pq} Z_p Z_q + \\ \sum_{p \neq q} \frac{T_{pq}}{2} (X_p Z_{p+1} \dots Z_{q-1} X_q + Y_p Z_{p+1} \dots Z_{q-1} Y_q) \\ f_{SWAP}^{p,q} = 1 + a_p^\dagger a_q + a_q^\dagger a_p - a_p^\dagger a_q - a_q^\dagger a_p.$$

$$F(p,q) = \exp \left(-iV_{pq}n_pn_q t \right) \exp \left(-iT_{pq}(a_p^\dagger a_q + a_q^\dagger a_p)t \right) f_{\text{swap}}^{p,q} \\ \equiv \exp \left(-\frac{i}{4}V_{pq}(1-Z_p-Z_q-Z_pZ_q)t \right) \exp \left(-\frac{i}{2}T_{pq}(X_pX_q + Y_pY_q)t \right) \\ \times \frac{1}{2}(X_pX_q + Y_pY_q + Z_p + Z_q) \\ \equiv \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -i\sin(T_{pq}t) & \cos(T_{pq}t) & 0 \\ 0 & \cos(T_{pq}t) & -i\sin(T_{pq}t) & 0 \\ 0 & 0 & 0 & -e^{-iV_{pq}t} \end{bmatrix}$$

$$\Gamma_{kl} = \frac{i}{2} \text{tr}(\rho[\gamma_k, \gamma_l])$$

$$\gamma_j = a_j^\dagger + a_j$$

$$\gamma_j^\dagger = -i(a_j^\dagger - a_j)$$

$$i^p \text{tr} \left(\rho \gamma_{j_1} \dots \gamma_{j_{2p}} \right) = \text{Pf} \left(\Gamma|_{j_1 \dots j_{2p}} \right)$$

$$1 \leq j_1 < \dots < j_{2p} \leq 2N, \Gamma|_{j_1 \dots j_{2p}}$$

$$\text{Pf}(\Gamma) = \frac{1}{2^N N!} \sum_{s \in S_{2N}} \text{sgn}(s) \prod_{j=1}^N \Gamma_{s(2j-1), s(2j)} \\ = \sqrt{\det(\Gamma)}$$

$$H = \sum_{pq} h_{pq} \gamma_p \gamma_q$$

$$|\psi\rangle = \prod_{k=1}^{2N} (u_k + v_k a_k^\dagger a_k^\dagger) |0\rangle$$

$$|v_k|^2 + |u_k|^2 = 1$$

$$|\psi_s\rangle = \mathcal{U} c_1^\dagger \cdots c_N^\dagger |vac\rangle$$

$$\phi_p = \sum_q \psi_q u_{pq}; \; a_p^\dagger = \sum_q c_q u_{pq}^*; \; a_p^\dagger = \sum_q c_q^\dagger u_{pq},$$

$$\mathcal{U} = \exp \left(\sum_{pq} u_{pq} (a_p^\dagger a_q - a_p a_q^\dagger) \right).$$

$$H = \sum_{j,k=1}^N \Sigma_{jk} c_j^\dagger c_k + \frac{1}{2} \sum_{j,k=1}^N (\Delta_{jk} c_j^\dagger c_k^\dagger + \text{h.c.}),$$

$$\Sigma = \Sigma^\dagger$$

$$\Delta = -\Delta^\dagger$$

$$H=\sum_j \epsilon_j b_j^\dagger b_j + C$$

$$\begin{bmatrix} \mathbf{b}^\dagger \\ \mathbf{b} \end{bmatrix} = W \begin{bmatrix} \mathbf{c}^\dagger \\ \mathbf{c} \end{bmatrix}.$$

$$|\Phi_0\rangle = C \prod_{k=1}^M b_k |\text{vac}\rangle$$

$$U_{\text{MG}}^{(k)} = \prod_{i \in \text{odd}} G_{i,i+1}^{(k)} \prod_{i \in \text{even}} G_{i,i+1}^{(k)}$$

$$U_{\text{MG}}^{\text{NN}} = \prod_{k=1}^{\lfloor \frac{M}{2} \rfloor} U_{\text{MG}}^{(k)}$$

$$W=U_{\text{MG}}^{\text{NN}}\prod_{i=1}^MR_i^Z$$

$$U_{\text{VarMG}}^{(k,l)}(\boldsymbol{\theta}^{(k,l)}) = \prod_{i \in \text{odd}} K_{i,i+1}^{(k,l)}\left(\boldsymbol{\theta}_{i,i+1}^{(k,l)}\right) \times \prod_{i \in \text{even}} K_{i,i+1}^{(k,l)}\left(\boldsymbol{\theta}_{i,i+1}^{(k,l)}\right).$$

$$U_{\text{VarMG}}^{\text{NN}(l)}(\boldsymbol{\theta}^{(l)}) = \prod_{k=1}^{\lfloor \frac{N}{2} \rfloor} U_{\text{VarMG}}^{(k,l)}(\boldsymbol{\theta}^{(k,l)})$$

$$U_{\text{VarMG}}(\boldsymbol{\Theta}) = \prod_{l=1}^L U_{\text{VarMG}}^{\text{NN}(l)}(\boldsymbol{\theta}^{(l)}) \prod_{i=1}^M R_i^Z(\theta_i^Z),$$

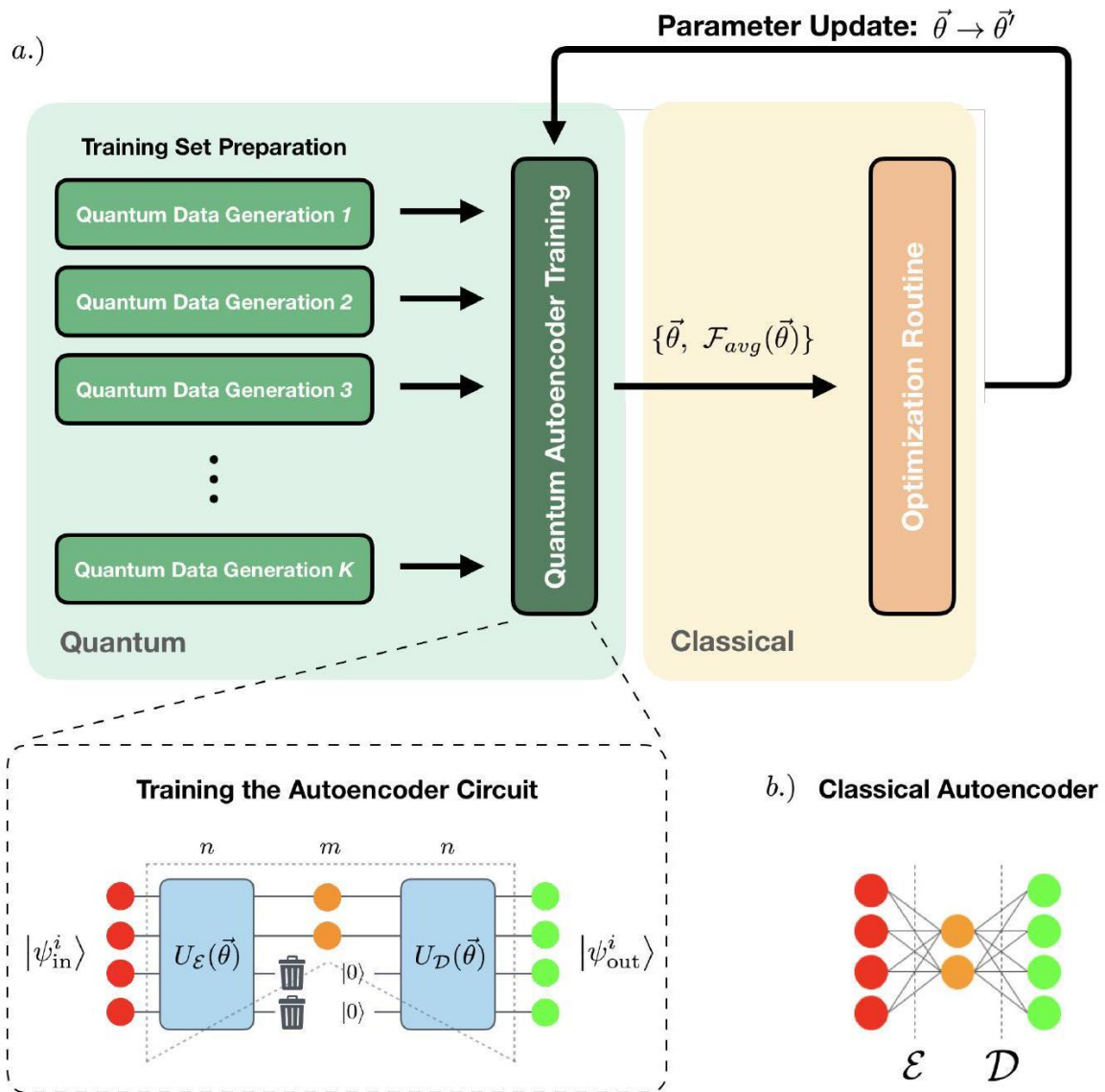
$$R_i^Z(\theta_i^Z) = e^{i\theta_i^Z\sigma_z^i}$$

$$|\Psi(\boldsymbol{\Theta})\rangle = U_{\text{Bog}}^\dagger U_{\text{VarMG}}(\boldsymbol{\Theta}) \prod_{i=1}^N X_i |0\rangle^{\otimes M},$$

$$|\Psi(\theta)\rangle = U^{(L)}(\theta^L) \ldots U^{(1)}(\theta^1) U^{(0)}(\theta^0) |\Psi_0\rangle$$

$$\theta = [\theta^0, \ldots, \theta^{L-1}, \theta^L], U^{(k)}$$

$$U^{(k)}(\theta^k) = \left(\prod_i^N R_i^Z(\theta_{i,1}^k) R_i^Z(\theta_{i,2}^k) R_i^Z(\theta_{i,3}^k) \right) E_{ent},$$



$$E(\vec{\theta}) = \langle \Psi(\vec{\theta}) | H | \Psi(\vec{\theta}) \rangle$$

$$H = \sum_{i_1 \alpha_1} h_{\alpha_1}^{i_1} \sigma_{\alpha_1}^{i_1} + \sum_{i_1 \alpha_1 i_2 \alpha_2} h_{\alpha_1 \alpha_2}^{i_1 i_2} \sigma_{\alpha_1 \alpha_2}^{i_1 i_2} + \dots,$$

$$\langle H \rangle = \sum_{i_1 \alpha_1} h_{\alpha_1}^{i_1} \langle \sigma_{\alpha_1}^{i_1} \rangle + \sum_{i_1 \alpha_1 i_2 \alpha_2} h_{\alpha_1 \alpha_2}^{i_1 i_2} \langle \sigma_{\alpha_1 \alpha_2}^{i_1 i_2} \rangle + \dots,$$

$$H = \sum_i^M h_i O_i$$

$$\text{Cov}(\langle O_i \rangle, \langle O_j \rangle) = 0 \forall i \neq j$$

$$\epsilon^2 = \sum_i^M |h_i|^2 \frac{\text{Var}(\langle O_i \rangle)}{\epsilon_i^2}$$

$$\epsilon_i^2 = \frac{\epsilon^2}{M}$$

$$\text{Var}(O_i) = 1 - \langle O_i \rangle^2 = \sigma_i$$

$$m = \frac{1}{\epsilon^2} \sum_i^M |h_i|^2 \sigma_i \leq \frac{1}{\epsilon^2} \sum_i^M |h_i|^2,$$

$$m = \left(\frac{1}{\epsilon} \sum_i^M |h_i| \sigma_i\right)^2 \leq \left(\frac{1}{\epsilon} \sum_i^M |h_i|\right)^2$$

$$O\left(\frac{N^{14/3}}{\epsilon^2\Omega^{2/3}}\left(1+\frac{1}{N^{4/3}\Omega^{2/3}}\right)\right)$$

$$m \in O\left(\frac{\langle V^2 \rangle + \langle T^2 \rangle}{\epsilon^2}\right) \subseteq O\left(\frac{\eta^{10/3} N^{2/3}}{\epsilon^2} + \frac{\eta^{2/3} N^{4/3}}{\epsilon^2}\right)$$

$$\delta_k = \sum_{i=1}^k |h_i|$$

$$(1-C)^2\epsilon^2\frac{1}{(1-C^2)\epsilon^2}\left(\sum_{i=k^*+1}^M|h_i|\sigma_i\right)^2\left\langle a_{i_1}^\dagger a_{j_1}\ldots a_{i_p}^\dagger a_{j_p}\right\rangle,$$

$$\hat{H} = H + \sum_{k=1}^K \beta_k C_k = \sum_{i=1}^M \left(h_i + \sum_k^K \beta_k c_{k,i} \right) O_i,$$

$$\min_{\beta} \left(\sum_{i=1}^M \left| h_i + \sum_k^K \beta_k c_{k,i} \right| \right) \text{ or } \min_{\beta} \left(\sum_{i=1}^M \left| h_i + \sum_k^K \beta_k c_{k,i} \right| \text{Var}(O_i) \right),$$

$$H(s) = (1-s)H_0 + sH_P$$

$$H_\lambda = (H - \lambda I)^2$$

$$L = H + \sum_i \lambda_i (S_i - s_i I)^2$$

$$\mathcal{F}_{obj}(\mathcal{P},E) = E - T \cdot \text{Tr}[\rho_C^2]$$

$$\langle E^1 \rangle = \sum_{pq} o_{pq} \langle a_p^\dagger a_q \rangle$$

$$\langle E^2 \rangle = \sum_{pqrs} o_{pqrs} \langle a_p^\dagger a_q^\dagger a_r a_s \rangle$$

$$(U(\overrightarrow{\theta_1})|\psi_0\rangle, U(\overrightarrow{\theta_2})|\psi_0\rangle, \ldots)(|\psi(t_1)\rangle, |\psi(t_2)\rangle, \ldots)$$

$$\int_{t_i}^{t_f} dt \langle \psi(\vec{\theta}(t)) | \left(i \frac{d}{dt} - H \right) | \psi(\vec{\theta}(t)) \rangle$$

$$\vec{\theta}_{i+1} = M^{-1} \vec{V}(t_{i+1} - t_i) + \vec{\theta}_i$$

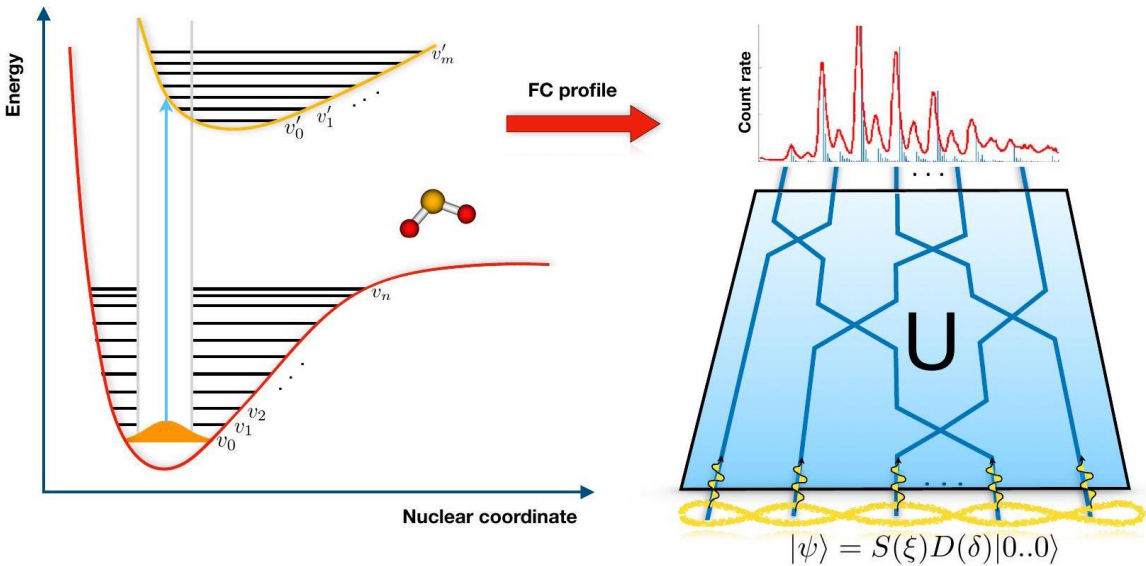
$$e^{-i(-i\tau)H}=e^{-\tau H}$$

$$\rho(T) = e^{-H/T}/\mathrm{tr}(e^{-H/T})$$

$$\tau = 1/(2T) e^{-\tau H} \cdot \frac{\mathbb{I}}{d} \cdot e^{-\tau H} \propto e^{-H/T}$$

$$|\psi_{\mathrm{gs}}\rangle\langle\psi_{\mathrm{gs}}| = \lim_{T\rightarrow 0} e^{-H/T}/\mathrm{tr}(e^{-H/T})$$

$$\begin{aligned} H_{\text{elec}} = & \mu_1 \mathbb{I} + \mu_2 Z_1 + \mu_3 Z_2 + \mu_4 Z_3 + \mu_5 Z_1 Z_2 \\ & + \mu_6 Z_1 Z_3 + \mu_7 Z_2 Z_4 + \mu_8 X_1 Z_2 X_3 + \mu_9 Y_1 Z_2 Y_3 \\ & + \mu_{10} Z_1 Z_2 Z_3 + \mu_{11} Z_1 Z_3 Z_4 + \mu_{12} Z_2 Z_3 Z_4 \\ & + \mu_{13} X_1 Z_2 X_3 Z_4 + \mu_{14} Y_1 Z_2 Y_3 Z_4 + \mu_{15} Z_1 Z_2 Z_3 Z_4 \end{aligned}$$



$$\Phi(\vec{r}) = R_{nl}(r)Y_{l,m}(\theta,\phi)$$

$$R_n^{STO}(r) = Nr^{n-1}e^{-\zeta r}$$

$$R_n^{GTO}(r) = Nr^{n-1}e^{-\zeta r^2}$$

$$\phi_v(r)=\sqrt{\frac{1}{V}}\exp\left(\frac{2\pi v r}{L}\right)$$

$$\mathrm{Sinc}(x) = \frac{\sin\left(\pi x\right)}{\pi x}$$

$$a_j^\dagger \leftrightarrow (\sigma_z)_1 \otimes \ldots \otimes (\sigma_z)_{j-1} \otimes (\sigma^+) _j \otimes \mathbb{I},$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \text{ and } \sigma^+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$



$$(a_K^\dagger)^{i_N} \dots (a_1^\dagger)^{i_1} |vac\rangle$$

$$|i_1\rangle\otimes|i_2\rangle\otimes\ldots\otimes|i_N\rangle$$

$$a_j^\dagger \leftrightarrow \mathbb{I} \otimes (\sigma_z)_{j-1} \otimes (\sigma^+)_{j} \otimes (\sigma_x)_{j+1} \otimes \dots \otimes (\sigma_x)_N$$

$$|i_1\rangle\otimes\ldots|i_N\rangle\rightarrow|i_1\rangle\otimes|i_1\oplus i_2\rangle\otimes\ldots|i_1\oplus\ldots\oplus i_N\rangle,$$

$$|i_1\rangle\otimes\ldots|i_N\rangle\rightarrow|b_1\rangle\otimes\ldots\otimes|b_N\rangle,$$

$$b_k=\sum_{l=1}^k[\boldsymbol{\beta}_r]_{kl}i_l\text{mod}2$$

$$\boldsymbol{\beta}_1=1,\\ \boldsymbol{\beta}_{r+1}=\begin{bmatrix} & 1 & \dots & 1 \\ \boldsymbol{\beta}_r & 0 & \dots & 0 \\ & \vdots & & \vdots \\ & 0 & \dots & 0 \\ \mathbf{0} & & \boldsymbol{\beta}_r & \end{bmatrix}.$$

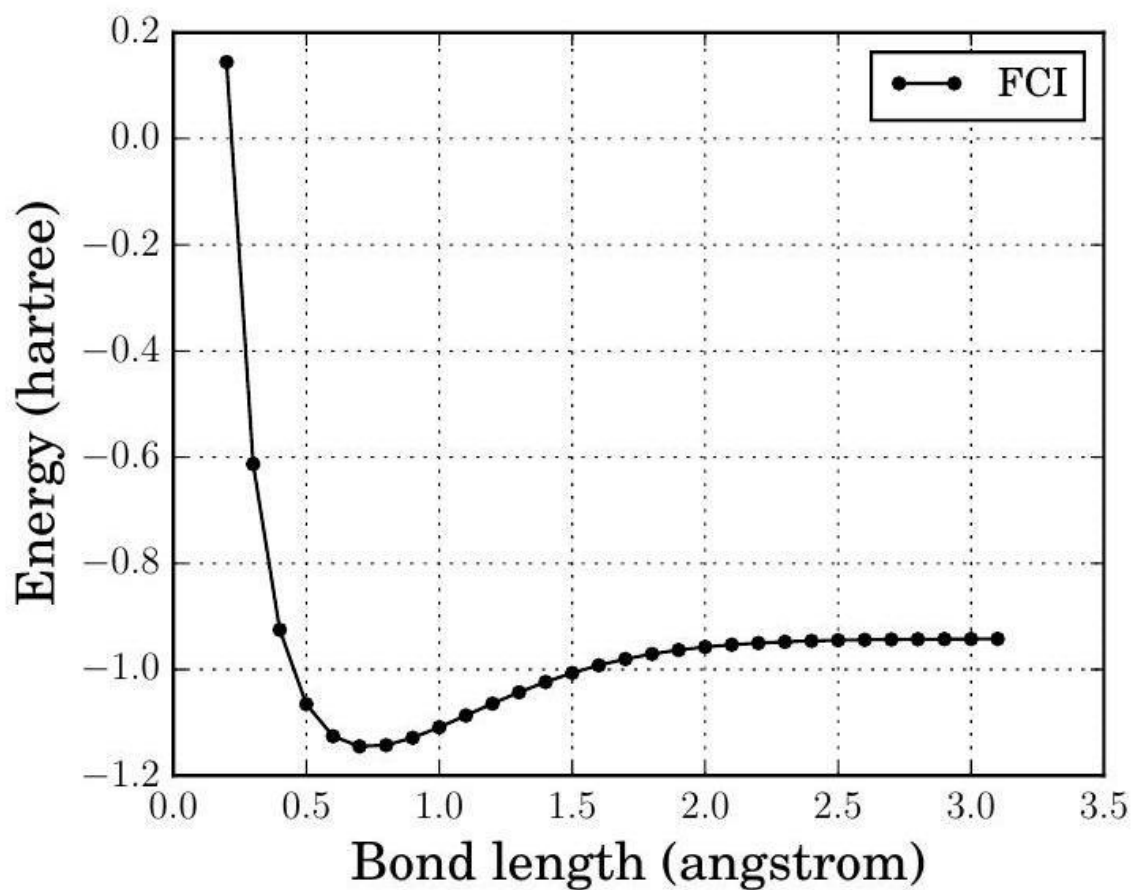
$$\boldsymbol{\beta}_3=\begin{bmatrix}1&1&1&1&1&1&1&1\\0&1&0&0&0&0&0&0\\0&0&1&1&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&1&1&1\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&1&1\\0&0&0&0&0&0&0&1\end{bmatrix}$$

$$H_{\rm elec} = -\sum_i \frac{\nabla_{\bf r_i}^2}{2} - \sum_{i,j} \frac{Z_i}{|{\bf R}_i - {\bf r}_j|} + \sum_{i,j>i} \frac{Z_i Z_j}{|{\bf R}_i - {\bf R}_j|} + \sum_{i,j>i} \frac{1}{|{\bf r}_i - {\bf r}_j|},$$

$$H=\sum_{pq}h_{pq}a_p^\dag a_q+\frac{1}{2}\sum_{pqrs}h_{pqrs}a_p^\dag a_q^\dag a_r a_s,$$

$$h_{pq}=\int\,dx\phi_p^*(x)\left(\frac{\nabla_r^2}{2}-\sum_i\frac{Z_i}{|{\bf R}_i-{\bf r}|}\right)\phi_q(x)$$

$$h_{pqrs}=\int\,dx_1dx_2\frac{\phi_p^*(x_1)\phi_q^*(x_2)\phi_s(x_1)\phi_r(x_2)}{|{\bf r}_1-{\bf r}_2|}$$



$$\begin{aligned}
 H_{\text{elec}} = & \mu_0 \mathbb{I} + \mu_1 Z_1 + \mu_2 Z_2 + \mu_3 Z_3 + \mu_4 Z_1 Z_2 \\
 & + \mu_5 Z_1 Z_3 + \mu_6 Z_2 Z_4 + \mu_7 X_1 Z_2 X_3 + \mu_8 Y_1 Z_2 Y_3 \\
 & + \mu_9 Z_1 Z_2 Z_3 + \mu_{10} Z_1 Z_3 Z_4 + \mu_{11} Z_2 Z_3 Z_4 \\
 & + \mu_{12} X_1 Z_2 X_3 Z_4 + \mu_{13} Y_1 Z_2 Y_3 Z_4 + \mu_{14} Z_1 Z_2 Z_3 Z_4
 \end{aligned}$$

$$X_1 = \sigma_x \otimes \mathbb{I} \otimes \mathbb{I} \otimes \mathbb{I}$$

$$\tilde{H}_{\text{elec}} = v_0 \mathbb{I} + v_1 Z_1 + v_2 Z_2 + v_3 Z_1 Z_2 + v_4 X_1 X_2 + v_5 Y_1 Y_2$$

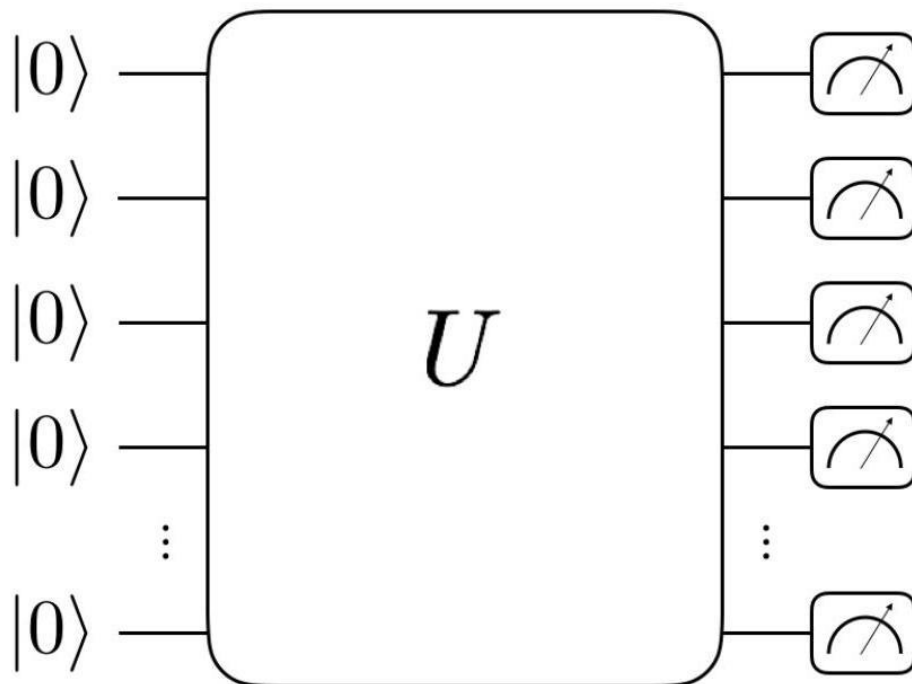
$$|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$$

$$Z(|0\rangle + |1\rangle)/\sqrt{2} = (|0\rangle - |1\rangle)/\sqrt{2} = |-\rangle$$

**1. Initialization
of qubits**

**2. Application
of gates**

**3. Measurement
of qubits**



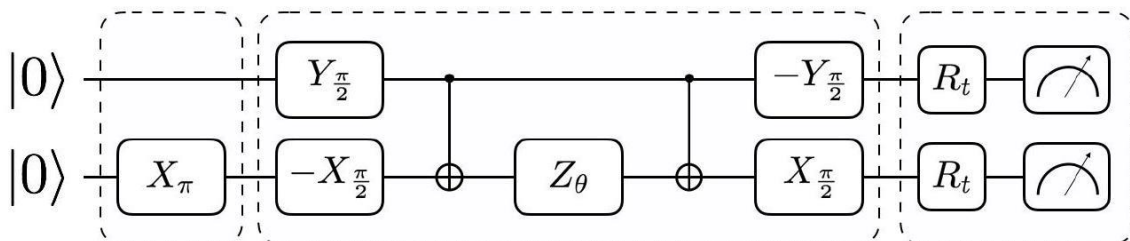
time 

$$|\psi(\vec{\theta})\rangle = U(\vec{\theta})|\phi_0\rangle$$

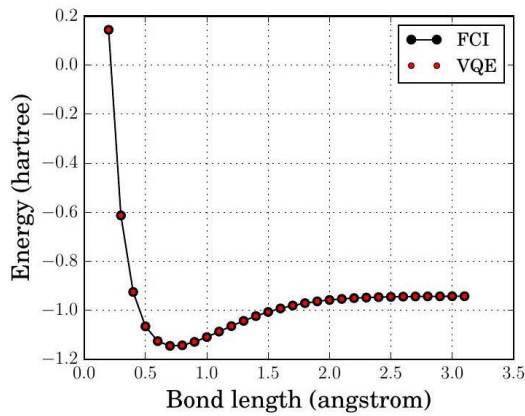
$$\langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle$$

$$\langle H\rangle = \sum_i h_i \langle O_i\rangle,$$

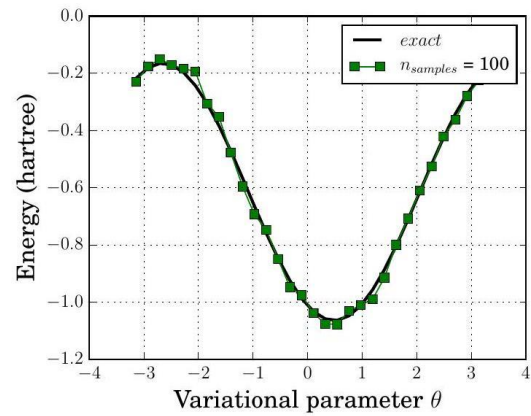
$$\langle H\rangle = v_0\mathbb{I} + v_1\langle Z_1\rangle + v_2\langle Z_2\rangle + v_3\langle Z_1Z_2\rangle + v_4\langle X_1X_2\rangle + v_5\langle Y_1Y_2\rangle.$$



a)



b)



$$\mathbf{x} \in \mathbb{R}^3 \times \{\uparrow, \downarrow\} \mathbf{r} \in \mathbb{R}^3 \sigma \in \{\uparrow, \downarrow\}$$

$$\Psi: (\mathbb{R}^3 \times \{\uparrow, \downarrow\})^N \rightarrow \mathbb{C}$$

$$\mathbf{x} \triangleq \mathbf{x}_1, \dots, \mathbf{x}_N$$

$$\int d\mathbf{x} |\Psi|^2(\mathbf{x}) = |\Psi|^2$$

$$\hat{H}\Psi(\mathbf{x}) = E\Psi(\mathbf{x})$$

$$\hat{H} = -\frac{1}{2} \sum_i \nabla_i^2 + \sum_{i>j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{il} \frac{Z_l}{|\mathbf{r}_i - \mathbf{R}_l|} + \sum_{l>j} \frac{Z_l Z_j}{|\mathbf{R}_l - \mathbf{R}_j|}$$

$$\nabla_i^2 = \sum_{j=1}^3 \frac{\partial^2}{\partial r_{ij}^2}$$

$$\Psi_{\theta}:(\mathbb{R}^3 \times \{\uparrow, \downarrow\})^N \rightarrow \mathbb{R}$$

$$\begin{aligned} \mathcal{L}_{\theta} &= \frac{\langle \Psi_{\theta} \hat{H} \Psi_{\theta} \rangle}{\langle \Psi_{\theta}^2 \rangle} = \frac{\int d\mathbf{x} \Psi_{\theta}(\mathbf{x}) \hat{H} \Psi_{\theta}(\mathbf{x})}{\int d\mathbf{x} \Psi_{\theta}^2(\mathbf{x})} \\ &= \mathbb{E}_{\mathbf{x} \sim \Psi_{\theta}^2} [\Psi_{\theta}^{-1}(\mathbf{x}) \hat{H} \Psi_{\theta}(\mathbf{x})] = \mathbb{E}_{\mathbf{x} \sim \Psi_{\theta}^2} [E_L(\mathbf{x})] \end{aligned}$$

$$E_L(\mathbf{x}) = \Psi^{-1}(\mathbf{x}) \hat{H} \Psi(\mathbf{x})$$

$$\Psi(\mathbf{x}) = \det[\mathbf{\Phi}(\mathbf{x})]$$

$$\Psi_{\theta}(\mathbf{x}) = \exp(\mathcal{J}_{\theta}(\mathbf{x})) \sum_{k=1}^{N_{\det}} \det[\mathbf{\Phi}_{\theta}^k(\mathbf{x})]$$

$$\mathcal{J}_{\theta}:(\mathbb{R}^3 \times \{\uparrow, \downarrow\})^N \rightarrow \mathbb{R}$$

$$\mathbf{\Phi}_{\theta}^k:(\mathbb{R}^3 \times \{\uparrow, \downarrow\})^{\mathcal{N}} \rightarrow \mathbb{R}^{N \times N}$$

$$|\mathbf{r}_i - \mathbf{R}_I|, I = 1, \dots, N_{\text{nuc}} \log(1 + |\mathbf{r}_i - \mathbf{R}_I|)/|\mathbf{r}_i - \mathbf{R}_I|$$

$$\begin{aligned}\mathbf{f}_i^{\ell+1} &= \mathbf{h}_i^\ell + \mathbf{W}_o^\ell \text{concat}_h[\\ &\quad \text{SELFATTN}_i(\mathbf{h}_1^\ell, \dots, \mathbf{h}_N^\ell; \mathbf{W}_q^{\ell h}, \mathbf{W}_k^{\ell h}, \mathbf{W}_v^{\ell h})] \\ \mathbf{h}_i^{\ell+1} &= \mathbf{f}_i^{\ell+1} + \tanh(\mathbf{W}^{\ell+1} \mathbf{f}_i^{\ell+1} + \mathbf{b}^{\ell+1})\end{aligned}$$

$$\begin{aligned}\text{SelfAttn}_i(\mathbf{h}_1, \dots, \mathbf{h}_N; \mathbf{W}_q, \mathbf{W}_k, \mathbf{W}_v) &= \\ \frac{1}{\sqrt{d}} \sum_j \sigma_j(\mathbf{q}_1^T \mathbf{k}_i, \dots, \mathbf{q}_N^T \mathbf{k}_i) \mathbf{v}_j \\ \mathbf{k}_i &= \mathbf{W}_k \mathbf{h}_i, \mathbf{q}_i = \mathbf{W}_q \mathbf{h}_i, \mathbf{v}_i = \mathbf{W}_v \mathbf{h}_i \\ \sigma_i(x_1, \dots, x_N) &= \frac{\exp(x_i)}{\sum_j \exp(x_j)}\end{aligned}$$

$$\Phi_{ij}^k = \Omega_{ij}^k \mathbf{w}_i^{kT} \mathbf{h}_j^L$$

$$\Omega_{ij}^k = \sum_I \pi_{iI}^k \exp\left(-\sigma_{iI}^k |\mathbf{r}_j - \mathbf{R}_I|\right)$$

$$\lim_{|\mathbf{r}|\rightarrow\infty}\Psi_{\theta}(\mathbf{r})=0$$

$$\begin{aligned}J_{\theta}(\boldsymbol{x}) &= \sum_{i < j; \sigma_i = \sigma_j} -\frac{1}{4} \frac{\alpha_{\text{par}}^2}{\alpha_{\text{par}} + |\mathbf{r}_i - \mathbf{r}_j|} \\ &+ \sum_{i, j; \sigma_i \neq \sigma_j} -\frac{1}{2} \frac{\alpha_{\text{anti}}^2}{\alpha_{\text{anti}} + |\mathbf{r}_i - \mathbf{r}_j|}\end{aligned}$$

$$E_L(\boldsymbol{x}) = -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^3 \left[\frac{\partial^2 \log|\Psi(\boldsymbol{x})|}{\partial r_{ij}^2} + \left(\frac{\partial \log|\Psi(\boldsymbol{x})|}{\partial r_{ij}} \right)^2 \right] + V(\boldsymbol{x})$$

$$\nabla \mathbb{E}_{\boldsymbol{x} \sim \Psi^2}[E_L(\boldsymbol{x})] = \frac{2 \mathbb{E}_{\boldsymbol{x} \sim \Psi^2}[(E_L(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{x}' \sim \Psi^2}[E_L(\boldsymbol{x}')]) \nabla \log|\Psi(\boldsymbol{x})|]}{2}$$

$$E_L(\boldsymbol{x}) = \Psi^{-1}(\boldsymbol{x}) \hat{H} \Psi(\boldsymbol{x})$$

$$E_L(\boldsymbol{x}) - \mathbb{E}_{\boldsymbol{x}' \sim \Psi^2}[E_L(\boldsymbol{x}')]$$

$$\text{MAD}_{\text{mean}}(E_L) = \frac{1}{N} \sum_i |E_L(\boldsymbol{x}_i) - \langle E_L \rangle_{\text{mean}}| \langle E_L \rangle_{\text{median}}$$

$$\text{MAD}_{\text{median}}(E_L) = \frac{1}{N} \sum_i |E_L(\boldsymbol{x}_i) - \langle E_L \rangle_{\text{median}}|$$

$$\mathbb{E}_{\boldsymbol{x}' \sim \Psi^2}[E_L(\boldsymbol{x}')] \langle E_L \rangle_{\text{mean}} \left[\langle \boldsymbol{x} \rangle_{\text{mean} / \text{median}} - \sigma, \langle \boldsymbol{x} \rangle_{\text{mean} / \text{median}} + \sigma \right]$$

$$\begin{aligned}\hat{E}_L(\boldsymbol{x}) &= \text{clip}_{\text{mean}}\left(E_L(\boldsymbol{x}); \rho \text{MAD}_{\text{mean}}(E_L)\right) \\ &\quad \langle (\hat{E}_L(\boldsymbol{x}) - \langle E_L \rangle_{\text{mean}}) \nabla \log|\Psi(\boldsymbol{x}) \rangle_{\text{mean}}\end{aligned}$$

$$\hat{E}_L(\boldsymbol{x}) = \text{clip}_{\text{median}}\left(E_L(\boldsymbol{x}); \rho \text{MAD}_{\text{median}}(E_L)\right) \\ \left\langle \left(\hat{E}_L(\boldsymbol{x}) - \langle \hat{E}_L \rangle_{\text{mean}}\right) \nabla \log |\Psi(\boldsymbol{x})| \right\rangle_{\text{mean}}$$

$$\det[\boldsymbol{\Phi}(\boldsymbol{x})] = \begin{vmatrix} \boldsymbol{\Phi}_{\uparrow}(\boldsymbol{x}_{\uparrow}) & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Phi}_{\downarrow}(\boldsymbol{x}_{\downarrow}) \end{vmatrix} \\ = \det[\boldsymbol{\Phi}_{\uparrow}(\boldsymbol{x}_{\uparrow})] \det[\boldsymbol{\Phi}_{\downarrow}(\boldsymbol{x}_{\downarrow})]$$

$$N \times N, N = N_{\uparrow} + N_{\downarrow}$$

$$\det[\boldsymbol{\Phi}(\boldsymbol{x})] = |\boldsymbol{\Phi}_{\uparrow}(\boldsymbol{x}_{\uparrow}) \; \boldsymbol{\Phi}_{\downarrow}(\boldsymbol{x}_{\downarrow})|$$

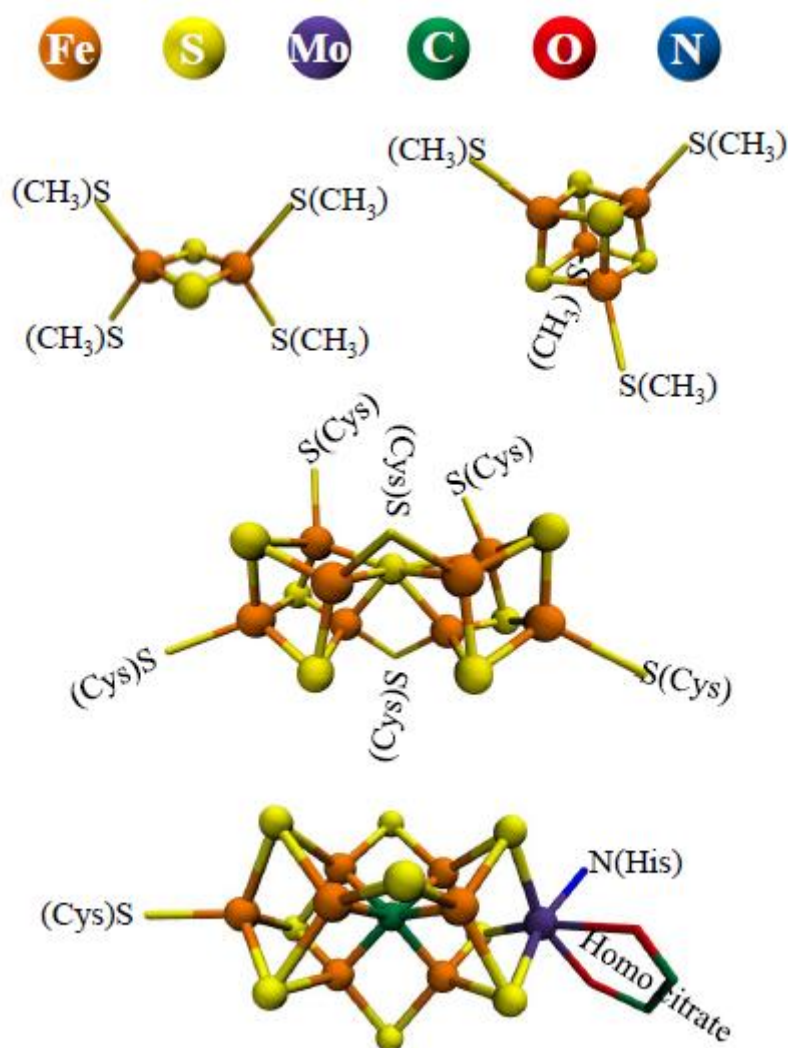
$$\lim_{L \rightarrow \infty} E(L) \propto L$$

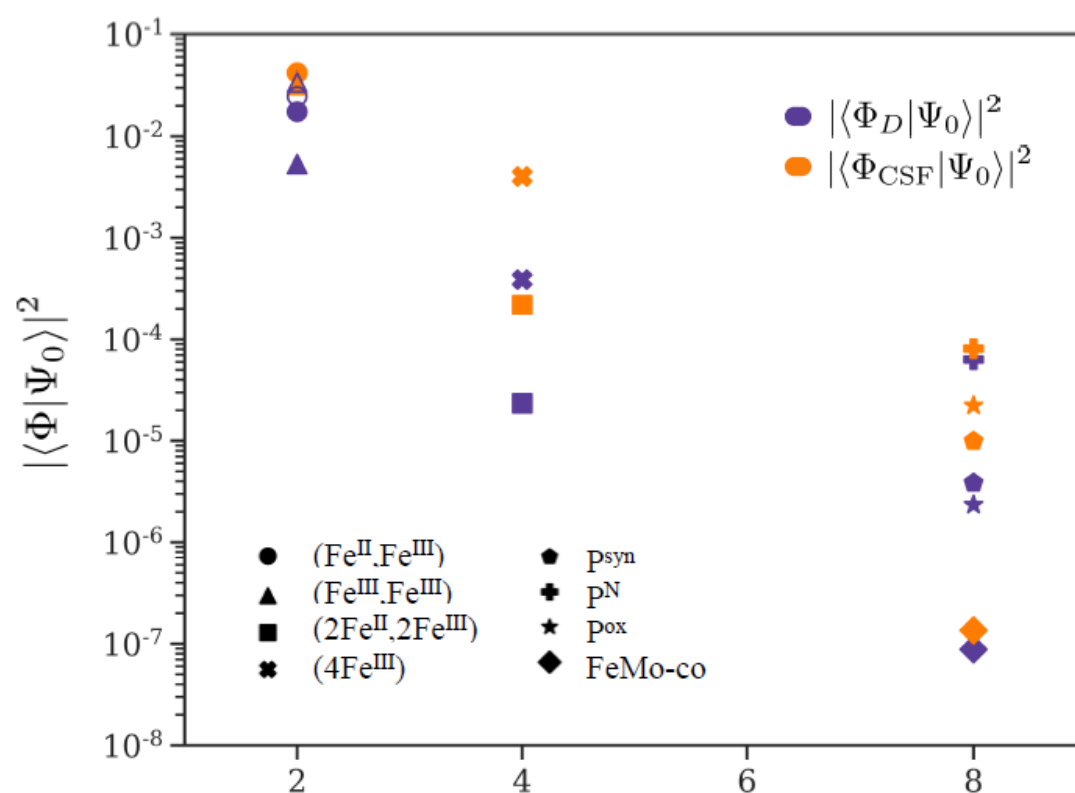
$$\bar{E} = E/L$$

$$\text{poly}(1/S)[\text{poly}(L)\text{poly}(1/\epsilon)+C]$$

$$\Delta_{\text{min}} \geq 1/\text{poly}(L)$$

$$\Delta_{\text{min}} \sim |\langle Y_0 \mid \Psi_0 \rangle|$$



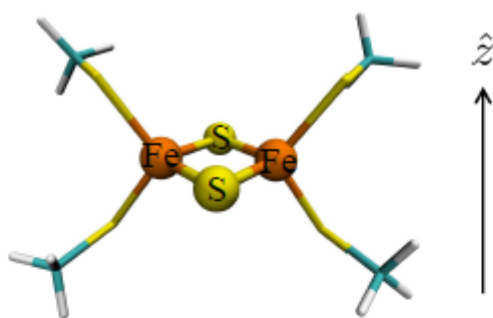
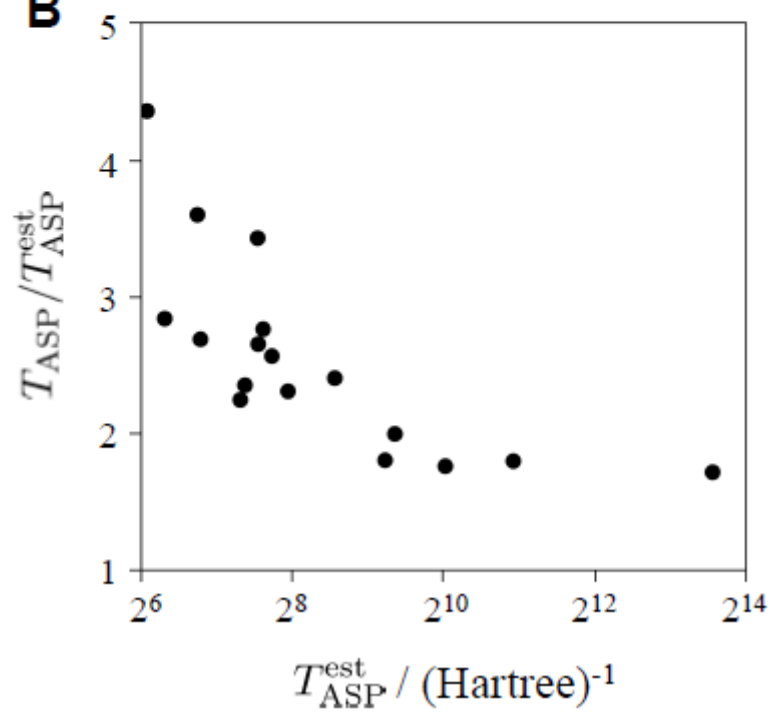


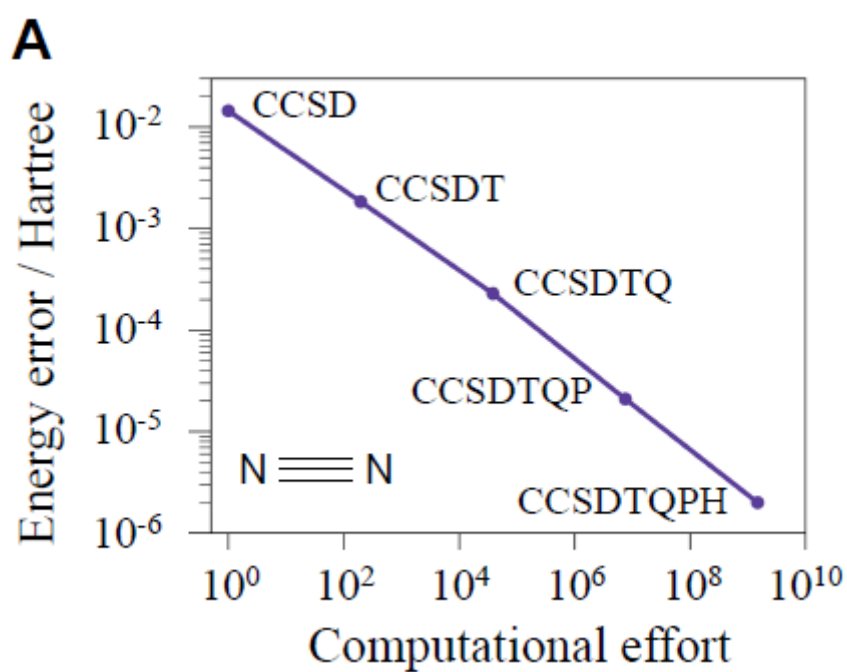
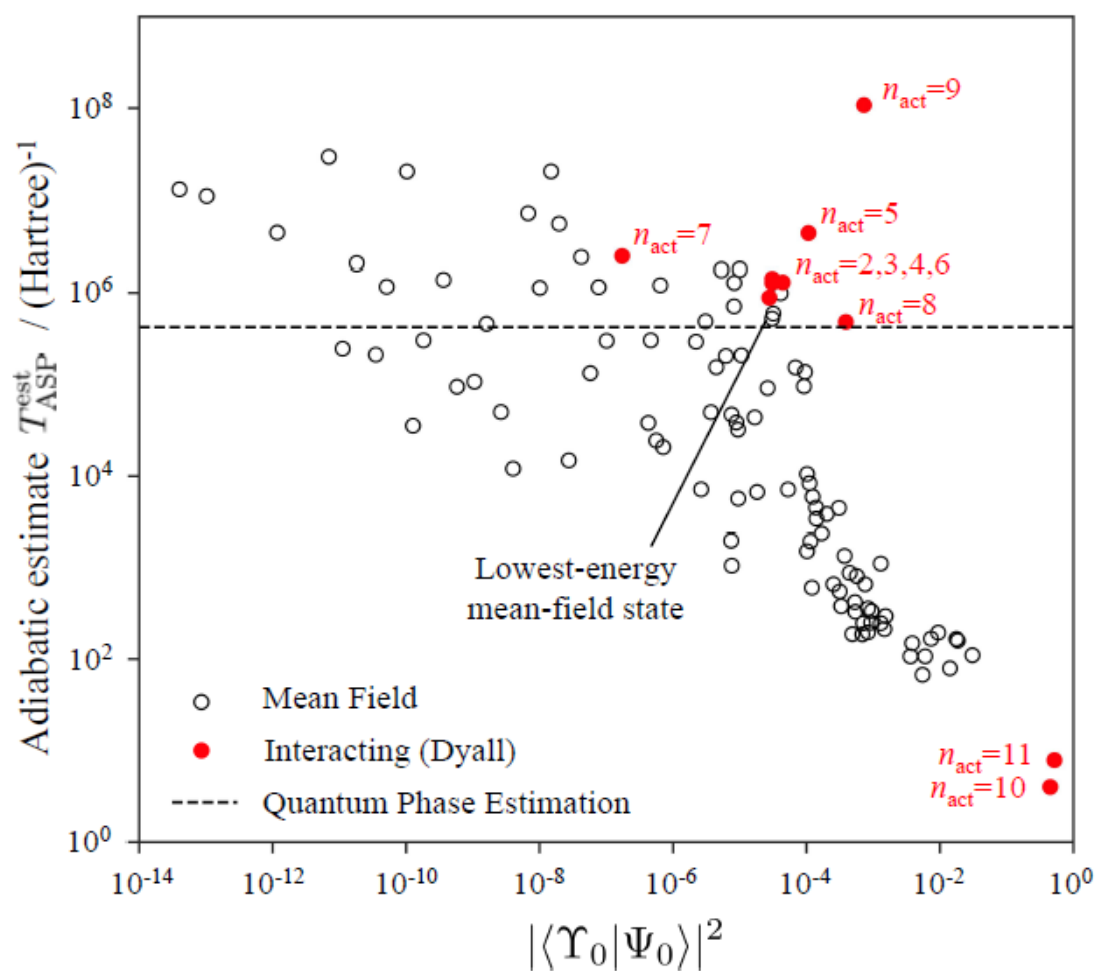
$$T_{\text{ASP}}^{\text{est}} \sim \max_s \tau(s)$$

$$\tau(s) = |\langle Y_0(s) | dH(s)/ds | Y_1(s) \rangle| / \Delta^2(s)$$

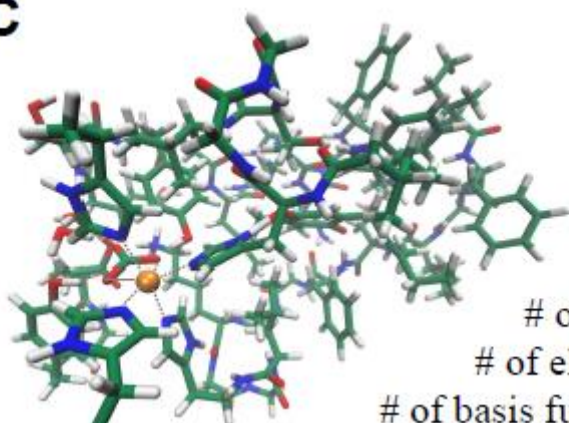
$$1/\left(\min_s \Delta(s)\right) \sim \text{poly}(1/|\langle Y_0 | \Psi_0 \rangle|)$$

$$T_{\text{ASP}} \sim \text{poly}(1/|\langle Y_0 | \Psi_0 \rangle|)$$

A
 $n_{\text{act}}=12$ (10 Fe $3d$ and 2 S $3p_z$)
B



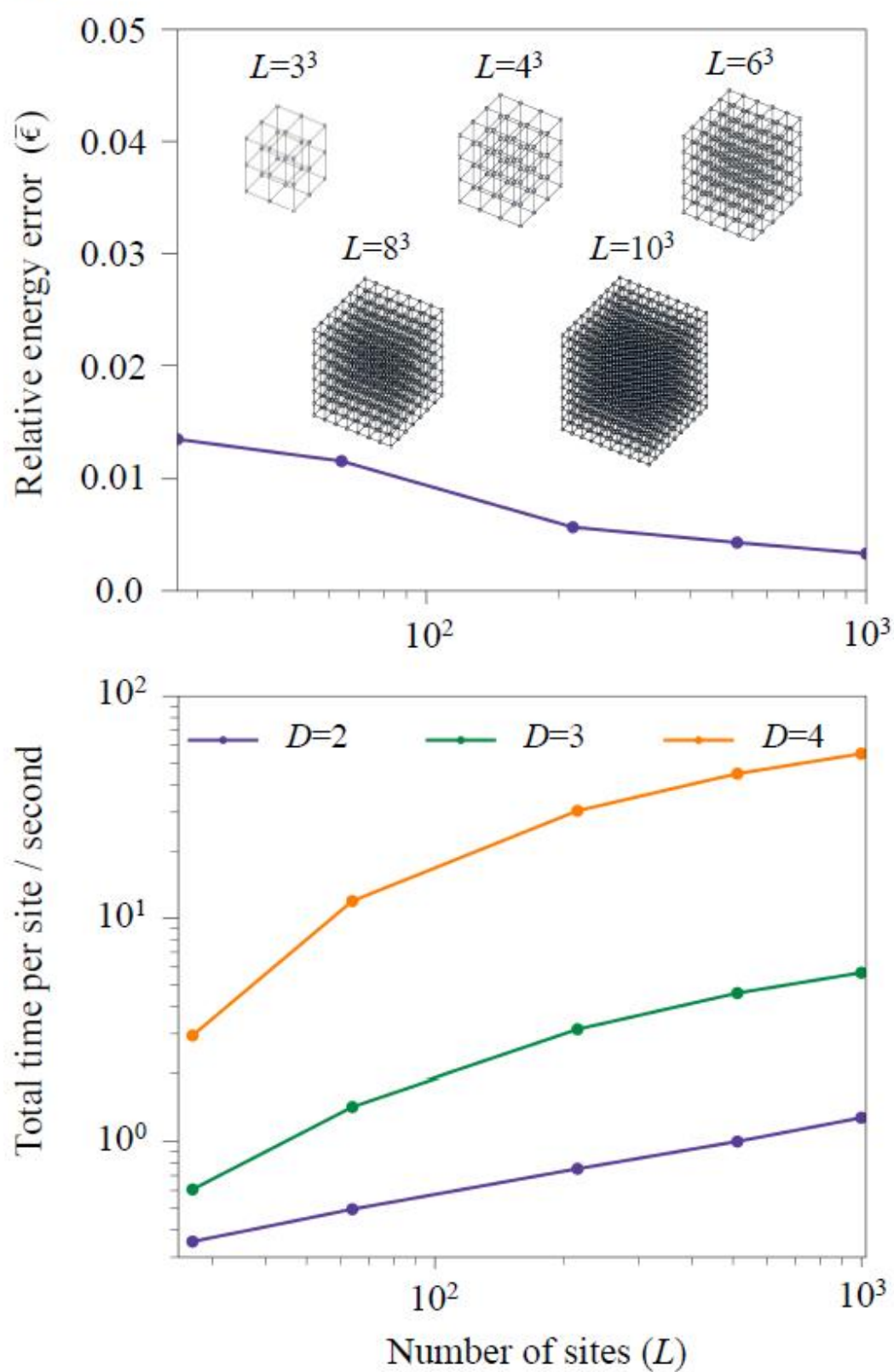
C

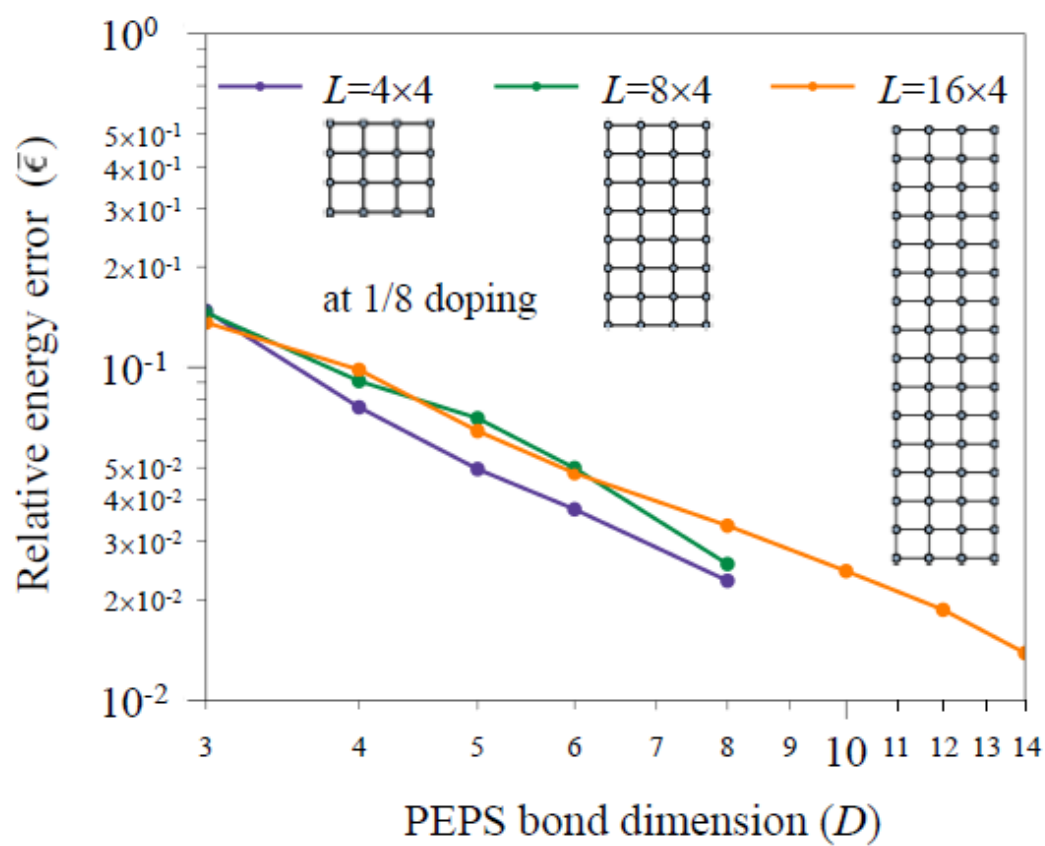
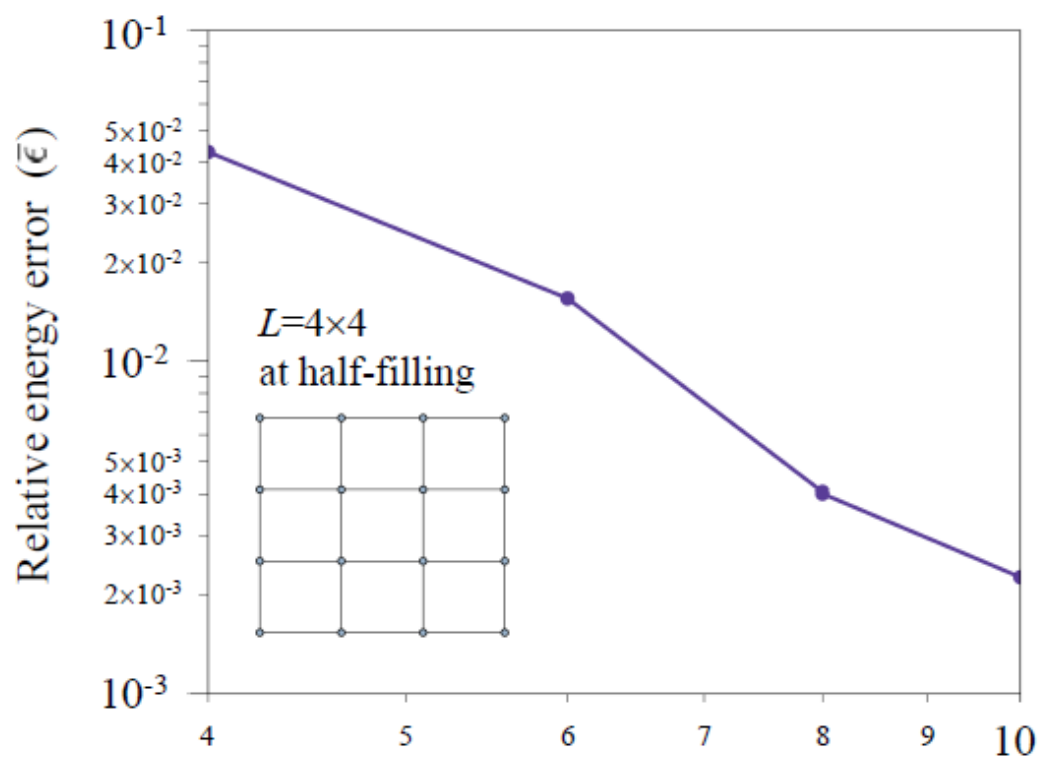


of atoms: 565

of electrons: 2170

of basis functions: 5420

A

B

$$H(s(t)) = (1 - s(t))H_{\text{init}} + s(t)H_{\text{final}}$$

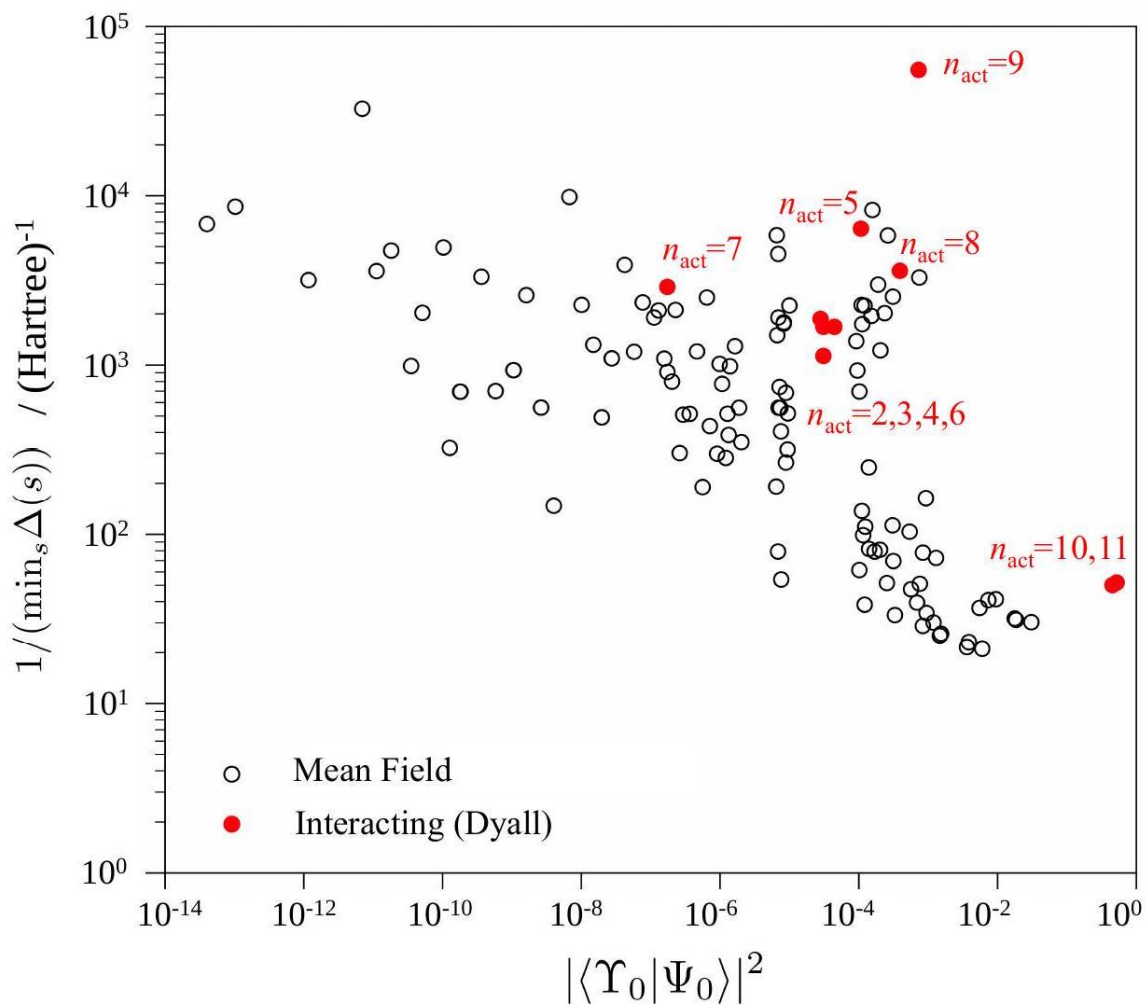
$$|\langle \Phi | \Psi_0 \rangle| \rightarrow 1, \text{ where } \Phi \equiv \Upsilon$$



$$T_{\text{ASP}} \gg \max_{s,i} |\langle Y_i(s) | dH/ds | Y_0(s) \rangle| / (E_i(s) - E_0(s))^2$$

$$T_{\text{ASP}} > K \left(\max_s \|dH/ds\| \right) \Delta^{-2} \log (\Delta^{-1})^{12}$$

$$I = 1 - |\langle \Psi_0(D) | \Psi_0(8000) \rangle|^2 \text{ and } \epsilon = E(D) - E(8000)$$

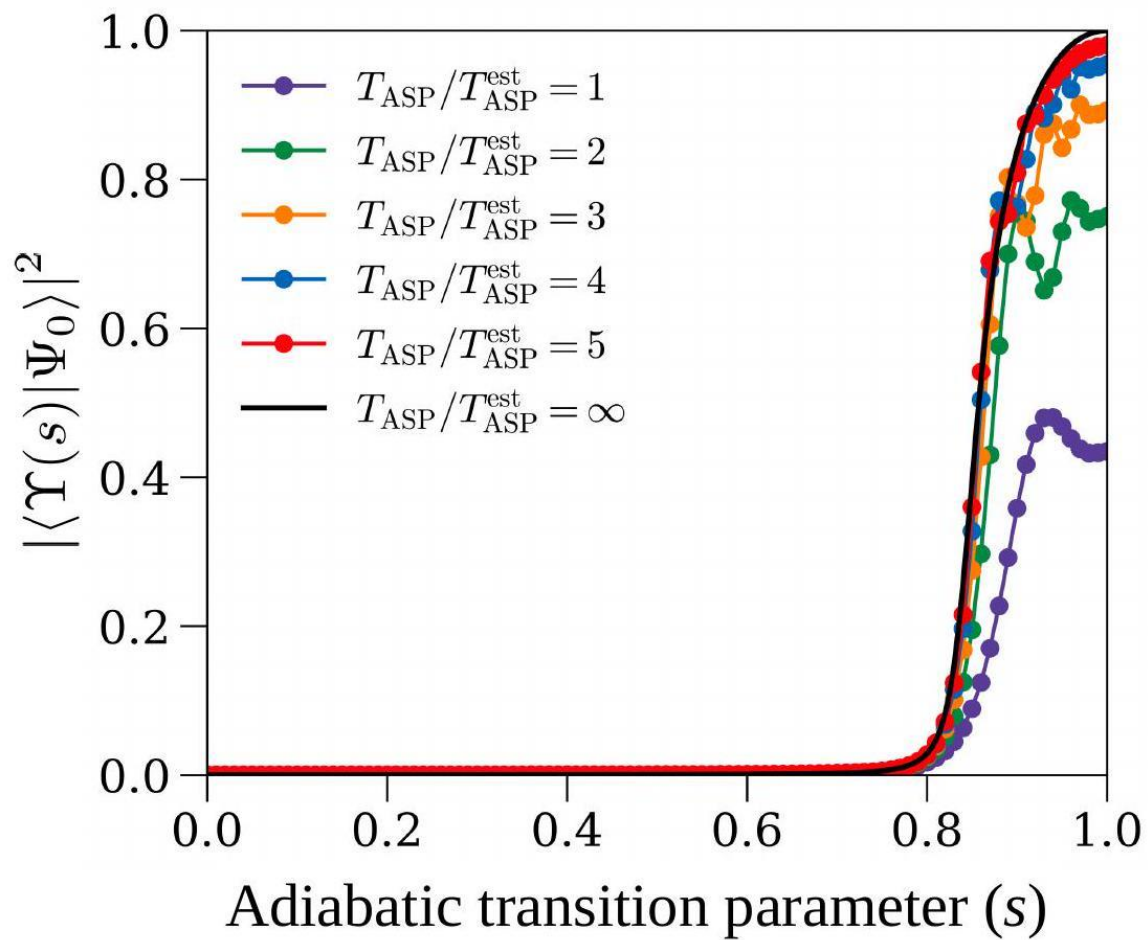


$$\left(1/\left(\min_s \Delta(s)\right)\right)$$

$$\Delta t = 0.01 E_h^{-1}$$

$$|Y(s(t+\Delta t))\rangle = e^{-iH(s(t+\Delta t/2))\Delta t}|Y(s(t))\rangle$$

$$T_{\text{ASP}}/T_{\text{ASP}}^{\text{est}} \approx 2$$



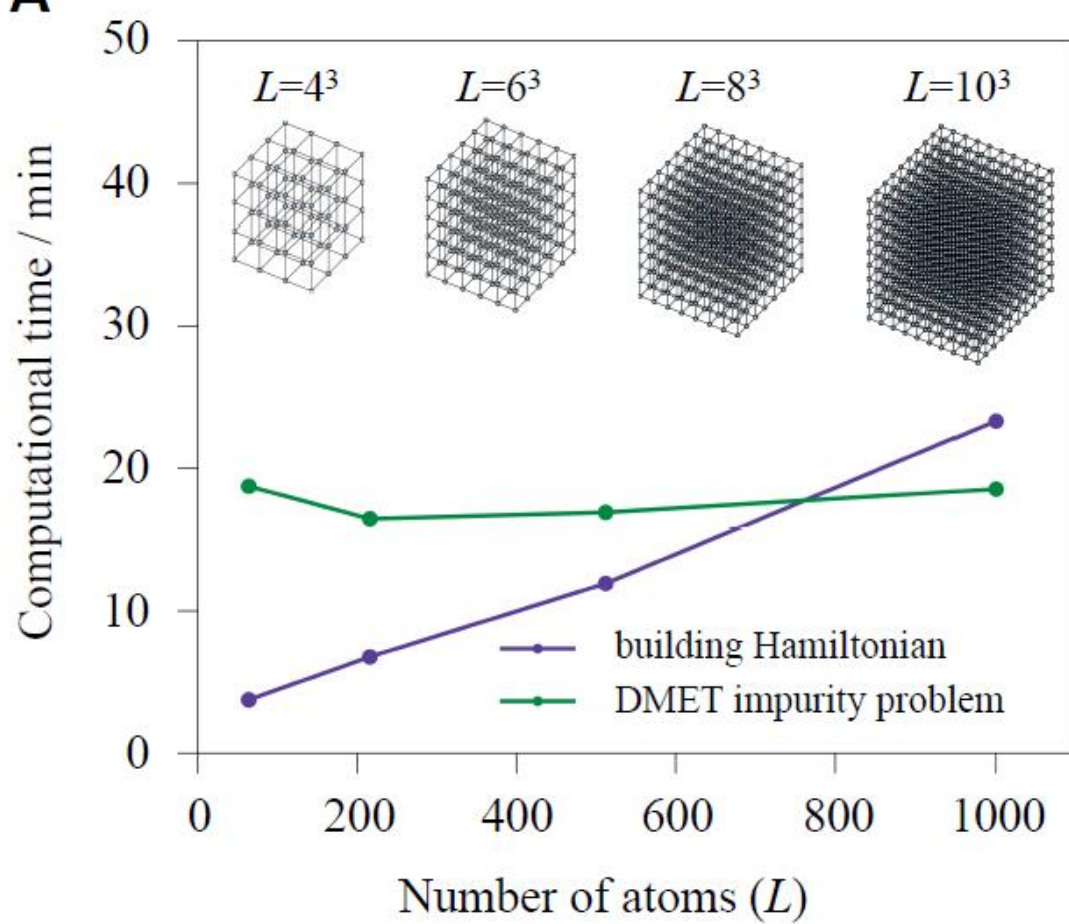
$$|\langle Y(s) | \Psi_0 \rangle|^2 e^{-iHt}$$

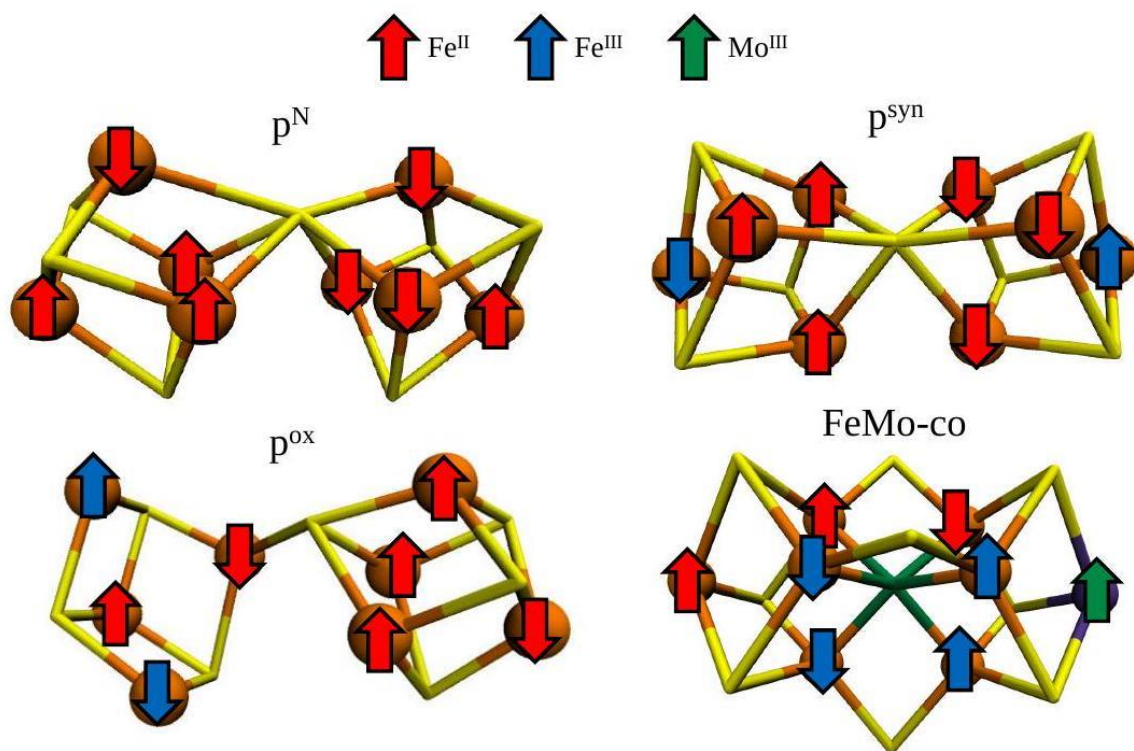
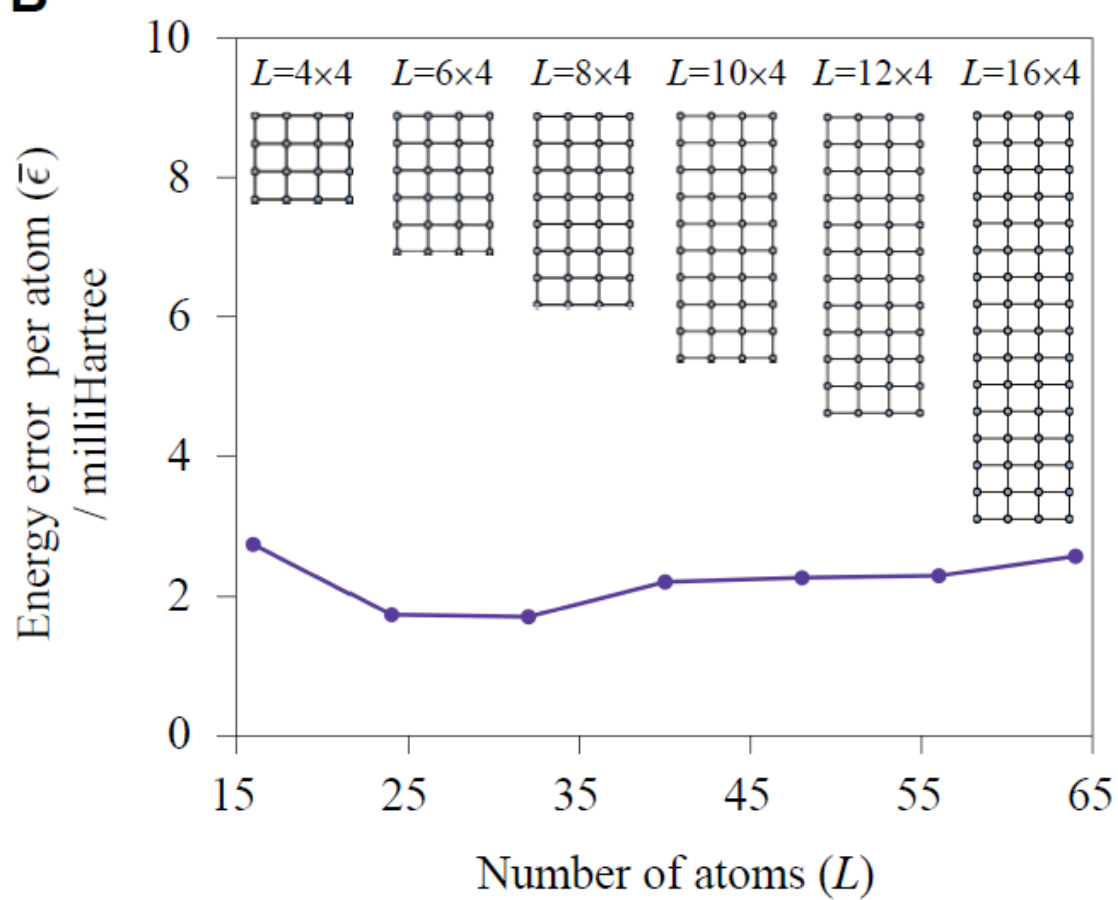
$$|\langle \Phi | \Psi_0 \rangle|^2 = p_0 > 1/2$$

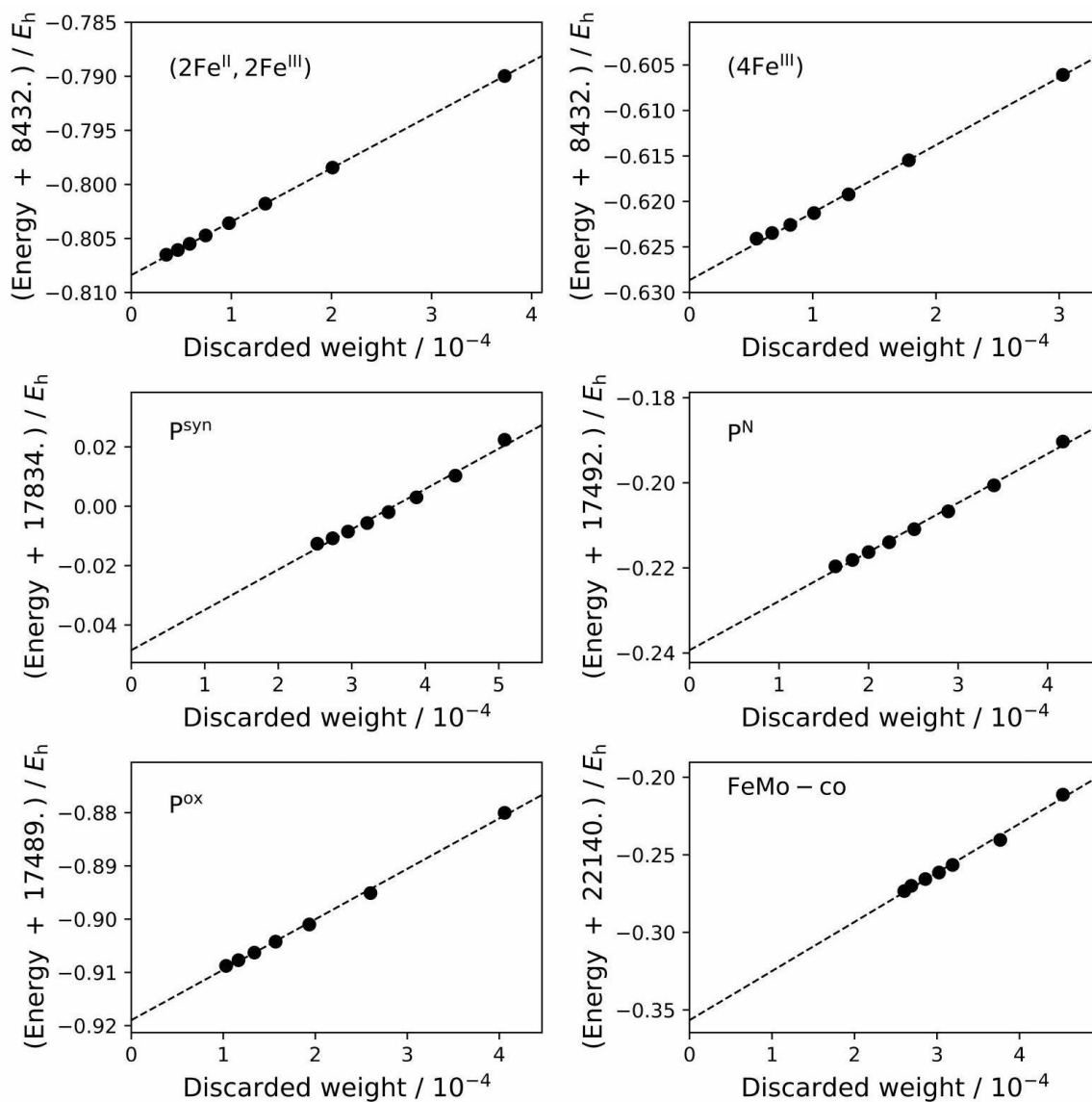
$$T = \frac{\pi}{\epsilon(1 - p_s/p_0)}$$

$$p_{\text{boosted}} = \sum_{m=(n_{\text{trial}}+1)/2}^{n_{\text{trial}}} \binom{n_{\text{trial}}}{m} p_s^m (1 - p_s)^{n_{\text{trial}}-m}$$

$$n_{\text{trial}} T = \frac{\pi n_{\text{trial}}}{\epsilon(1 - p_s/p_0)}$$

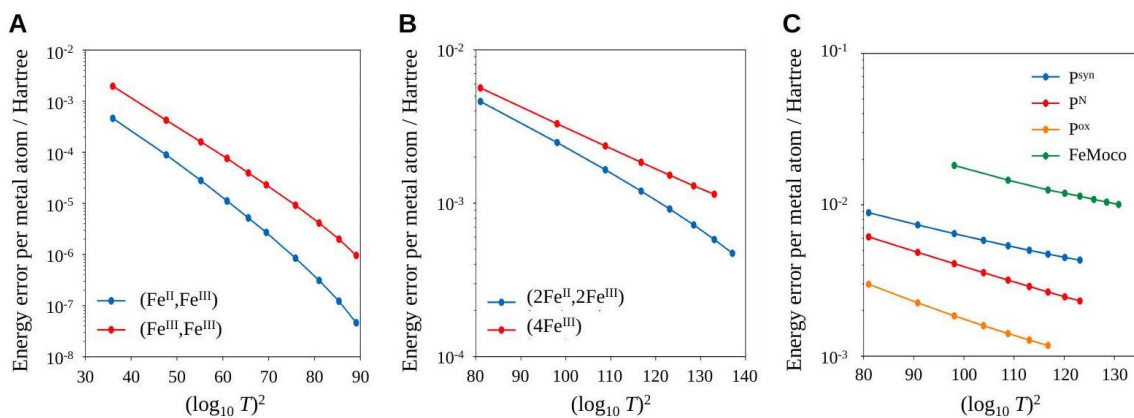
A

B



D	Discarded weight	Energy / E_h	D	Discarded weight	Energy / E_h
2 Fe (II)-2Fe(III)			4Fe(III)		
1000	3.73×10^{-4}	-8432.789966	1000	3.03×10^{-4}	-8432.606085
2000	2.01×10^{-4}	-8432.798444	2000	1.78×10^{-4}	-8432.615484
3000	1.34×10^{-4}	-8432.801780	3000	1.29×10^{-4}	-8432.619229
4000	9.76×10^{-5}	-8432.803590	4000	1.01×10^{-4}	-8432.621279
5000	7.43×10^{-5}	-8432.804722	5000	8.18×10^{-5}	-8432.622578
6000	5.84×10^{-5}	-8432.805500	6000	6.70×10^{-5}	-8432.623476
7000	4.65×10^{-5}	-8432.806069	7000	5.44×10^{-5}	-8432.624094
8000	3.50×10^{-5}	-8432.806502	∞		-8432.6287(9)

∞		-8432.8084(4)			
	p ^{syn}			p ^N	
1000	5.08×10^{-4}	-17833.977588	1000	4.17×10^{-4}	-17492.190311
1500	4.41×10^{-4}	-17833.989684	1500	3.40×10^{-4}	-17492.200594
2000	3.88×10^{-4}	-17833.996979	2000	2.89×10^{-4}	-17492.206725
2500	3.50×10^{-4}	-17834.001975	2500	2.51×10^{-4}	-17492.210894
3000	3.21×10^{-4}	-17834.005658	3000	2.23×10^{-4}	-17492.213953
3500	2.95×10^{-4}	-17834.008503	3500	2.00×10^{-4}	-17492.216294
4000	2.74×10^{-4}	-17834.010764	4000	1.82×10^{-4}	-17492.218146
4500	2.53×10^{-4}	-17834.012610	4500	1.63×10^{-4}	-17492.219644
5000	2.27×10^{-4}	-17834.014051	5000	1.36×10^{-4}	-17492.220847
∞		-17834.049(7)	∞		-17492.239(4)
pox			FeMo-co		
500	4.06×10^{-4}	-17489.880043	2000	4.53×10^{-4}	-22140.21120
1000	2.60×10^{-4}	-17489.895112	3000	3.77×10^{-4}	-22140.24039
1500	1.94×10^{-4}	-17489.901003	4000	3.19×10^{-4}	-22140.25652
2000	1.57×10^{-4}	-17489.904229	4500	3.02×10^{-4}	-22140.26141
2500	1.34×10^{-4}	-17489.906285	5000	2.86×10^{-4}	-22140.26562
3000	1.17×10^{-4}	-17489.907715	5500	2.69×10^{-4}	-22140.26995
3500	1.03×10^{-4}	-17489.908781	6000	2.60×10^{-4}	-22140.27335
4000	8.70×10^{-5}	-17489.909590	6500	2.55×10^{-4}	-22140.27633
∞		-17489.919(2)	7000	2.47×10^{-4}	-22140.27881
			∞		-22140.36(2)



$$\log(1/\bar{\epsilon}) \sim (\log T)^2$$

$$O(D^3 L^3) + O(D^2 L^4)$$

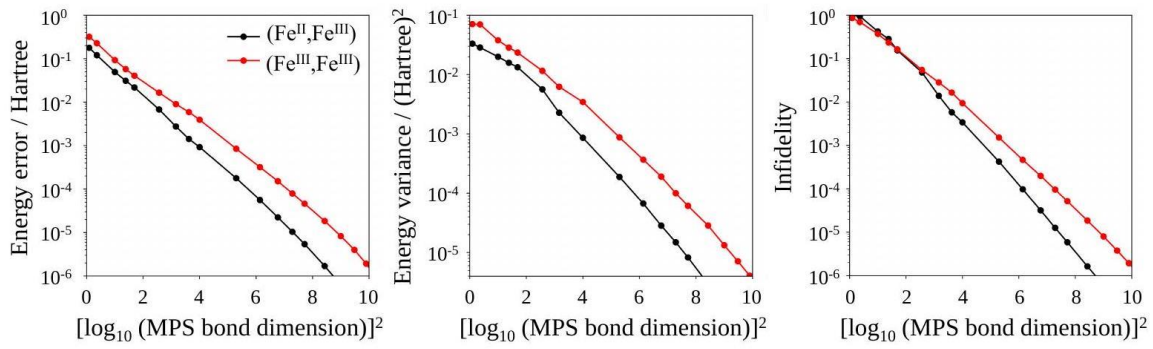
$$(|\langle \Phi_D | \Psi_0 \rangle|)(|\langle \Phi_{\text{CSF}} | \Psi_0 \rangle|)$$

$$S(D) = c/D + S(\infty)$$

D	Overlap (S)		D	Overlap (S)	
	CSF	DET		CSF	DET
2 Fe (II)-2Fe(III)			4Fe(III)		
2000	1.66×10^{-2}	3.54×10^{-3}	2000	7.12×10^{-2}	2.15×10^{-2}
3000	1.61×10^{-2}	3.44×10^{-3}	3000	6.89×10^{-2}	2.08×10^{-2}
4000	1.58×10^{-2}	4.99×10^{-3}	4000	6.75×10^{-2}	2.03×10^{-2}
5000	1.56×10^{-2}	4.93×10^{-3}	5000	6.65×10^{-2}	2.01×10^{-2}
6000	1.54×10^{-2}	4.88×10^{-3}	6000	6.59×10^{-2}	1.99×10^{-2}
7000	1.53×10^{-2}	4.84×10^{-3}	7000	6.54×10^{-2}	1.97×10^{-2}
∞	1.47×10^{-2}	4.65×10^{-3}	∞	6.34×10^{-2}	1.90×10^{-2}
p ^{syn}			p ^N		
1000	4.51×10^{-3}	1.97×10^{-3}	1000	2.44×10^{-2}	1.10×10^{-2}
1500	4.32×10^{-3}	2.05×10^{-3}	1500	2.05×10^{-2}	1.03×10^{-2}
2000	4.09×10^{-3}	2.04×10^{-3}	2000	1.80×10^{-2}	9.73×10^{-3}
2500	3.93×10^{-3}	2.02×10^{-3}	2500	1.62×10^{-2}	9.22×10^{-3}
3000	3.80×10^{-3}	2.00×10^{-3}	3000	1.49×10^{-2}	8.81×10^{-3}
3500	3.69×10^{-3}	1.99×10^{-3}	3500	1.39×10^{-2}	8.48×10^{-3}
4000	3.59×10^{-3}	1.98×10^{-3}	4000	1.32×10^{-2}	8.24×10^{-3}
4500	3.51×10^{-3}	1.97×10^{-3}	4500	1.27×10^{-2}	8.07×10^{-3}
5000	3.45×10^{-3}	1.96×10^{-3}	5000	1.23×10^{-2}	7.95×10^{-3}



∞	3.15×10^{-3}	1.92×10^{-3}	∞	8.63×10^{-3}	6.83×10^{-3}
Pox			FeMo-co		
500	5.66×10^{-3}	1.94×10^{-3}	6000	3.68×10^{-4}	
1000	5.33×10^{-3}	1.78×10^{-3}	7000		9.88×10^{-5}
1500	5.33×10^{-3}	1.70×10^{-3}			
2000	5.08×10^{-3}	1.65×10^{-3}			
2500	5.00×10^{-3}	1.61×10^{-3}			
3000	4.94×10^{-3}	1.57×10^{-3}			
3500	4.90×10^{-3}	1.55×10^{-3}			
4000	4.86×10^{-3}	1.53×10^{-3}			
∞	4.72×10^{-3}	1.44×10^{-3}			



$$(E_{\text{DMRG}} - E_{\text{FCI}})(\langle \Phi_{\text{DMRG}} | (H - E_{\text{DMRG}})^2 | \Phi_{\text{DMRG}} \rangle) (1 - |\langle \Phi_{\text{DMRG}} | \Psi_{\text{FCI}} \rangle|^2)$$

$$H = \sum_{pq} h_{pq}^c \hat{E}_{pq} + \frac{1}{2} \sum_{pqrs} (pq | rs) (\hat{E}_{pq} \hat{E}_{rs} - \delta_{qr} \hat{E}_{ps}) + K_C$$

$$\hat{E}_{pq} = \hat{a}_{p\alpha}^\dagger \hat{a}_{q\alpha} + \hat{a}_{p\beta}^\dagger \hat{a}_{q\beta},$$

$$h_{pq}^c = h_{pq} + \sum_I (2(pq | II) - (pI | Iq)),$$

$$K_C = 2 \sum_I h_{II} + \sum_{IJ} (2(II | JJ) - (IJ | JI)),$$

$$H_{\text{Fock}} = \sum_p (\epsilon_p + \delta(n_p)) \hat{E}_{pp} + K_{\text{C,Fock}}$$

$$K_{\text{C,Fock}} = 2 \sum_I \epsilon_I(n_p)$$

$$\delta(n_p = 2) = 0 \text{ and } \delta(n_p = 0) = 0.5 \text{ (Hartree)}$$

$$H_{\text{Dyall}} = \sum_{ij} f_{ij} \hat{E}_{ij} + \sum_{ab} f_{ab} \hat{E}_{ab} \\ + \sum_{uv} h_{uv}^{\text{eff}} \hat{E}_{uv} + \frac{1}{2} \sum_{uvwx} (uv \mid wx) (\hat{E}_{uv} \hat{E}_{wx} - \delta_{vw} \hat{E}_{ux}) + K_{\text{C,Dyall}}$$

$$h_{pq}^{\text{eff}} = h_{pq}^{\text{C}} + \sum_i (2(pq \mid ii) - (pi \mid iq)),$$

$$f_{pq} = h_{pq}^{\text{eff}} + \sum_{uv} D_{uv} ((pq \mid uv) - 0.5(pu \mid vq)),$$

$$K_{\text{C,Dyall}} = K_{\text{C}} + 2 \sum_i h_{ii}^{\text{C}} + \sum_{ij} (2(ii \mid jj) - (ij \mid ji)) - 2 \sum_i f_{ii}.$$

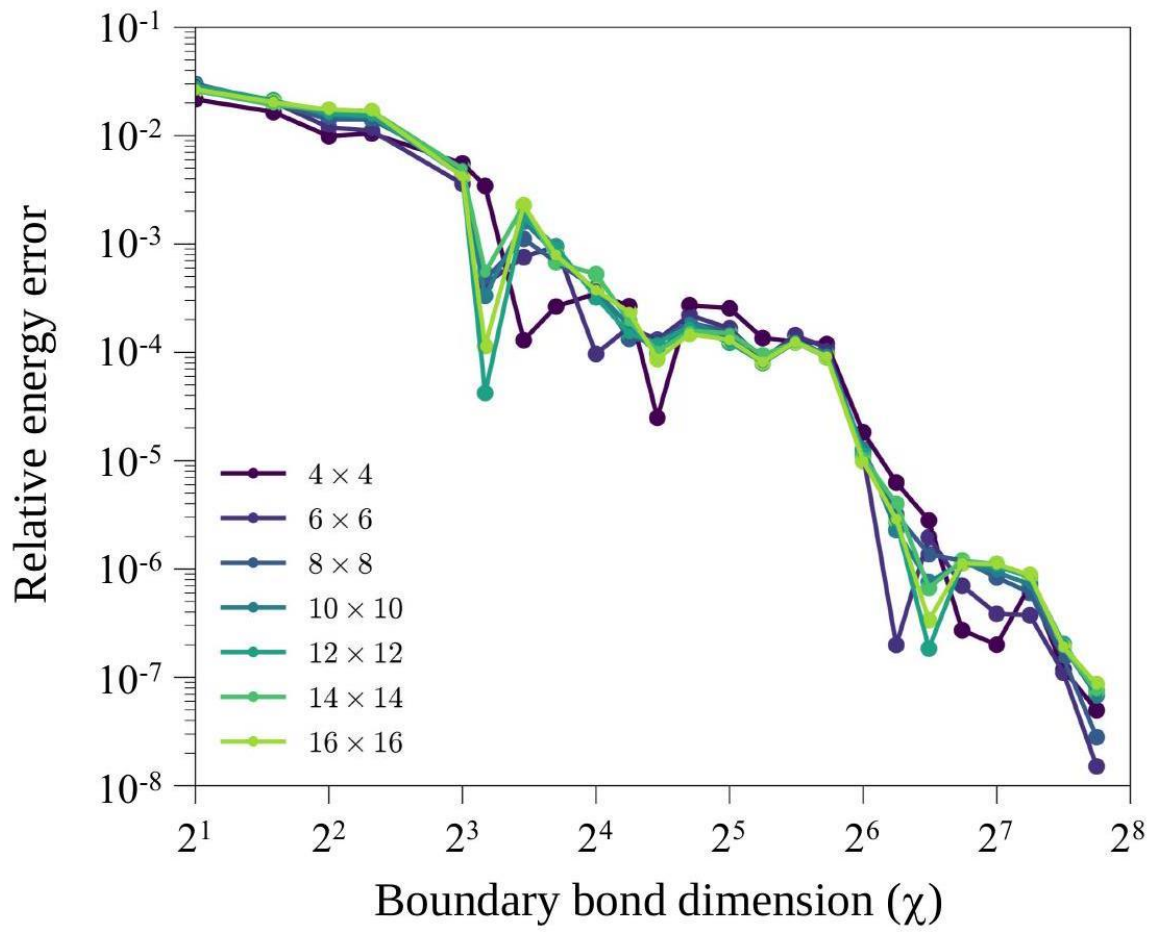
$$|\Psi_0\rangle = \exp(\hat{T})|\Phi_0\rangle$$

$$\Delta E_{\text{CC}}(\text{C}_m\text{H}_{2m+2}) = mE_{\text{CC}}(\text{C}) + (2m+2)E_{\text{HF}}(\text{H}) - E_{\text{CC}}(\text{C}_m\text{H}_{m+2}),$$

$$E_{\text{CC}} = E_{\text{DLPNO-CCSD(T)-F12(fc)/cc-pVTZ-F12}} + (E_{\text{DLPNO-CCSD(T)(ae)/cc-pCVTZ}} - E_{\text{DLPNO-CCSD(T)(fc)/cc-pCVTZ}})$$

$$\Delta_f H_{\text{CC}}^{\ominus}(\text{C}_m\text{H}_{2m+2}; 298.15 \text{ K}) = \Delta E_{\text{CC}}(\text{C}_m\text{H}_{2m+2}) - \Delta E_{\text{ZPE}}(\text{C}_m\text{H}_{2m+2}) \\ + m(\Delta_f H_{\text{exp}}^{\ominus}(\text{C}; 0 \text{ K}) + \Delta H_{\text{exp}}^{\ominus}(\text{C}(\text{cr}); 0 \text{ K} \rightarrow 298.15 \text{ K})) \\ + (2m+2)(\Delta_f H_{\text{exp}}^{\ominus}(\text{H}; 0 \text{ K}) + \Delta H_{\text{exp}}^{\ominus}(\text{H}_2; 0 \text{ K} \rightarrow 298.15 \text{ K})) \\ + \Delta H_{\text{B3LYP/pc-2}}^{\ominus}(\text{C}_m\text{H}_{2m+2}; 0 \text{ K} \rightarrow 298.15 \text{ K}),$$

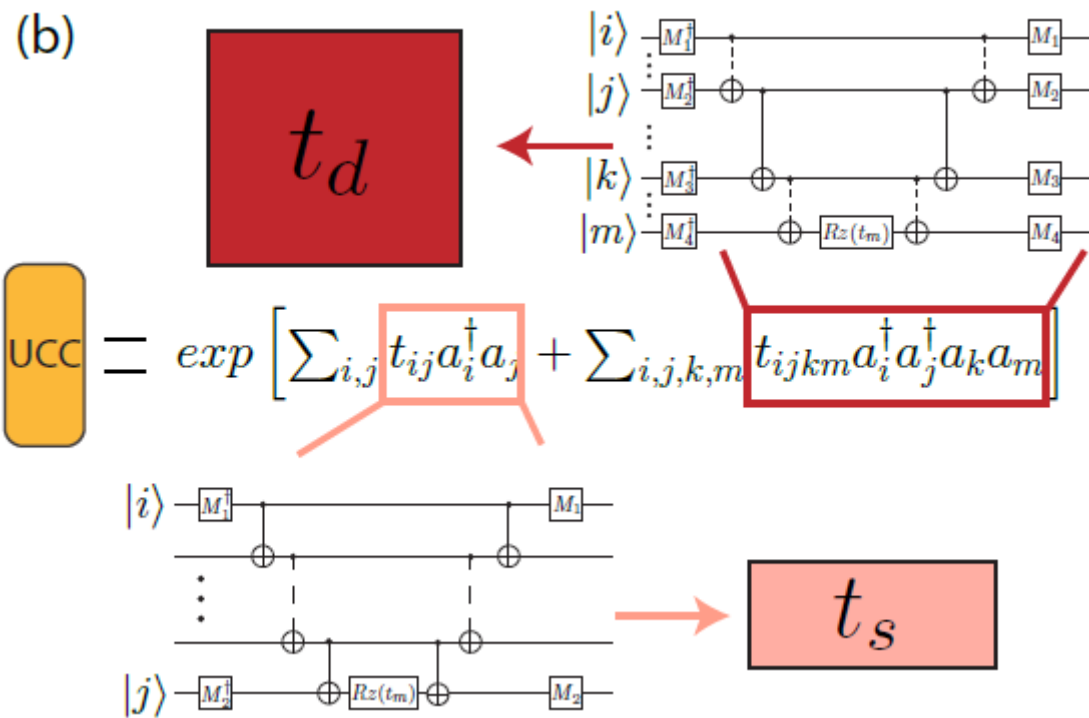
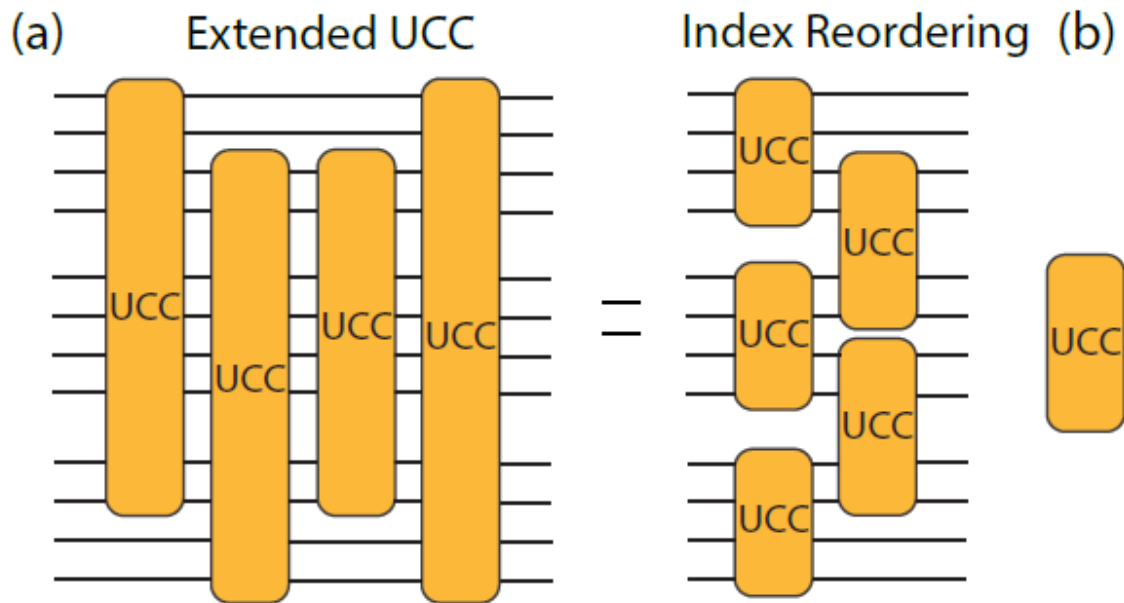
$$\Delta H_{\text{B3LYP/pc-2}}^{\ominus}(\text{C}_m\text{H}_{2m+2}; 0 \text{ K} \rightarrow 298.15 \text{ K})$$

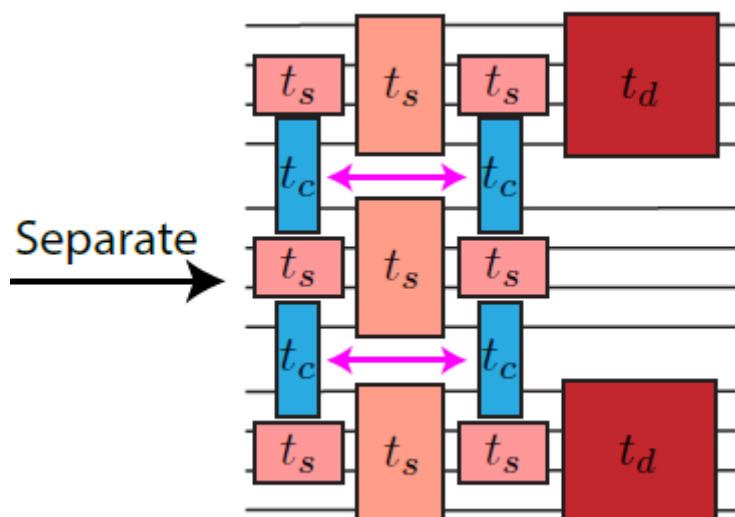
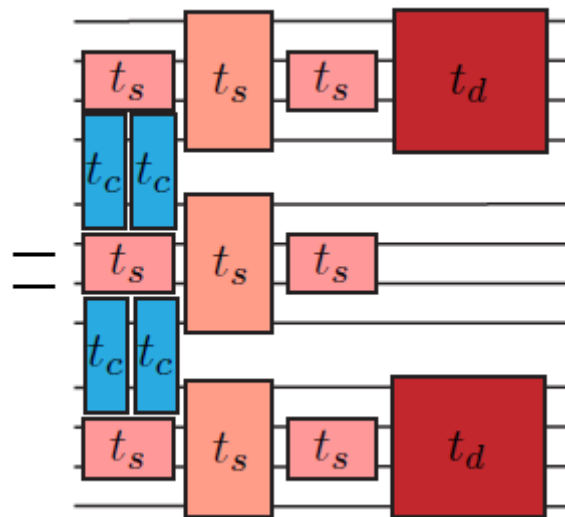
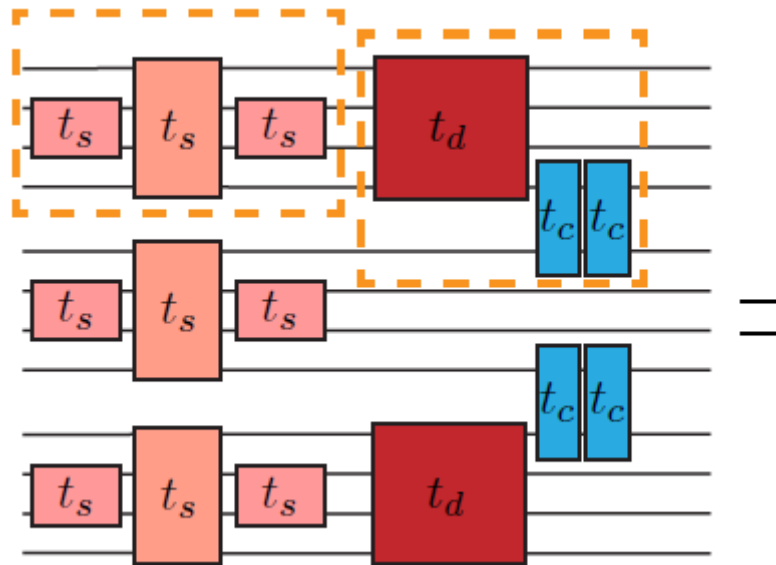


D	4 × 4, half-filling		4 × 4, 1/8 doped		4 × 8, 1/8 doped		4 × 16, 1/8 doped		
	SU	DMR G	SU	DMR G	SU	DMR G	SU	DMR G	VMC
3			- 0.525 6	- 0.539 3	- 0.554 3	- 0.572 7	- 0.570 4	- 0.592 2	
4	- 0.405 4	- 0.407 3	- 0.557 6	- 0.584 7	- 0.586 5	- 0.60 95	- 0.596 2	- 0.618 2	- 0.6182(2)
5	- 0.410 5	- 0.414 6	- 0.569 4	- 0.601 3	- 0.598 6	- 0.623 3	- 0.60 91	- 0.641 4	
6	- 0.415 4	- 0.418 9	- 0.583 8	- 0.608 9	- 0.617 1	- 0.637 0	- 0.631 3	- 0.652 6	- 0.6526(1)

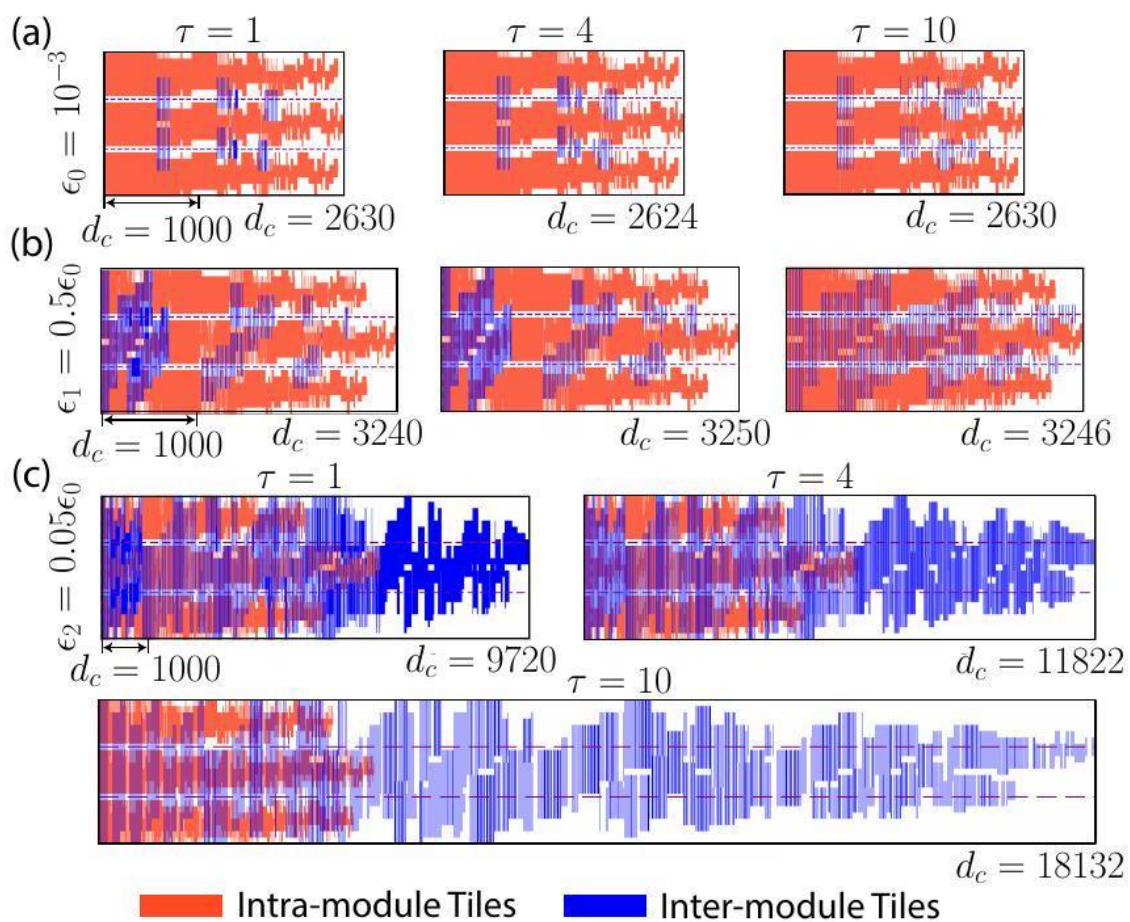
7	- 0.417 7	- 0.423 0							
8	- 0.418 0	- 0.423 8	- 0.597 9	- 0.618 1	- 0.628 5	- 0.653 2	- 0.641 5	- 0.662 4	- 0.6626(2)
1 0	- 0.420 8	- 0.424 6	- 0.605 6	- 0.622 0					- 0.6688(1)
1 2									- 0.6727(1)
1 4									- 0.6760(1)

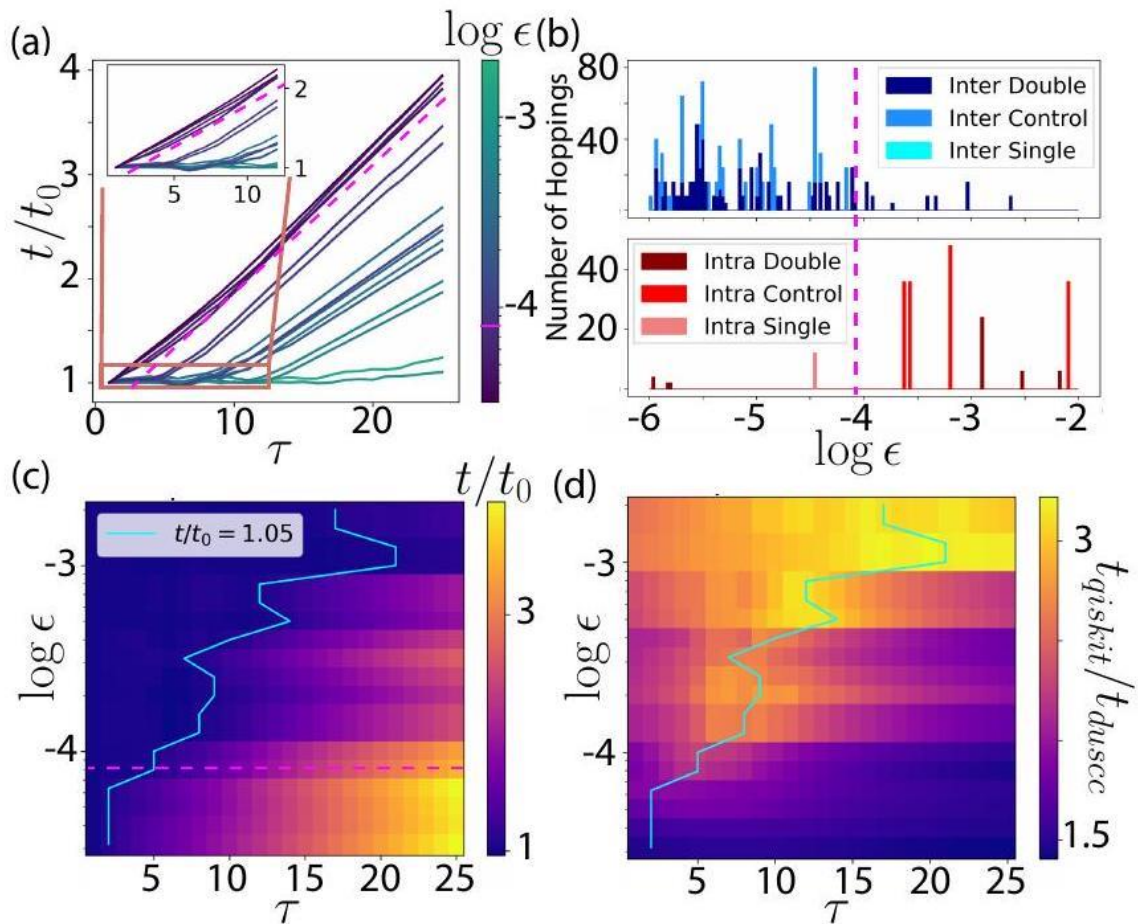
D	Discarded weight	Energy per site	D	Discarded weight	Energy per site
4 × 4 at half-filling			4 × 4 at 1/8 doped		
500	3.59×10^{-6}	-0.42551504	500	7.30×10^{-5}	-0.63241788
1000	2.61×10^{-7}	-0.42552519	1000	5.40×10^{-6}	-0.63260460
1500	5.80×10^{-8}	-0.42552583	1500	1.01×10^{-6}	-0.63261660
2000	1.50×10^{-8}	-0.42552589	2000	2.50×10^{-7}	-0.63261805
2500	4.12×10^{-9}	-0.42552590	2500	7.55×10^{-8}	-0.63261830
∞		- 0.42552596(1)	∞		-0.6326190(1)
4 × 8 at 1/8 doped			4 × 16 at 1/8 doped		
500	3.66×10^{-4}	-0.66601570	6000	2.27×10^{-5}	-0.68515566
1000	1.87×10^{-4}	-0.66842805	7000	1.87×10^{-5}	-0.68522094
1500	1.13×10^{-4}	-0.66918879	8000	1.62×10^{-5}	-0.68526802
2000	7.59×10^{-5}	-0.66952323	9000	1.41×10^{-5}	-0.68530352
2500	5.38×10^{-5}	-0.66969776	∞		-0.68555(5)
∞		-0.67047(15)			





$$\tau \equiv \frac{t_{\text{Bell pairs}}}{t_{\text{intra-CNOT}}}$$





$$|\Psi_{LAS}\rangle = \prod_K |\Psi_K\rangle \otimes |\Phi_D\rangle$$

$$|\Psi_{LAS-USCC}(\mathbf{t})\rangle = \hat{U}_{USCC}(\mathbf{t})|\Psi_{QLAS}\rangle$$

$$\hat{U}_{USCC}(\mathbf{t}) = \exp [t_{ij}(a_i^\dagger a_j - \text{h.c.}) + t_{ijkm}(a_i^\dagger a_j^\dagger a_k a_m - \text{h.c.})]$$

$$\mathbf{t} = [t_{ij}, t_{ijkm}]$$

$$\left| \frac{\partial E_{USCC}}{2 \partial t_\beta} \right|_{t_\beta=0} \geq \epsilon$$

$$\hat{U}_{aUSCC} = \prod_{ij} M_{ij}^\dagger \exp \left[t_{ij} \prod_k \sigma_k^z \right] M_{ij} +$$

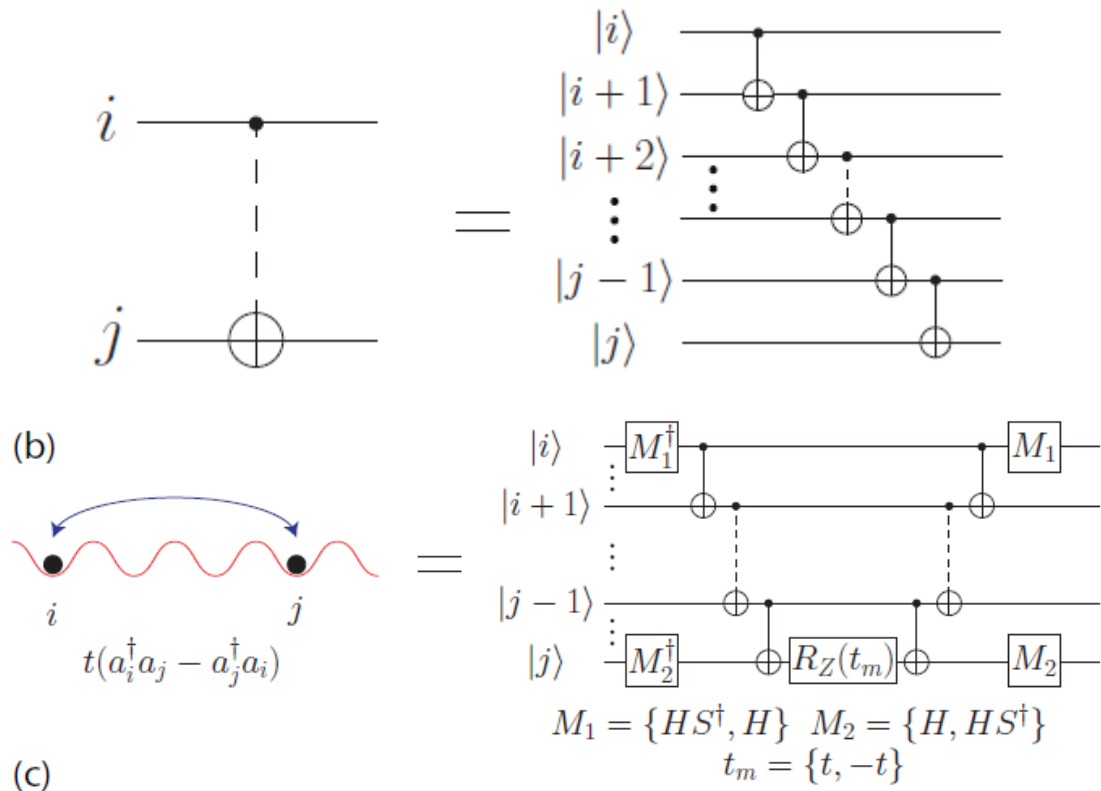
$$\prod_{ij} M_{ijkm}^\dagger \exp \left[t_{ijkm} \prod_k \sigma_k^z \right] M_{ijkm}$$

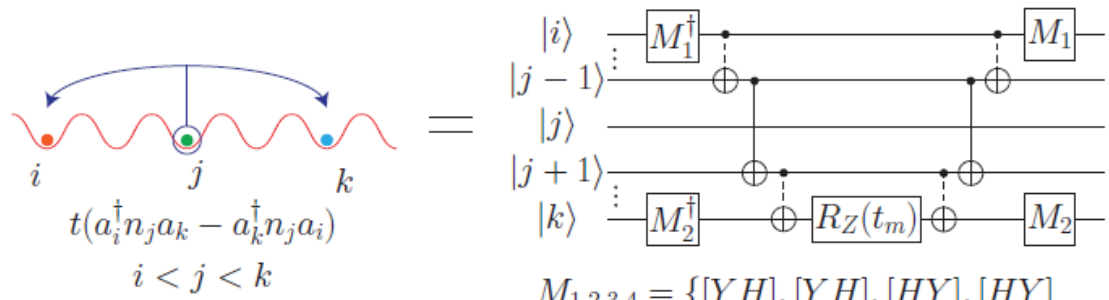
$$\hat{U}_{USCC} = \prod_{ij} \exp (t_{ij} a_i^\dagger a_j - h.c.) +$$

$$\prod_{ijkm} \exp (t_{ijkm} a_i^\dagger a_j^\dagger a_k a_m - h.c.) + O(t^2)$$

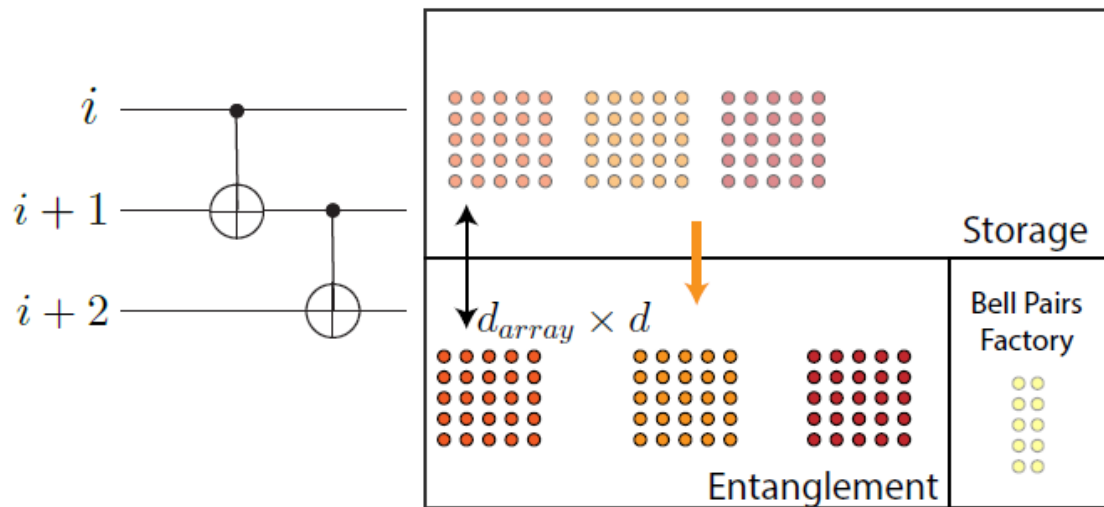
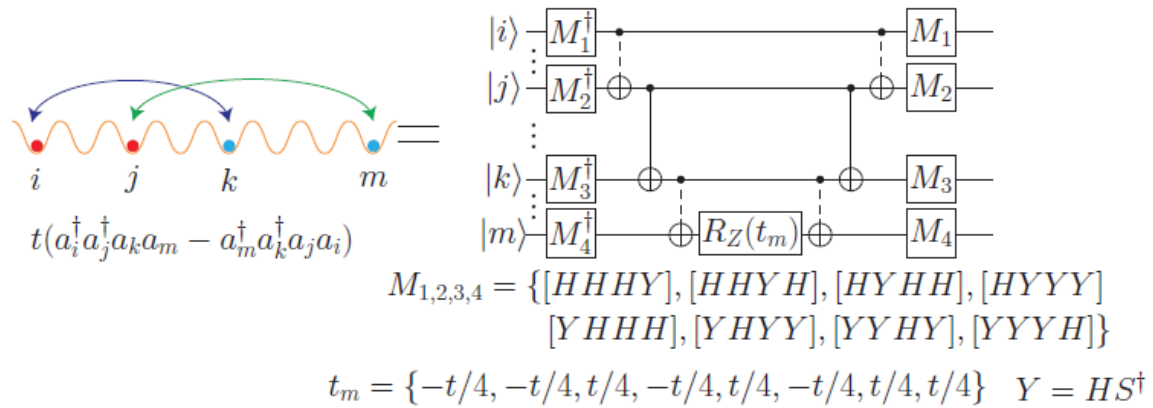
$$\begin{aligned}
a_i &= \left(\prod_{j=1}^{i-1} \sigma_j^z \right) Q_i^+ a_i^\dagger = \left(\prod_{j=1}^{i-1} \sigma_j^z \right) Q_i^- \\
Q^+ &= \frac{1}{2}(\sigma^x - i\sigma^y)Q^- = \frac{1}{2}(\sigma^x + i\sigma^y) \\
&\exp [t_{ij} a_i^\dagger a_j - h.c.] \\
&= \exp \left[t_{ij} \left(Q_i^- \prod_{k=i+1}^L \sigma_k^z \right) \left(Q_j^+ \prod_{k=j+1}^L \sigma_k^z \right) - h.c. \right] \\
&= \exp \left[t_{ij} Q_i^- \left(\prod_{k=i+1}^{j-1} \sigma_k^z \right) (\sigma_j^z Q_j^+) - h.c. \right] \\
&= \exp \left[it_{ij}/2 \left[\sigma_i^x \left(\prod_{k=i+1}^{j-1} \sigma_k^z \right) \sigma_j^y - \sigma_i^y \left(\prod_{k=i+1}^{j-1} \sigma_k^z \right) \sigma_j^x \right] \right] \\
&= H_i (HS^\dagger)_j^\dagger \exp \left[it_{ij}/2 \prod_{k=i}^j \sigma^z \right] H_i (HS^\dagger)_j \\
&\times (HS^\dagger)_i^\dagger H_j \exp \left[-it_{ij}/2 \prod_{k=i}^j \sigma^z \right] (HS^\dagger)_i H_j
\end{aligned}$$

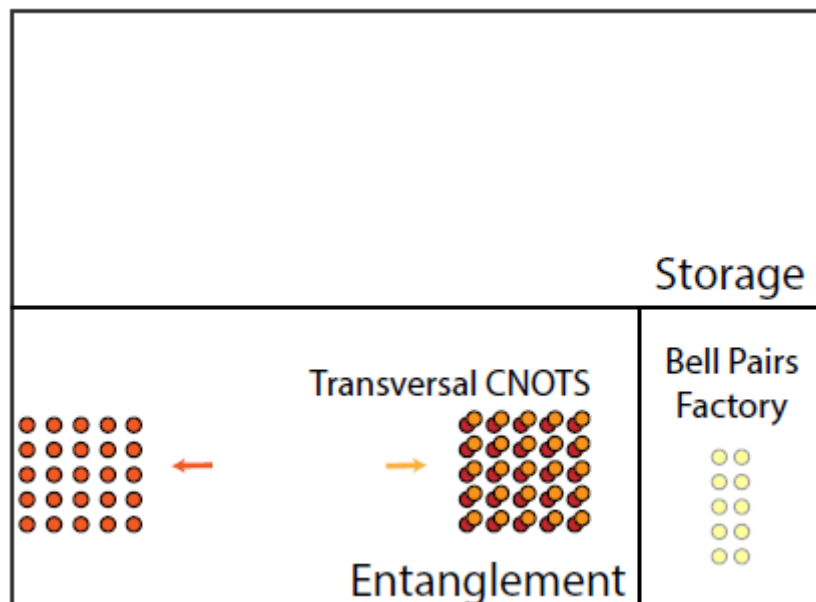
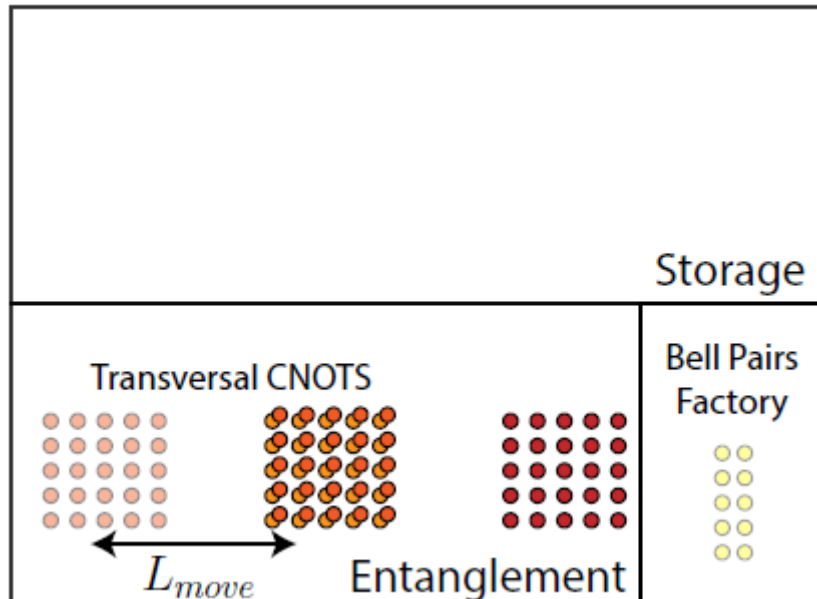
$$\exp(U^\dagger M U) = U^\dagger \exp(M) U$$

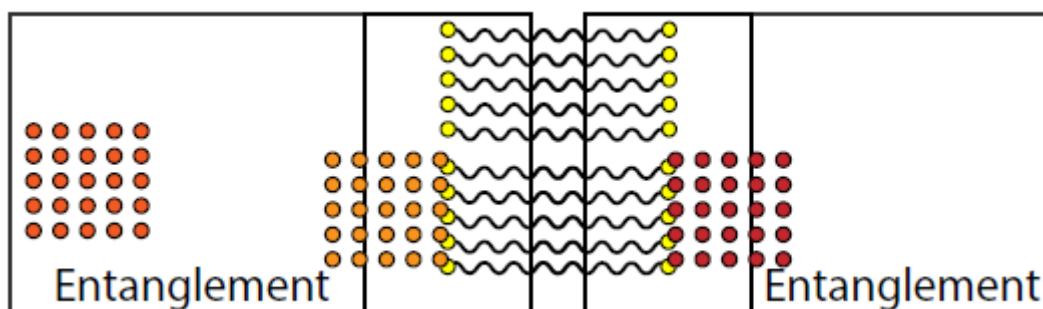
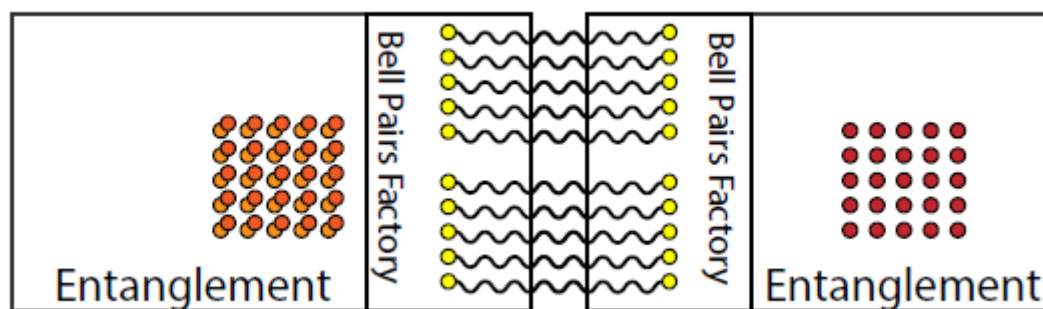
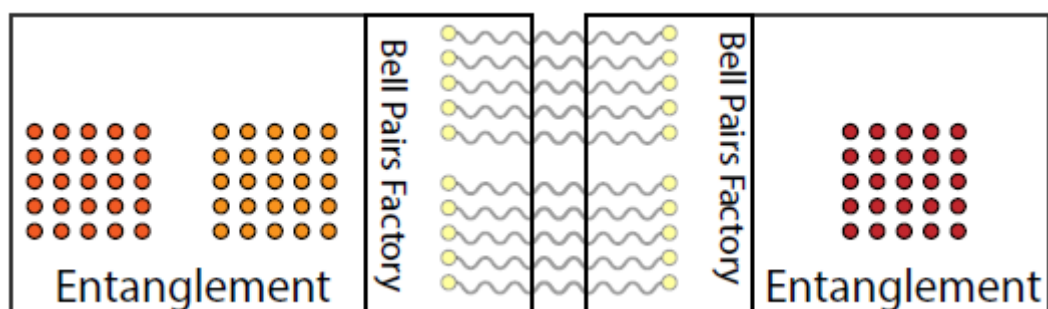
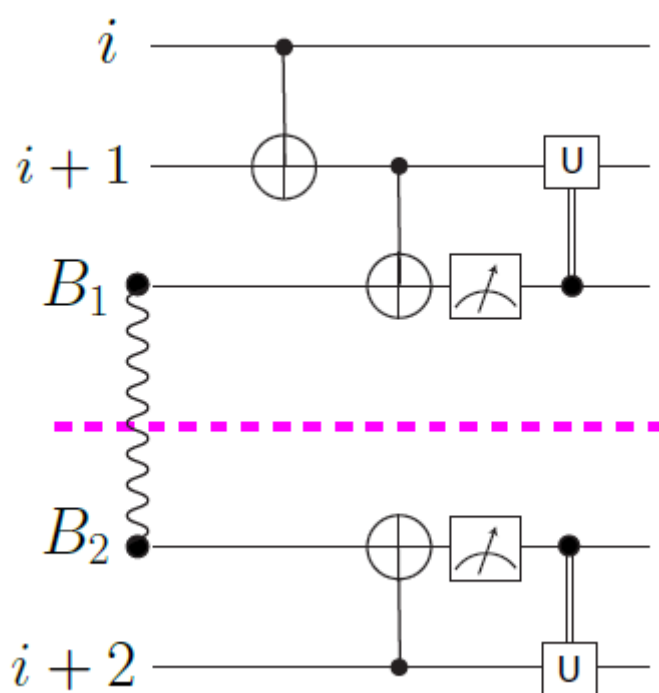


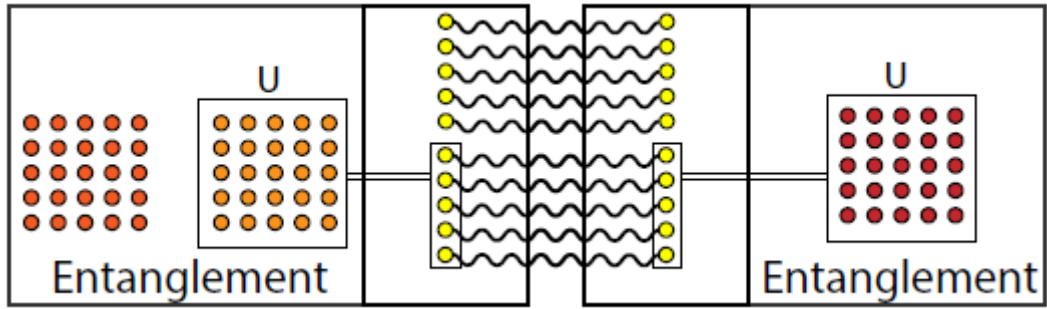


(d)





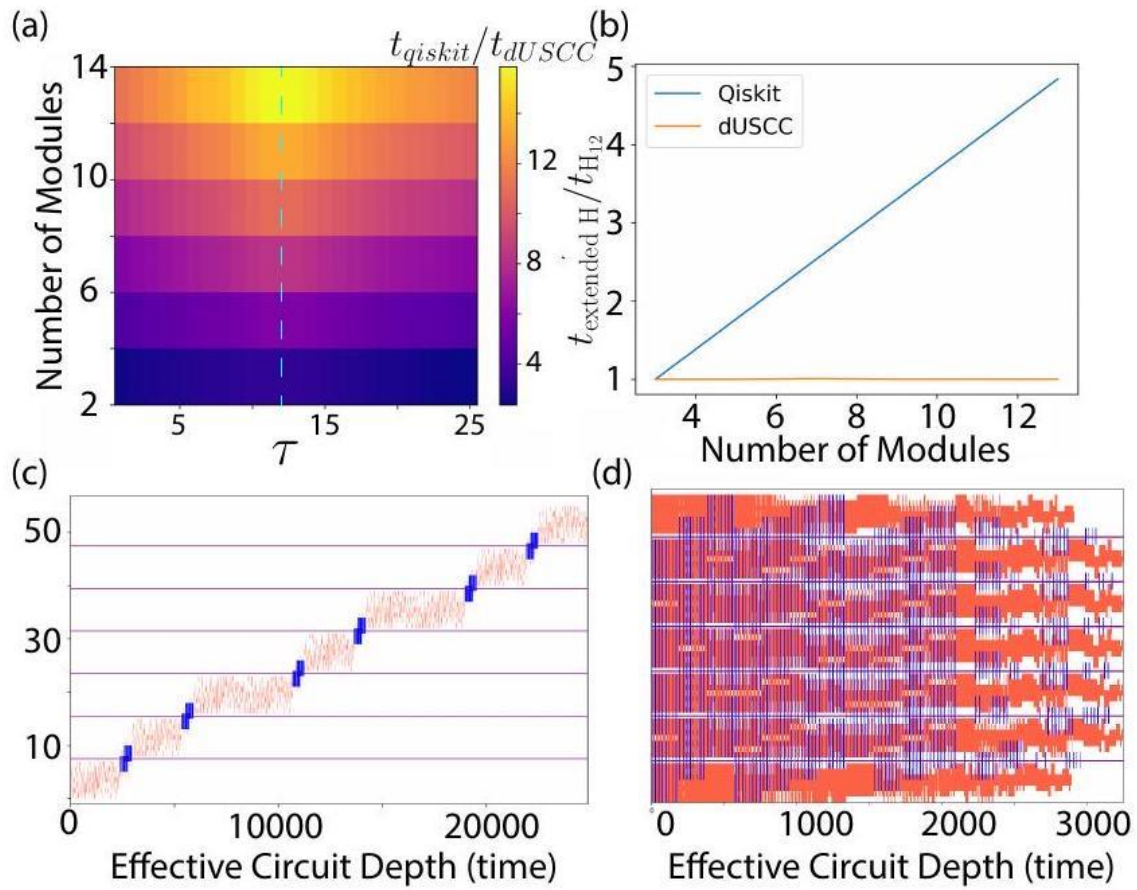




$$t_{\text{intra}}^{\text{ladder}} = \frac{d_{\text{array}} \cdot d + L_{\text{move}} \cdot N_L^{\text{row}}}{v_{\text{avg}}} + t_{\text{intra}}^{\text{bare}} \cdot N_L^{\text{row}}$$

$$\approx \frac{L_{\text{move}} \cdot N_L^{\text{row}}}{v_{\text{avg}}}$$

$$L_{\text{move}} = d \cdot d_{\text{array}} = 5 \cdot 5 \mu\text{m}$$



$$t_{\text{intra}} \approx \frac{t_{\text{intra}}^{\text{ladder}}}{N_L^{\text{row}}} = 25 \mu$$

$$M_{ij}^{\dagger} \exp \left[t_{ij} \prod_k \sigma_k^z \right] M_{ij}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & a & c & 0 \\ 0 & b & d & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a & c & 0 \\ 0 & 0 & 0 & 0 & 0 & b & d & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\sigma^{\dagger}=(X+iY)/2$$

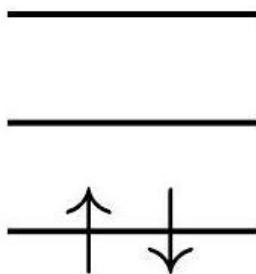
$$\sigma=(X-iY)/2$$

$$N=\sum_i\sigma_i^{\dagger}\sigma_i$$

$$N|x\rangle=w(x)|x\rangle$$

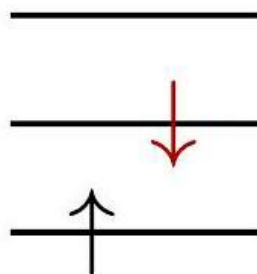
$$[U,N]=0$$

Reference



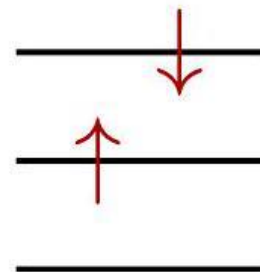
$|110000\rangle$

Single excitation



$|100100\rangle$

Double excitation



$|001001\rangle$

$$G(\theta)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos{(\theta)} & -\sin{(\theta)} & 0 \\ 0 & \sin{(\theta)} & \cos{(\theta)} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$G=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & a & c & 0 \\ 0 & b & d & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$|a|^2+|c|^2=|b|^2+|d|^2=1$$

$$G^{(2)}|0011\rangle=a|0011\rangle+b|1100\rangle,$$

$$G^{(2)}|1100\rangle=d|1100\rangle+c|0011\rangle,$$



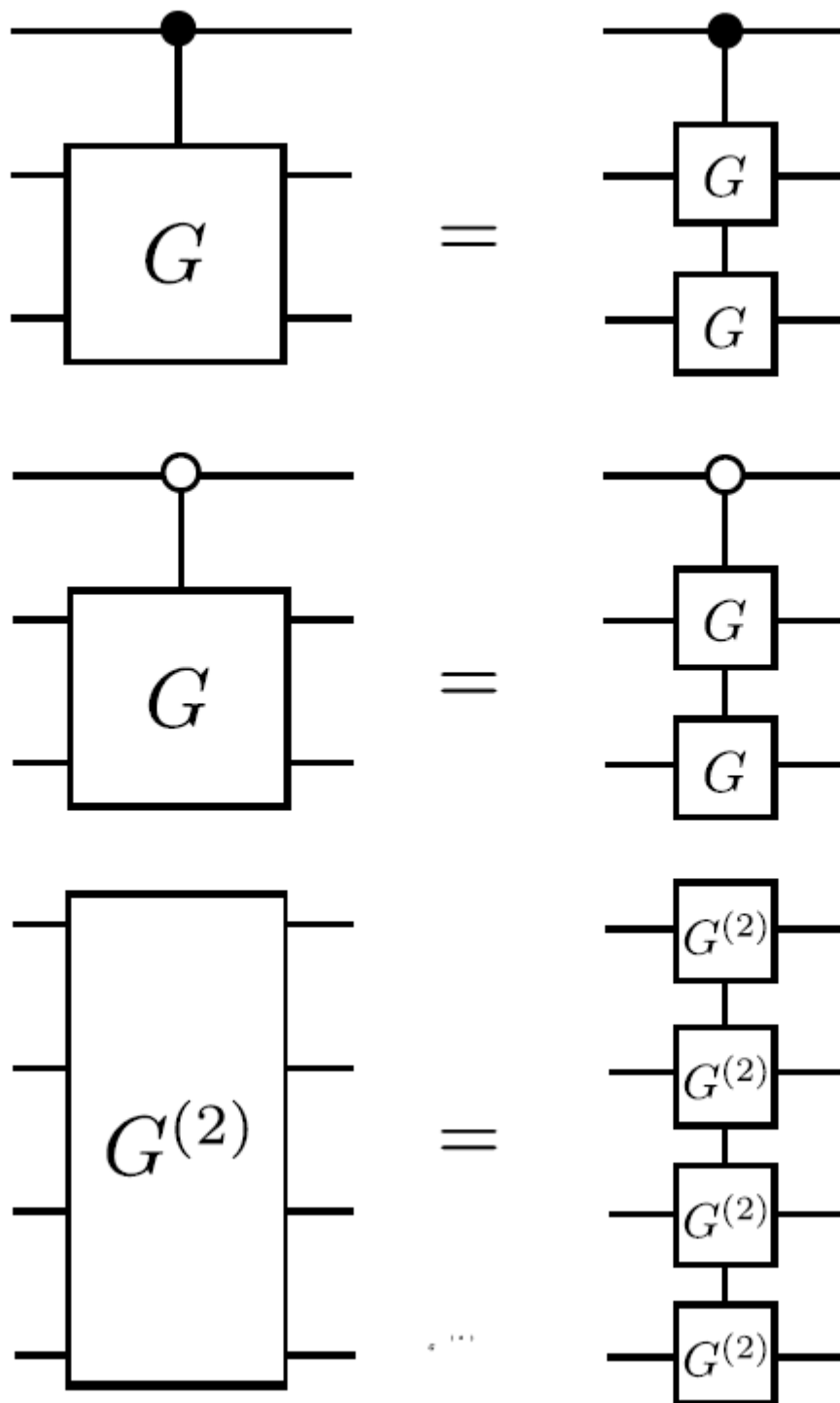
$$|\mathbf{1}_\ell \mathbf{0}_\ell\rangle := |1\rangle^{\otimes \ell} |0\rangle^{\otimes \ell} |\mathbf{0}_\ell \mathbf{1}_\ell\rangle := |0\rangle^{\otimes \ell} |1\rangle^{\otimes \ell}$$

$$G^{(\ell)}|\mathbf{0}_\ell \mathbf{1}_\ell\rangle = a|\mathbf{0}_\ell \mathbf{1}_\ell\rangle + b|\mathbf{1}_\ell \mathbf{0}_\ell\rangle$$

$$G^{(\ell)}|\mathbf{1}_\ell \mathbf{0}_\ell\rangle = d|\mathbf{1}_\ell \mathbf{0}_\ell\rangle + c|\mathbf{0}_\ell \mathbf{1}_\ell\rangle$$

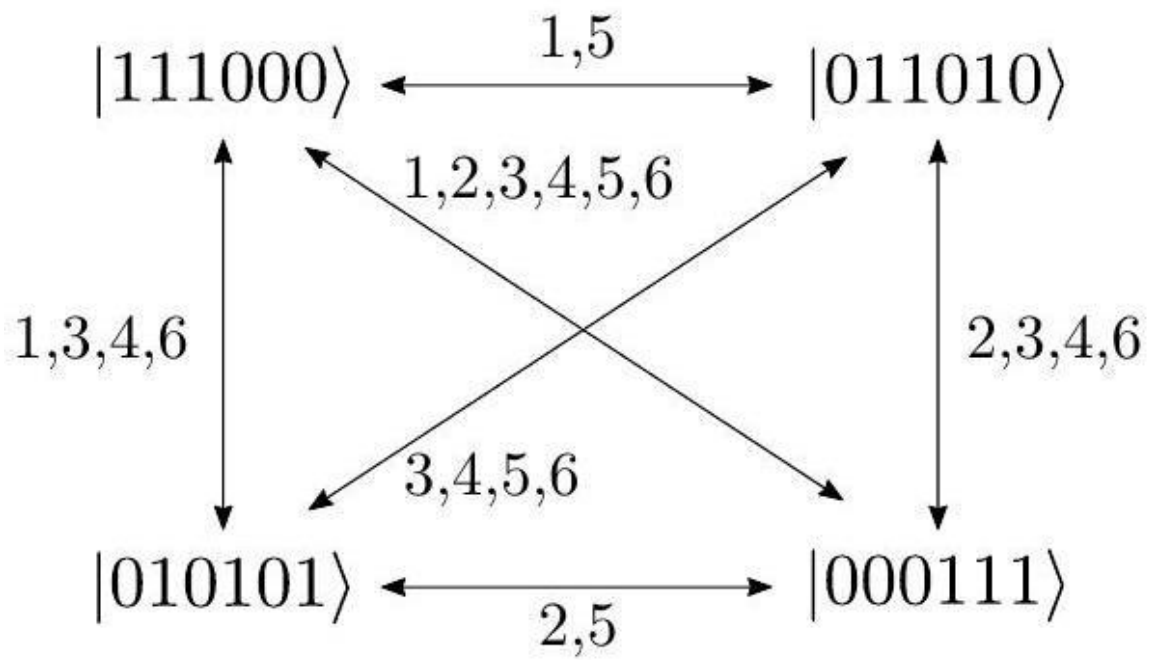
$$CG = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a & c & 0 \\ 0 & 0 & 0 & 0 & 0 & b & d & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

$$F = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$



$$\exp [-i\theta(a_i^\dagger a_j - a_j^\dagger a_i)] a_i^\dagger \rightarrow \sigma_i^+ \prod_{j<i} z_j$$

$$\sigma^\pm = (X \pm iY)$$



$$U|x\rangle = a|x\rangle + b|y\rangle,$$

$$U|y\rangle = d|y\rangle + c|x\rangle,$$

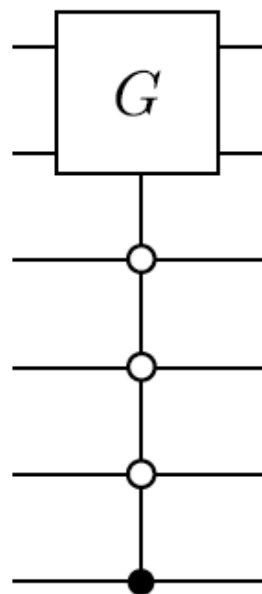
$$G^{(\ell)}|z\rangle|x\rangle = a|z\rangle|x\rangle + b|z\rangle|y\rangle,$$

$$C^{(m)}G^{(\ell)}|x'\rangle = a|x'\rangle + b|y'\rangle,$$

$$C^{(m)}G^{(\ell)}|y'\rangle = d|y'\rangle + c|x'\rangle,$$

$$C^{(4)}G|\textcolor{red}{1}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{1}\rangle = a|\textcolor{red}{1}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{1}\rangle + b|\textcolor{red}{0}\textcolor{red}{1}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{1}\rangle$$

$$C^{(4)}G|\textcolor{red}{0}\textcolor{red}{1}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{1}\textcolor{green}{0}\rangle = |\textcolor{red}{0}\textcolor{red}{1}\textcolor{green}{0}\textcolor{green}{0}\textcolor{green}{1}\textcolor{green}{0}\rangle$$



$$\text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$|g_1\rangle = |x\rangle = |101001\rangle$$

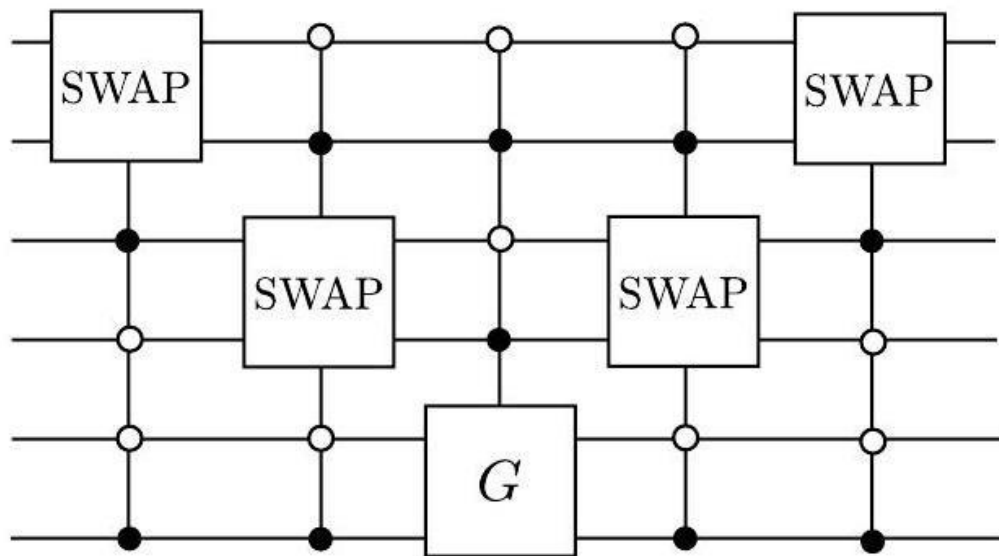
$$C^{(4)}\text{SWAP}|g_1\rangle = |\mathbf{01}1001\rangle = |g_2\rangle$$

$$C^{(4)}\text{SWAP}|g_2\rangle = |01\mathbf{01}01\rangle = |g_3\rangle$$

$$C^{(4)}G|g_3\rangle = a|g_3\rangle + b|0101\mathbf{10}\rangle = a|g_3\rangle + b|y\rangle$$

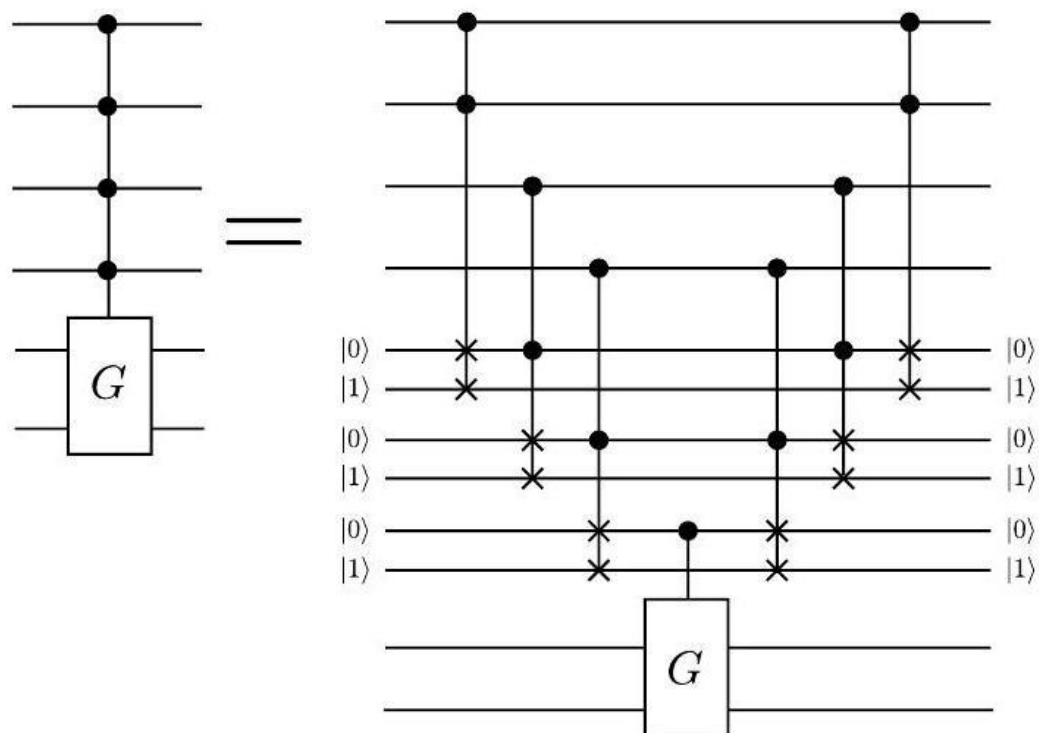
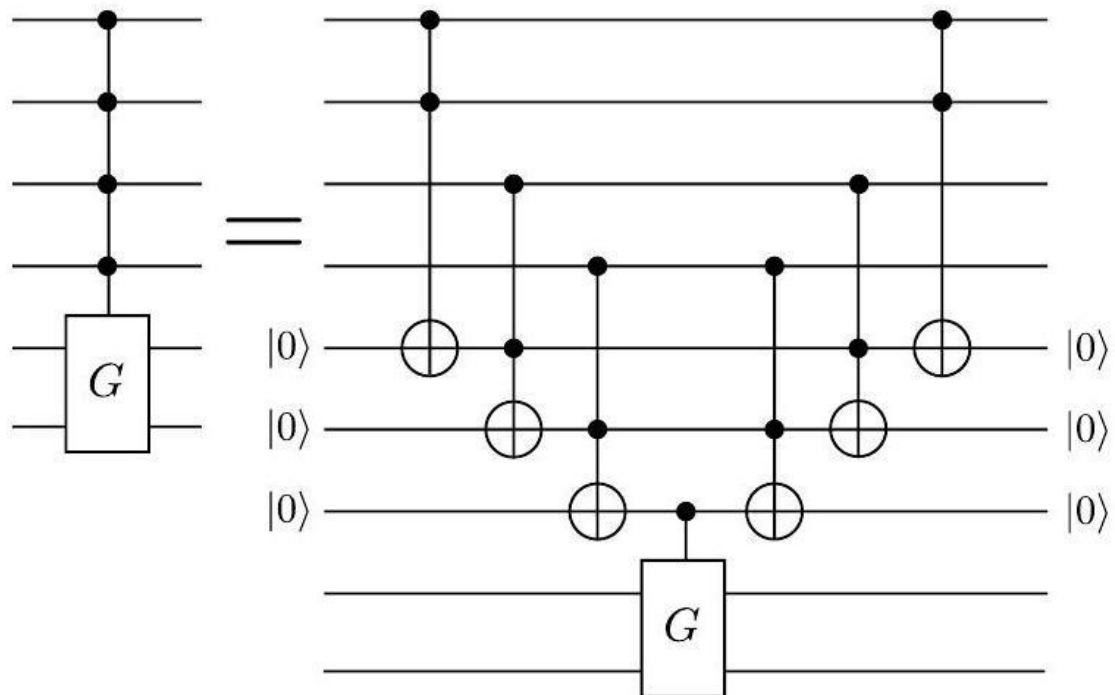
$$C^{(4)}\text{SWAP}(a|g_3\rangle + b|y\rangle) = a|g_2\rangle + b|y\rangle$$

$$C^{(4)}\text{SWAP}(a|g_2\rangle + b|y\rangle) = a|x\rangle + b|y\rangle$$



$$|\psi\rangle = \sum_x c_x |x\rangle$$

$$|x_1\rangle = |011\rangle, |x_2\rangle = |101\rangle, |x_3\rangle = |110\rangle$$



$$|\psi\rangle = \sum_{i=1}^d c_i |x_i\rangle$$

$$|x_1\rangle \rightarrow \alpha_1 |x_1\rangle + c_2 |x_2\rangle$$

$$\alpha_1 = \sqrt{1 - |c_2|^2}$$

$$\alpha_1 |x_1\rangle + c_2 |x_2\rangle \rightarrow \alpha_1 \alpha_2 |x_1\rangle + c_2 |x_2\rangle + \alpha_1 c'_3 |x_3\rangle$$

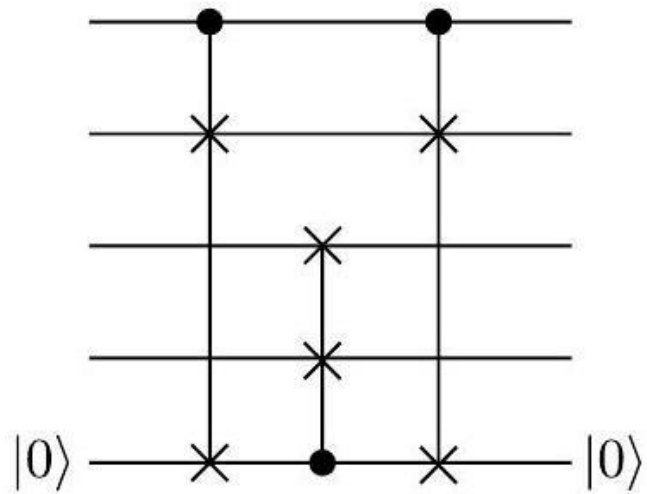
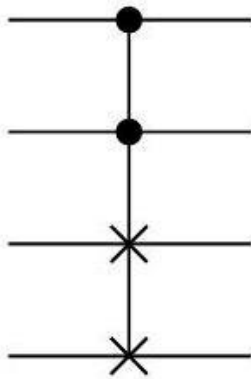
$$c_3' = c_3/\alpha_1$$

$$\alpha_2 = \sqrt{1 - |c_3'|^2}$$

$$|\psi\rangle = \alpha|x_1\rangle + \sum_{i=2}^d c_i|x_i\rangle,$$

$$\alpha = \prod_{i=1}^{d-1} \alpha_i$$

$$|\alpha|^2 = |c_1|^2$$



$$\alpha = c_1 = |c_1|e^{i\theta}$$

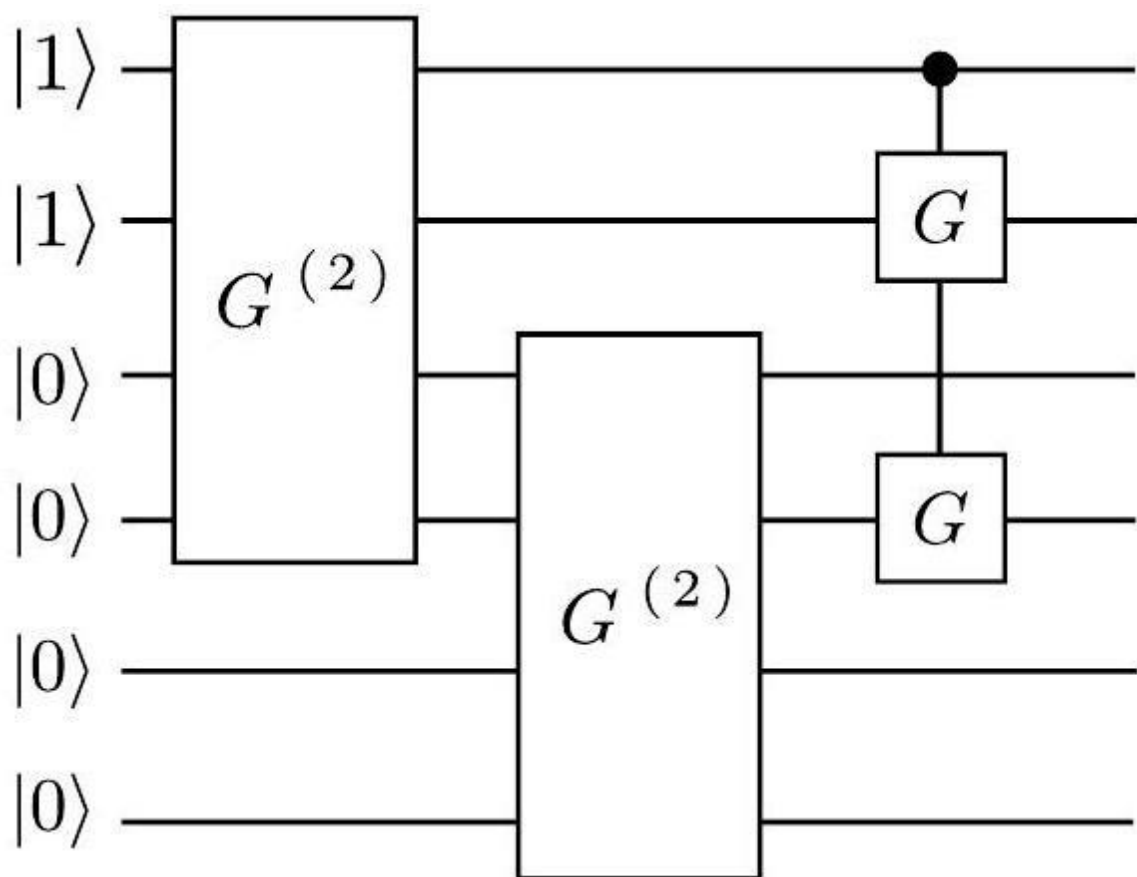
$$\alpha_{d-1} = |\alpha_{d-1}|e^{i\theta}$$

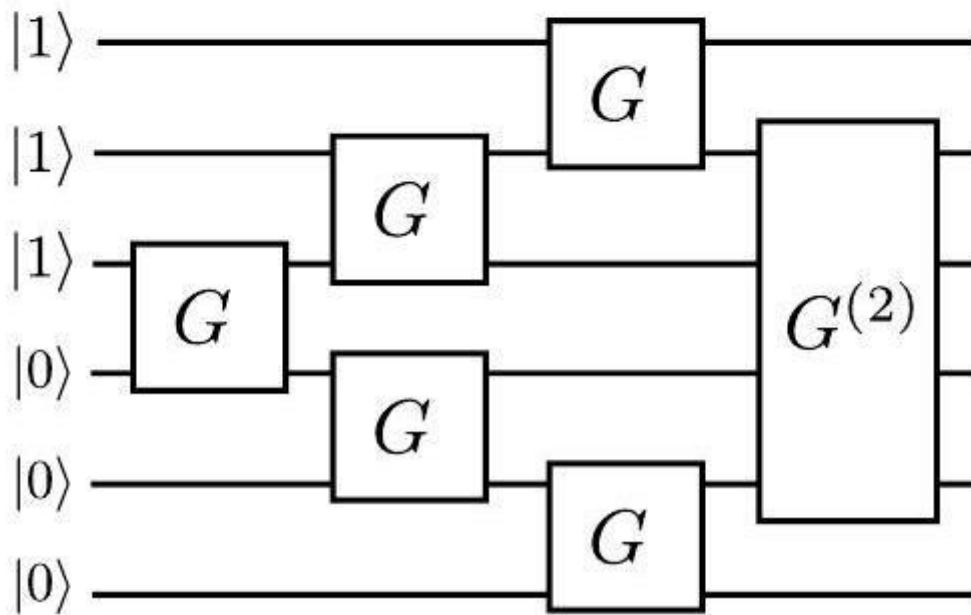
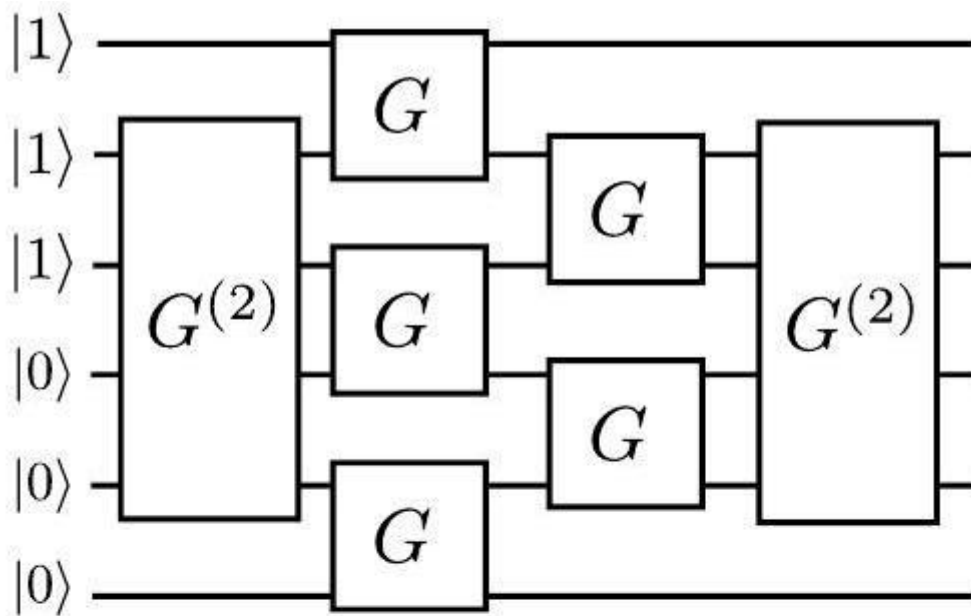
$$U = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

$$d = -\sqrt{1 - |c|^2}$$

$$b^* = \frac{c\sqrt{1 - |c|^2}}{a}$$

$$c_1|110000\rangle + c_2|001100\rangle + c_3|000011\rangle + c_4|100100\rangle,$$



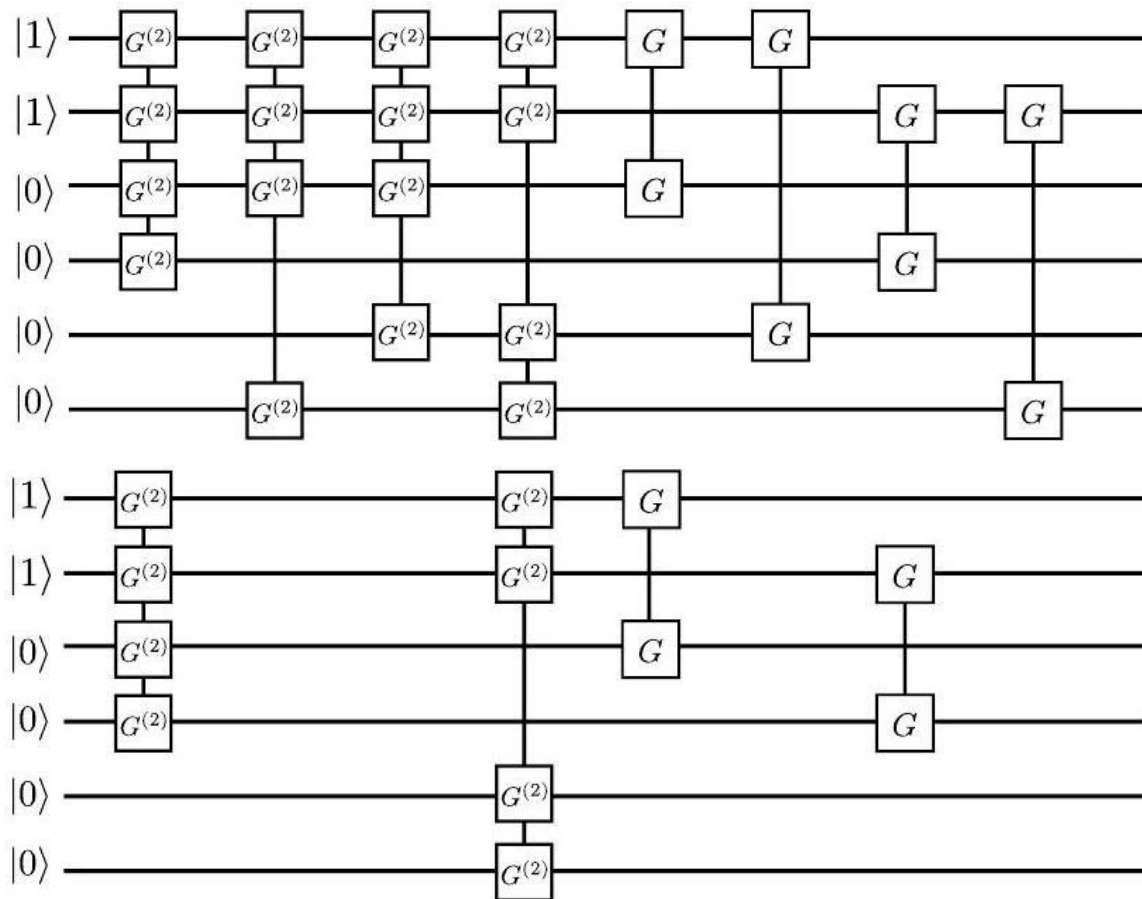


$$U(\theta) = \mathbb{1} \oplus \tilde{U}(\theta) \text{ is } H = \mathbf{0} \oplus \tilde{H}$$

$$H = \frac{1}{2}(H_+ + H_-),$$

$$H_{\pm} = (\pm \mathbb{1}) \oplus \tilde{H}.$$

$$U(\theta) = e^{i\theta G_+/2} e^{i\theta G_-/2},$$



$$U_{\pm}(\theta) = e^{i\theta G_{\pm}}.$$

$$H_{\pm}^2 = \mathbb{1}$$

$$[H_+, H_-] = 0.$$

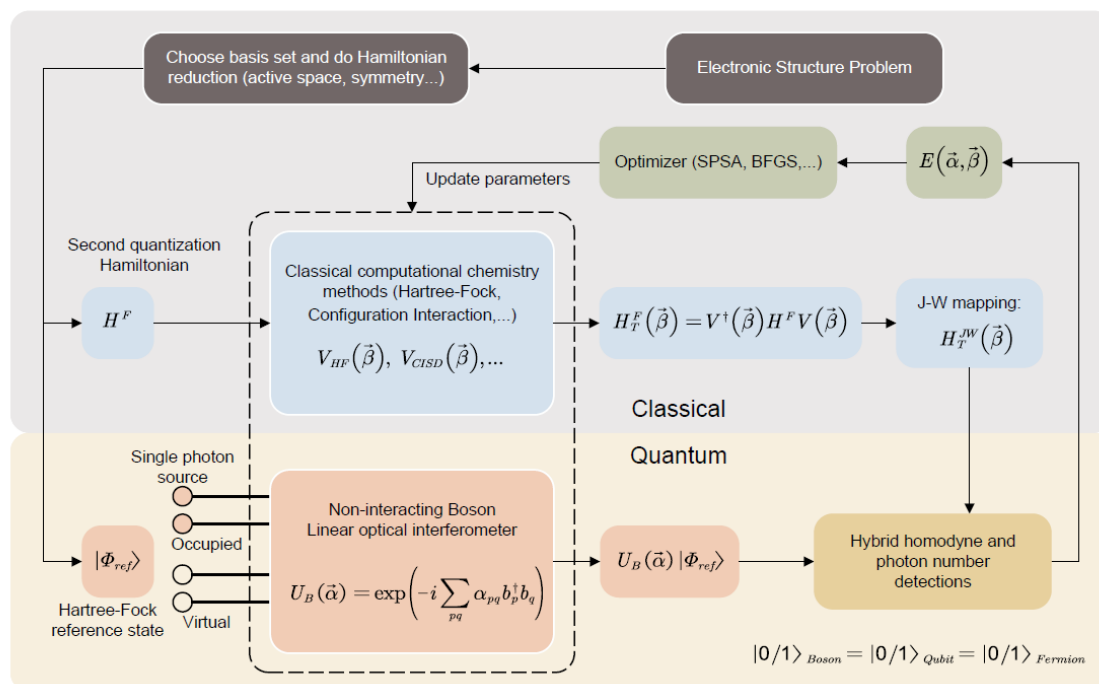
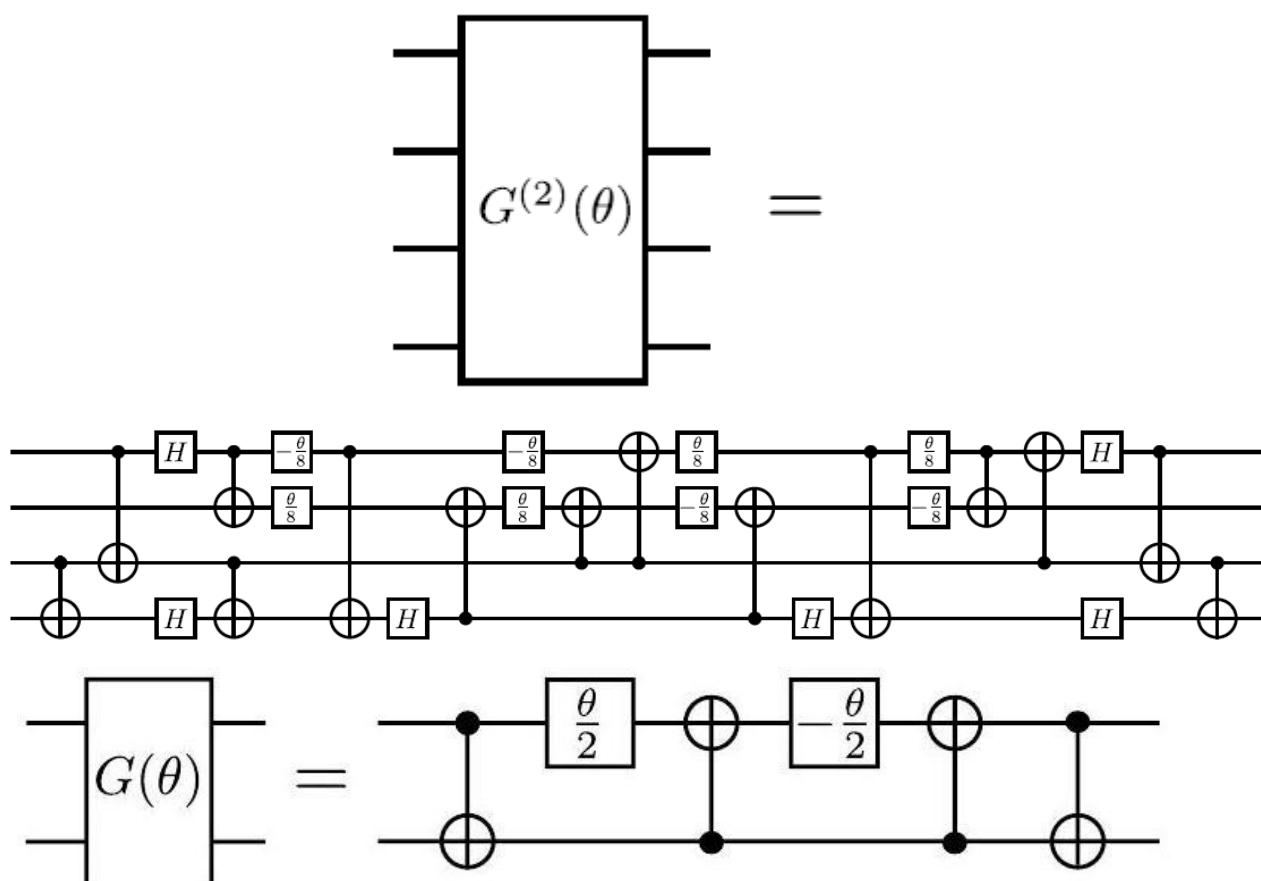
$$\frac{\partial C(\theta)}{\partial \theta} = \frac{C(\theta + s) - C(\theta - s)}{2\sin(s)},$$

$$C(\theta) = \langle \psi | U^\dagger(\theta) K U(\theta) | \psi \rangle$$

$$U(\theta) = U_+(\theta/2)U_-(\theta/2)$$

$$G(\theta) = G_+(\theta/2)G_-(\theta/2)$$

$$G_{\pm}(\theta) = \begin{pmatrix} e^{\pm i\theta} & 0 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta & 0 \\ 0 & \sin \theta & \cos \theta & 0 \\ 0 & 0 & 0 & e^{\pm i\theta} \end{pmatrix},$$



$$H^F = \sum_{pq} h_{pq} f_p^\dagger f_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} f_p^\dagger f_q^\dagger f_r f_s$$

$$U_F(\vec{\beta}) = \exp \left(-i \sum_{pq} \beta_{pq} f_p^\dagger f_q \right)$$

$$|HF\rangle = U_F(\vec{\beta}_{hf})|\phi_0\rangle, \vec{\beta}_{hf} = \operatorname{argmin}_{\vec{\beta}} \langle \phi_0 | U_F^\dagger(\vec{\beta}) H^F U_F(\vec{\beta}) | \phi_0 \rangle$$

$$(1+T)|\Phi_{\rm ref}\rangle e^T|\Phi_{\rm ref}\rangle$$

$$T=T_1+T_2=\sum_{pq}\beta_{pq}f_p^\dagger f_q+\sum_{pqrs}\beta_{pqrs}f_p^\dagger f_q^\dagger f_r f_s$$

$$U_B(\vec{\alpha}) = \exp \left(-i \sum_{pq} \alpha_{pq} b_p^\dagger b_q \right)$$

$$|S\rangle = |s_1 s_2 \ldots s_M\rangle$$

$$|T\rangle = |t_1 t_2 \ldots t_M\rangle$$

$$\langle T|U_B(\vec{\alpha})|S\rangle=\frac{\operatorname{Per}(U_{B,ST}(\vec{\alpha}))}{\sqrt{\Pi_p s_p! \Pi_p t_p!}}$$

$$\langle T|U_F(\vec{\beta})|S\rangle = \operatorname{Det}(U_{F,ST}(\vec{\beta}))$$

$$U_{B,ST}(\vec{\alpha})(U_{F,ST}(\vec{\beta}))$$

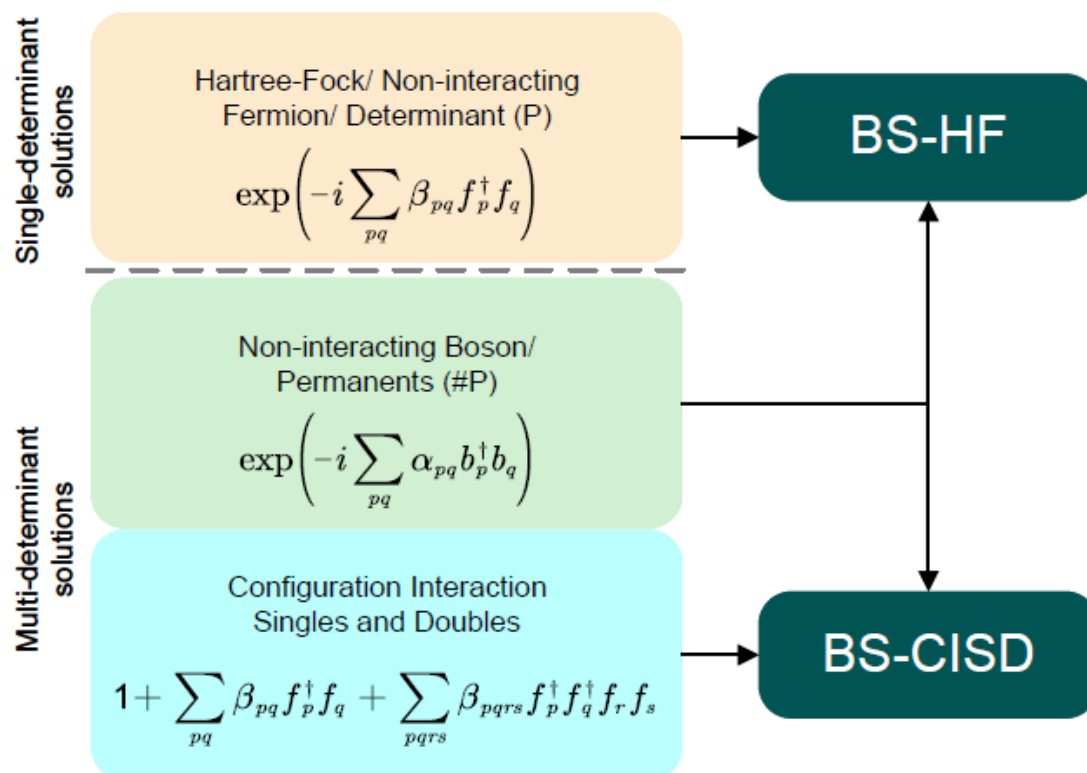
$$e^{i\alpha}(e^{i\beta})U_B(\vec{\alpha})(U_F(\vec{\beta}))$$

$$|\Phi_{BS-C}\rangle = V_C(\vec{\beta})|\Phi(\vec{\alpha})\rangle = V_C(\vec{\beta})U_B(\vec{\alpha})|\Phi_{ref}\rangle$$

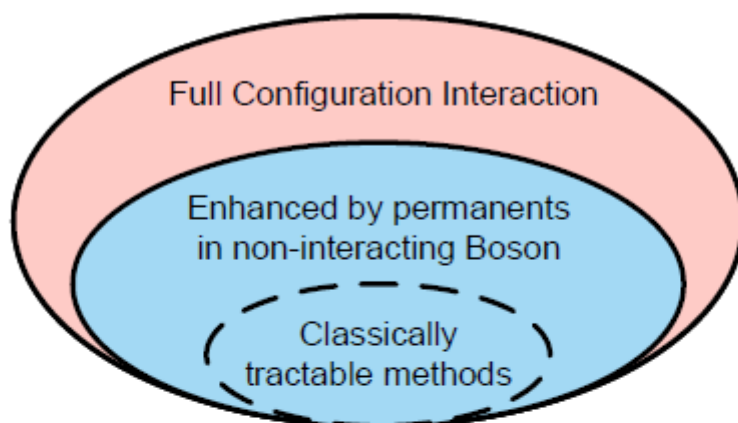
$$V_{HF}(\vec{\beta}) = U_B(\vec{\beta})$$

$$V_{\text{CISD}}\left(\vec{\beta}\right)=1+T_1+T_2$$

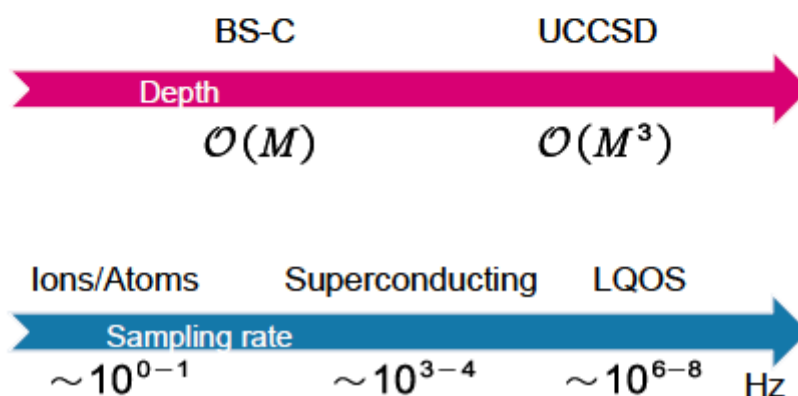
Resources for exploring electron states



b



c



$$H_T^F(\vec{\beta}) = V_C^\dagger(\vec{\beta}) H^F V_C(\vec{\beta})$$

$$\langle \Phi(\vec{\alpha}) | H_T^{JW}(\vec{\beta}) | \Phi(\vec{\alpha}) \rangle | \Phi_{BS-C} \rangle$$

$$E(\vec{\alpha}, \vec{\beta}) = \frac{\langle \Phi(\vec{\alpha}) | H_T^{JW}(\vec{\beta}) | \Phi(\vec{\alpha}) \rangle}{\langle \Phi(\vec{\alpha}) | V_C^\dagger(\vec{\beta}) V_C(\vec{\beta}) | \Phi(\vec{\alpha}) \rangle}$$

$$H_T^{JW}(\vec{\beta}) V_C(\vec{\beta}) \binom{M}{N} V_{HF}(\vec{\beta}) E(\vec{\alpha}, \vec{\beta}) \langle \Phi(\vec{\alpha}) | H_T^{JW}(\vec{\beta}) | \Phi(\vec{\alpha}) \rangle \\ / \langle \Phi(\vec{\alpha}) | Q | \Phi(\vec{\alpha}) \rangle \binom{M+N-1}{N} \binom{M}{N} | \Phi(\vec{\alpha}) \rangle \langle \Phi(\vec{\alpha}) | Q | \Phi(\vec{\alpha}) \rangle$$

$$H_i = Z_1 Z_2 \sigma_{+,3} \sigma_{-,4}$$

$$\text{Tr}(H_i \rho) = \sum_{jk} q_{jk} \langle j | Z_1 | j \rangle \langle k | Z_2 | k \rangle \int_0^\pi \frac{d\phi_3 d\phi_4}{\pi^2} \\ \int_{-\infty}^{\infty} dx_3 dx_4 p_{jk}(\phi_3, \phi_4, x_3, x_4) K(\phi_3, \phi_4, x_3, x_4, \sigma_{+,3} \sigma_{-,4})$$

$$q_{jk} p_{jk}(\phi_3, \phi_4, x_3, x_4) = \langle jk | \langle x_{\phi_3} x_{\phi_4} | \rho | jk \rangle | x_{\phi_3} x_{\phi_4} \rangle$$

$$X_{p,\phi_p} = (a_p^\dagger e^{i\phi_p} + a_p e^{-i\phi_p})/2$$

$$K(\phi_1, \dots, \phi_M, x_1, \dots, x_M, \vec{\beta})$$

$$\{2.07317^k, \epsilon^{-2}, m_H, m_V, \chi^{-2}\}$$

$$H_T^{JW}(\vec{\beta}), m_V V_C^\dagger(\vec{\beta}) V_C(\vec{\beta})$$

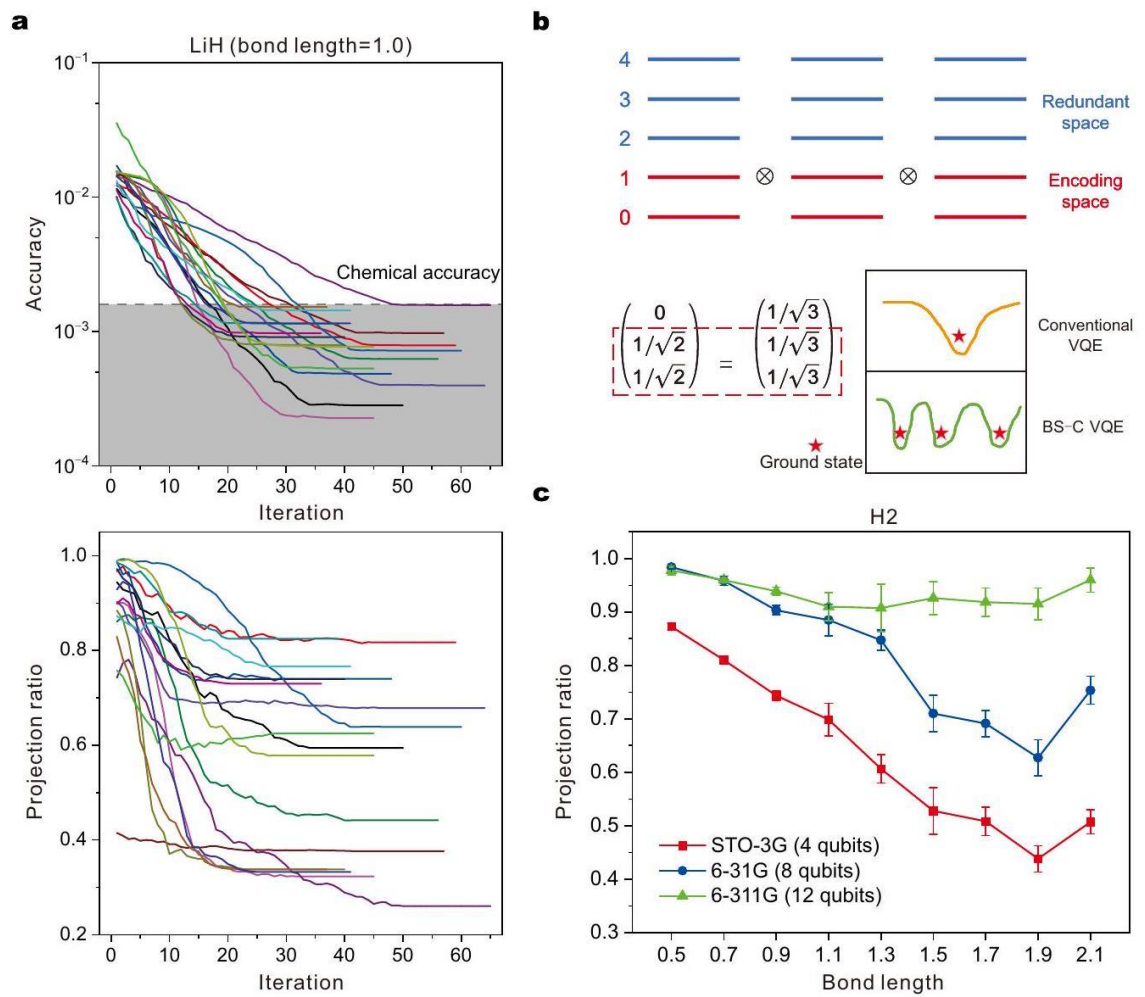
$$\frac{n_3}{n_1}\frac{n_2}{n_3}\langle H_i\rangle_{\text{raw}}$$

$$\langle \Phi(\vec{\alpha}) | H_T^{JW}(\vec{\beta}) | \Phi(\vec{\alpha}) \rangle =$$

$$\sum_{ij} H_T^{JW}(\vec{\beta})_{ij} \text{Per}(U_{B,0i}(\vec{\alpha})) \text{Per}(U_{B,0j}(\vec{\alpha}))$$

$$|\Phi_{ref}\rangle \mathcal{O}(M^3) \langle \Phi(\vec{\alpha}) | Q | \Phi(\vec{\alpha}) \rangle E(\vec{\alpha}, \vec{\beta})$$

$$E(\vec{\alpha}, \vec{\beta}) \mathcal{O}(\langle Q \rangle^{-2}) E(\vec{\alpha}, \vec{\beta})$$



$$|\Phi(\vec{\alpha})\rangle - \lambda \langle Q \rangle$$

$$r(M,N)=\binom{M}{N}/\binom{M+N-1}{N}$$

$$H = \int \frac{d^2\alpha}{\pi} \text{Tr}[HD^\dagger(\alpha)]D(\alpha) = \int_0^\pi \frac{d\phi}{\pi} \int_{-\infty}^\infty dr \frac{|r|}{4} \text{Tr}(He^{irX_\phi})e^{-irX_\phi}$$

$$D(\alpha) = e^{(\alpha b^\dagger - \alpha^* b)}$$

$$\alpha = -ir e^{i\phi}/2$$

$$X_\phi = (b^\dagger e^{i\phi} + b e^{-i\phi})/2$$

$$\begin{aligned}\langle H \rangle &= \text{Tr}(H\rho) \\ &= \text{Tr}\left(\int \frac{d^2\alpha}{\pi} \text{Tr}(HD^\dagger(\alpha))D(\alpha)\rho\right) \\ &= \int_0^\pi \frac{d\phi}{\pi} \int_{-\infty}^\infty dr \frac{|r|}{4} \text{Tr}(He^{irX_\phi})\text{Tr}(\rho e^{-irX_\phi}) \\ &= \int_0^\pi \frac{d\phi}{\pi} \int_{-\infty}^\infty dx \int_{-\infty}^\infty dr \frac{|r|}{4} \text{Tr}(He^{irX_\phi})p(\phi,x)e^{-irx} \\ &= \int_0^\pi \frac{d\phi}{\pi} \int_{-\infty}^\infty dx p(\phi,x) \int_{-\infty}^\infty dr \frac{|r|}{4} \text{Tr}(He^{ir(X_\phi-x)}) \\ &= \int_0^\pi \frac{d\phi}{\pi} \int_{-\infty}^\infty dx p(\phi,x)K(\phi,x,H)\end{aligned}$$

$$p(\phi,x) = \langle x_\phi | \rho | x_\phi \rangle$$

$$\langle X_\phi | \rho | X_\phi \rangle K(\phi,x,H)$$

$$K(\phi,x,H) = \int_{-\infty}^\infty dr \frac{|r|}{4} \text{Tr}(He^{ir(X_\phi-x)})$$

$$H = |n+\lambda\rangle\langle n|$$

$$\begin{aligned}K(\phi,x,|n+\lambda\rangle\langle n|) &= 2e^{-i\lambda\phi} \sqrt{\frac{n!}{(n+\lambda)!}} e^{-x^2} \sum_{v=0}^n \frac{(-1)^v}{v!} \binom{n+\lambda}{n-v} \\ &\quad \times (2v+\lambda+1)! \text{Re}[(-i)^\lambda \mathcal{D}_{-(2v+\lambda+2)}(-2ix)]\end{aligned}$$

$$\begin{aligned}\langle H \rangle &= \int_0^\pi \frac{d\phi_1 d\phi_2 \dots d\phi_M}{\pi^M} \int_{-\infty}^\infty dx_1 dx_2 \dots dx_M \\ &\quad p(\phi_1, \phi_2, \dots, \phi_M, x_1, x_2, \dots, x_M) K(\phi_1, \phi_2, \dots, \phi_M, x_1, x_2, \dots, x_M, H)\end{aligned}$$

$$\begin{aligned}K(\phi_1, \phi_2, \dots, \phi_M, x_1, x_2, \dots, x_M, H) &= \\ \int_{-\infty}^\infty dr_1 dr_2 \dots dr_M \Pi_{m=1}^M \frac{|r_m|}{4} \text{Tr}(He^{ir_m(X_{\phi_m}-x_m)}) \frac{(b-a)^2}{4}\end{aligned}$$

$$E(\vec{\alpha},\vec{\beta})=\frac{\langle \Phi(\vec{\alpha})|H_T^{JW}(\vec{\beta})|\Phi(\vec{\alpha})\rangle}{\langle \Phi(\vec{\alpha})|V_C^\dagger(\vec{\beta})V_C(\vec{\beta})|\Phi(\vec{\alpha})\rangle}$$

$$\begin{aligned}E\left[\frac{\bar{X}}{\bar{Y}}\right] &\approx \frac{E[X]}{E[Y]} + \frac{E[X]}{E[Y]^3} \text{Var}[\bar{Y}] \\ \text{Var}\left[\frac{\bar{X}}{\bar{Y}}\right] &\approx \frac{E[X]^2 \text{Var}[\bar{Y}] + E[Y]^2 \text{Var}[\bar{X}]}{E[Y]^4}\end{aligned}$$

$$\langle H_T^{JW} \rangle \langle \Phi(\vec{\alpha}) | H_T^{JW}(\vec{\beta}) | \Phi(\vec{\alpha}) \rangle$$

$$\langle V_C^\dagger V_C \rangle \langle \Phi_{\text{ref}} | V_C^\dagger(\vec{\beta}) V_C(\vec{\beta}) | \Phi_{\text{ref}} \rangle$$

$$H_T^{JW}(\vec{\beta}) = \sum_{i=1}^{m_H} h_i H_i$$

$$\text{Var}[\overline{H_T^{JW}}] \leq \sum_{i=1}^{m_H} \frac{2.07317^{4k_h} m_H h_i^2}{N_H}$$

$$V_C^\dagger V_C = \sum_{i=1}^{m_V} g_i V_i$$

$$\text{Var}[\overline{V_C^\dagger V_C}] \leq \sum_{i=1}^{m_V} \frac{2.07317^{4k_v} m_V g_i^2}{N_V}$$

$$\langle \Phi(\vec{\alpha}) | Q | \Phi(\vec{\alpha}) \rangle \langle Q \rangle \geq \chi \langle H_T^{JW} \rangle_r = \langle H_T^{JW} \rangle / \langle Q \rangle$$

$$\langle V_C^\dagger V_C \rangle_r = \langle V_C^\dagger V_C \rangle / \langle Q \rangle E(\vec{\alpha}, \vec{\beta})$$

$$\begin{aligned} \text{Bias}[E(\vec{\alpha}, \vec{\beta})]^2 &\leq \left(\frac{\langle H_T^{JW} \rangle}{\langle V_C^\dagger V_C \rangle} - \frac{\overline{H_T^{JW}}}{\overline{V_C^\dagger V_C}} \right)^2 \approx \left(\frac{\langle H_T^{JW} \rangle}{\langle V_C^\dagger V_C \rangle^3} \text{Var}[\overline{V_C^\dagger V_C}] \right)^2 \\ &= \left(\frac{E(\vec{\alpha}, \vec{\beta})}{\langle V_C^\dagger V_C \rangle^2} \sum_{i=1}^{m_V} \frac{2.07317^{4k_v} m_V g_i^2}{N_V} \right)^2 \\ &= \left(\frac{E(\vec{\alpha}, \vec{\beta})}{\chi^2 \langle V_C^\dagger V_C \rangle_r^2} \frac{2.07317^{4k_v} m_V}{N_V} \sum_{i=1}^{m_V} g_i^2 \right)^2 \\ &\leq \frac{2.07317^{4k_v} m_V^2 (\sum_{i=1}^{m_V} g_i^2)^2 \|H_T^{JW}\|_2^2}{\chi^4 N_V^2} \end{aligned}$$

$$\begin{aligned} \text{Var}[E(\vec{\alpha}, \vec{\beta})] &\leq \frac{\langle H_T^{JW} \rangle^2 \text{Var}[\overline{V_C^\dagger V_C}] + \langle V_C^\dagger V_C \rangle^2 \text{Var}[\overline{H_T^{JW}}]}{\langle V_C^\dagger V_C \rangle^4} \\ &= \frac{E(\vec{\alpha}, \vec{\beta})^2 \sum_{i=1}^{m_V} \frac{2.07317^{4k_v} m_V g_i^2}{N_V} + \sum_{i=1}^{m_H} \frac{2.07317^{4k_h} m_H h_i^2}{N_H}}{\langle V_C^\dagger V_C \rangle^2} \\ &= \frac{E(\vec{\alpha}, \vec{\beta})^2 \frac{2.07317^{4k_v} m_V}{N_V} \sum_{i=1}^{m_V} g_i^2 + \frac{2.07317^{4k_h} m_H}{N_H} \sum_{i=1}^{m_H} h_i^2}{\langle V_C^\dagger V_C \rangle^2} \\ &\leq \frac{2.07317^{4k_v} m_V (\sum_{i=1}^{m_V} g_i^2)^2 \|H_T^{JW}\|_2^2}{\chi^2 N_V} + \frac{2.07317^{4k_h} m_H \sum_{i=1}^{m_H} h_i^2}{\chi^2 N_H} \end{aligned}$$

$$|\psi\rangle = \sum_{i=0}^N c_i |\psi_{N-i}\rangle |i\rangle_e$$

$$\mathfrak{t} \, |\psi_N\rangle = d_F |\psi_{N,F}\rangle + \cdots \text{ where } |\psi_{N,F}\rangle$$

$$\langle \psi_{N,F} | H_i | \psi_{N,F} \rangle$$

$$\langle \phi_{N-k,T} | H_i | \phi_{N-k,T} \rangle \text{ where } |\phi_{N-k,T}\rangle$$

$$|\phi_{N-k}\rangle = \alpha |\phi_{N-k,T}\rangle + \beta |\phi_{N-k,W}\rangle$$

$$|\phi_{N-k,W}\rangle \langle H_i \rangle_{raw} = \langle \phi_{N-k} | H_i | \phi_{N-k} \rangle = |\alpha|^2 \langle \phi_{N-k,T} | H_i | \phi_{N-k,T} \rangle 1/|\alpha|^2$$

$$|\phi_{N-k,T}\rangle |\psi_{N,F}\rangle |\psi_{N,F}\rangle = \gamma |\phi_{N-k,T}\rangle + \sum_i \kappa_i |\phi_{i \neq N-k,T}\rangle$$

$$\langle \psi_{N,F} | H_i | \psi_{N,F} \rangle = \frac{|\gamma|^2}{|\alpha|^2} \langle \phi_{N-k} | H_i | \phi_{N-k} \rangle$$

$$|\gamma^2| = \frac{n_3}{n_1} \text{ and } |\alpha|^2 = \frac{n_3}{n_2}$$

$$\langle \psi_{N,F} | H_i | \psi_{N,F} \rangle \approx \frac{n_3}{n_1} \frac{n_2}{n_3} \langle H_i \rangle_{raw}$$

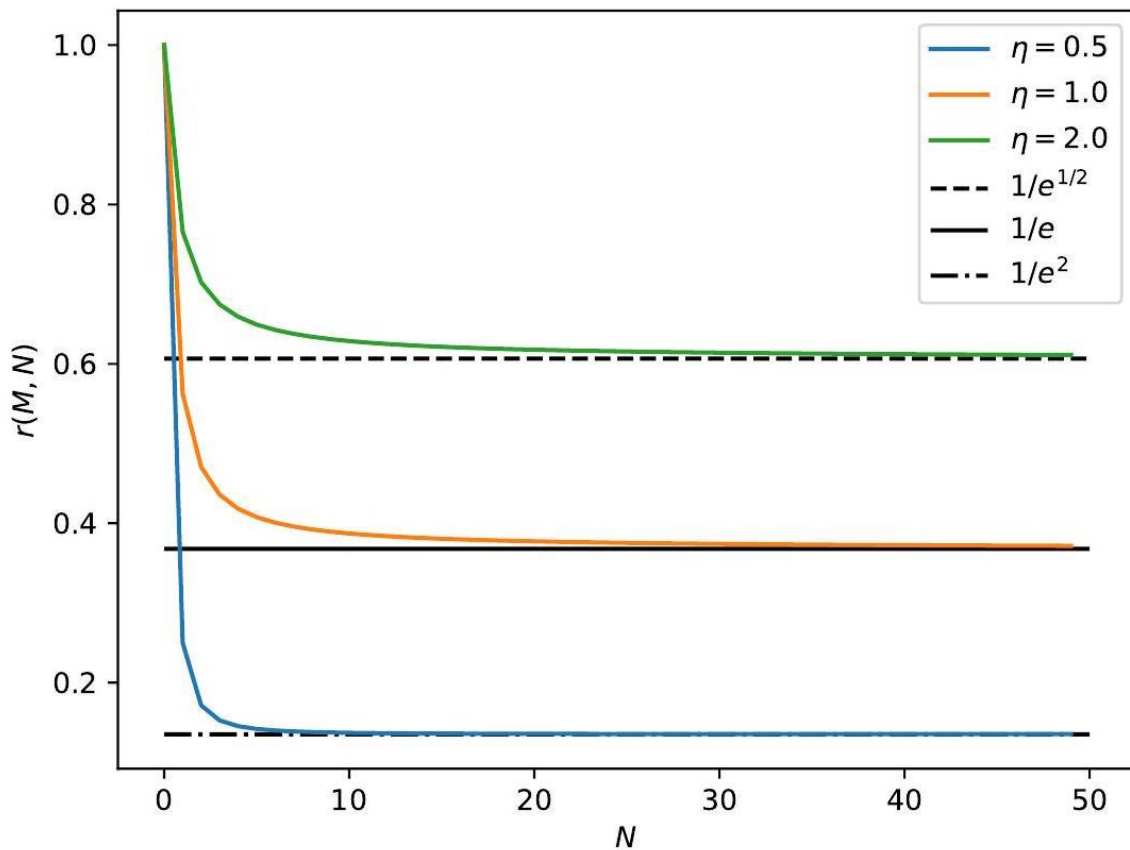
$$r(M,N) = \binom{M}{N} / \binom{M+N-1}{N}$$

$$M=\eta N^2, r(M,N)e^{1/\eta}$$

$$r(M,N)=\frac{M}{M+N-1}\frac{M-1}{M+N-2}\cdots\frac{M-N+1}{M}$$

$$r(M,N) > \left(\frac{M-N+1}{M}\right)^N$$

$$\left(\frac{M-N+1}{M}\right)^N = \frac{1}{\left(\frac{\eta N^2}{\eta N^2 - N + 1}\right)^N} = \frac{1}{\left(1 + \frac{N-1}{\eta N^2 - N + 1}\right)^N}$$



$$\lim_{N \rightarrow \infty} \frac{1}{\left(1 + \frac{N-1}{\eta N^2 - N + 1}\right)^N} = \lim_{N \rightarrow \infty} \left(\frac{1}{\left(1 + \frac{1}{\eta N}\right)^{\eta N}} \right)^{\frac{1}{\eta}} = e^{\frac{1}{\eta}}$$

$$H = -\frac{1}{2m_{12}}\nabla_{\mathbf{r}_1}^2 - \frac{1}{2m_{13}}\nabla_{\mathbf{r}_2}^2 - \frac{1}{m_1}\nabla_{\mathbf{r}_1} \cdot \nabla_{\mathbf{r}_2} + \frac{Z_1Z_2}{r_1} + \frac{Z_1Z_3}{r_2} + \frac{Z_2Z_3}{R},$$

$$m_{ij}=m_i m_j/(m_i+m_j), \mathbf{r}_1=\mathbf{R}_2-\mathbf{R}_1, \mathbf{r}_2=\mathbf{R}_3-\mathbf{R}_1 \text{ and } \mathbf{R}=\mathbf{R}_3-\mathbf{R}_2$$

$$\mathbf{L}=\mathbf{l}_1+\mathbf{l}_2, \mathbf{l}_i=-i\mathbf{r}_i\times\nabla_{\mathbf{r}_i}.$$

$$\psi_{LM}^{\Pi}=\sum_{l_1+l_2=L_{\Pi}}r_1^{l_1}r_2^{l_2}\{Y_{l_1}(\hat{\mathbf{r}}_1)\otimes Y_{l_2}(\hat{\mathbf{r}}_2)\}_{LM}F_{l_1l_2}^{L\Pi}(r_1,r_2,R).$$

$$L(L+1), M(-1)^{l_1+l_2}$$

$$L_{\Pi}=L\Pi=(-1)^L$$

$$L_{\Pi}=L+1\Pi=-(-1)^L$$

$$\Pi=(-1)^L$$

$$F_{00}^{01}(r_1,r_2,R)\equiv F(r_1,r_2,R)$$

$$F(r_1,r_2,R)=\sum_{i=1}^N\left[C_i\mathrm{Re}\big(e^{-\alpha_ir_1-\beta_ir_2-\gamma_iR}\big)+D_i\mathrm{Im}\big(e^{-\alpha_ir_1-\beta_ir_2-\gamma_iR}\big)\right],$$

$$|\Psi\rangle=\prod_l e^{\theta_l \hat{T}_l}|\psi_0\rangle$$

$$\{V_j\}_n=\{Z_n\{V_k\}_{n-1},iY_n,iY_{n-1}\}$$

$$X\equiv\sigma_x,Y\equiv\sigma_y,Z\equiv\sigma_z$$

$$\hat{U}(\vec{\theta})=\prod_{l=1}^{2n-2}e^{i\theta_l\hat{P}_l}$$

$$|\Psi(\vec{\theta})\rangle=\left[\prod_{m=1}^k\left(\prod_{l=1}^{2n-2}e^{i\theta_l\hat{P}_l}\right)\right]|\psi_0\rangle$$

$$F(r_1,r_2,R)=\sum_{i=1}^N c_i\phi_i(r_1,r_2,R)$$

$$\phi_i(r_1,r_2,R)=[\text{Re or Im}](e^{-\alpha_i r_1-\beta_i r_2-\gamma_i R})\pm (r_1\leftrightarrow r_2)$$

$$\mathbf{H}\mathbf{c} = E\mathbf{O}\mathbf{c}$$

$$H_{ij}=\langle\phi_i|H|\phi_j\rangle$$

$$O_{ij}=\langle\phi_i\mid\phi_j\rangle$$

$$H=\sum_{i,j=1}^N H_{ij}|\phi_i\rangle\langle\phi_j|$$

$$|\phi_1\rangle\langle\phi_2|=|00\dots00\rangle\langle10\dots00|=(|0\rangle\langle1|)\otimes(|0\rangle\langle0|)\otimes\dots\otimes(|0\rangle\langle0|)$$

$$|0\rangle\langle0|=\frac{1}{2}(I+Z),|0\rangle\langle1|=\frac{1}{2}(X+iY),|1\rangle\langle0|=\frac{1}{2}(X-iY),|1\rangle\langle1|=\frac{1}{2}(I-Z)$$

$$g_j=|\langle\psi(\boldsymbol{\theta})|[\hat{H},\hat{A}_j]|\psi(\boldsymbol{\theta})\rangle|\,$$

$$g=\|\vec{g}\|=\sqrt{\sum_j|g_j|^2}$$

$$D_{ij}=\langle\phi_i'|\delta(\mathbf{r}_a)|\phi_j'\rangle,a=1,2$$

$$\langle\phi|\delta(\mathbf{r}_a)|\phi\rangle=\sum_{i,j=1}^N c_i'c_j'D_{ij}=2\sum_{i>j}c_i'c_j'D_{ij}+\sum_ic_i'^2D_{ii}.$$

$$Ax=aBx$$

$$A'x'=ax'$$

$$U^TB U=I$$

$$U=\Delta D$$

$$U^T A U U^T x = a U^T B U U^T x.$$

$$A'x'=ax'$$

$$A' = U^T A U, \text{ and } x' = U^T x$$

$$\hat{H} = h_q^p \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} h_{qs}^{pr} \hat{a}_p^\dagger \hat{a}_r^\dagger \hat{a}_s \hat{a}_q$$

$$|\mathrm{LAS}\rangle = \bigwedge_K |\Psi_K\rangle \wedge |\Phi\rangle$$

$$E_{\mathrm{LAS}} = \langle \mathrm{LAS} | \hat{H} | \mathrm{LAS} \rangle,$$

$$|\mathrm{LAS}\rangle \rightarrow \hat{U}_{\mathrm{orb}} \prod_K \hat{U}_{\mathrm{Cl},K} |\mathrm{LAS}\rangle$$

$$\hat{U}_{\mathrm{orb}} = \exp\{x_l^k(\hat{a}_k^\dagger \hat{a}_l - \hat{a}_l^\dagger \hat{a}_k)\},$$

$$\hat{U}_{\mathrm{Cl},K} = \exp\{x_{\vec{k}}(|\vec{k}\rangle\langle\Psi_K| - |\Psi_K\rangle\langle\vec{k}|)\},$$

$$\hat{U}_{\mathrm{UCC}} \equiv \exp\{\hat{T}_{\mathrm{UCC}}\}$$

$$\hat{T}_{\mathrm{UCC}} \equiv x_l^k(\hat{a}_k^\dagger \hat{a}_l - \text{h.c.}) + \frac{1}{4} x_{ln}^{km}(\hat{a}_k^\dagger \hat{a}_m^\dagger \hat{a}_n \hat{a}_l - \text{h.c.}) + \cdots$$

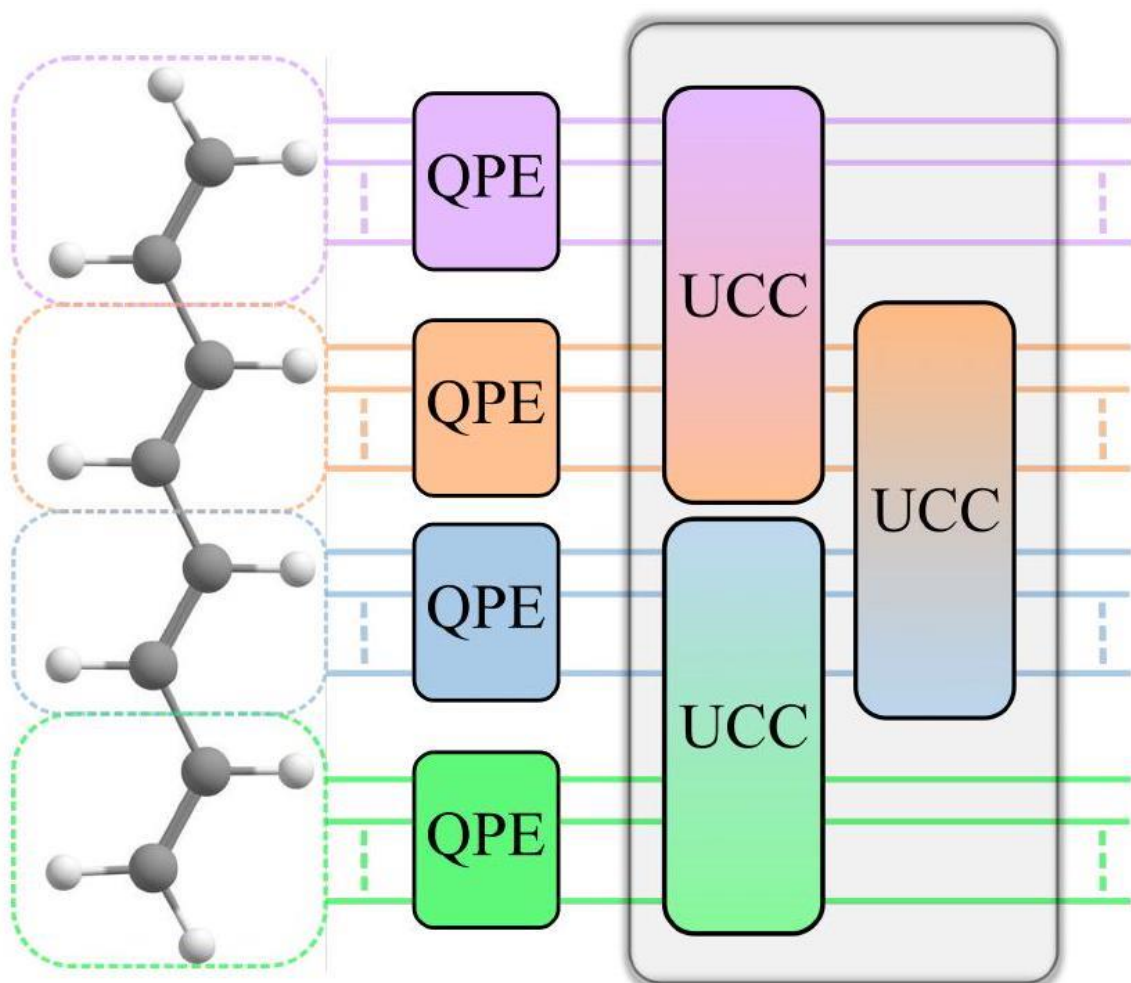
$$\hat{H}_{\mathrm{eff}} = \sum_K^{n_f} \left(\tilde{h}_{k_2}^{k_1} \hat{a}_{k_1}^\dagger \hat{a}_{k_2} + \frac{1}{4} h_{k_2 k_4}^{k_1 k_3} \hat{a}_{k_1}^\dagger \hat{a}_{k_3}^\dagger \hat{a}_{k_4} \hat{a}_{k_2} \right),$$

$$\tilde{h}_{k_2}^{k_1} = h_{k_2}^{k_1} + h_{k_2 i}^{k_1 i} + \sum_{L \neq K} h_{k_2 l_2}^{k_1 l_1} \gamma_{l_2}^{l_1},$$

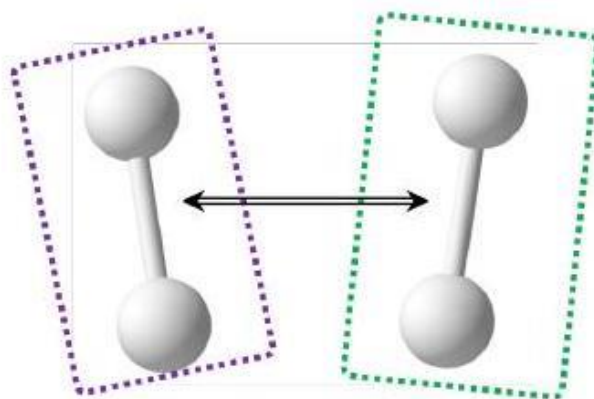
$$\gamma_{l_2}^{l_1} \equiv \langle \mathrm{LAS} | \hat{a}_{l_1}^\dagger \hat{a}_{l_2} | \mathrm{LAS} \rangle = \langle \Psi_L | \hat{a}_{l_1}^\dagger \hat{a}_{l_2} | \Psi_L \rangle.$$

$$|\mathrm{QLAS}(x)\rangle \rightarrow \prod_{\zeta} \hat{U}_{\mathrm{UCCSD},\zeta}(x) |\mathrm{QLAS}\rangle$$

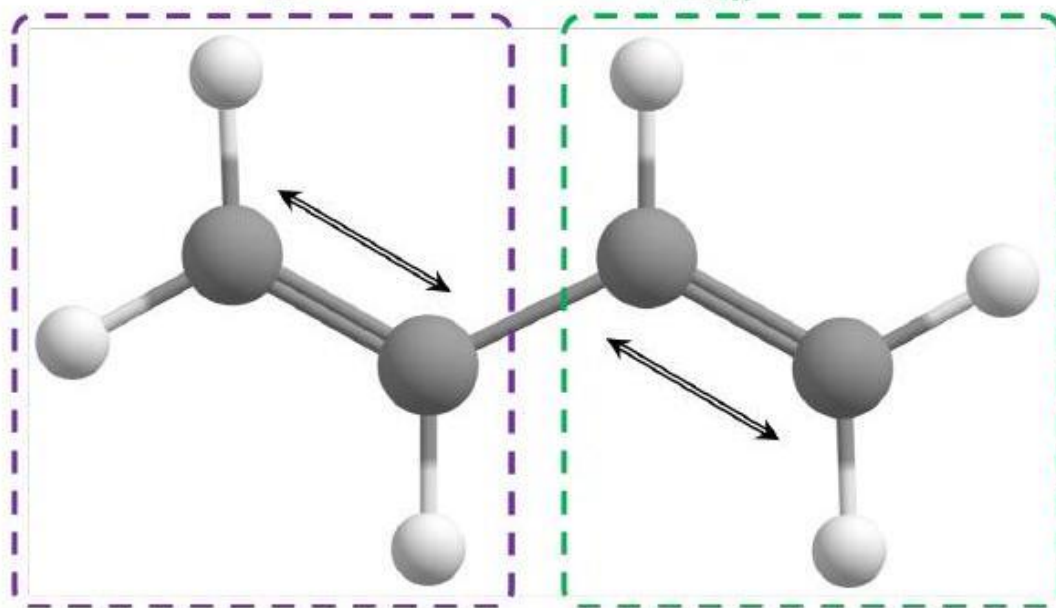
$$E = \min_x \langle \mathrm{QLAS}(x) | \hat{H} | \mathrm{QLAS}(x) \rangle$$



a



b



$$U|v_k\rangle = e^{-i\hat{H}\tau}|v_k\rangle = e^{i2\pi\phi}|v_k\rangle,$$

$$E = -2\pi\phi/\tau$$

$$U = e^{-i\hat{H}\tau}$$

$$E = \min_{\theta} \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle$$

$$|\psi_{\text{UCCSD}}\rangle = \hat{U}_{\text{UCCSD}}|\text{HF}\rangle = \exp\{\hat{T}_{\text{UCCSD}}\}|\text{HF}\rangle,$$

$$\frac{\partial E_{\text{LAS}}}{\partial x_{\vec{k}}} = \langle \Phi | \bigwedge_{L \neq K} \langle \Psi_L | \wedge \langle \vec{k} | \hat{H} - E_{\text{LAS}} | \Psi_K \rangle \bigwedge_{M \neq K} | \Psi_M \rangle \wedge | \Phi \rangle,$$

$$\hat{H}_K|\Psi_K\rangle=E_{\text{LAS}}|\Psi_K\rangle$$

$$\begin{aligned} \hat{H}_K &\equiv \langle \Phi | \bigwedge_{L \neq K} \langle \Psi_L | \hat{H} \bigwedge_{M \neq K} | \Psi_M \rangle \wedge | \Phi \rangle \\ &= \tilde{h}_{k_2}^{k_1} \hat{a}_{k_1}^\dagger \hat{a}_{k_2} + \frac{1}{4} h_{k_2 k_4}^{k_1 k_3} \hat{a}_{k_1}^\dagger \hat{a}_{k_3}^\dagger \hat{a}_{k_4} \hat{a}_{k_2} \end{aligned}$$

$$(\hat{H}_A + \hat{H}_B)|\Psi_A\rangle \wedge |\Psi_B\rangle = (E_A + E_B)|\Psi_A\rangle \wedge |\Psi_B\rangle.$$

$$\hat{H}_{\text{eff}} = \sum_K \hat{H}_K,$$

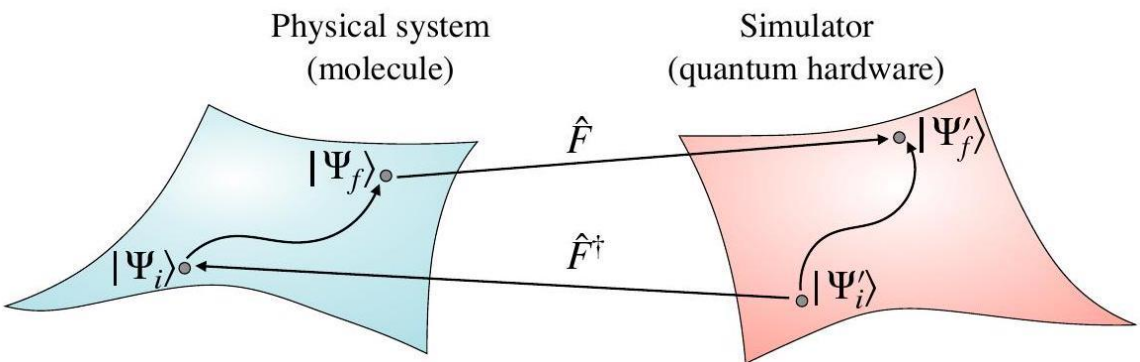
$$\hat{H}_{\text{eff}} \bigwedge_K |\Psi_K\rangle = n_f \times E_{\text{LAS}} \bigwedge_K |\Psi_K\rangle.$$

$$|\text{QLAS}\rangle \equiv \bigwedge_K |\Psi_K\rangle$$

$$\tilde{a}_j^\dagger = Z^{\otimes j-1} \otimes \frac{X-iY}{2} \otimes I^{\otimes N-1},$$

$$Z^{\otimes 4} = Z \otimes Z \otimes Z \otimes Z$$

$$\tilde{a}_j^\dagger \tilde{a}_k = I^{\otimes k-1} \otimes \frac{Z(X-iY)}{2} \otimes Z^{\otimes j-k-1} \otimes \frac{X-iY}{2} \otimes I^{\otimes N-j}$$



$$\mathcal{H}_n = \mathcal{H}^{\otimes n}$$

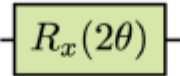
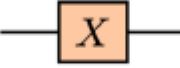
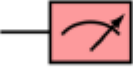
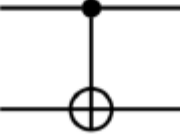
$$|\mathbf{z}\rangle = \bigotimes_{\ell=0}^{n-1} |z_\ell\rangle = |z_{n-1} \dots z_0\rangle = |\mathbf{z}\rangle, \mathbf{z} \in \{0,1\}^n, z = \sum_{\ell=0}^{n-1} z_\ell 2^\ell \in \{0 \dots 2^n - 1\}$$

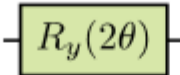
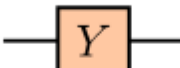
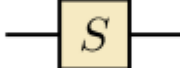
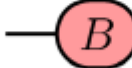
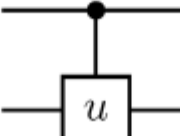
$$\hat{\sigma}_{\mathbf{m}} = \hat{\sigma}_{m_{n-1}} \otimes \cdots \otimes \hat{\sigma}_{m_0}, \hat{\sigma}_m \in \{\mathbb{1}, X, Y, Z\}$$

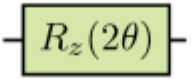
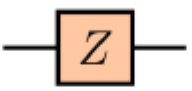
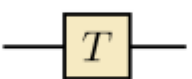
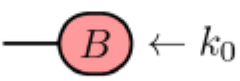
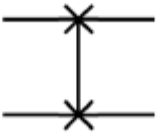
$$\hat{R}_{\hat{\sigma}_{\mathbf{m}}}(\theta) = e^{-\frac{i\theta}{2}\hat{\sigma}_{\mathbf{m}}} = \hat{V}^\dagger e^{-\frac{i\theta}{2}Z\otimes\cdots\otimes Z}\hat{V}, \hat{V} = \bigotimes_{\ell=0}^{n-1} \hat{A}_{m_\ell}, \hat{A}_m^\dagger \hat{\sigma}_m \hat{A}_m = Z$$

$$\hat{\sigma}_{\mathbf{m}} = \hat{V}^\dagger (Z \otimes \cdots \otimes Z) \hat{V} = \sum_{\mathbf{z}} f(\mathbf{z}) \hat{V}^\dagger |\mathbf{z}\rangle \langle \mathbf{z}| \hat{V}, f(\mathbf{z}) = \prod_{\ell=0}^{n-1} (-1)^{z_\ell}$$



name	symbol	matrix
X rotation		$\begin{bmatrix} \cos(\theta) & -i \sin(\theta) \\ -i \sin(\theta) & \cos(\theta) \end{bmatrix}$
Pauli X		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Hadamard		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Z measurement		$p(z) = \langle z \Psi \rangle ^2$
CNOT		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$

name	symbol	matrix
Y rotation		$\begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$
Pauli Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
S gate		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
general measurement		$p(k) = \langle \varphi_k \Psi \rangle ^2$
controlled- U		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & u_{00} & 0 & u_{10} \\ 0 & 0 & 1 & 0 \\ 0 & u_{10} & 0 & u_{11} \end{bmatrix}$

name	symbol	matrix
Z rotation		$\begin{bmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{bmatrix}$
Pauli Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
T gate		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix}$
post-selection		$k = k_0$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

$$R_x(\theta) = \exp(-i\theta X/2)$$

$$X = R_x(\pi/2)$$

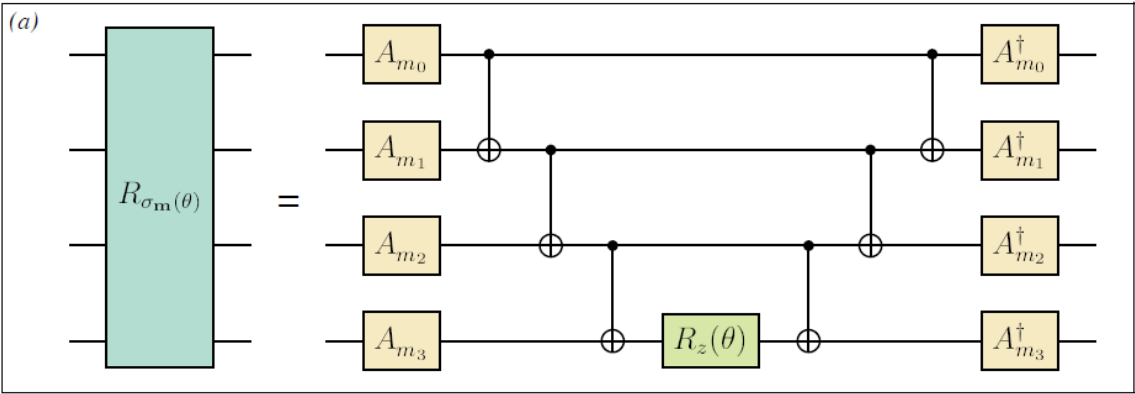
$$S = R_z(\pi/2)$$

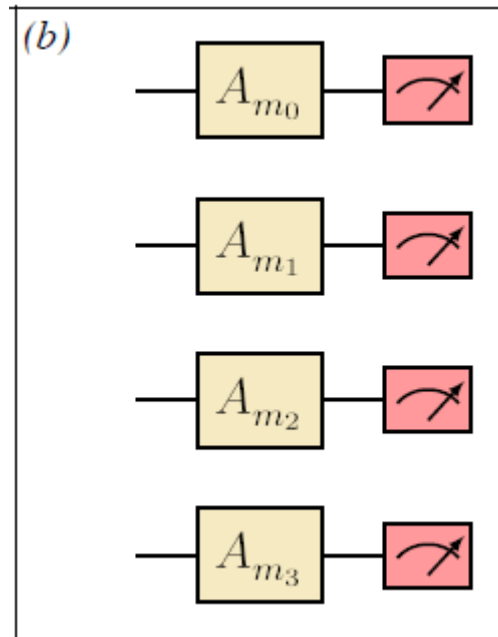
$$T = R_z(\pi/4)$$

$$H = \exp(-i\pi/2(X + Z))$$

$$B = \sum_k b_k |\varphi_k\rangle \langle \varphi_k|$$

$$G_{zw} = \langle z | \hat{G} | w \rangle = \langle z_{n-1} \dots z_0 | \hat{G} | w_{n-1} \dots w_0 \rangle$$





$$\otimes_{\ell=0}^3 \sigma_{m_\ell} A_X = H, A_Y = HS \text{ and } A_Z = I$$

$$\hat{H}\Psi=\left[\sum_{a<b}^{N_n}\frac{Z_aZ_b}{|\mathbf{R}_a-\mathbf{R}_b|}\right]\Psi-\frac{1}{2}\sum_{i=1}^N\frac{\partial^2\Psi}{\partial\mathbf{r}_i^2}-\left[\sum_{i=1}^N\sum_{a=1}^{N_n}\frac{Z_a}{|\mathbf{r}_i-\mathbf{R}_a|}\right]\Psi+\left[\sum_{i<j}^N\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}\right]\Psi\{\varphi_p\}_{p=1}^M$$

$$|\Psi\rangle=\sum_{i_1<\dots<i_N}^M\psi_{i_1\dots i_N}|i_1\dots i_N\rangle$$

$$\hat{H}=\sum_{a<b}^{N_n}\frac{Z_aZ_b}{|\mathbf{R}_a-\mathbf{R}_b|}+\sum_{pr}h_{pr}\hat{a}_p^\dagger\hat{a}_r+\sum_{prqs}\frac{(pr\mid qs)}{2}\hat{a}_p^\dagger\hat{a}_q^\dagger\hat{a}_s\hat{a}_r$$

$$D_{0\rightarrow f}\propto (E_f-E_0)\sum_{\alpha=x,y,z}|\langle\Psi_f|\hat{\mu}_\alpha|\Psi_0\rangle|^2$$

$$S_{\mu_{\alpha},\mu_{\beta}}(\omega)=\sum_l\langle\Psi_0|\hat{\mu}_{\alpha}|\Psi_l\rangle\delta(\hbar\omega-(E_l-E_0))\langle\Psi_l|\hat{\mu}_{\beta}|\Psi_0\rangle$$

$$D_{0\rightarrow f}=\sum_{\alpha}S_{\mu_{\alpha},\mu_{\alpha}}(E_f-E_0)$$

$$C_{\mu_{\alpha},\mu_{\beta}}(t)=\langle\Psi_0|\hat{\mu}_{\alpha}e^{\frac{t}{i\hbar}(\hat{H}-E_0)}\hat{\mu}_{\beta}|\Psi_0\rangle=\sum_f\langle\Psi_0|\hat{\mu}_{\alpha}|\Psi_f\rangle e^{\frac{t}{i\hbar}(E_f-E_0)}\langle\Psi_f|\hat{\mu}_{\beta}|\Psi_0\rangle$$

$$\hat{V}(t)=\sum_kf_k(t)\hat{O}_k^+$$

$$O_j(t)=\langle\Psi(t)|\hat{O}_{j,S}(t)|\Psi(t)\rangle\,,|\Psi(t)\rangle=\hat{U}(t)|\Psi_0\rangle\,,\hat{U}(t)=\sum_{n=0}^\infty\int_0^t\frac{dt_1}{i\hbar}\dots\int_0^{t_{n-1}}\frac{dt_n}{i\hbar}\hat{V}_S(t_1)\dots\hat{V}_S(t_n)$$

$$\hat{V}_S(t) = e^{-\frac{t\hat{H}_S}{i\hbar}}\hat{V}e^{\frac{t\hat{H}_S}{i\hbar}}$$

$$O_j(t)=O_j(0)+\int_0^t\frac{dt'}{i\hbar}\sum_kf_k(t)\alpha_{jk}(t-t'),\alpha_{jk}(t)=\langle\Psi_0|[\hat{O}_{j,S}(t),\hat{O}_k^{\dagger}]|\Psi_0\rangle$$

$$\hat{H}_{nuc} = -\frac{1}{2}\sum_{a=1}^{N_n}\frac{1}{M_a}\frac{\partial^2}{\partial \mathbf{R}_a^2} + V(\mathbf{R}_1\ldots \mathbf{R}_{N_n})$$

$$\hat{H}_{nuc}=\frac{1}{2}\sum_{\alpha\beta}(\hat{J}_{\alpha}-\hat{\pi}_{\alpha})\mu_{\alpha\beta}(\hat{J}_{\beta}-\hat{\pi}_{\beta})-\frac{1}{2}\sum_k\frac{\partial^2}{\partial Q_k^2}-\frac{1}{8}\sum_{\alpha}\mu_{\alpha\alpha}+V(\mathbf{Q}),V(\mathbf{Q})=\frac{\kappa}{2}\mathbf{Q}^2$$

$$\hat{F}\colon \mathcal{F}_-\rightarrow \mathcal{H}^{\otimes M}, |\Psi\rangle \mapsto \hat{F}|\Psi\rangle \equiv |\Psi'\rangle$$

$$\left(\hat{a}_{M-1}^\dagger\right)^{x_{M-1}}\ldots\left(\hat{a}_0^\dagger\right)^{x_0}|\emptyset\rangle\mapsto|\mathbf{x}\rangle,$$

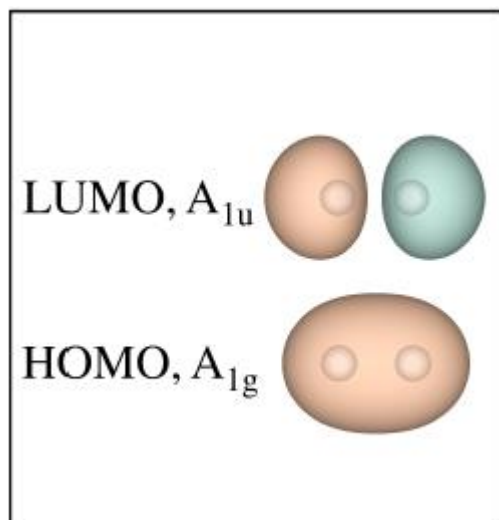
$$\hat{a}_k^\dagger \mapsto \frac{X_k-iY_k}{2} \otimes Z_{k-1} \otimes \cdots \otimes Z_0 \equiv S_{+,k} Z_0^{k-1}, \hat{a}_k \mapsto \frac{X_k+iY_k}{2} Z_0^{k-1} \equiv S_{-,k} Z_0^{k-1}$$

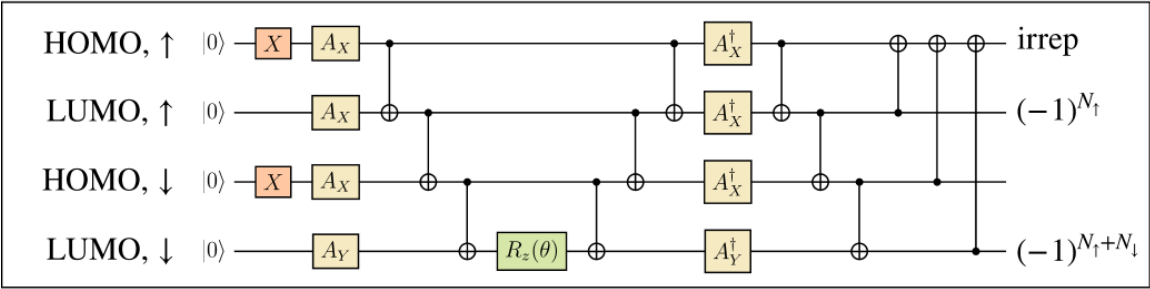
$$p_k=\sum_{j=0}^{k-1}x_j\mathrm{mod}2$$

$$\left(\hat{a}_{M-1}^\dagger\right)^{x_{M-1}}\ldots\left(\hat{a}_0^\dagger\right)^{x_0}|\emptyset\rangle\mapsto|\mathbf{p}\rangle,\hat{a}_k^\dagger\mapsto X_{M-1}\otimes\cdots\otimes X_{k+1}\otimes\frac{X_k-iY_k}{2}\equiv X_{k+1}^{M-1}\otimes S_{+,k}$$

$$|p_3,p_2,p_1,p_0\rangle \text{ with } p_k=x_0+\cdots+x_k$$

$$\left(\hat{a}_{M-1}^\dagger\right)^{x_{M-1}}\ldots\left(\hat{a}_0^\dagger\right)^{x_0}\mapsto|\mathbf{b}\rangle,b_k=\sum_{j=0}^{M-1}A_{kj}x_j\mathrm{mod}2,$$





configuration	irrep	JW	parity (2QR)	tapering	configuration	irrep	JW	parity (2QR)	tapering
	A _{lg}	0000⟩	0000⟩	0000⟩		A _{lu}	1000⟩	1000⟩	1001⟩
	A _{lg}	0001⟩	1111⟩	1110⟩		A _{lu}	1001⟩	0111⟩	0111⟩
	A _{lu}	0010⟩	1110⟩	1111⟩		A _{lg}	1010⟩	0110⟩	0110⟩
	A _{lu}	0011⟩	0001⟩	0001⟩		A _{lg}	1011⟩	1001⟩	1000⟩
	A _{lg}	0100⟩	1100⟩	1100⟩		A _{lu}	1100⟩	0100⟩	0101⟩
	A _{lg}	0101⟩	0011⟩	0010⟩		A _{lu}	1101⟩	1011⟩	1011⟩
	A _{lu}	0110⟩	0010⟩	0011⟩		A _{lg}	1110⟩	1010⟩	1010⟩
	A _{lu}	0111⟩	1101⟩	1101⟩		A _{lg}	1111⟩	0101⟩	0100⟩

$$(-1)^{N_{\uparrow}+N_{\downarrow}}, (-1)^{N_{\uparrow}}$$

$$x_1+x_3=p_0+p_1+p_2+p_3\text{mod}2$$

$$\hat{H}=\sum_j c_j P_j$$

$$\tau_i=U^\dagger Z_i U$$

$$Z_iU|\Psi\rangle=s_iU|\Psi\rangle,\text{i.e. }U|\Psi\rangle=|\Phi_{\mathbf{s}}\rangle\otimes|\mathbf{s}\rangle$$

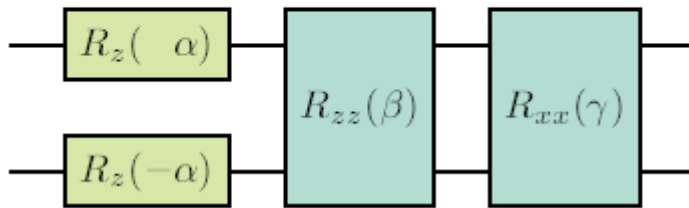
$$\hat{H}_{\mathbf{s}}=\text{Tr}_{1\dots k}[(\mathbb{1}\otimes|\mathbf{s}\rangle\langle\mathbf{s}|)U^\dagger H U]$$

$$l=\sum_{i=0}^{n_q-1}x_i2^i$$

$$\mathbf{x}_l=\left(x_0\ldots x_{n_q-1}\right)$$



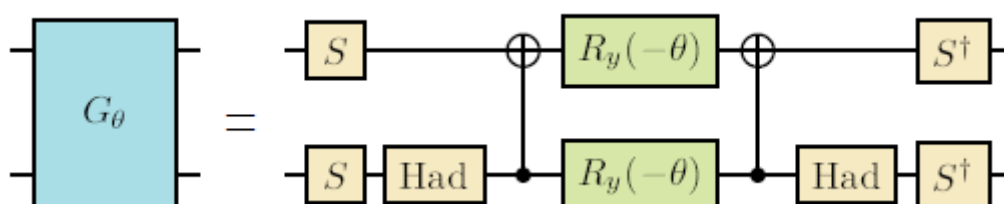
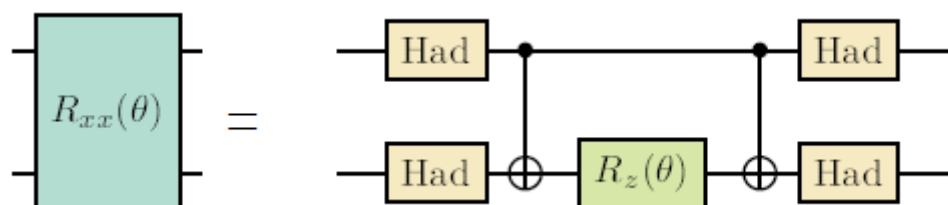
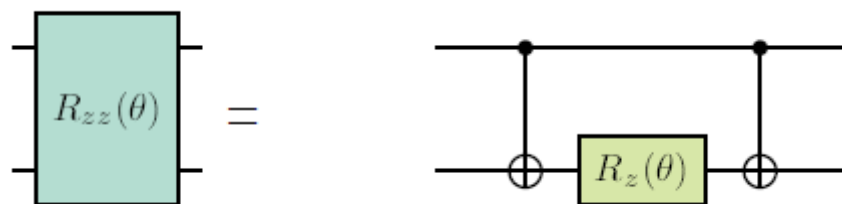
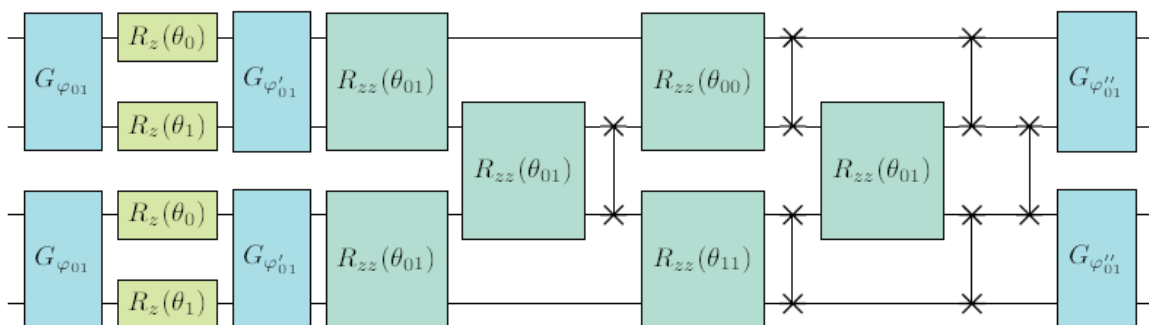
$$\Delta t \hat{H} = \frac{\alpha}{2}(\mathbb{I} \otimes Z - Z \otimes \mathbb{I}) + \frac{\beta}{2}Z \otimes Z + \frac{\gamma}{2}X \otimes X$$



$$\Delta t \hat{H} = -\alpha Z - \frac{\gamma}{2}X$$



$$\Delta t \hat{H} = \hat{V}_0^\dagger \left[\sum_k \alpha_k Z_k \right] \hat{V}_0 + \hat{V}_1^\dagger \left[\sum_{kl} \beta_{kl} Z_k Z_l \right] \hat{V}_1$$



$$\|\hat{U}-e^{-it\hat{H}}\|<\varepsilon$$

$$\hat{H}=\sum_{\ell=1}^L\hat{h}_{\ell}$$

$$\hat{U}(t)=e^{-it\hat{H}}=\prod_{i=0}^{n_T-1}\hat{U}(\Delta t),\Delta t=\frac{t}{n_T}$$

$$\hat{U}(\Delta t)=\prod_{\ell}e^{-i\Delta t\hat{h}_{\ell}}+\mathcal{O}(\Delta t^2),\hat{U}_p(\Delta t)\equiv\prod_{\ell}e^{-i\Delta t\hat{h}_{\ell}}.$$

$$\|\hat{U}(t)-\hat{U}_p(\Delta t)^{n_T}\|=\gamma_p n_T \Delta t^2+\mathcal{O}(t^3/n_T^2),\gamma_p=\frac{1}{2}\sum_{\ell<\ell'}\|[\hat{h}_{\ell},\hat{h}_{\ell'}]\|$$

$$n_T=\mathcal{O}(\gamma_p t^2/\varepsilon)$$

$$\hat{U}_{2k+2}(\Delta t)=\hat{U}_{2k}^2(a_{2k}\Delta t)\hat{U}_{2k}((1-4a_{2k})\Delta t)\hat{U}_{2k}^2(a_{2k}\Delta t)\\ \hat{U}_2(\Delta t)=\left[\prod_{\ell=L}^1e^{-i\frac{\Delta t}{2}\hat{h}_{\ell}}\right]\left[\prod_{\ell=1}^Le^{-i\frac{\Delta t}{2}\hat{h}_{\ell}}\right],a_{2k}=\frac{1}{4-\frac{1}{4^{2k+1}}}$$

$$\hat{U}_{2k}(\Delta t)=e^{-i\Delta t\hat{H}}+\mathcal{O}(\Delta t^{2k+1})$$

$$n_T=t^{1+\frac{1}{2k}}\varepsilon^{-\frac{1}{2k}}e^{-i\Delta t\hat{h}_{\ell}}$$

$$\hat{H}=\sum_{\ell=1}^L c_{\ell} \hat{P}_{\ell}$$

$$(pr \mid qs) = \sum_{\gamma=1}^{N_{\gamma}} L_{pr}^{\gamma} L_{qs}^{\gamma}$$

$$\hat{H}=E_0+\hat{V}_0^{\dagger}\left[\sum_pt_p\hat{n}_p\right]\hat{V}_0+\sum_{\gamma}\hat{V}_{\gamma}^{\dagger}\left[\sum_{pq}v_{pq}^{\gamma}\hat{n}_p\hat{n}_q\right]\hat{V}_{\gamma},\hat{V}_{\gamma}=e^{\sum_{pq}A_{pq}^{\gamma}\hat{a}_p^{\dagger}\hat{a}_q}$$

$$e^{-i\Delta t\hat{H}}\simeq\prod_{\gamma}\left[\hat{V}_{\gamma}^{\dagger}\left(\prod_{pq}e^{-i\Delta tv_{pq}^{\gamma}\hat{n}_p\hat{n}_q}\right)\hat{V}_{\gamma}\right]\prod_pe^{-i\Delta t\hat{n}_p}$$

$$R_z(\varphi)=\exp\left(-i\varphi/2Z\right)\text{ and }R_{zz}(\varphi)=\exp\left(-i\varphi/2Z\otimes Z\right)$$

$$\mathcal{O}(N_{\gamma}M^2)=\mathcal{O}(M^3)$$

$$\hat{H}=\sum_{\lambda}\lambda|\lambda\rangle\langle\lambda|$$

$$\zeta\geq\|\hat{H}\|$$

$$\hat{W}=i\hat{S}(2\hat{T}\hat{T}^{\dagger}-\mathbb{1})$$

$$\hat{T}\colon\mathcal{H}\rightarrow\mathcal{H}_e$$

$$\hat{S}\colon\mathcal{H}_e\rightarrow\mathcal{H}_e$$

$$\hat{T}^\dagger \hat{S} \hat{T} = \hat{H}$$

$$\mathcal{S}_\lambda=\text{span}\{\hat{T}|\lambda\rangle,\hat{S}\hat{T}|\lambda\rangle\}$$

$$\hat{W}|\mu_{\pm}(\lambda)\rangle=\mu_{\pm}(\lambda)|\mu_{\pm}(\lambda)\rangle\,,\mu_{\pm}(\lambda)=\pm e^{\pm i\arcsin{(\lambda)}}\,,|\mu_{\pm}(\lambda)\rangle=\frac{\mathbb{1}+i\mu_{\pm}(\lambda)\hat{S}}{\sqrt{2(1-\lambda^2)}}\hat{T}|\lambda\rangle$$

$$|\Psi\rangle\mapsto\frac{\hat{X}|\Psi\rangle}{\|\hat{X}\Psi\|}\equiv|\Psi_X\rangle,\hat{X}=\sum_{\ell=0}^{L-1}\alpha_{\ell}\hat{U}_{\ell}$$

$$\hat{W}_p|0\rangle=\sum_{\ell=0}^{L-1}\sqrt{\frac{|\alpha_{\ell}|}{\alpha}}|\ell\rangle\,,\alpha=\sum_{\ell=0}^{L-1}\alpha_{\ell}$$

$$\hat{W}_s=\sum_{\ell=0}^{L-1}\hat{U}_{\ell}\otimes|\ell\rangle\langle\ell|$$

$$p=\|\hat{X}\psi\|^2/\alpha^2$$

$$n_A=\lceil \log_2\left(L\right)\rceil$$

$$L=\text{poly}(n)$$

$$2^{n_A}=\text{poly}(n)$$

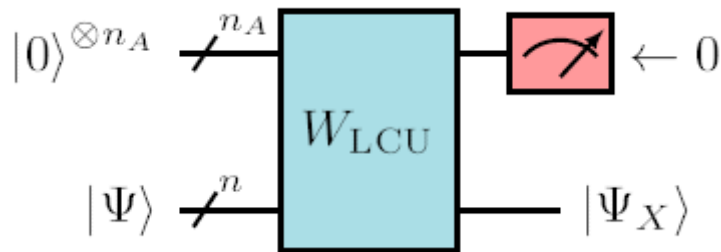
$$c_\ell=\text{poly}\left(n\right)$$

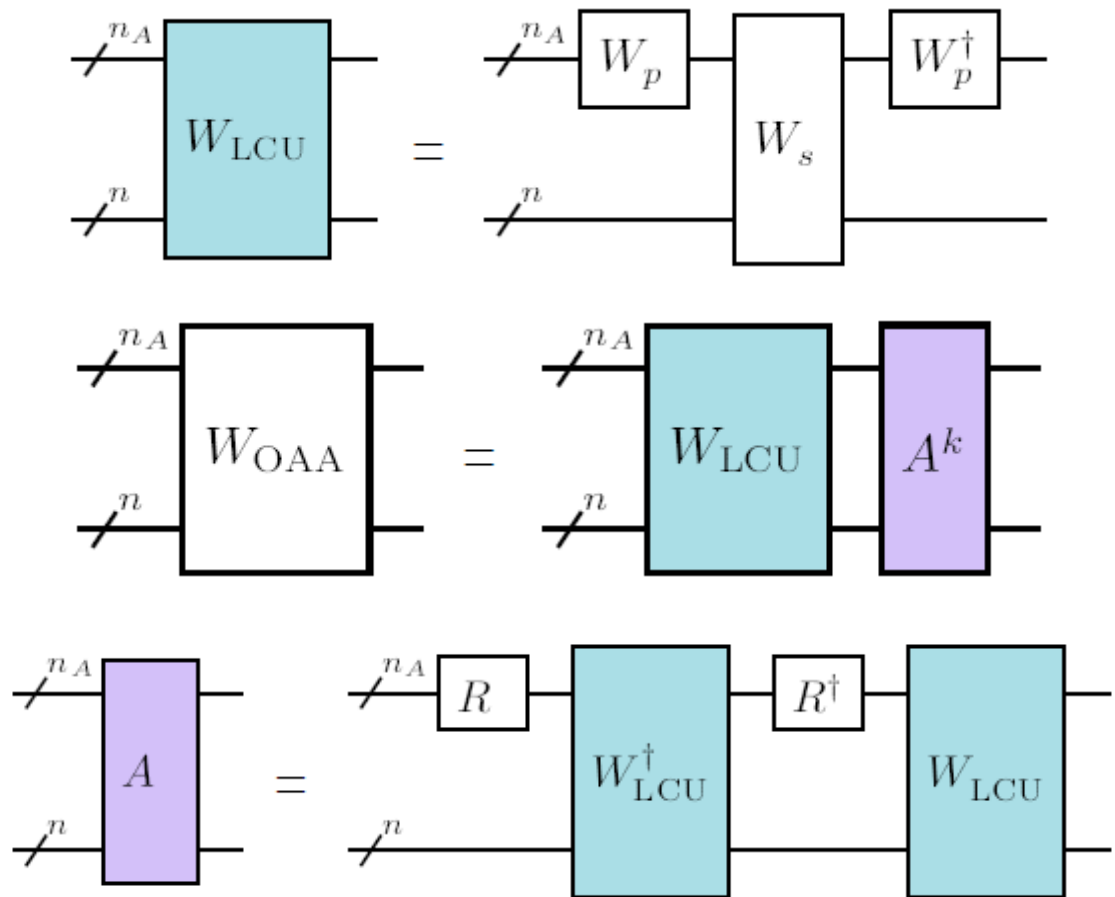
$$1-(1-p)^k=2^{-\mathcal{O}(k)}$$

$$\hat{W}_{\text{LCU}}=\hat{W}_p^\dagger \hat{W}_s \hat{W}_p$$

$$\hat{R}=\mathbb{1}\otimes\left(\mathbb{1}-2\left|0\right\rangle\left\langle 0\right|\right)$$

$$\hat{U}|0\rangle|\Psi\rangle=\sqrt{p_k}\frac{\hat{X}|\Psi\rangle}{\|\hat{X}\Psi\|}\otimes|0\rangle^{\otimes n_A}+\sqrt{1-p_k}|\Phi^\perp\rangle\,,p_k=\sin^2\left((2k+1)\theta\right)\,,\theta=\arcsin\sqrt{p}\,,$$





$$\hat{H} = \sum_{\ell=0}^{L-1} \alpha_{\ell} \hat{U}_{\ell}$$

$$C = \sum_{\ell} \alpha_{\ell} = 1$$

$$\hat{H} \rightarrow C^{-1} \hat{H} \text{ and } t \rightarrow Ct$$

$$\Delta t = t/re^{-i\Delta t \hat{H}}$$

$$e^{-i\Delta t \hat{H}} \simeq \hat{V}_K(\Delta t) = \sum_{m=0}^K \frac{(-i\Delta t)^m}{m!} \hat{H}^m = \sum_{m=0}^K \sum_{\ell_0 \dots \ell_m=0}^{L-1} \frac{(-i\Delta t)^m}{m!} \alpha_{\ell_0} \dots \alpha_{\ell_m} \hat{U}_{\ell_0} \dots \hat{U}_{\ell_m}.$$

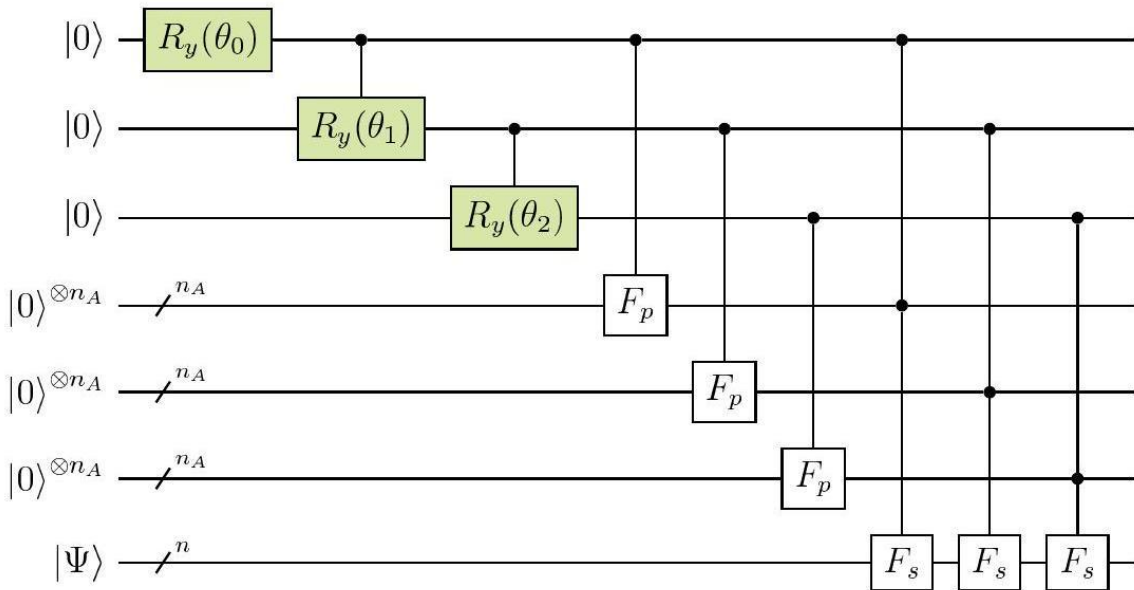
$$\sum_m \sqrt{\Delta t^m/m!} \, |0\rangle^{K-m} |1\rangle^m$$

$$\sum_{\ell} \sqrt{\alpha_{\ell}} |\ell\rangle$$

$$\mathcal{O}(KL)|\psi\rangle|\ell_k\rangle \dots |\ell_1\rangle|k\rangle \text{ to } (-i)^k \hat{U}_{\ell_1} \dots \hat{U}_{\ell_k} |\psi\rangle|\ell_k\rangle \dots |\ell_1\rangle|k\rangle$$

$$\mathcal{O}(L(n+\log_2 L)K)e^{-i\Delta t \hat{H}} \varepsilon/K$$

$$K = \mathcal{O}\left(\frac{\log\left(\frac{t}{\varepsilon}\right)}{\log\log\left(\frac{t}{\varepsilon}\right)}\right)$$



$$K=3n_A=\log_2\left(L\right)$$

$$\sum_m \sqrt{\Delta t^m/m!} \, |0\rangle^{K-m} |1\rangle^m$$

$$c\hat{F}_p|0\rangle|k\rangle=V^k|0\rangle|k\rangle$$

$$V|0\rangle=\sum_{\ell}\sqrt{\alpha_{\ell}}|\ell\rangle$$

$$c\hat{F}_s|\psi\rangle|\ell\rangle|k\rangle = (-i\hat{U}_{\ell})^k|\psi\rangle|\ell\rangle|k\rangle$$

$$\langle\phi|\langle g|\hat{U}|\psi\rangle|g\rangle=\langle\phi|\hat{H}|\psi\rangle \text{ for some } |g\rangle\in\mathcal{H}' \text{ and any } |\phi\rangle, |\psi\rangle\in\mathcal{H}.$$

$$\hat{H},\hat{H}|\lambda\rangle=\lambda|\lambda\rangle$$

$$\hat{W}_{\rm Q}|g_{\lambda}\rangle=\lambda|g_{\lambda}\rangle-\sqrt{1-\lambda^2}|g_{\lambda}^{\perp}\rangle,\hat{W}_{\rm Q}|g_{\lambda}^{\perp}\rangle=\lambda|g_{\lambda}^{\perp}\rangle+\sqrt{1-\lambda^2}|g_{\lambda}\rangle$$

$$|g_{\lambda}\rangle=|\lambda\rangle|g\rangle|g_{\lambda}^{\perp}\rangle$$

$$\hat{W}_{\rm Q}=\bigoplus_{\lambda}e^{-i\theta_{\lambda}Y_{\lambda}},\theta_{\lambda}=\arccos\left(\lambda\right)e^{-it\hat{H}}\hat{V}_{\vec{\varphi}}$$

$$\hat{V}_{\vec{\varphi}}=\prod_{m=0}^K\hat{U}_{\varphi_{2m+2}+\pi}^{\dagger}\hat{U}_{\varphi_{2m+1}},\hat{U}_{\varphi}=[1\otimes R_z(-\varphi)\text{Had}]c(iW_{\rm Q})[1\otimes\text{Had}R_z(\varphi)]$$

$$\hat{V}_{\vec{\varphi}}=\sum_{\lambda,\pm}|\lambda_{\pm}\rangle\langle\lambda_{\pm}| \otimes u(\vec{\varphi},\theta_{\lambda,\pm})$$

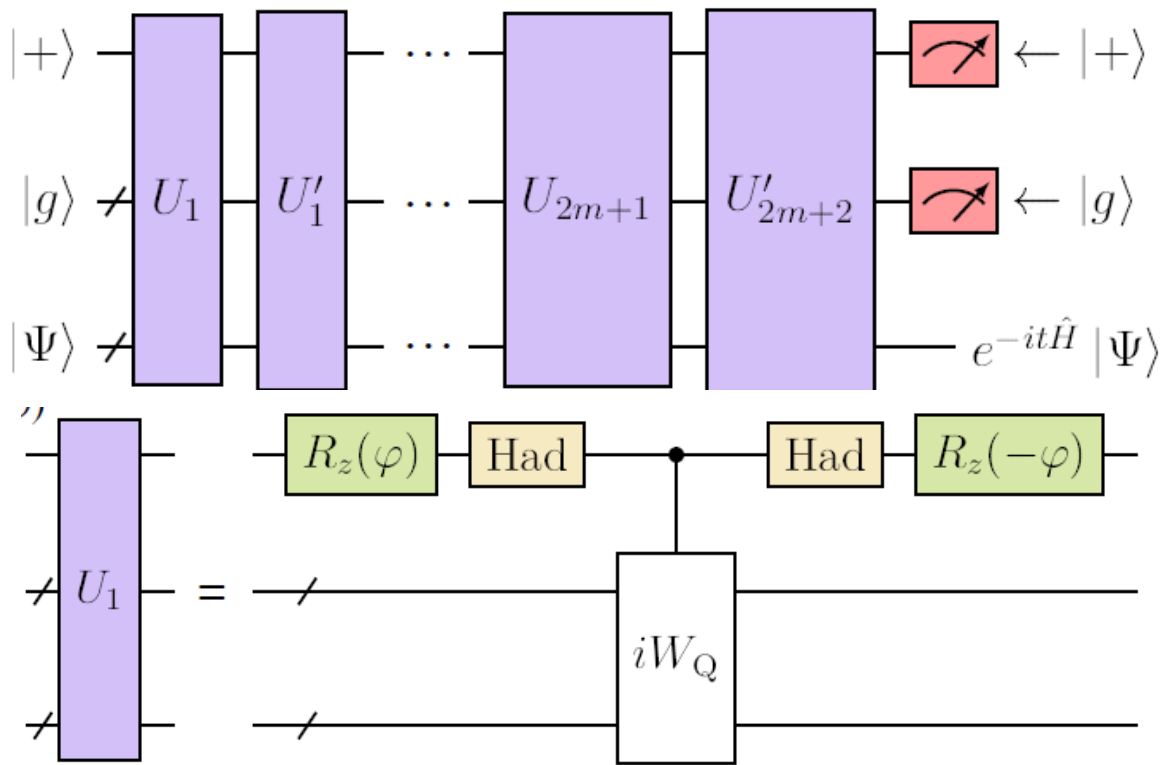
$$K=\mathcal{O}(t+\log\,\varepsilon^{-1})$$

$$\langle\chi|\langle g|\langle +|\hat{V}_{\vec{\varphi}}|\psi\rangle|g\rangle|+\rangle\simeq\langle\chi|e^{-it\hat{H}}|\psi\rangle$$



$$\Psi(t) \rightarrow \Psi_I(t) = e^{\frac{t}{i\hbar}\hat{T}}\Psi_t$$

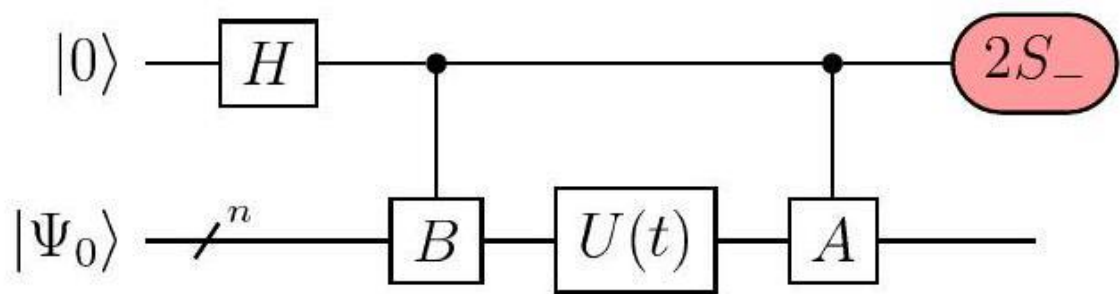
$$\hat{V}_I(t) = e^{\frac{t}{i\hbar}\hat{T}}\hat{V}e^{-\frac{t}{i\hbar}\hat{T}}$$



$$U'_k=U_{\varphi_k+\pi}^\dagger$$

$$d_{\mu\nu}(t)=\langle\Psi_0|\hat{d}_\mu(t)\hat{d}_\nu|\Psi_0\rangle$$

$$\hat{d}_\mu=\sum_jc_{j\mu}\hat{P}_j$$

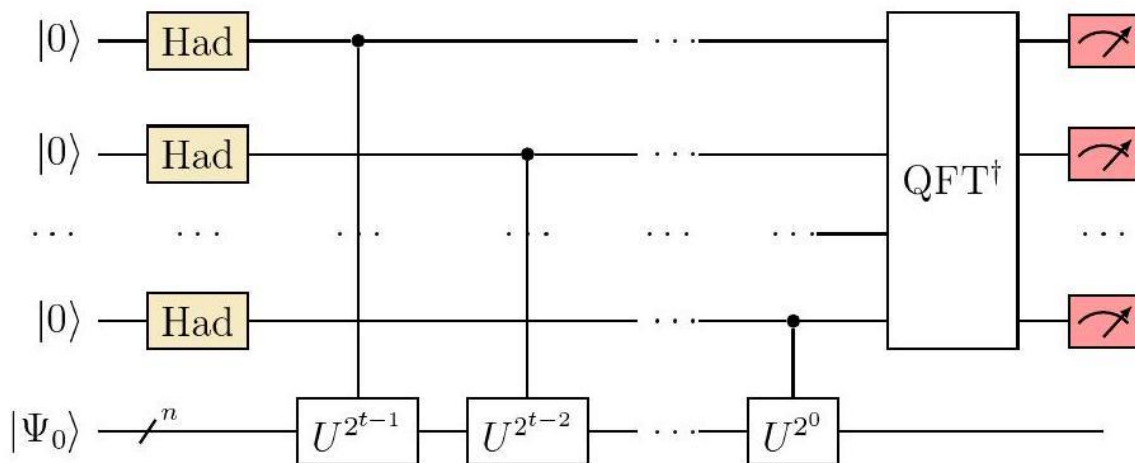


$$\langle\Psi_0|\hat{U}^\dagger(t)\hat{A}\hat{U}(t)\hat{B}|\Psi_0\rangle$$

$$\hat{A},\hat{B},S_-=\frac{X+iY}{2}$$

$$u=e^{i2\pi\theta},0<\theta<1$$

$$\hat{H}'=2\pi(\hat{H}-E_1)/(E_2-E_1)e^{-i\lambda\hat{H}}$$



$$|\Psi\rangle = \sum_{z=0}^{2^t-1} \left(\sum_{k=0}^{2^t-1} \frac{e^{\frac{2\pi iz(2^t\theta-k)}{2^t}}}{2^t} \right) |z\rangle \otimes |u\rangle = \sum_{z=0}^{2^t-1} \Delta(z,\theta) |z\rangle \otimes |u\rangle$$

$$|\Psi\rangle = |k_0\rangle \otimes |\psi\rangle$$

$$k_0=2^t\theta$$

$$p(z)=|\Delta(z,\theta)|^2$$

$$2^t\theta, p(k_0) \geq 4/\pi^2 \simeq 0.4[247].p(k_0)$$

$$t=\mathcal{O}(\log \varepsilon^{-1})$$

$$\hat{H}_0=\hat{F}+\langle\Psi_{\rm HF}|\hat{H}-\hat{F}|\Psi_{\rm HF}\rangle$$

$$\hat{H}(s), 0\leq s\leq 1$$

$$\hat{H}(s=0)=\hat{H}_0 \text{ and } \hat{H}(s=1)=\hat{H}$$

$$\hat{H}(s)=\hat{H}_0+s\hat{H}_1$$

$$i\frac{d}{dt}|\Psi_t\rangle=\hat{H}(t/T)|\Psi_t\rangle,0\leq t\leq T,|\Psi_0\rangle=|\Phi_0(0)\rangle$$

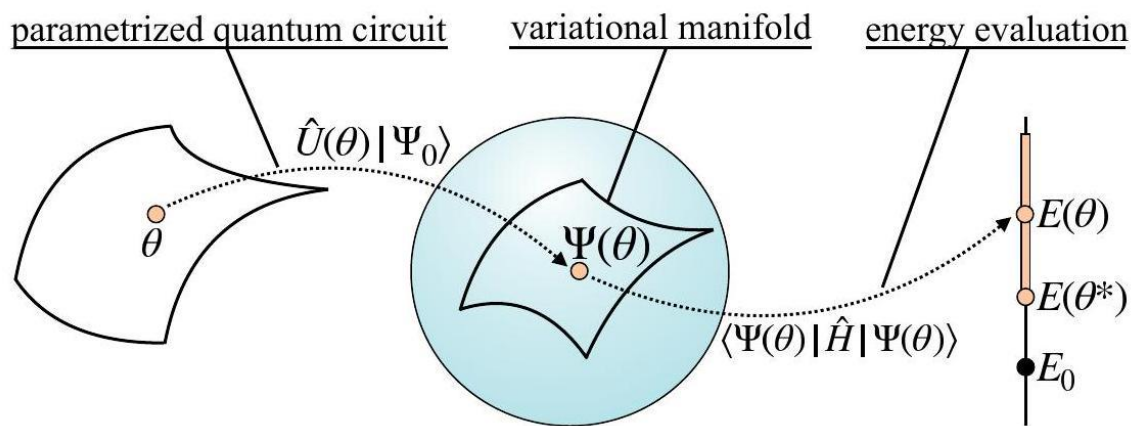
$$\lim_{T\rightarrow\infty}|\Psi(T)\rangle=|\Phi_0(1)\rangle$$

$$\varepsilon^{-1}F(\gamma(s),f_1(s),f_2(s))$$

$$\gamma(s)\hat{H}(s)f_k(s)=\left\|\frac{d^k\hat{H}}{ds^k}\right\|(s)$$

$$\hat{H}|\Phi_\mu\rangle=E_\mu|\Phi_\mu\rangle$$

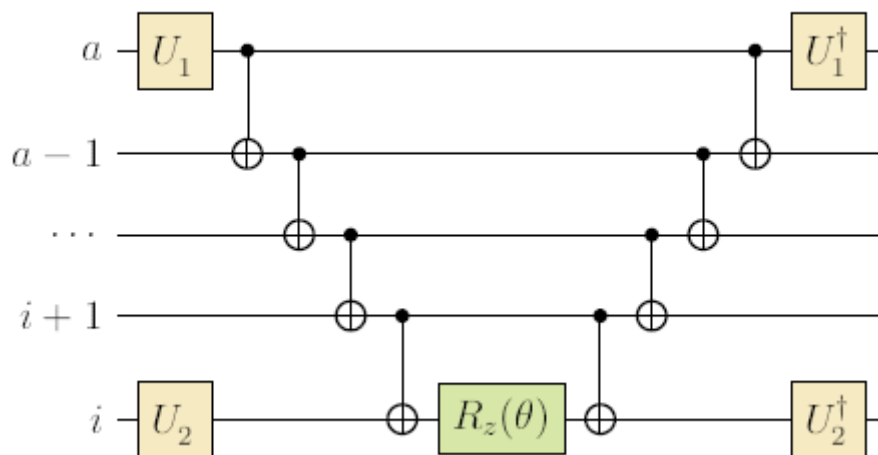
$$|\Psi(\theta)\rangle=\hat{U}(\theta)|\Psi_0\rangle,\hat{U}(\theta)=\hat{u}_{n_g-1}\left(\theta_{n_g-1}\right)\ldots\hat{u}_0(\theta_0)$$

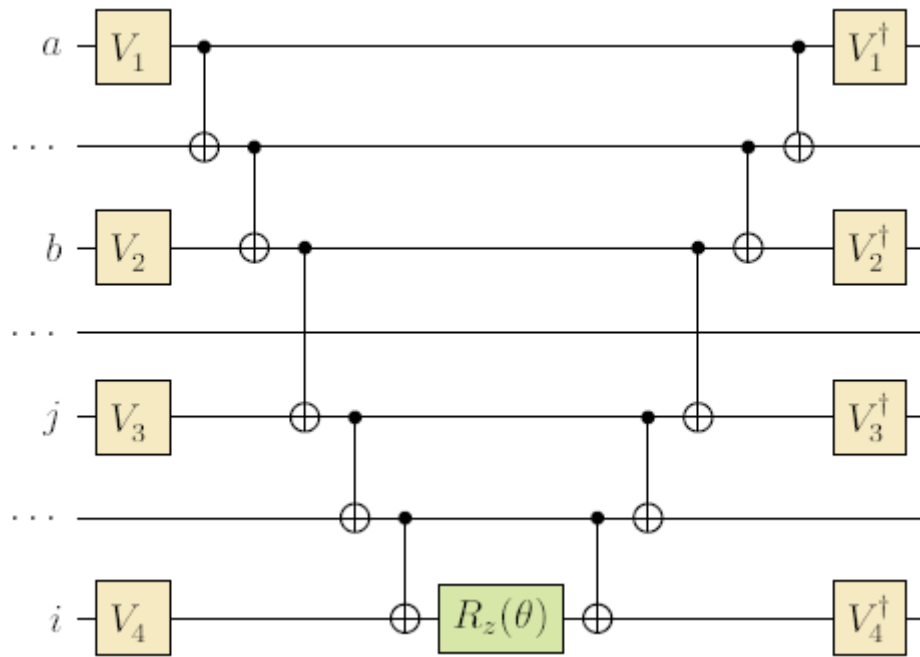


$$E(\theta) = \langle \Psi(\theta) | \hat{H} | \Psi(\theta) \rangle$$

$$E(\theta) \sim \mu \pm \sigma$$

$$\theta_{n+1} = \theta_n - a_n g(\theta_n)$$





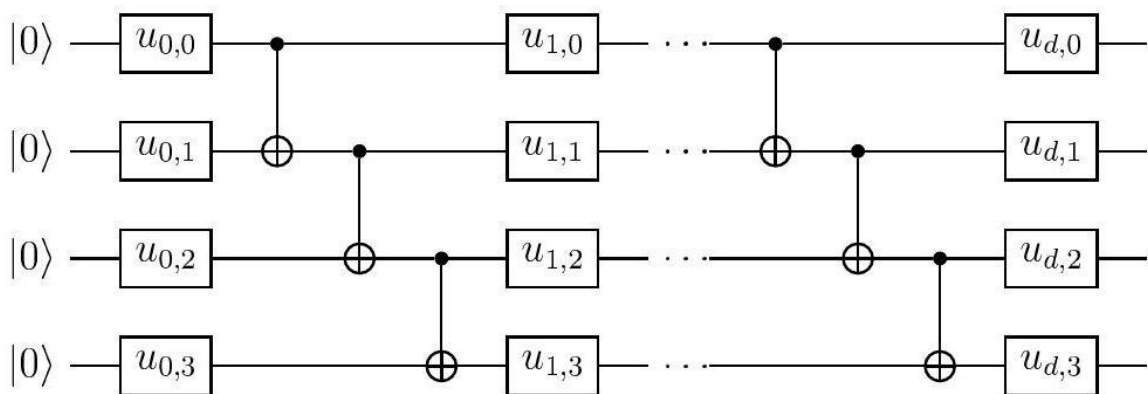
$$(U_1, U_2) = \{(A_Y, A_X), (A_X, A_Y)\}$$

$$(V_1, V_2, V_3, V_4) = (A_X, A_X, A_Y, A_X), (A_Y, A_X, A_Y, A_Y), (A_X, A_Y, A_Y, A_Y), (A_X, A_X, A_X, A_Y), (A_Y, A_X, A_X, A_X), (A_X, A_Y, A_X, A_X), (A_Y, A_Y, A_Y, A_X), (A_Y, A_Y, A_X, A_Y)\}$$

$$|\Psi\rangle = e^{\hat{T}-\hat{T}^\dagger}|\Psi_0\rangle, \hat{T} = \sum_{l=1}^k \hat{T}_l, \hat{T}_l = \sum_{a_0 \dots a_{l-1}} \sum_{i_0 \dots i_{l-1}} t_{i_0 \dots i_{l-1}}^{a_0 \dots a_{l-1}} \hat{a}_{a_0}^\dagger \dots \hat{a}_{a_{l-1}}^\dagger \hat{a}_{i_{l-1}} \dots \hat{a}_{i_0},$$

$$e^{\hat{T}-\hat{T}^\dagger} \simeq \prod_{\mu} e^{\theta_{\mu}(\hat{t}_{\mu}-\hat{t}_{\mu}^\dagger)}$$

$$e^{\hat{T}-\hat{T}^\dagger} \simeq \prod_{ia} e^{\theta_i^a(\hat{a}_a^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_a)} \prod_{ijab} e^{\theta_{ij}^{ab}(\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i - \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_b \hat{a}_a)}$$



$$|\Psi_{\theta}\rangle = \exp\left(\theta_n \hat{A}_{i_n}\right) \dots \exp\left(\theta_1 \hat{A}_{i_1}\right) |\Psi_0\rangle$$

$$g_i = \langle \Psi_{\theta} | [\hat{H}, \hat{A}_i] | \Psi_{\theta} \rangle$$

$$|\Delta\rangle = \frac{d}{dt}|\Psi_{\theta_t}\rangle + i\hat{H}|\Psi_{\theta_t}\rangle = \sum_k \frac{d\theta_k}{dt}|\Psi_{\theta_t}^k\rangle + i\hat{H}|\Psi_{\theta_t}\rangle, |\Psi_{\theta_t}^k\rangle = \frac{\partial}{\partial\theta_k}|\Psi_{\theta_t}\rangle,$$

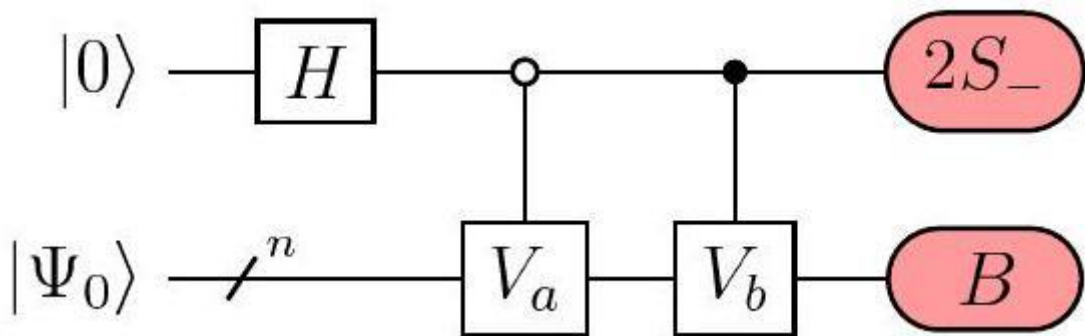
$$b_r = \sum_k A_{rk} \frac{d\theta_k}{dt}, A_{rk} = \text{Re}(\langle \Psi_{\theta_t}^r | \Psi_{\theta_t}^k \rangle), b_r = \text{Im}(\langle \Psi_{\theta_t}^r | \hat{H} | \Psi_{\theta_t} \rangle) \{|\mathbf{v}_a\rangle\}_{a=0}^{d-1},$$

$$S_{ab} = \langle \mathbf{v}_a | \mathbf{v}_b \rangle, H_{ab} = \langle \mathbf{v}_a | \hat{H} | \mathbf{v}_b \rangle$$

$$H\mathbf{c}_\mu = E_\mu S\mathbf{c}_\mu$$

$$|\psi_\mu\rangle = \sum_a c_{a\mu} |\mathbf{v}_a\rangle$$

$$|\mathbf{v}_a\rangle = \hat{V}_a |\Psi_0\rangle, a = 0 \dots d-1$$



$$B_{ab} = \langle \mathbf{v}_a | \hat{B} | \mathbf{v}_b \rangle$$

$$|\psi_\mu\rangle = \sum_a c_{a\mu} \hat{E}_a |\Psi_0\rangle, \text{ where } \{\hat{E}_a\}_a$$

$$P_k = \{ \hat{\sigma}_{\mathbf{m}} = \hat{\sigma}_{m_{n-1}} \otimes \cdots \otimes \hat{\sigma}_{m_0}, \sigma_{m_i} \neq \mathbb{1} \text{ for at most } k \text{ indices} \}$$

$$F_k = \{ \hat{a}_{i_0}^\dagger \dots \hat{a}_{i_{l-1}}^\dagger \hat{a}_{j_{l-1}} \dots \hat{a}_{j_0}, l \leq k \}.$$

$$\Delta E_\mu = \frac{\langle \Psi_0 | [\hat{O}_\mu, \hat{H}, \hat{O}_\mu^\dagger] | \Psi_0 \rangle}{\langle \Psi_0 | [\hat{O}_\mu, \hat{O}_\mu^\dagger] | \Psi_0 \rangle},$$

$$2[\hat{O}_\mu, \hat{H}, \hat{O}_\mu^\dagger] = \left[[\hat{O}_\mu, \hat{H}], \hat{O}_\mu^\dagger \right] + \left[\hat{O}_\mu, [\hat{H}, \hat{O}_\mu^\dagger] \right]$$

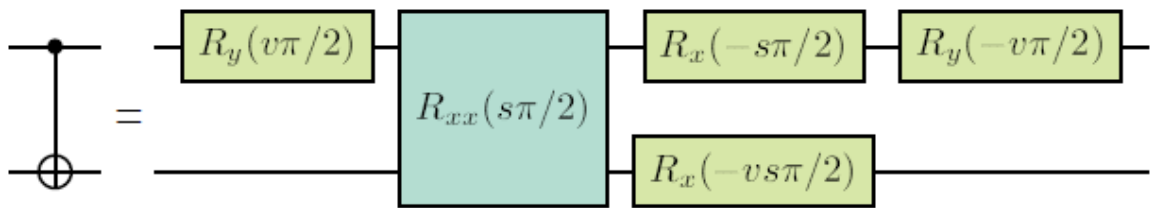
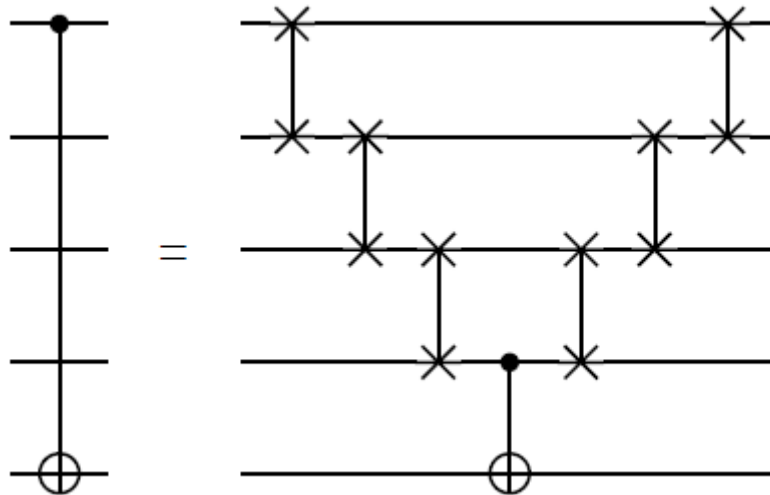
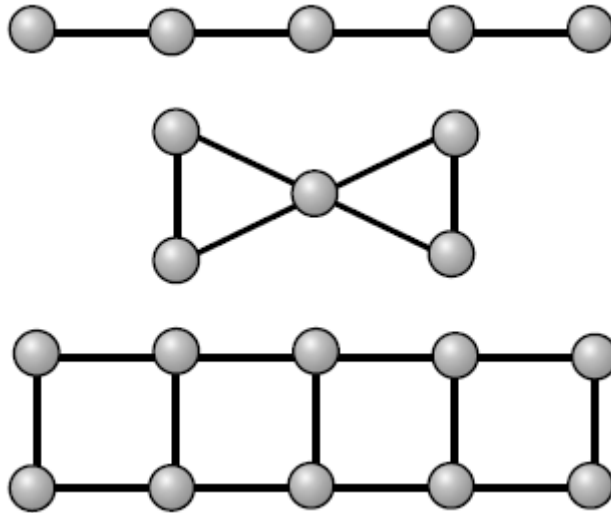
$$\hat{H}\hat{O}_\mu^\dagger|\Psi_0\rangle = [\hat{H}, \hat{O}_\mu^\dagger]|\Psi_0\rangle + E_0\hat{O}_\mu^\dagger|\Psi_0\rangle$$

$$[\hat{H}, \hat{O}_\mu^\dagger]|\Psi_0\rangle = (E_\mu - E_0)\hat{O}_\mu^\dagger|\Psi_0\rangle = \Delta E_\mu \hat{O}_\mu^\dagger|\Psi_0\rangle$$

$$|\mathbf{v}_k\rangle = \frac{e^{-k\Delta\tau\hat{H}}|\Psi_0\rangle}{\|e^{-k\Delta\tau\hat{H}}|\Psi_0\rangle\|}, k = 0 \dots d-1,$$

$$e^{-\Delta\tau\hat{h}_m}|\Psi\rangle\propto e^{i\hat{A}_m}|\Psi\rangle$$

$$\hat{A}_m = \sum_i x_{im} \hat{P}_{im}$$



$$i\hbar \frac{d\rho_{\text{hw}}}{dt} = [\hat{H}_{\text{hw}}(t) + \hat{H}_{\text{c}}(t), \rho_{\text{hw}}] + \mathcal{L}_{\text{i}}(t, \rho_{\text{hw}})$$

$$\mathcal{L}_{\text{a}}(\rho) = \gamma_{\text{a}} \mathcal{V}_{\text{S}_{-}}(\rho) , \mathcal{L}_{\text{p}}(\rho) = \gamma_{\text{p}} \mathcal{V}_{\text{Z}}(\rho) , \mathcal{L}_{\text{d}}(\rho) = \gamma_{\text{d}} \sum_m \mathcal{V}_{\sigma_m}(\rho)$$

$$\mathcal{V}_A(\rho) = A\rho A^\dagger - A^\dagger A\rho - \rho A^\dagger A$$

$$\Lambda_0, \mathbf{\Delta}_0 = \operatorname{argmin}_{\Lambda, \mathbf{\Delta}} \sum_k \left\| \mathbf{p}_{\text{exp}}\left(k\right) - \Lambda \mathbf{p}_{\text{ideal}}\left(k\right) - \mathbf{\Delta} \right\|$$

$$\mathbf{p}_{\text{ideal}} \simeq \Lambda_0^{-1}[\mathbf{p}_{\text{exp}} - \mathbf{\Delta}_0]$$

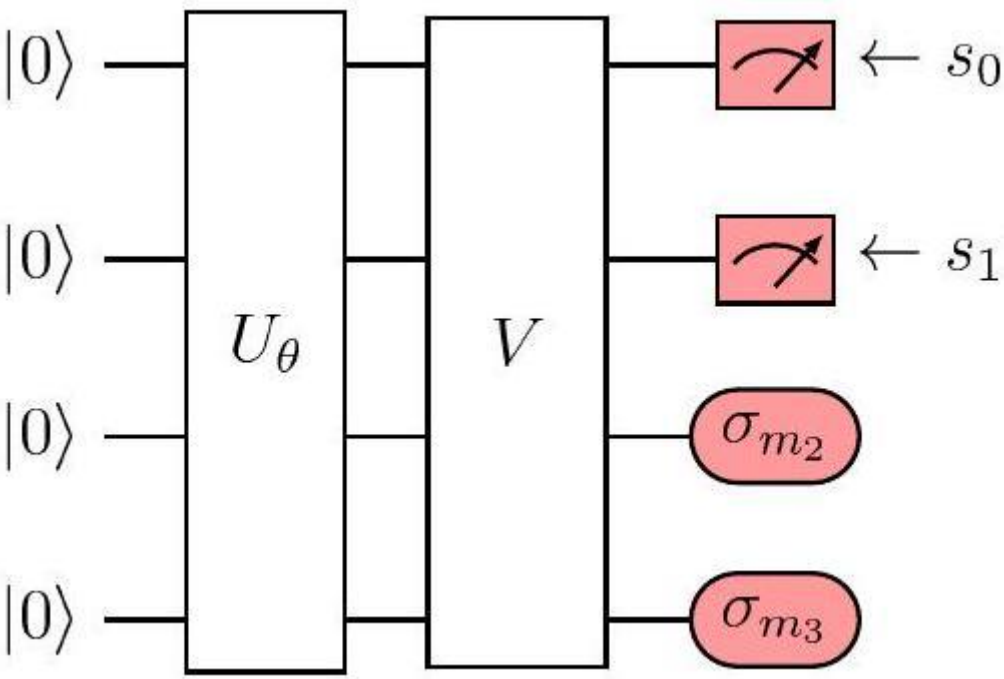
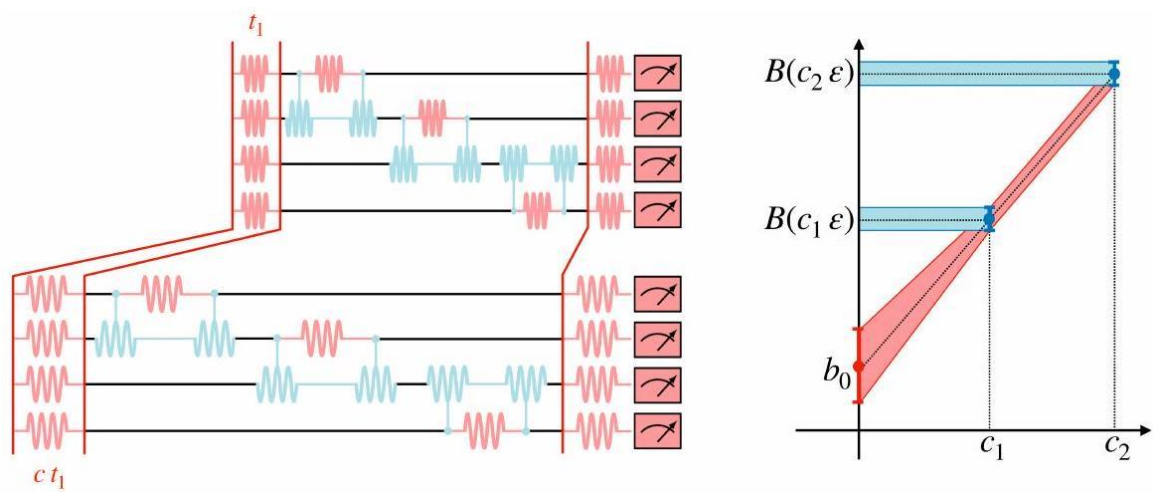
$$\hat{H}_{\text{hw}}(t) = \sum_{\alpha} J_{\alpha}(t) \hat{P}_{\alpha}$$

$$B(\varepsilon) = b_0 + \sum_{k=1}^n b_k \varepsilon^k + \mathcal{O}(\varepsilon^{n+1})$$

$$J_{\alpha}(t) \rightarrow c_i^{-1} J_{\alpha}(c_i^{-1} t)$$

$$B_i(\varepsilon) = B(c_i\varepsilon) = b_0 + \sum_k b_k (c_i\varepsilon)^k$$

$$|\Psi\rangle = \hat{U}^\dagger \sum_{\mathbf{s}} c_{\mathbf{s}} |\Phi_{\mathbf{s}}\rangle \otimes |\mathbf{s}\rangle$$



$$[a_j,a_k]_+=0\;[a_j^{\dagger},a_k^{\dagger}]_+=0\;[a_j,a_k^{\dagger}]_+=\delta_{jk}$$

$$[a,b]_+\equiv ab+ba$$

$$H = h_{nuc} + \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$$h_{pq} = \int d\sigma \varphi_p^*(\sigma) \left(-\frac{\nabla_{\vec{r}}^2}{2} - \sum_i \frac{Z_i}{|\vec{R}_i - \vec{r}|} \right) \varphi_q(\sigma)$$

$$h_{pqrs} = \int d\sigma_1 d\sigma_2 \frac{\varphi_p^*(\sigma_1) \varphi_q^*(\sigma_2) \varphi_s(\sigma_1) \varphi_r(\sigma_2)}{|\vec{r}_1 - \vec{r}_2|}$$

$$h_{nuc} = \frac{1}{2} \sum_{i \neq j} \frac{Z_i Z_j}{|\vec{R}_i - \vec{R}_j|}$$

$$\text{rate} \propto \frac{e^{-\beta \Delta G^\ddagger}}{\beta},$$

$$T = \sum_{i=1}^{\eta} T_i$$

$$T_1 = \sum_{\substack{i \in \text{occ} \\ a \in \text{virt}}} t_a^i a_a^\dagger a_i$$

$$T_2 = \sum_{\substack{i > j \in \text{occ} \\ a > b \in \text{virt} \\ \dots}} t_{ab}^{ij} a_a^\dagger a_b^\dagger a_i a_j$$

$$|\text{FCI}\rangle = (1+T)|\text{HF}\rangle$$

$$E_{\text{FCI}} = \min_{\tilde{t}} \frac{\langle \text{FCI} | H | \text{FCI} \rangle}{\langle \text{FCI} | \text{FCI} \rangle}$$

$$O(\eta^k(N-\eta)^{k+2})$$

$$|\Psi\rangle = e^T |\text{HF}\rangle$$

$$|\text{CCSD}\rangle = e^{T_1+T_2} |\text{HF}\rangle.$$

$$e^{-T} H e^T |\text{HF}\rangle = E_{\text{CC}} |\text{HF}\rangle$$

$$\langle \text{HF} | e^{-T} H e^T | \text{HF} \rangle = E$$

$$\langle \mu | e^{-T} H e^T | \text{HF} \rangle = 0$$

$$\begin{aligned} e^{-T} H e^T = & H + [H, T] + \frac{1}{2} [[H, T], T] \\ & + \frac{1}{3!} [[[H, T] T], T] + \frac{1}{4!} [[[[H, T] T], T], T] \end{aligned}$$

$$|\Psi\rangle = e^{T-T^\dagger} |\text{HF}\rangle.$$

$$E = \min_{\tilde{t}} \langle \text{HF} | e^{-(T-T^\dagger)} H e^{T-T^\dagger} | \text{HF} \rangle$$

$$U_1(\vec{t})=\prod_j\exp\left(it_j\sum_k^{2^{2l_k-1}}P_j^k\right)$$

$$U_1(\vec{t})=\prod_j\prod_k^{2^{2l_k-1}}\exp\left(it_jP_k^j\right)\|t_j(\tau_j-\tau_j^\dagger)\|$$

$$T\approx T_1+T_2$$

$$\binom{N-\eta}{2}\binom{\eta}{2}+\binom{N-\eta}{1}\binom{\eta}{1}<O(N^2\eta^2)$$

$$U_{\text{MS}}(\theta,\phi)=\exp\left(-i\frac{\theta}{2}\sum_{j<k}\sigma_j^\phi\sigma_k^\phi\right),$$

$$\sigma_j^\phi = \cos{(\phi)}\sigma_j^x + \sin{(\phi)}\sigma_j^y$$

$$\ket{q_3} \text{---} \boxed{\text{meter}}$$

$$\ket{q_2} \text{---} \boxed{R_x\left(\frac{\pi}{2}\right)} \text{---} \boxed{\text{meter}}$$

$$\ket{q_1} \text{---} \boxed{\text{meter}}$$

$$\ket{q_0} \text{---} \boxed{H} \text{---} \boxed{\text{meter}}$$

$$\sigma_3^z\sigma_2^y\sigma_1^z\sigma_0^xHR_x\left(-\frac{\pi}{2}\right)$$

$$|\Phi_0\rangle = a_{\eta}^{\dagger}a_{\eta-1}^{\dagger} \ldots a_1^{\dagger} | \rangle$$

$$|0\rangle^{\otimes N-\eta}\otimes |1\rangle^{\otimes \eta}$$

$$E=\langle \Phi_0|e^{-(T-T^\dagger)}He^{T-T^\dagger}|\Phi_0\rangle$$

$$E=\sum_i^M h_i\langle O_i\rangle$$

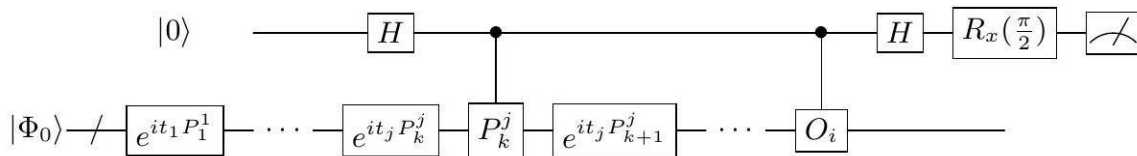
$$\epsilon_i^2=\frac{|h_i|^2\mathrm{Var}[\langle O_i\rangle]}{m_i}$$

$$\text{Var}[\langle O_i \rangle] \epsilon_i^2 = \frac{|h_i|}{\sum_j^M |h_j|} \epsilon^2$$

$$m = \frac{\sum_j^M |h_j| \sum_i^M |h_i| \text{Var}[\langle O_i \rangle]}{\epsilon^2} \leq \frac{(\sum_j^M |h_j|)^2}{\epsilon^2}$$

$$t_i^a = 0; \quad t_{ij}^{ab} = \frac{h_{ijba} - h_{ijab}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

$$U(\vec{t}) = \prod_j^{N_P} \prod_k^{N_S^j} \exp\left(i c_k^j t_j P_k^j \right)$$



$$\Psi(\vec{t}) = \langle \Phi_0 | V_k^{j\dagger}(\vec{t}) O_i U(\vec{t}) | \Phi_0 \rangle \frac{\partial E(\vec{t})}{\partial t_j} R_x\left(\frac{\pi}{2}\right) U(\vec{t}) | \Phi_0 \rangle$$

$$E(\vec{t}) = \langle \Psi(\vec{t}) | H | \Psi(\vec{t}) \rangle$$

$$\frac{\partial E(\vec{t})}{\partial t_j} = \langle \Phi_0 | U^\dagger(\vec{t}) H \frac{\partial U(\vec{t})}{\partial t_j} | \Phi_0 \rangle + \langle \Phi_0 | \frac{\partial U(\vec{t})^\dagger}{\partial t_j} H U(\vec{t}) | \Phi_0 \rangle$$

$$= i \sum_k^{N_S^j} \langle \Phi_0 | U^\dagger(\vec{t}) H V_k^j(\vec{t}) | \Phi_0 \rangle - \langle \Phi_0 | V_k^{j\dagger}(\vec{t}) H U(\vec{t}) | \Phi_0 \rangle$$

$$= 2 \sum_k^{N_S^j} c_k^j \text{Im}(\langle \Phi_0 | V_k^{j\dagger}(\vec{t}) H U(\vec{t}) | \Phi_0 \rangle)$$

$$V_k^j(\vec{t}) \exp\left(it_j P_{k-1}^j\right) \exp\left(it_j P_k^j\right)$$

$$V_k^j(\vec{t}) = \exp\left(it_j P_1^1\right) \cdots \exp\left(it_j P_{k-1}^j\right) P_k^j \exp\left(it_j P_k^j\right)$$

$$\exp\left(it_j P_{k+1}^j\right) \cdots \exp\left(it_{N_P} P_{N_S^{N_P}}^{N_P}\right) \frac{\partial E(\vec{t})}{\partial t_j}$$

$$\frac{\partial E(\vec{t})}{\partial t_j} = 2 \sum_i^M h_i \left(\sum_k^{N_S^j} c_k^j \text{Im}(\langle \Phi_0 | V_k^{j\dagger}(\vec{t}) O_i U(\vec{t}) | \Phi_0 \rangle) \right)$$

$$\langle \Phi_0 | V_k^{j\dagger} H_i U(\vec{t}) | \Phi_0 \rangle \exp\left(it_j P_k^j\right)$$

$$\frac{|0\rangle \otimes (U|\Phi_0\rangle + O_i V_k^j(\vec{t})|\Phi_0\rangle) + |1\rangle \otimes (U|\Phi_0\rangle - O_i V_k^j(\vec{t})|\Phi_0\rangle)}{2} \langle \Phi_0 | V_k^{j\dagger}(\vec{t}) O_i U(\vec{t}) | \Phi_0 \rangle$$

$$\mathrm{Var}\left[\frac{\partial E(\vec{t})}{\partial t_j}\right] = 4 \sum_i^M |h_i|^2 \sum_k^{N_S^j} |c_k^j|^2 \mathrm{Var}\left[\langle \sigma^y \rangle_{O_{i,P_k^j}}\right]$$

$$\langle \sigma^y \rangle_{O_{i,P_k^j}} = \langle 0 \otimes \Phi_0 | C_{O_{i,P_k^j}}^\dagger (\sigma^y \otimes I) C_{O_{i,P_k^j}} | 0 \otimes \Phi_0 \rangle$$

$$\tilde{m}_{j,k}^i = \frac{|c_k^j|^2 \mathrm{Var}\left[\langle \sigma^y \rangle_{O_{i,P_k^j}}\right]}{(\tilde{\epsilon}_{j,k}^i)^2}$$

$$|c_{j,k}^i| = |c_j|$$

$$\sum_k^{N_S^j} |c_{j,k}^i| = 1$$

$$(\tilde{\epsilon}_{j,k}^i)^2 = |c_j|(\tilde{\epsilon}_j^i)^2$$

$$(\tilde{\epsilon}_j^i)^2 = \frac{|h_i|\tilde{\epsilon}_j^2}{\sum_l^M |h_l|}$$

$$\tilde{m}_j = \left(4 \sum_l^M |h_l|\right) \frac{\sum_i^M \sum_k^{N_S^j} |h_i| |c_k^j| \mathrm{Var}\left[\langle \sigma^y \rangle_{O_{i,P_k^j}}\right]}{\tilde{\epsilon}_j^2}$$

$$\tilde{m}_j \leq 4 \frac{(\sum_i^M |h_i|)^2}{\tilde{\epsilon}_j^2}$$

$$\frac{\partial E(\vec{t})}{\partial t_j} \approx \frac{E(t_1,\dots,t_j+\delta,\dots,t_{N_P})-E(t_1,\dots,t_j-\delta,\dots,t_{N_P})}{2\delta}$$

$$\epsilon_j = \frac{2\delta\tilde{\epsilon}_j}{\sqrt{2}}$$

$$\tilde{m}_j \leq 4 \left(\frac{(\sum_i^M |h_i|)^2}{(2\delta)^2 \tilde{\epsilon}_j^2} \right)$$

$$\tilde{\epsilon}_j^2 = \frac{\tilde{\epsilon}^2}{N_P}$$

$$\tilde{m} \leq C N_P \left(\frac{(\sum_i^M |h_i|)^2}{\tilde{\epsilon}^2} \right),$$

$$C = \frac{4}{(2\delta)^2}$$

$$T^A = \sum_i^{\eta_A} T_i$$

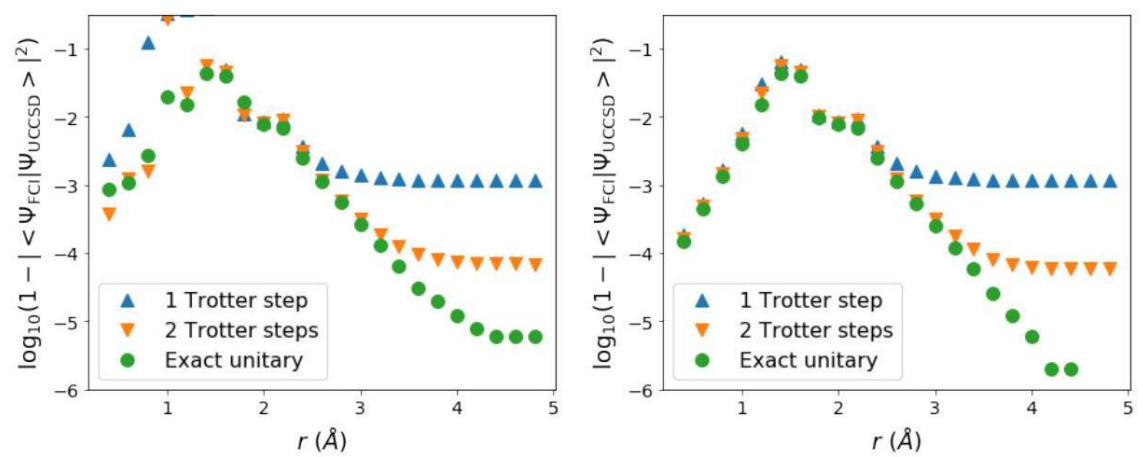
$$|\Phi_0\rangle = |\Phi_0^A\rangle \otimes |\Phi_0^I\rangle, \text{ where } |\Phi_0^I\rangle \text{ and } |\Phi_0^A\rangle$$

$$E = \langle \Phi_0^A | e^{-(T^A - T^{A\dagger})} \tilde{H}^A e^{T^A - T^{A\dagger}} | \Phi_0^A \rangle$$

$$\tilde{H}^A = \langle \Phi_0^I | H | \Phi_0^I \rangle$$

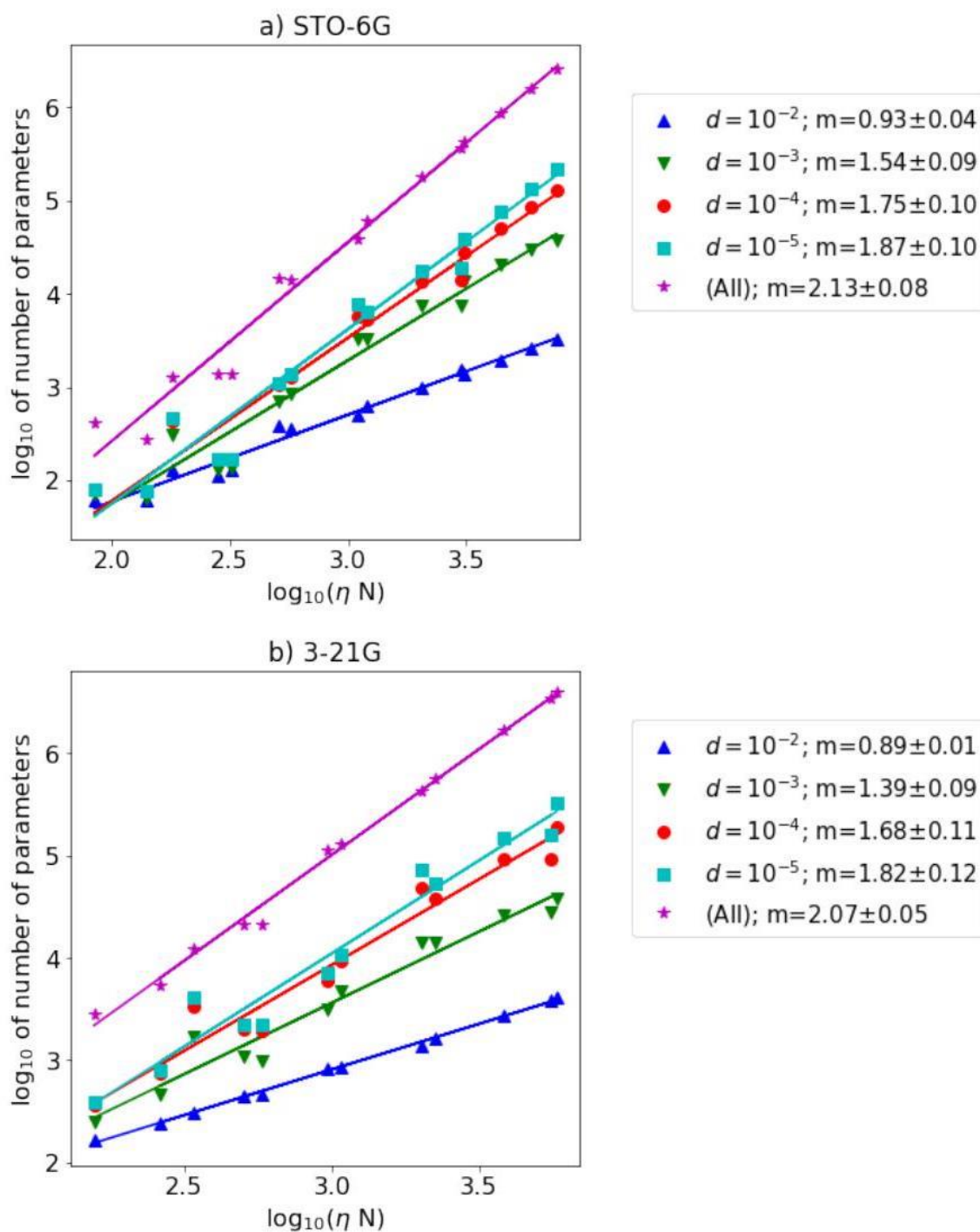
$$\left(1 - |\langle \Psi_{\text{VQE}} | \Psi_{\text{FCI}} \rangle|^2\right)$$

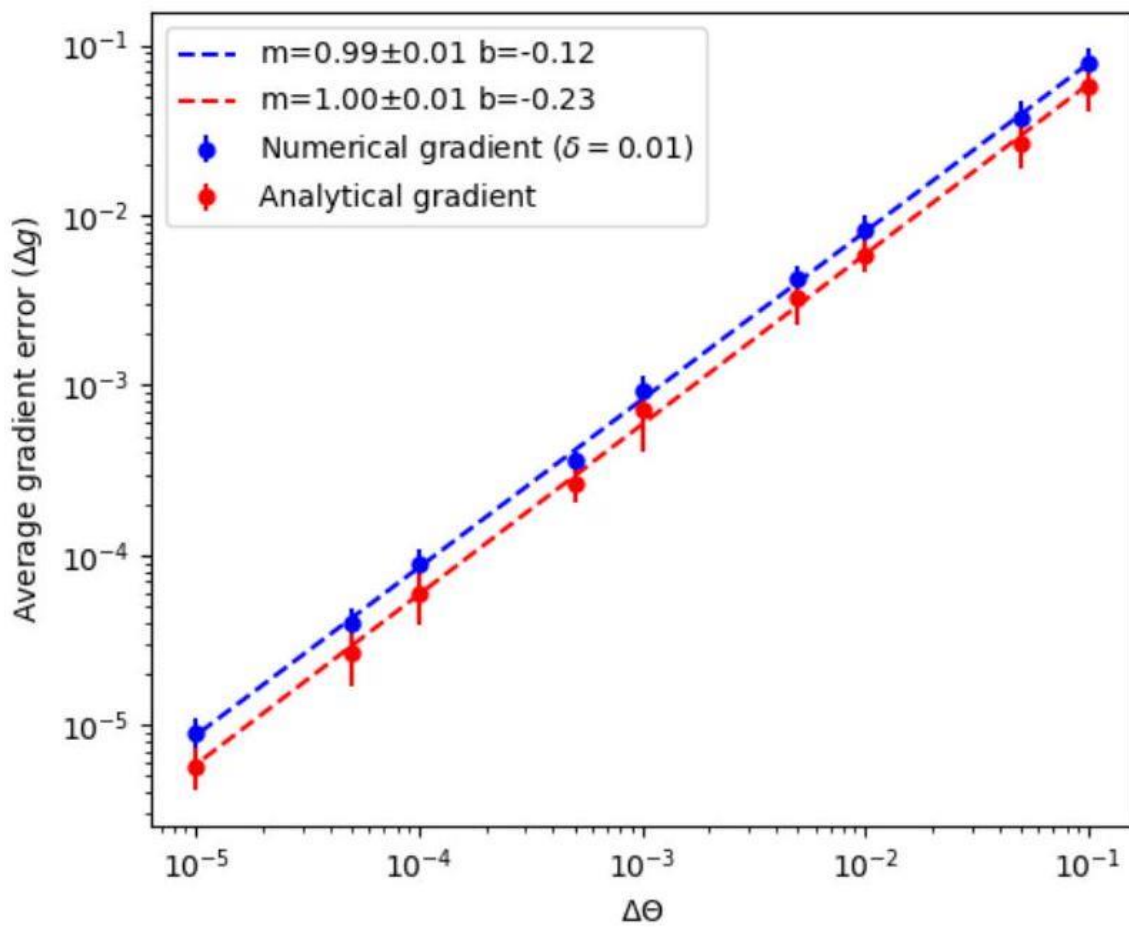
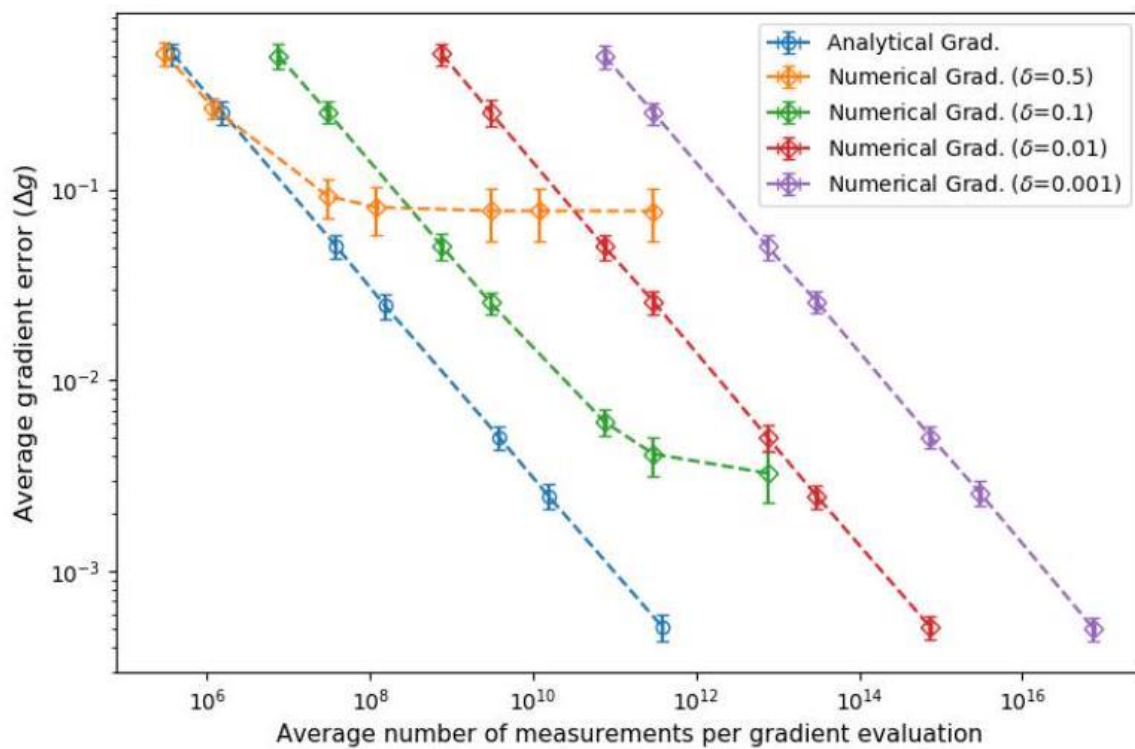
$$\text{NPE} = \max(E_{\text{UCCSD}} - E_{\text{FCI}}) - \min(E_{\text{UCCSD}} - E_{\text{FCI}})$$



$$1 - |\langle \Psi_{\text{UCCSD}} | \Psi_{\text{FCI}} \rangle| \left\{ t_{ij}^{ab(\text{MP2})} \right\} \left| t_{ij}^{ab(\text{MP2})} \right| < d$$







$$\tilde{U}(\vec{p}) = U(\vec{p} + \Delta \vec{p})$$

$$t_i^a (a_a^\dagger a_i - h.c.) \equiv \frac{it_i^a}{2} \bigotimes_{k=i+1}^{a-1} \sigma_k^z (\sigma_i^y \sigma_a^x - \sigma_i^x \sigma_a^y)$$

$$t_{ij}^{ab} (a_b^\dagger a_a^\dagger a_j a_i - h.c.) \equiv \frac{it_{ij}^{ab}}{8} \bigotimes_{k=i+1}^{j-1} \sigma_k^z \bigotimes_{l=a+1}^{b-1} \sigma_l^z$$

$$(\sigma_i^x \sigma_j^x \sigma_a^y \sigma_b^x + \sigma_i^y \sigma_j^x \sigma_a^y \sigma_b^y$$

$$+ \sigma_i^x \sigma_j^y \sigma_a^y \sigma_b^y + \sigma_i^x \sigma_j^x \sigma_a^x \sigma_b^y$$

$$- \sigma_i^y \sigma_j^x \sigma_a^x \sigma_b^x - \sigma_i^x \sigma_j^y \sigma_a^x \sigma_b^x$$

$$- \sigma_i^y \sigma_j^y \sigma_a^y \sigma_b^x - \sigma_i^y \sigma_j^y \sigma_a^x \sigma_b^y)$$

$$2n, P_A = \bigotimes_{i=1}^{2n} \sigma_i^{a_i}$$

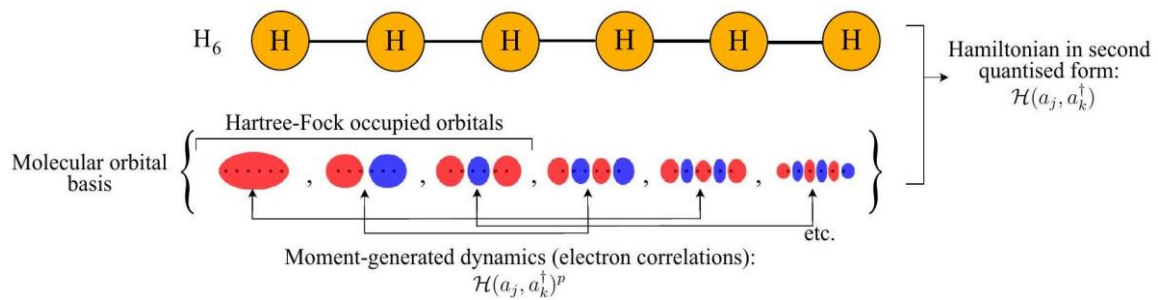
$$P_B = \bigotimes_{i=1}^{2n} \sigma_i^{b_i}$$

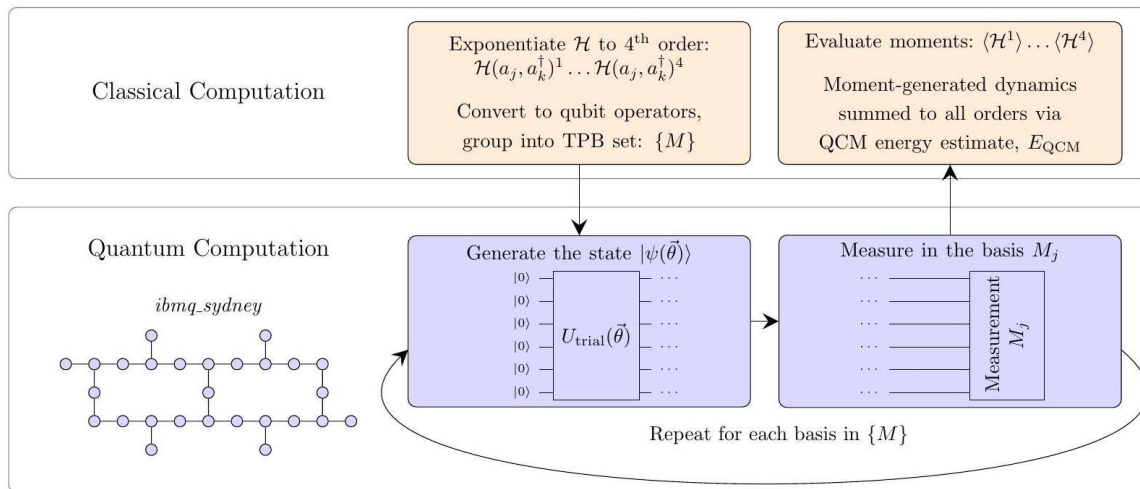
$$[P_A, P_B] = \bigotimes_{i=1}^{2n} (\sigma_i^{a_i} \sigma_i^{b_i}) - \bigotimes_{i=1}^{2n} (\sigma_i^{b_i} \sigma_i^{a_i})$$

$$\sigma_i^{a_i} \sigma_i^{b_i} = \begin{cases} 1 & \text{if } a_i = b_i \\ i\sigma_z & \text{if } a_i = x, b_i = y \\ -i\sigma_z & \text{if } a_i = y, b_i = x \end{cases}$$

$$[P_A, P_B] = \left[(-i)^{n_y^A - c_y} (i)^{n_x^A - c_x} - (-i)^{n_y^B - c_y} (i)^{n_x^B - c_x} \right] P,$$

$$[P_A, P_B] = (-1)^{n_y^A - c_y} \left(1 - (-1)^{n_y^B - n_y^A} \right) i^{2n - c_x - c_y} P$$

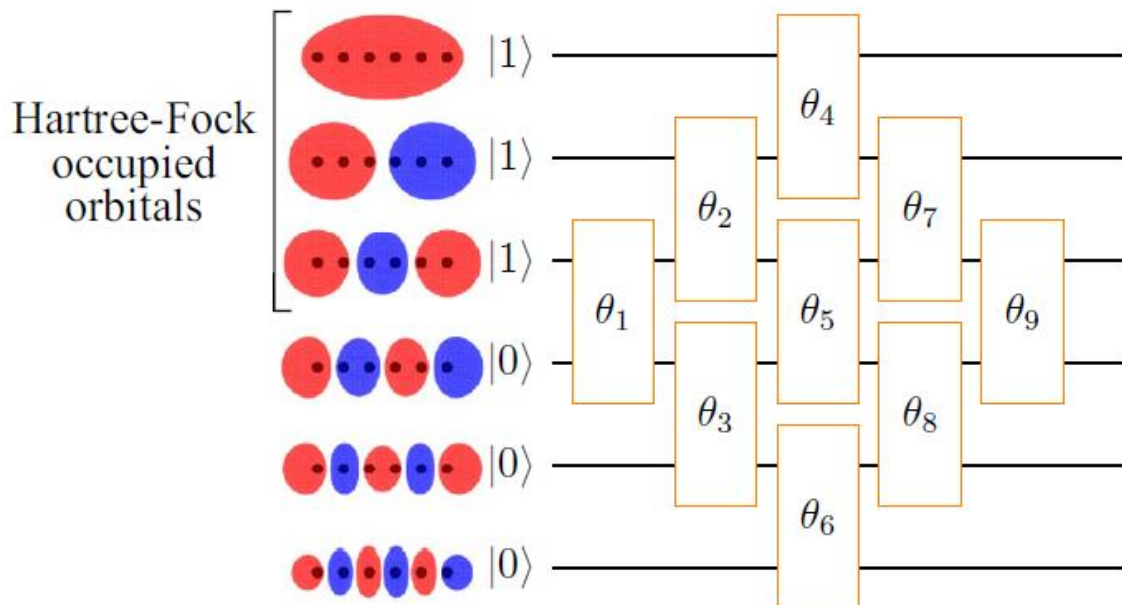


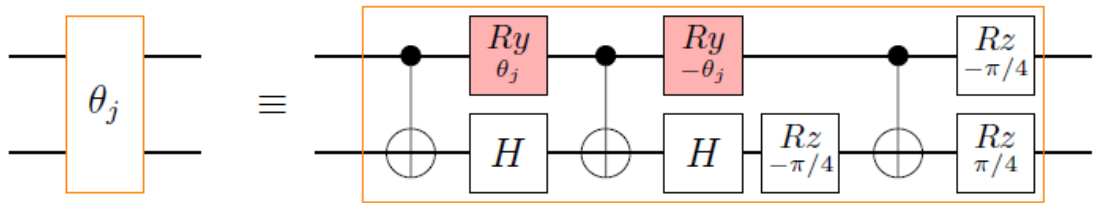


$$\mathcal{H} = \sum_{jk} h_{jk} a_j^\dagger a_k + \sum_{jklm} g_{jklm} a_j^\dagger a_k^\dagger a_l a_m,$$

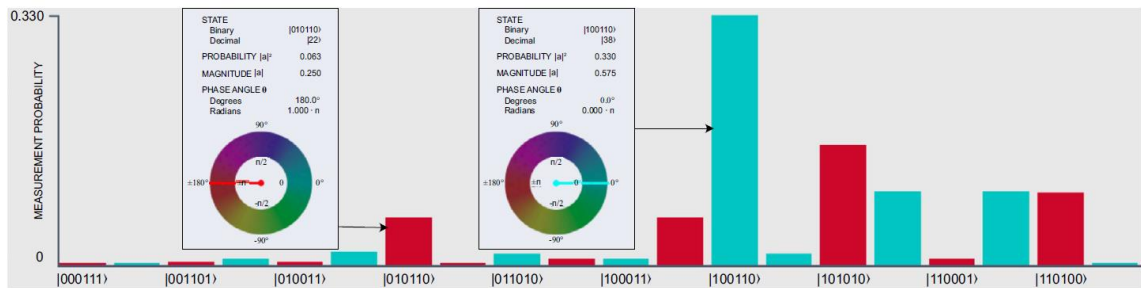
$$E_{\text{QCM}} \equiv c_1 - \frac{c_2^2}{c_3^2 - c_2 c_4} \left(\sqrt{3c_3^2 - 2c_2 c_4 - c_3} \right)$$

$$c_p = \langle \mathcal{H}^p \rangle - \sum_{j=0}^{p-2} \binom{p-1}{j} c_{j+1} \langle \mathcal{H}^{p-1-j} \rangle$$





$$[\theta_j] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta_j) & -\sin(\theta_j) & 0 \\ 0 & \sin(\theta_j) & \cos(\theta_j) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$



$$\langle \Psi_P | a_j^\dagger a_k^\dagger \dots a_{k'} a_{j'} | \Psi_P \rangle = \begin{vmatrix} \langle a_j^\dagger a_{j'} \rangle & \langle a_j^\dagger a_{k'} \rangle & \dots \\ \langle a_k^\dagger a_{j'} \rangle & \langle a_k^\dagger a_{k'} \rangle & \dots \\ \vdots & \vdots & \ddots \end{vmatrix}.$$

$$R_{j+1}=3R_j^2-2R_j^3,$$

$$\{\phi_1(\boldsymbol{x}),\ldots,\phi_M(\boldsymbol{x})\}$$

$$H_{\rm elec} = \sum_{p,q=1}^M h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s=1}^M g_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$$\{a_p^\dagger,a_q\}=\delta_{pq}$$

$$h_{pq}=\int \phi_p^*(x)\left(-\frac{\nabla^2}{2}-\sum_A\frac{Z_A}{r_A}\right)\phi_q(x)dx$$

$$g_{pqrs} = \iint \frac{\phi_p^*(\boldsymbol{x}_1)\phi_q^*(\boldsymbol{x}_2)\phi_r(\boldsymbol{x}_2)\phi_s(\boldsymbol{x}_1)}{r_{12}}d\boldsymbol{x}_1d\boldsymbol{x}_2$$

$$\hat{a}_j \mapsto \frac{1}{2} \big(\sigma_j^x + i \sigma_j^y \big) \sigma_1^z \cdots \sigma_{j-1}^z$$

$$H_{\rm elec} = \sum_i \gamma_i P_i$$

$$P_i = \otimes_{j=1}^M \sigma_{i,j} \text{ for } \sigma_{i,j} \in \{I, \sigma^x, \sigma^y, \sigma^z\}$$

$$\langle \psi_g | H_{\text{elec}} | \psi_g \rangle = E_g$$

$$\min_{\boldsymbol{\theta}} \langle \psi(\boldsymbol{\theta}) | H_{\text{elec}} | \psi(\boldsymbol{\theta}) \rangle \geq E_g,$$

$$\langle \psi(\boldsymbol{\theta}^*) | H_{\text{elec}} | \psi(\boldsymbol{\theta}^*) \rangle$$

$$H_{\text{Ising}} = \sum_{i=1}^M h_i \sigma_i^z + \sum_{j>i=1}^M J_{ij} \sigma_i^z \sigma_j^z$$

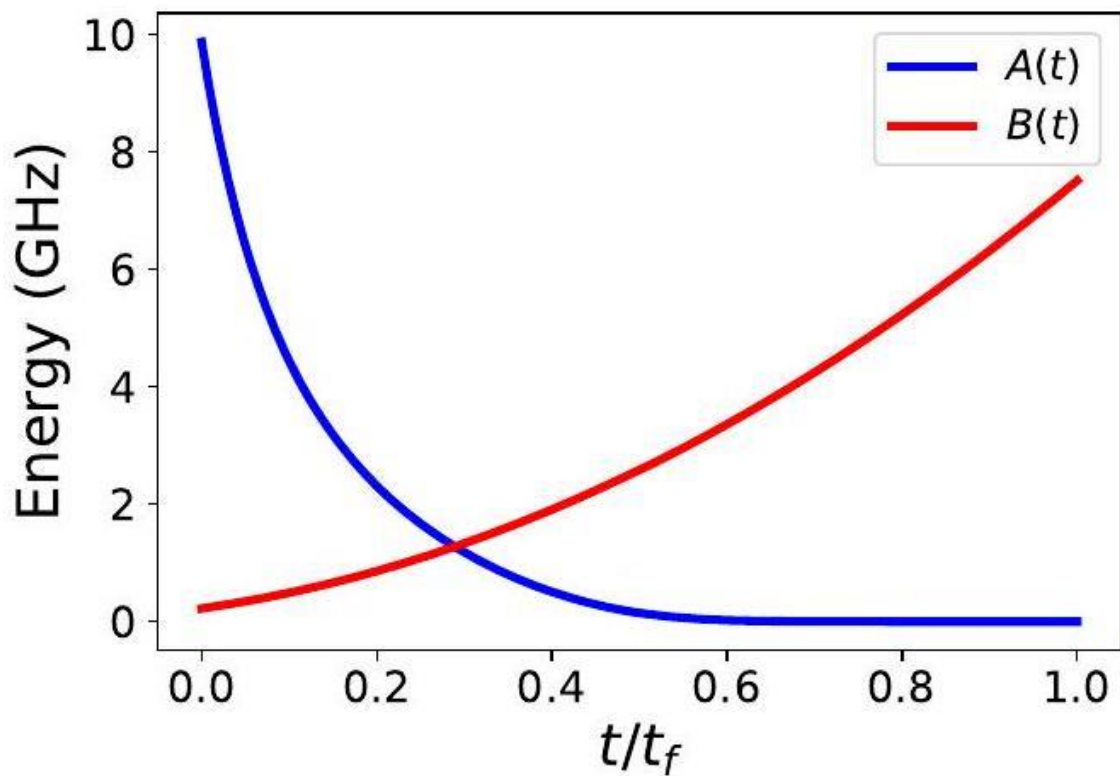
$$\nu = M(M+1)/2 + 1$$

$$H(\boldsymbol{\theta}) = \sum_{i=1}^M \theta_i \sigma_i^z + \sum_{j>i=1}^M \theta_{ij} \sigma_i^z \sigma_j^z + \theta_0 I,$$

$$\boldsymbol{\theta} = \{\theta_0, \boldsymbol{\theta}_i, \boldsymbol{\theta}_{ij}\} \in \mathbb{R}^\nu$$

$$H(t,\boldsymbol{\theta})=-\frac{A(t)}{2}\left(\sum_{i=1}^M\sigma_i^x\right)+\frac{B(t)}{2}H(\boldsymbol{\theta})$$

$$|\psi(0)\rangle = \bigotimes_{i=1}^M |+\rangle, \text{ where } |+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$



$$\rho(t_f,\boldsymbol{\theta})=\Phi(t_f,\boldsymbol{\theta})[\rho(0)]$$

$$\rho(0)=|\psi(0)\rangle\langle\psi(0)|$$

$$\Phi(t_f, \boldsymbol{\theta}) = \mathcal{T} \exp \left[\int_0^{t_f} \mathcal{L}(t, \boldsymbol{\theta}) dt \right]$$

$$\mathcal{L}(t, \boldsymbol{\theta}) = -i[H(t, \boldsymbol{\theta}), \cdot] + \mathcal{D}(t, \boldsymbol{\theta}),$$

$$t=t_f\rightarrow\infty$$

$$\mathcal{L}(t_f,\boldsymbol{\theta})\rho_{\text{ss}}(t_f,\boldsymbol{\theta})=0$$

$$\rho_{\text{ss}}(t_f,\boldsymbol{\theta})=\frac{e^{-\beta H(\boldsymbol{\theta})}}{\text{Tr}(e^{-\beta H(\boldsymbol{\theta})})}$$

$$|\psi(\boldsymbol{\theta})\rangle\rho(t_f,\boldsymbol{\theta})$$

$$\rho(t_f,\boldsymbol{\theta})\{A_m\}A_m^\dagger A_m\sum_m A_m^\dagger A_m=I$$

$$p(m)=\text{Tr}\left(A_m^\dagger A_m\rho(t_f,\boldsymbol{\theta})\right).$$

$$|\psi(\boldsymbol{\theta})\rangle_{\pm}=\sum_m \varepsilon_m \sqrt{p(m)}|m\rangle, \text{ where } \varepsilon_m=\pm 1$$

$$p(m)=\langle m|\rho(t_f,\boldsymbol{\theta})|m\rangle,$$

$$\rho(t_f,\boldsymbol{\theta})=\frac{e^{-\beta H(\boldsymbol{\theta})}}{\text{Tr}(e^{-\beta H(\boldsymbol{\theta})})},$$

$$p(m)=\frac{e^{-\beta E_m(\boldsymbol{\theta})}}{\sum_me^{-\beta E_m(\boldsymbol{\theta})}},$$

$$H(\boldsymbol{\theta})=\sum_mE_m(\boldsymbol{\theta})|m\rangle\langle m|,$$

$$\min_{\boldsymbol{\theta},\pm}\pm\langle\psi(\boldsymbol{\theta})|H_{\text{elec}}|\psi(\boldsymbol{\theta})\rangle_{\pm}$$

$$\text{s.t. }\boldsymbol{\theta}\in\mathbb{R}^{\nu},\nu=M(M+1)/2+1$$

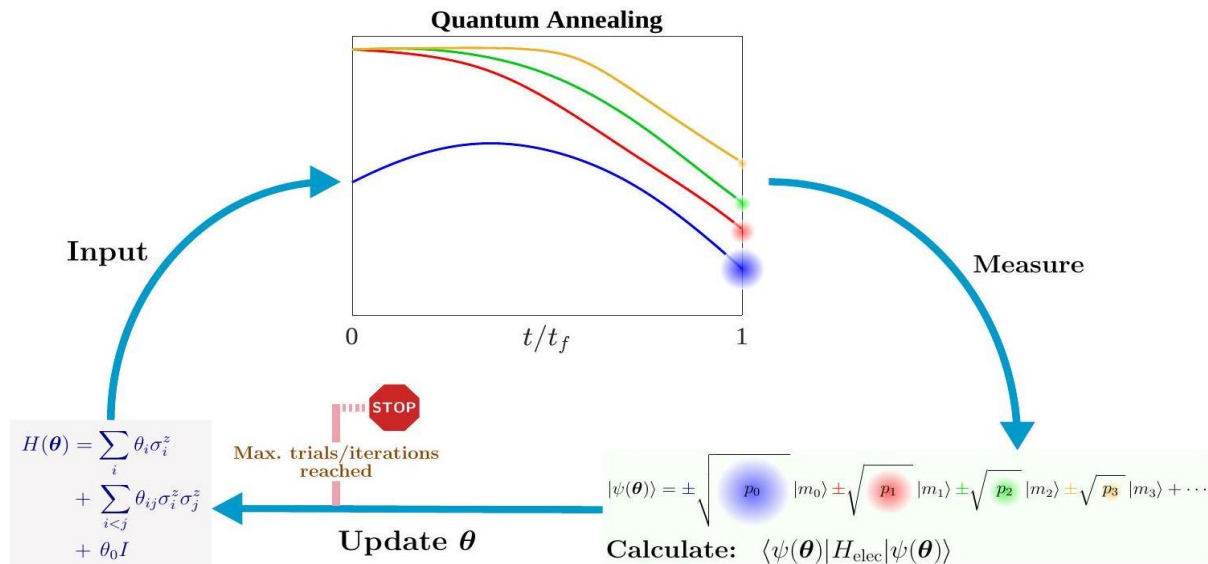
$$\mathcal{D}_1=\{-1,1\}^{\otimes \nu},$$

$$\mathcal{D}_2=\{-1,0,1\}^{\otimes \nu}.$$

$$|\psi(\boldsymbol{\theta})\rangle_{\pm}=\sum_m \varepsilon_m \sqrt{\frac{\sum_{s=1}^S[m^s=m]}{S}}|m\rangle, \varepsilon_m=\pm 1.$$

$$\pm \langle \psi(\boldsymbol{\theta}) | H_{\text{elec}} | \psi(\boldsymbol{\theta}) \rangle_{\pm}$$

$$\langle \psi(\boldsymbol{\theta}^*) | H_{\text{elec}} | \psi(\boldsymbol{\theta}^*) \rangle$$



$$H^k = H + \sum_{i=0}^{k-1} \alpha_i |e_i\rangle \langle e_i|$$

$$v = M(M+1)/2 + 1$$

$$\boldsymbol{\Theta} = (\theta^1, \theta^2, \dots, \theta^\alpha).$$

$$H(\boldsymbol{\theta}^k) = \sum_{i=1}^M \theta_i^k \sigma_i^z + \sum_{j>i=1}^M \theta_{ij}^k \sigma_i^z \sigma_j^z + \theta_0^k I,$$

$$|\psi(\boldsymbol{\Theta})\rangle_{\pm} = \sum_m \varepsilon_m \sqrt{\sum_{k=1}^{\alpha} \frac{p^k(m)}{\alpha}} |m\rangle, \varepsilon_m = \pm 1.$$

$$\boldsymbol{\theta}^* = \{\theta_1^* = 0, \theta_2^* = 0, \theta_3^* = 1, \theta_4^* = 0, \theta_{12}^* = 1, \theta_{13}^* = -1, \theta_{14}^* = 1, \theta_{23}^* = 1, \theta_{24}^* = -1, \theta_{34}^* = 1, \theta_0^* = 1\}$$

$$|\psi_g\rangle_{\text{H}_2} = \alpha|0101\rangle + \beta|1010\rangle,$$

$$|\psi(\boldsymbol{\theta})\rangle_{\pm} = \sum_m \varepsilon_m \sqrt{p(m)} |m\rangle, \text{ where } \varepsilon_m = \pm 1.$$

$$|\psi(\boldsymbol{\theta})\rangle_{\pm} = \sum_m \varepsilon_m \sqrt{\frac{\sum_{s=1}^S [m^s = m]}{S}} |m\rangle, \varepsilon_m = \pm 1.$$

$$\begin{aligned} \pm \langle \psi(\boldsymbol{\theta}) | H_{\text{elec}} | \psi(\boldsymbol{\theta}) \rangle_{\pm} &= \sum_{m,n}^I |\langle m | \psi(\boldsymbol{\theta}) \rangle|^2 |\langle n | \psi(\boldsymbol{\theta}) \rangle|^2 \frac{\langle m | H_{\text{elec}} | n \rangle}{\langle m | \psi(\boldsymbol{\theta}) \rangle \langle \psi(\boldsymbol{\theta}) | n \rangle} \\ &= \sum_{m,n}^I \varepsilon_m \varepsilon_n \sqrt{p(m)} \sqrt{p(n)} \langle m | H_{\text{elec}} | n \rangle \end{aligned}$$

$$H_{\text{elec}} = \sum_i \gamma_i P_i$$

$$\langle m | H_{\text{elec}} | n \rangle = \sum_i \gamma_i \langle m | P_i | n \rangle$$

$$p(m) = \langle m | \rho(t_f, \boldsymbol{\theta}) | m \rangle$$

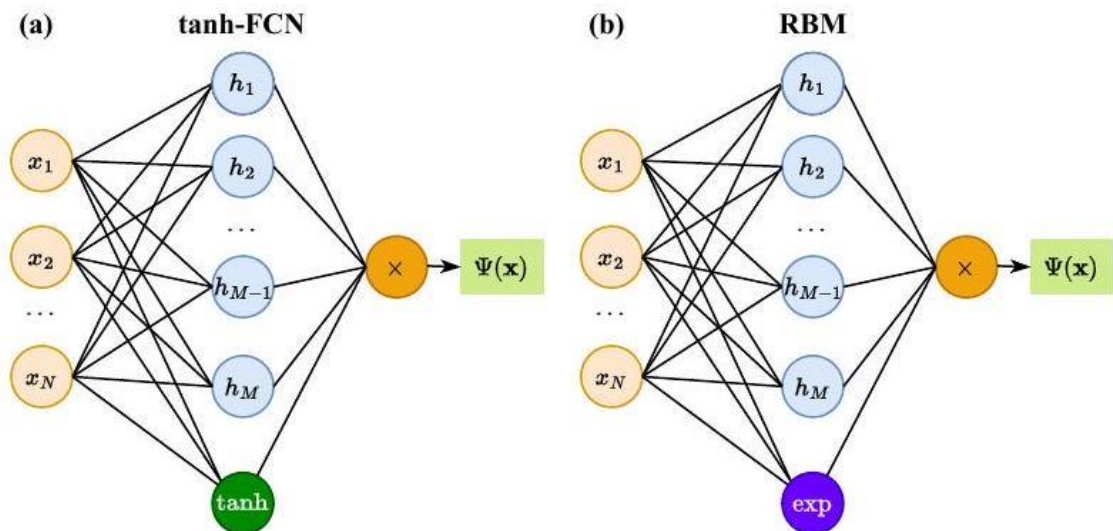
$$\pm \langle \psi(\boldsymbol{\theta}) | H_{\text{elec}} | \psi(\boldsymbol{\theta}) \rangle_{\pm} = \sum_{m,n}^i \varepsilon_m \varepsilon_n \sqrt{\langle m | \rho(t_f, \boldsymbol{\theta}) | m \rangle} \sqrt{\langle n | \rho(t_f, \boldsymbol{\theta}) | n \rangle} \langle m | H_{\text{elec}} | n \rangle,$$

$$\mathcal{H} = \sum_{j=1}^{N_v} a_j x_j + \sum_{i=1}^{N_h} b_i h_i + \sum_{i,j} W_{ij} h_i x_j,$$

$$\mathcal{Z} = \sum_{\mathbf{x}} p(\mathbf{x}),$$

$$p(\mathbf{x}) = \sum_{\mathbf{h}} e^{\mathcal{H}} \\ = e^{\sum_{j=1}^{N_v} a_j x_j} \times \prod_{i=1}^{N_h} 2 \cosh \left(b_i + \sum_{j=1}^{N_v} W_{ij} x_j \right).$$

$$p(\mathbf{x}) = \tanh \left(\sum_{j=1}^{N_v} a_j x_j \right) \times \prod_{i=1}^{N_h} 2 \cosh \left(b_i + \sum_{j=1}^{N_v} W_{ij} x_j \right).$$



$$\hat{H}^e = \sum_{p,q} h_q^p a_p^\dagger a_q + \frac{1}{2} \sum_{\substack{p,q \\ r,s}} g_{rs}^{pq} a_p^\dagger a_q^\dagger a_r a_s$$

$$\hat{H} = \sum_i c_i \prod_{j=1}^N \sigma_j^{v_{i,j}}$$

$$E(\theta)=\frac{\langle\Psi_\theta|\hat{H}|\Psi_\theta\rangle}{\langle\Psi_\theta|\Psi_\theta\rangle}=\frac{\sum_{\mathbf{x}}E_{\text{loc}}(\mathbf{x})|\Psi_\theta(\mathbf{x})|^2}{\sum_{\mathbf{y}}|\Psi_\theta(\mathbf{y})|^2}$$

$$E_{\text{loc}}(\mathbf{x})=\sum_{\mathbf{x}'}\frac{\Psi_\theta(\mathbf{x}')}{\Psi_\theta(\mathbf{x})}H_{\mathbf{x}'\mathbf{x}}$$

$$H_{\mathbf{x}'\mathbf{x}}=\langle\mathbf{x}'|\hat{H}|\mathbf{x}\rangle$$

$$\tilde{E}(\theta)=\langle E_{\text{loc}}\rangle,$$

$$|\Psi_\theta(\mathbf{x})|^2\otimes\tilde{E}(\theta)$$

$$\boldsymbol{\theta}^{k+1}=\boldsymbol{\theta}^k-\alpha S^{-1}F,$$

$$S_{ij}(k)=\langle O_i^*O_j\rangle-\langle O_i^*\rangle\langle O_j\rangle,$$

$$F_i(k)=\langle E_{\text{loc}}O_i^*\rangle-\langle E_{\text{loc}}\rangle\langle O_i^*\rangle$$

$$O_i(\mathbf{x})=\frac{1}{\Psi_\theta(\mathbf{x})}\frac{\partial\Psi_\theta(\mathbf{x})}{\partial\theta_i}.$$

$$H=\sum_{pq}t_{pq}c_p^\dagger c_q+\frac{1}{2}\sum_{pqrs}V_{pqrs}c_p^\dagger c_q^\dagger c_r c_s$$

$$\langle\psi\mid\psi_0\rangle>1/2$$

$$|\psi_{\text{HF}}\rangle=\prod_{i=1}^{N_e}c_i^\dagger|0\rangle$$

$$\langle\psi_{\text{HF}}\mid\psi_0\rangle$$

$$|\psi\rangle=\sum_ic_i|\phi_i\rangle|0\rangle$$

$$\sum_i c_i|\phi_i\rangle|E_i\rangle$$

$$|\psi(t)\rangle=\exp{(-iHt)}|\psi(0)\rangle$$

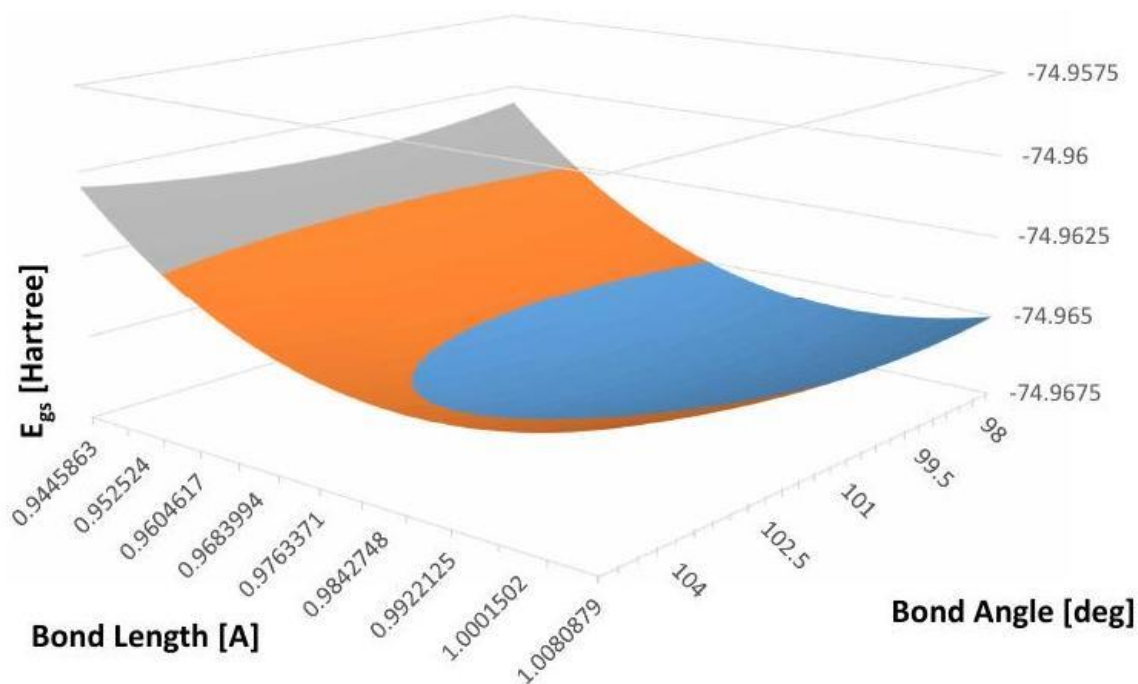
$$\Delta_t=t/M$$

$$\exp\left(-it\sum_k h_k\right)=U(\Delta_t)^M+\mathcal{O}(\Delta_t)$$

$$U(\Delta_t)=\prod_k\exp{(-i\Delta_th_k)}$$

$$U_k(\Delta_t)=\exp{(-i\Delta_th_k)}\mathcal{O}(\Delta_t^2)$$

$$H_{\text{eff}}=\ln U(\Delta_t)/(-i\Delta_t)$$



$$H = \sum_{i=1}^m H_i$$

$$\mathcal{O}(d^{2/3}((\log \log d)t\|H\|)^{4/3})$$

$$d=N^4$$

$$\mathcal{O}\left(N^{8/3}((\log \log N^4)\|H\|)^{4/3}\right)\mathcal{O}(d\Lambda_{\max}t)\Lambda_{\max}$$

$$h_{pp}c_p^\dagger c_p, h_{pq}c_p^\dagger c_q, h_{pqqp}c_p^\dagger c_q^\dagger c_q c_p, h_{pqqr}c_p^\dagger c_q^\dagger c_q c_r \text{ and } h_{pqrs}c_p^\dagger c_q^\dagger c_r c_s$$

$$p(h_{pp})=u_{[-10,0]}(h_{pp})$$

$$p(h_{pq})=u_{[-1,1]}(h_{pq})$$

$$p(h_{pqqp})=u_{[-0.5,0.5]}(h_{pqqp})$$

$$p(h_{pqqr})=\frac{1}{2\cdot 0.2}e^{-|h_{pqqr}|/0.2}$$

$$p(h_{pqrs})=\frac{1}{2\cdot 0.1}e^{-|h_{pqrs}|/0.1}$$

$$N_e=N/2$$

$$N_e=N/3\epsilon(\Delta_t)$$

$$N_{\mathrm{Trotter}}=\left(\frac{\epsilon(\Delta_t)}{\Delta_t^2\epsilon_t}\right)^{1/2}$$

$$\epsilon(\Delta_t)\sim\Delta_t^2$$

$$H = \sum_{i=1}^m H_i \exp(-iH\Delta_t)$$

$$U^{TS} \equiv \exp(-iH_1\Delta_t/2) \dots \exp(-iH_m\Delta_t/2) \\ \times \exp(-iH_m\Delta_t/2) \dots \exp(-iH_1\Delta_t/2)$$

$$U = \exp(-iH\Delta_t)(m\Lambda\Delta_t)^3\|H_i\|t(m\Lambda)^3\Delta_t^2\Delta_t \ll m^{-3/2}$$

$$K=\mathcal{O}(N^3)$$

$$\|U-U^{TS}\|\leq \mathcal{O}(mK^2\Lambda^3\Delta_t^3)$$

$$\mathcal{O}(m^3\Lambda^3\Delta_t^3), m=\mathcal{O}(N^4), K=\mathcal{O}(N^3)\mathcal{O}(N^5)\mathcal{O}(mk\Delta^3t^3)$$

$$\mathcal{O}(mK^2\Delta_t^3)\circledast \mathcal{O}(mK^2\Delta_t^3)$$

$$[H_{i_a},H_{i_b}]\mathcal{O}(m^{q-2}K^2(\Lambda\Delta_t)^q)\mathcal{O}(mK^2\Lambda^3\Delta_t^3)m\Lambda\Delta_t$$

$$\Delta_t=1$$

$$H(x)=B+(1-x)A$$

$$\left\|\exp\left(-i\frac{A}{2}\right)\exp(-iB)\exp\left(-i\frac{A}{2}\right)-\exp(-iH(0))\right\| \\ =\left\|\int_0^1\partial_x\left(\exp\left(-ix\frac{A}{2}\right)\exp(-iH(x))\exp\left(-ix\frac{A}{2}\right)\right)dx\right\|$$

$$A(t,x)=\exp(iH(x)t)A\exp(-iH(x)t)$$

$$\left\|\partial_x\left(\exp\left(-ix\frac{A}{2}\right)\exp(-iH(x))\exp\left(-ix\frac{A}{2}\right)\right)\right\| \\ =\left\|\exp\left(-ix\frac{A}{2}\right)\exp(-iH(x))\left(-i\frac{A}{2}-i\frac{A(1,x)}{2}\right.\right. \\ \left.\left.+i\int_0^1A(t,x)dt\right)\exp\left(-ix\frac{A}{2}\right)\right\| \\ =\left\|-\frac{A(0,x)}{2}-\frac{A(1,x)}{2}+\int_0^1A(t,x)dt\right\|$$

$$A(t,x)=A(0,x)+tA'(0,x)+\int_0^t(t-s)A''(s,x)ds$$

$$\left\|\partial_x\left(\exp\left(-ix\frac{A}{2}\right)\exp(-iH(x))\exp\left(-ix\frac{A}{2}\right)\right)\right\| \\ \leq\left\|\int_0^1((1-s)-(1-s)^2/2)A''(t,s)ds\right\| \\ \leq\int_0^1\|A''(t,s)\|ds$$

$$\|A''(t,s)\|=\|[[A,H(x)],H(x)]\|\leq \|[[A,B],A]+[[A,B],B]\|$$

$$\left\| \exp \left(-i \frac{A}{2} \right) \exp (-iB) \exp \left(-i \frac{A}{2} \right) - \exp (-i(A+B)) \right\| \\ \leq \| [[A,B],A] \| + \| [[A,B],B] \|.$$

$$U-U^{TS}$$

$$U_j = \exp \left(-i \sum_{j \leq k \leq m} H_k \right)$$

$$U_j^{TS} = \exp \left(-iH_j \frac{\Delta_t}{2} \right) \ldots \exp \left(-iH_m \frac{\Delta_t}{2} \right) \\ \times \exp \left(-iH_m \frac{\Delta_t}{2} \right) \ldots \exp \left(-iH_j \frac{\Delta_t}{2} \right)$$

$$\|U_{j-1}-U_{j-1}^{TS}\| \\ \leq \left\|U_{j-1}-\exp\left(iH_{j-1}\frac{\Delta_t}{2}\right)U_j\exp\left(-iH_{j-1}\frac{\Delta_t}{2}\right)\right\| \\ +\left\|\exp\left(iH_{j-1}\frac{\Delta_t}{2}\right)U_j\exp\left(-iH_{j-1}\frac{\Delta_t}{2}\right)-U_{j-1}^{TS}\right\| \\ =\left\|U_{j-1}-\exp\left(iH_{j-1}\frac{\Delta_t}{2}\right)U_j\exp\left(-iH_{j-1}\frac{\Delta_t}{2}\right)\right\| \\ +\|U_j-U_j^{TS}\|.$$

$$A=H_{j-1}\Delta_t$$

$$B=\sum_{j\leq k\leq m}H_k\Delta_t$$

$$\|U_{j-1}-U_{j-1}^{TS}\|\leq \text{const.}\times \Lambda^3\Delta_t^3K^2+\|U_j-U_j^{TS}\|$$

$$\|U-U^{TS}\|=\|U_1-U_1^{TS}\|$$

$$\Delta_t^{(k)}\cdot \|h_k\|$$

$$U=\left(\prod U_k\right)^{T/\Delta_t},$$

$$H=\sum_i H_i$$

$$\|H_i\|\leq \Lambda_a$$

$$U=\exp\left(-iHt\right)$$

$$\exp\left(-i\theta H_i\right)$$

$$\epsilon \leq \sum_a O\left(\frac{S_a^3 + T_{a-1}S_a^2 + T_{a-1}^2S_a}{(2^{k-a})^2}\right)$$

$$S_a=N_a\Lambda_at$$

$$T_a=\sum_{b\leq a}S_b$$

$$K_a=\sum_{i\in B_a}H_i$$

$$O\left(S_a^3/(2^{k-a})^2\right)\exp{(-iK_at)}\exp{\left(-iK_a\frac{t}{2^{k-a}}\right)}2^{k-a}(2^{k-1})^2(2^{k-a})^2$$

$$J_a=\sum_{b\leq a}\sum_{i\in B_b}H_i$$

$$U_a=\exp\left(-iJ_a\frac{t}{2^{k-a}}\right)$$

$$\epsilon_a=\|V_a-U_a\|$$

$$W_a=\prod_{i\in B_1}\exp\left(-i\frac{1}{2}H_i\frac{t}{2^{k-a}}\right)$$

$$W_a'=W_a^T$$

$$V_1=W_1W_1'$$

$$\epsilon_1\leq O\left(\frac{S_1}{2^{k-1}}\right)^3$$

$$V_{a+1}=W_{a+1}V_a^2W_{a+1}'$$

$$\|V_{a+1}-W_{a+1}U_a^2W_{a+1}'\|\leq 2\epsilon_a$$

$$\|U_{a+1}-W_{a+1}U_a^2W_{a+1}'\|\\ \leq O\left(\frac{S_{a+1}^3+\|J_a\|S_{a+1}^2+\|J_a\|^2S_{a+1}}{(2^{k-a-1})^3}\right)$$

$$\epsilon_{a+1}\leq 2\epsilon_a+O\left(\frac{S_{a+1}^3+T_aS_{a+1}^2+T_a^2S_{a+1}}{(2^{k-a-1})^3}\right),$$

$$\|J_a\|\leq T_a$$

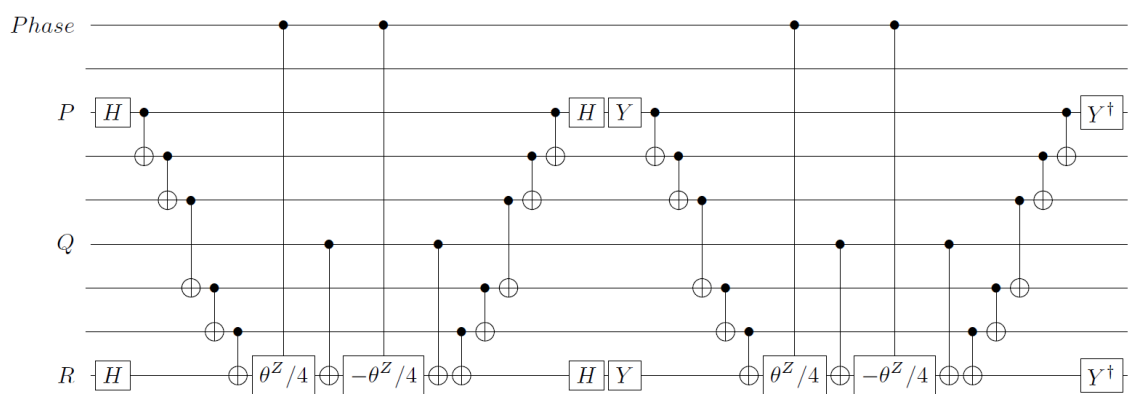
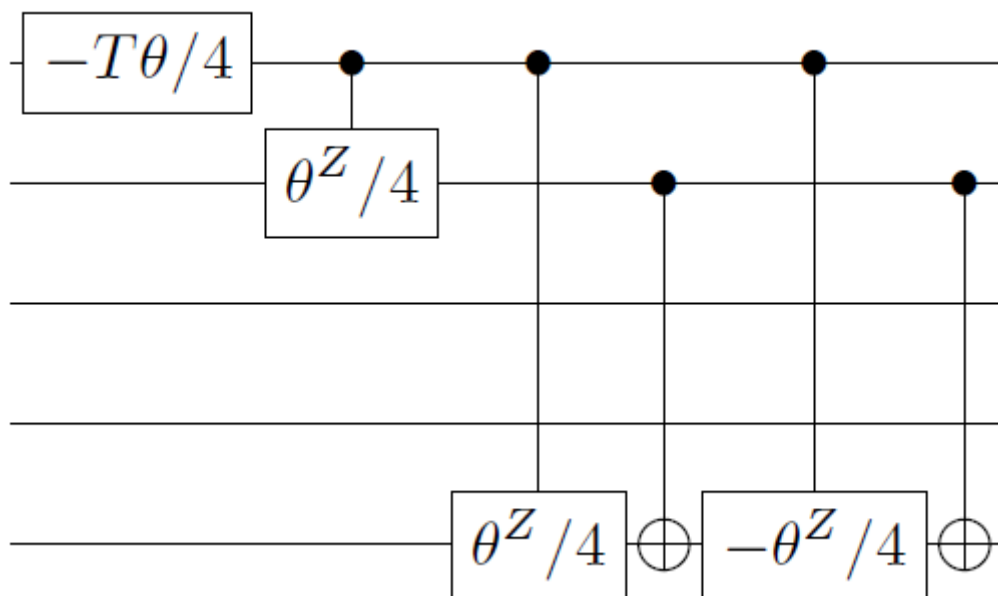
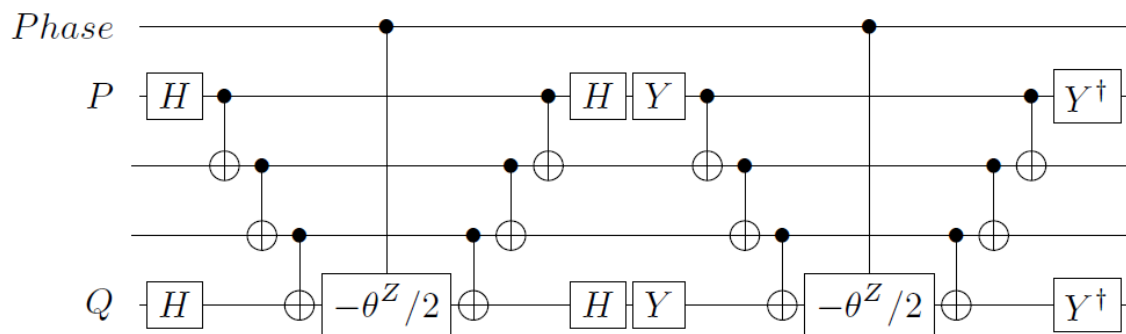
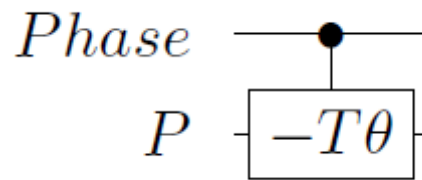
$$\epsilon_a\leq \sum_{b\leq a}2^{a-b}O\left(\frac{S_b^3+T_{b-1}S_b^2+T_{b-1}^2S_b}{(2^{k-b-1})^3}\right)$$

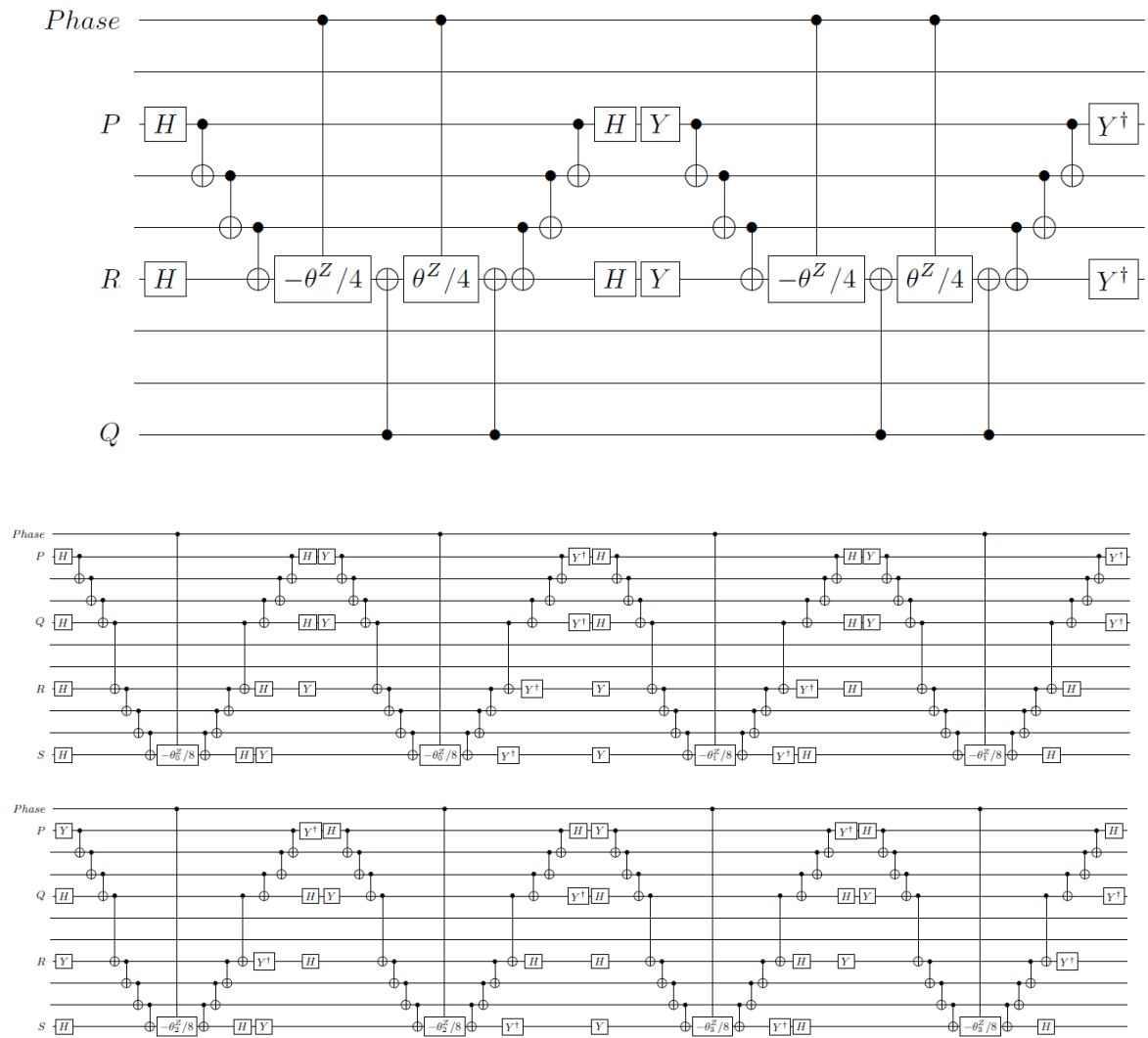
$$\epsilon_k\leq \sum_aO\left(\frac{S_a^3+T_{a-1}S_a^2+T_{a-1}^2S_a}{(2^{k-a})^2}\right)$$

$$\mathbf{H}=\frac{1}{\sqrt{2}}\begin{bmatrix}1&1\\1&-1\end{bmatrix}\mathbf{Y}=\frac{1}{\sqrt{2}}\begin{bmatrix}1&i\\i&1\end{bmatrix}$$

$$H_{pqqr}V_{pqrs}\frac{1}{2}\sum_{pqrs}V_{pqrs}c_p^\dagger c_q^\dagger c_r c_sO(N^3)$$

$$\hat{P} \sum_p \sum_q W_{pq} c_p^\dagger c_p c_q^\dagger c_q \hat{P} + \text{single body terms}$$





Sequential Circuit	Global R_z	H, Y, $Y^\dagger$	CNOT	CR_z	BSM	Total
H_{pp} H_{pq} H_{pqqp} $H_{pqqr}, p < q < r$ $H_{pqqr}, q < p \text{ or } r < q$ H_{pqrs}	1	8 8 8 8.8		1		1
			$2(q - p)$	4		$12 + 2(q - p)$
			2	3		1 + 5
			$4(r - p)$	4		$12 + 4(r - p)$
			$4(r - p + 1)$	4		$16 + 4(r - p)$

			$8 \cdot 2(q - p + s - r + 1)$	$8 \cdot 1$		$8 \cdot 9 + 8 \cdot 2(q - p + s - r + 1)$
Parallel Circuit	Global $\mathbf{R}_z$	$\mathbf{H}, \mathbf{Y}, \mathbf{Y}^\dagger$	CNOT	$\mathbf{C}\mathbf{R}_z$	BSM	Total
H_{pp}	1			1		1
H_{pq}		8	2	4	4	18
H_{pqqp}			2	3		1 + 5
H_{pqqr}		4	8	4	4	24
H_{pqrs}		$8 \cdot 2$	$8 \cdot 2$	$8 \cdot 1$	$8 \cdot 2$	$8 \cdot 7$

$$\frac{1}{2} \sum_{pqrs} V_{pqrs} c_p^\dagger c_r c_q^\dagger c_s + \text{single body terms.}$$

$$\sum_a \lambda_a O(a) O(a) + \text{single body terms}$$

$$O(a) = \sum_{p,q} A(p,q,a) c_p^\dagger c_q$$

$$k = O(N^2)$$

$$\frac{1}{\sqrt{k}} \begin{pmatrix} U(1) \\ U(1) \\ \cdots \\ U(k) \end{pmatrix}$$

$$W_{pq} = \sqrt{k} \lambda(a) \Lambda(a)_{bb} \Lambda(a)_{dd}$$

$$\alpha_k = |\langle \varphi \mid k \rangle|^2$$

$$\sigma_{E_k} = O((\tau M)^{-1})e^{-iH\tau}$$

$$O(\text{poly}(\eta)\text{polylog}(N,1/\epsilon))O(\text{polylog}(1/\delta))\tilde{O}(\eta^2)\tilde{O}(\eta^3)$$

$$O(\eta \log^c \eta \log N)$$

$$O(\log^c \eta \log \log N)$$

$$O(\eta^2 \log N)$$

$$|\varphi\rangle O(\text{polylog}(1/\epsilon))$$

$$|r_1 \cdots r_\eta\rangle \mapsto \sum_{\sigma \in S_\eta} (-1)^{\pi(\sigma)} |\sigma(r_1, \cdots, r_\eta)\rangle$$



$$r_p < r_{p+1} | r_1 \cdots r_\eta \rangle$$

$$O(\eta^2\log N)O(\eta\log \eta\log N)O(\log \eta\log \log N)$$

$$f(\eta)\geq \eta^2\tilde{O}(\eta^2)\tilde{O}(\eta)$$

$$O(\eta\log^2 \eta) \, O(\log^2 \eta)O(\eta\log \eta)O(\eta\log \eta)O(\eta\log \eta)$$

$$O(\log \eta\log \log N)O(\eta\log \eta\log N)O(\eta\log \eta)O(\log \eta)O(\log N)O(\log \log N)O(\log \log \eta)O(\eta\log \eta\log N)$$

$$O(\log \eta\log \log N)$$

$$O(\eta\log \eta)O(\eta)O(\eta\log \eta)O(\log \log \eta)$$

$$O(\eta\log \eta)O(\log \eta)$$

$$\tilde{O}(\eta)\tilde{O}(\eta^3)$$

$$\log_2(\eta!)=O(\eta\log \eta)$$

$$O(\log \eta)O(\eta\log \eta)O(\eta\log N)$$

$$O(\log^2 \eta\log \log N)O(\eta\log \eta\log N)O(\eta\log \eta)\tilde{O}(\eta^2)$$

$$O(\eta\log \eta\log N)O(\log \eta\log \log N)$$

$$\alpha_k=|\langle \varphi \mid k \rangle|^2$$

$$E_0 \leq \tilde{E}_0 < E_1$$

$$1/\epsilon E_1-\tilde{E}_0 1/(E_1-\tilde{E}_0)E_1-\tilde{E}_0$$

$$1/[\alpha_0(E_1-E_0)]$$

$$O\left(\frac{1}{\alpha_0(E_1-\tilde{E}_0)}+\frac{1}{\epsilon_f}\right)$$

$$O\left(1/(\alpha_0\epsilon_f)\right)\alpha_0(E_1-\tilde{E}_0)>\epsilon_f$$

$$\tilde{E}_1-\tilde{E}_0 1/\sqrt{\alpha_0}1/\alpha_0$$

$$E^*=\min_{k>0}E_k \text{ subject to } |\langle \varphi \mid k \rangle|^2>0$$

$$E_0 \leq \tilde{E}_0 < E^* \pm e^{\pm i \arcsin{(E_k/\lambda)}}$$

$$(|0\rangle\langle 0|_a\otimes\mathbb{1}_s)V(|0\rangle\langle 0|_a\otimes\mathbb{1}_s)=|0\rangle\langle 0|_a\otimes H/\lambda$$

$$H=\sum_{j=0}^{d-1}a_jU_j\,a_j>0$$

$$U=(A^\dagger\otimes\mathbb{1})\text{SELECT}-\text{U}(A\otimes\mathbb{1})$$

$$A|0\rangle=\sum_{j=0}^{d-1}\sqrt{a_j/\lambda}|j\rangle$$



$$\lambda=\sum_{j=0}^{d-1}a_j$$

$$\text{SELECT-U}=\sum_{j=0}^{d-1}|j\rangle\langle j|\otimes U_j$$

$$V=|+\rangle\langle -|\otimes U+|-\rangle\langle +|\otimes U^\dagger$$

$$|\pm\rangle=\frac{1}{\sqrt{2}}(|0\rangle\pm|1\rangle)$$

$$W=i(2|0\rangle\langle 0|_a\otimes\mathbb{1}_s-\mathbb{1})V$$

$$W|0\rangle_a|k\rangle_s=i\frac{E_k}{\lambda}|0\rangle_a|k\rangle_s+i\sqrt{1-\left|\frac{E_k}{\lambda}\right|^2}|0k^\perp\rangle_{as}$$

$$W|0k^\perp\rangle_{as}=i\frac{E_k}{\lambda}|0k^\perp\rangle_{as}-i\sqrt{1-\left|\frac{E_k}{\lambda}\right|^2}|0\rangle_a|k\rangle_s$$

$$|0k^\perp\rangle_{as}|0\rangle_a|k\rangle_s|0k^\perp\rangle_{as}$$

$$W|\pm k\rangle_{as}=\mp e^{\mp i\arcsin{(E_k/\lambda)}}|\pm k\rangle_{as}$$

$$|\pm k\rangle_{as}=\frac{1}{\sqrt{2}}(|0\rangle_a|k\rangle_s\pm|0k^\perp\rangle_{as})$$

$$(2|0\rangle\langle 0|_a\otimes\mathbb{1}_s-\mathbb{1})$$

$$\arcsin{(E_k/\lambda)}\pi-\arcsin{(E_k/\lambda)}E_k/\lambda\geq\|H\||E_k/\lambda|\leq 1e^{if(H)}$$

$$f(\cdot)\colon\mathbb{R}\rightarrow(-\pi,\pi)$$

$$\sigma_{E_k}=\left|\left(\frac{df}{dx}\Big|_{x=E_k}\right)\right|^{-1}\sigma_{f(E_k)}$$

$$\sigma_{E_k}=\sigma_{\text{phase}}\sqrt{\lambda^2-E_k^2}\leq\lambda\sigma_{\text{phase}}$$

$$\{B'[1],\ldots,B'[i-1]\}$$

$$\tilde{O}(\eta^3)\tilde{O}(\eta^2)$$

$$\frac{1}{f(\eta)^{\eta/2}}\sum_{\ell_0,\ldots,\ell_{\eta-1}=0}^{f(\eta)-1}|\ell_0,\ldots,\ell_{\eta-1}\rangle$$

$$\text{span}\{\lvert \ell_0,\ldots,\ell_{\eta-1}\rangle\mid \forall i\neq j\colon \ell_i\neq \ell_j\}$$

$$\frac{1}{f(\eta)^{\eta/2}}\sum_{0\leq \ell_0<\cdots<\ell_{\eta-1}<f(\eta)}\sum_{\sigma\in S_\eta}|\sigma(\ell_0,\ldots,\ell_{\eta-1})\rangle.$$

$$\frac{\eta!}{f(\eta)^\eta} \binom{f(\eta)}{\eta}$$

$$1 - C(f(\eta), \eta)$$

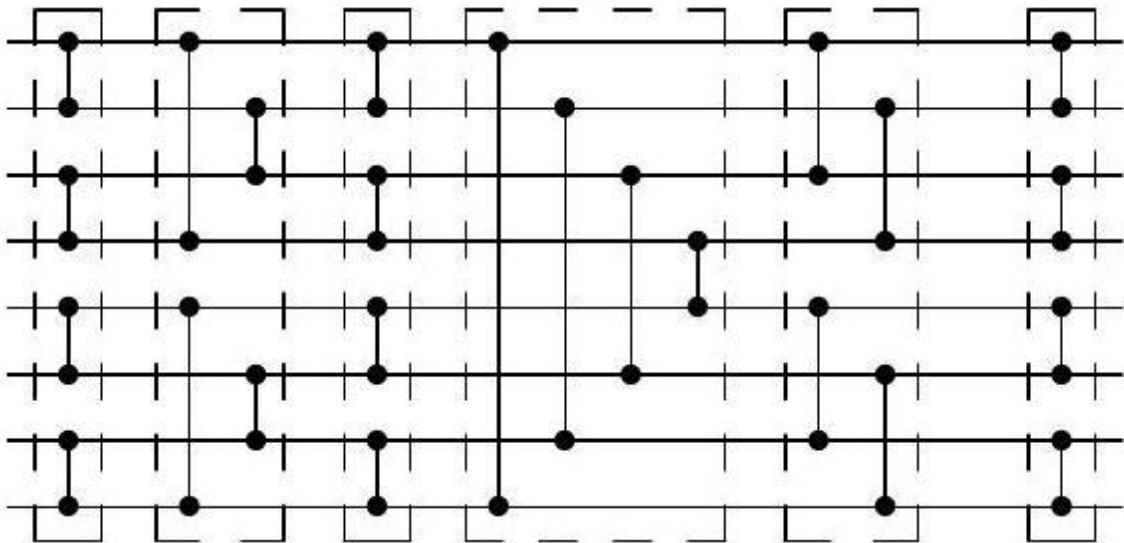
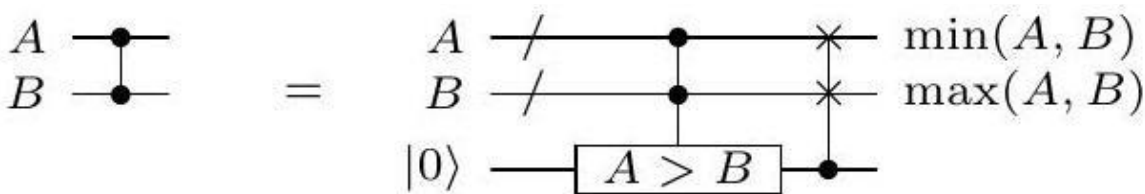
$$\Pr(\text{repetition}) = C(f(\eta), \eta) \leq \frac{\eta(\eta-1)}{2f(\eta)}$$

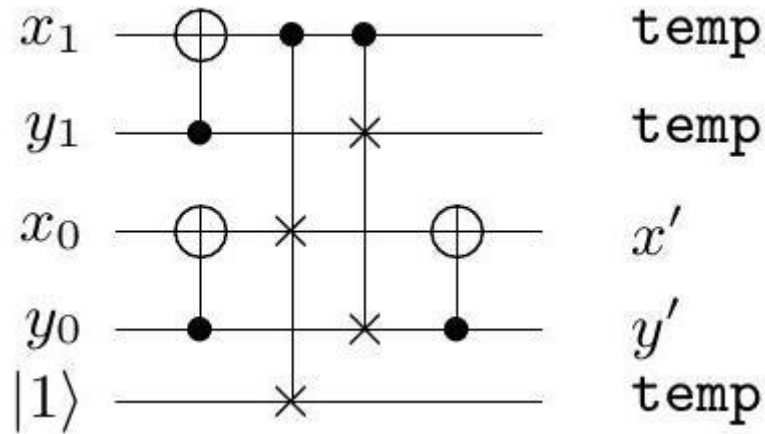
$$\sum_{0 \leq \ell_0 < \dots < \ell_{\eta-1} < f(\eta)} \sum_{\sigma \in S_\eta} |\sigma(\ell_0, \dots, \ell_{\eta-1})\rangle_{\text{seed}} |l\rangle_{\text{record}}.$$

$$\sigma_T \circ \dots \circ \sigma_1 \circ \sigma(\ell_0, \dots, \ell_{\eta-1}) = (\ell_0, \dots, \ell_{\eta-1})$$

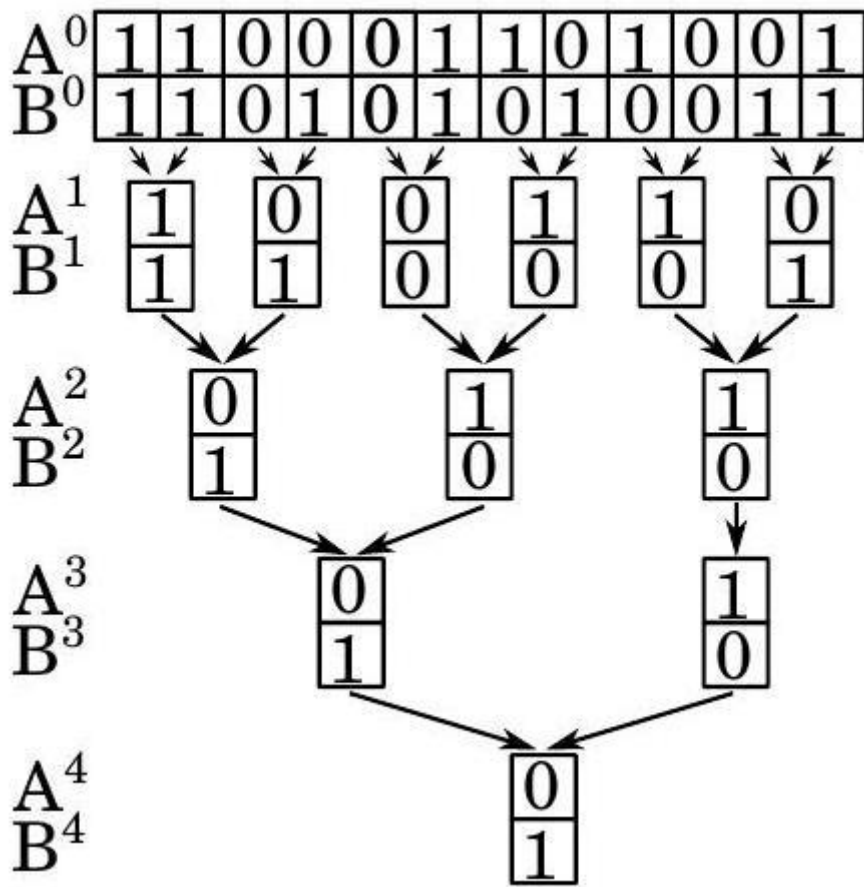
$$\sigma_T \circ \dots \circ \sigma_1 \circ \sigma = \iota.$$

$$\sum_{0 \leq \ell_0 < \dots < \ell_{\eta-1} < f(\eta)} |\ell_0, \dots, \ell_{\eta-1}\rangle_{\text{seed}} \sum_{\sigma \in S_\eta} |\sigma_1, \dots, \sigma_T\rangle_{\text{record}}.$$





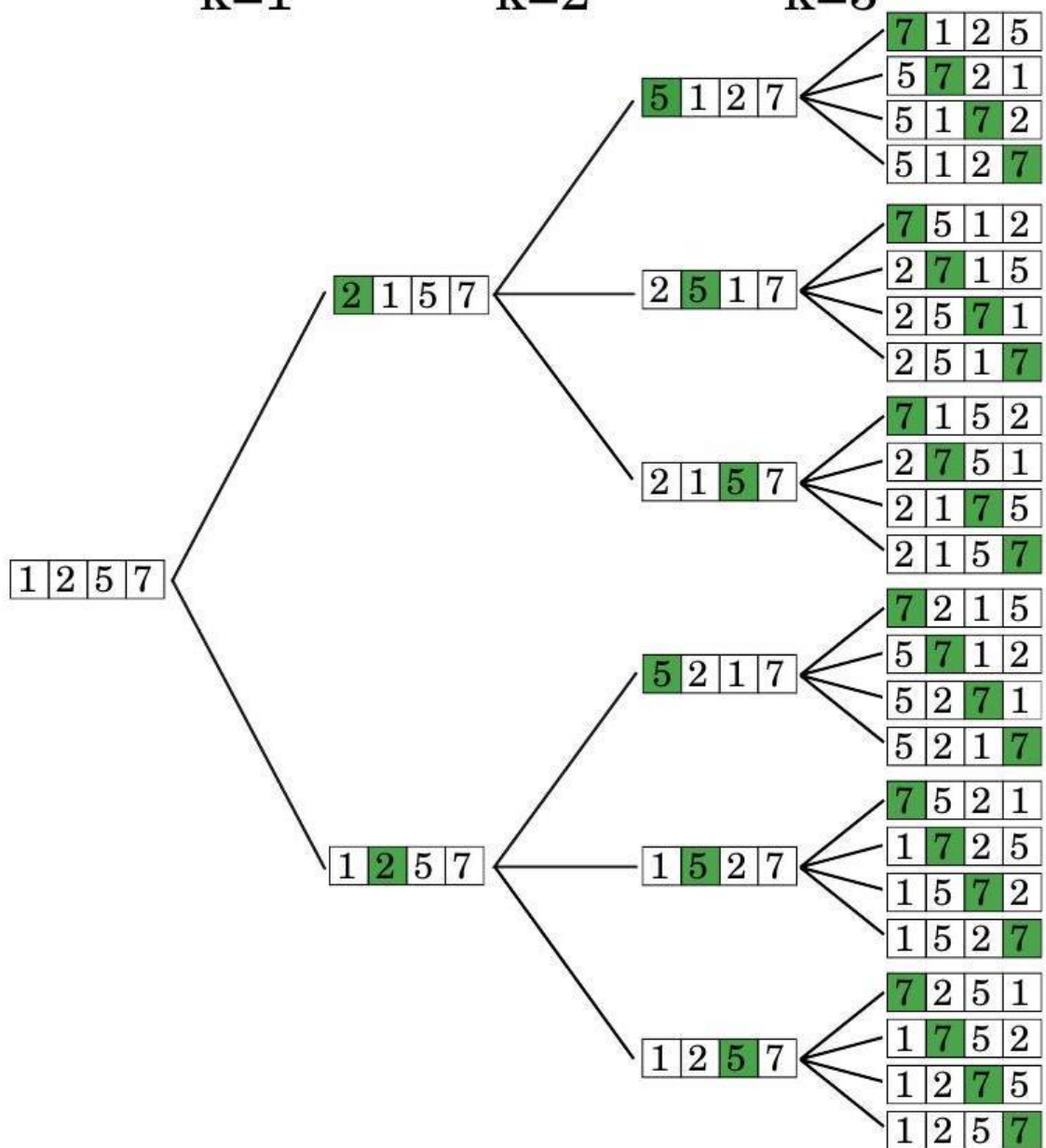
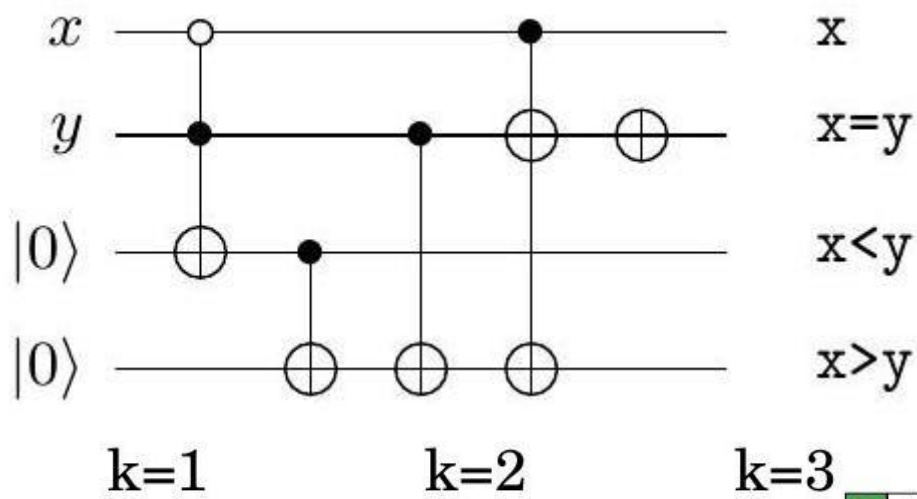
$$(A^{j+1}[i], B^{j+1}[i]) = \text{Compare2}(A^j[2i], B^j[2i], A^j[2i+1], B^j[2i+1])$$



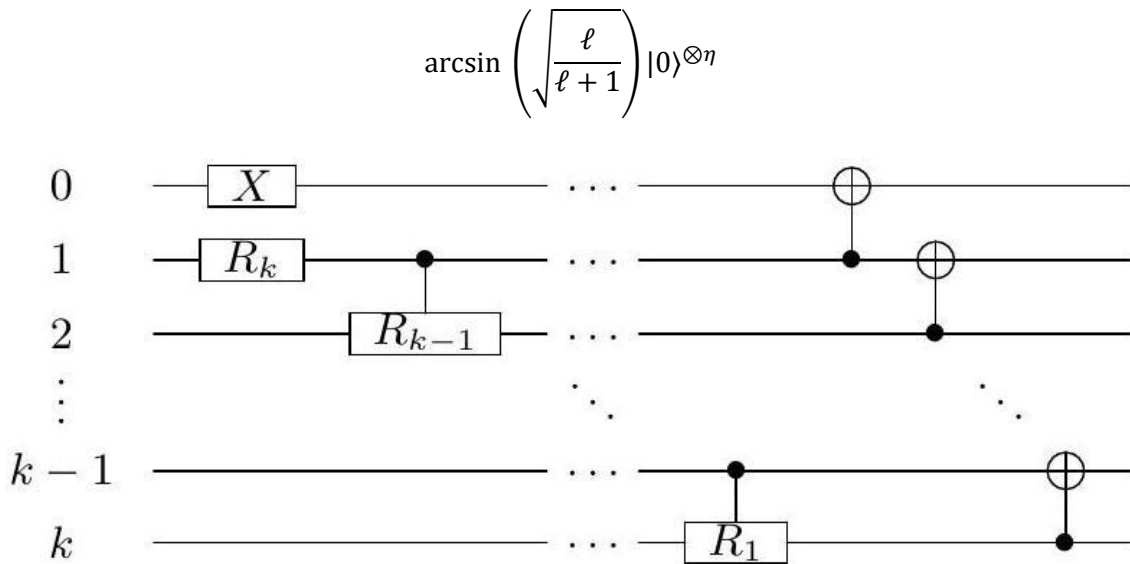
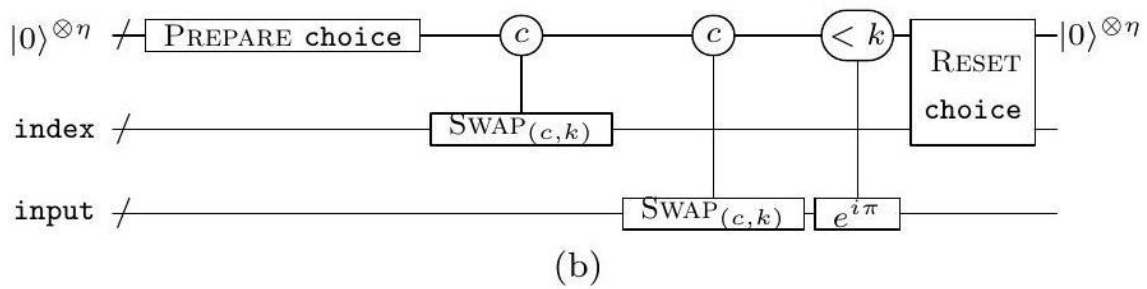
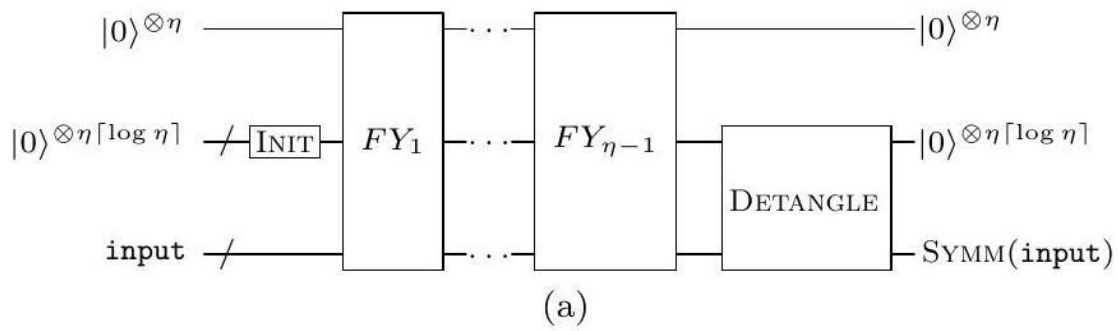
```

for  $j = 0, \dots, \log d - 1$  do
  for  $i = 0, \dots, \text{size}(A^j)/2 - 1$  do
     $(A^{j+1}[i], B^{j+1}[i]) = \text{COMPARE2}(A^j[2i], B^j[2i],$ 
                                    $A^j[2i+1], B^j[2i+1])$ 
  end for
end for
return  $(A^{\log d-1}[0], B^{\log d-1}[0])$ 

```



$$\frac{1}{\sqrt{k+1}} \sum_{\ell=0}^k |\ell\rangle$$



$$|\text{null}\rangle = |0\rangle^{\otimes \eta}$$

$$|\ell\rangle = X_\ell |\text{null}\rangle,$$

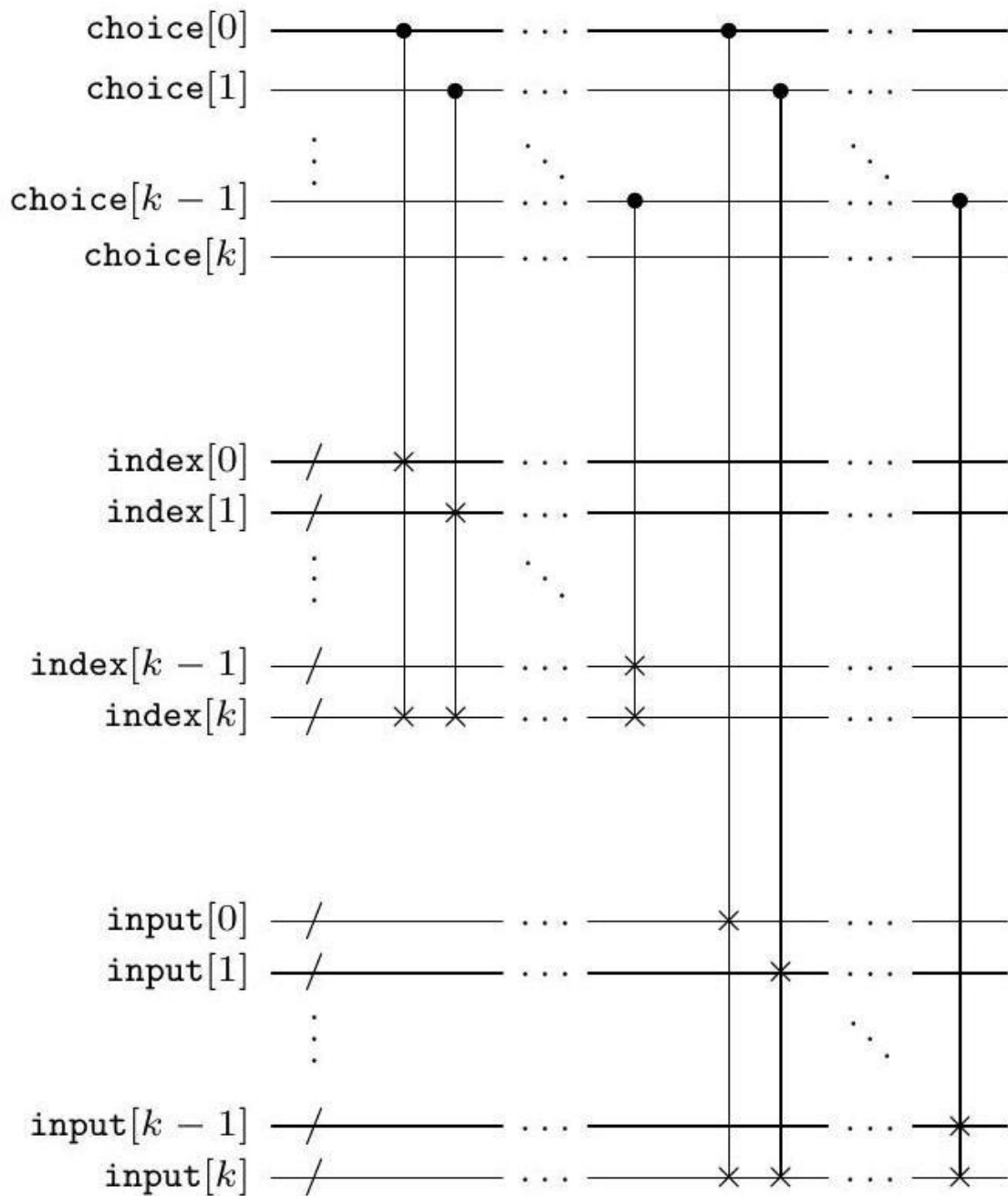
$$|W_k\rangle := \frac{1}{\sqrt{k+1}} \sum_{\ell=0}^k |\ell\rangle$$

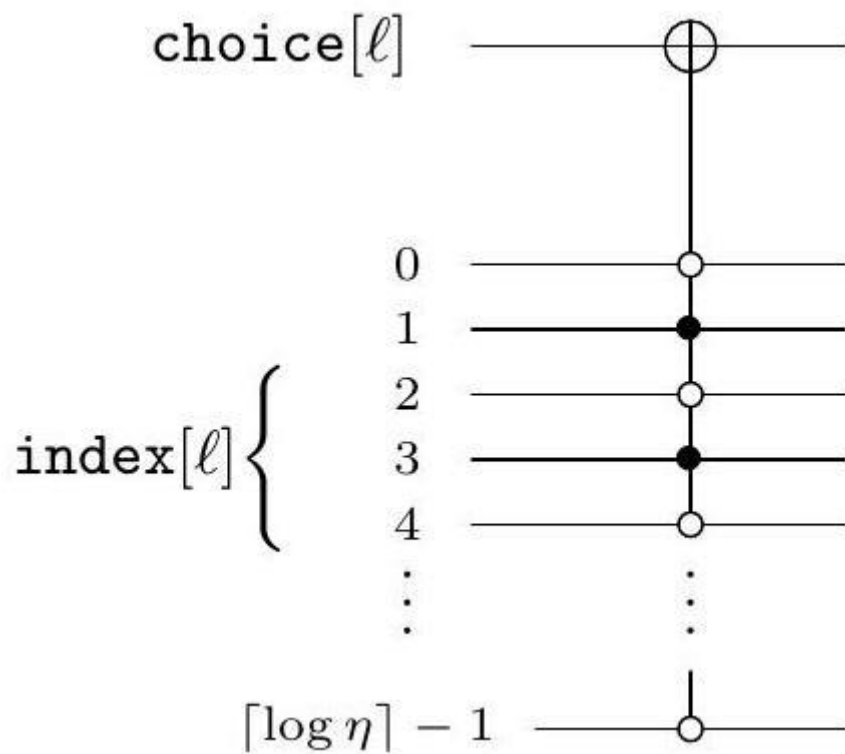
$$\frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$$

$$|\ell\rangle = \left(\prod_{\ell'=0}^{\ell} X_{\ell'} \right) |\text{null}\rangle$$

$$R_\ell := \frac{1}{\sqrt{\ell+1}} \begin{pmatrix} 1 & -\sqrt{\ell} \\ \sqrt{\ell} & 1 \end{pmatrix}.$$

$$\text{SELSWAP}_k := \sum_{c=0}^{\eta-1} |c\rangle\langle c|_{\text{choice}} \otimes \text{SWAP}(c, k)_{\text{target}}$$

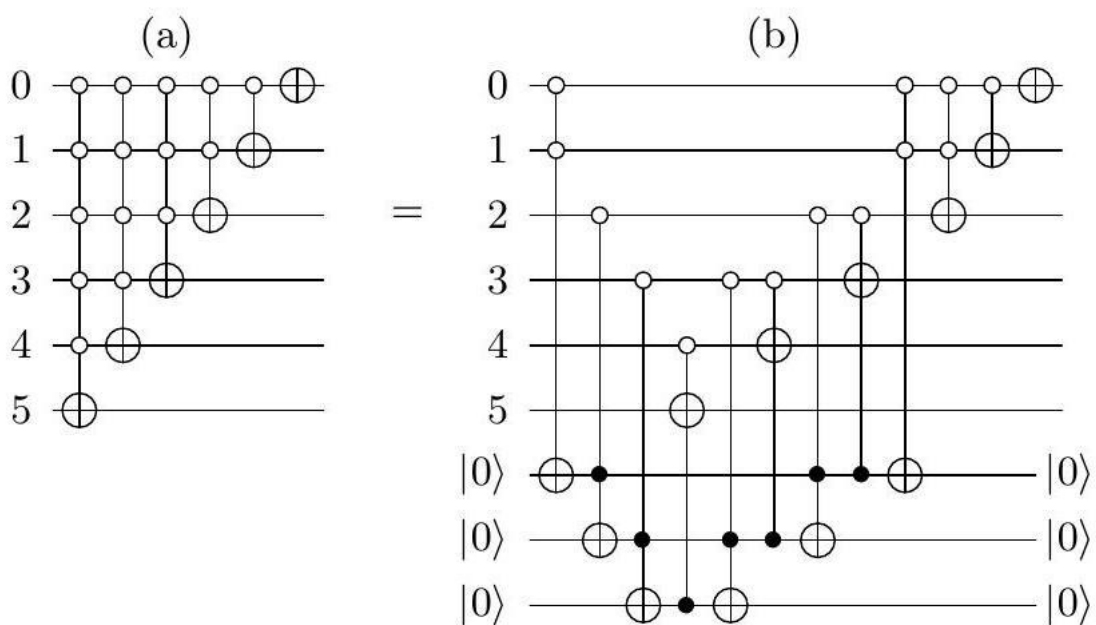




$$|0\rangle^{\otimes \eta \lceil \log \eta \rceil} [\ell'] (\ell' \neq \ell) \eta (\eta - 1)$$

$$O(\log \eta) O(\log^2 \eta)$$

$$O(\eta (\eta - 1) [\log N + \log \eta])$$



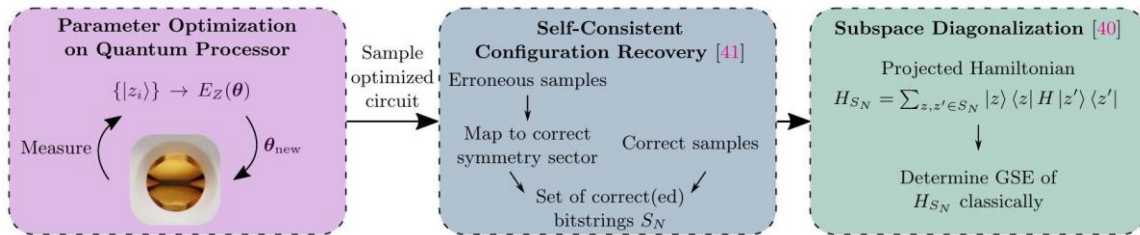
$$O(\eta^2 \log N) O(\eta^2 [\log \log N + \log \eta])$$

$$e^{-\beta \Delta A} / \beta$$

$$C(\boldsymbol{\theta}), |\psi_{\boldsymbol{\theta}}\rangle = C(\boldsymbol{\theta})|\psi_0\rangle$$

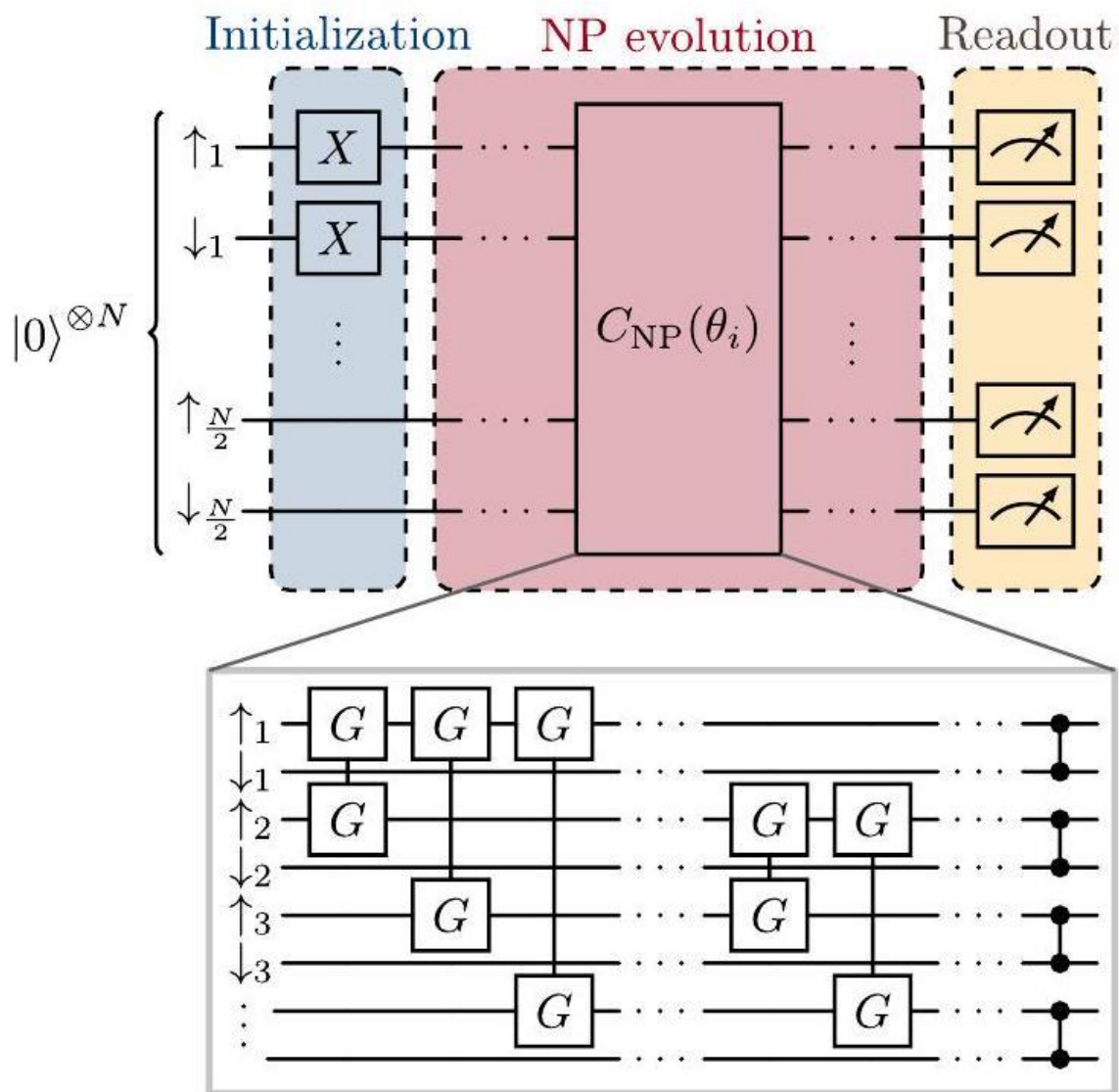
$$E_Z(\boldsymbol{\theta}) = \frac{1}{N_{\text{tot}}} \sum_{j=1}^{N_u} N_j \langle z_j | H | z_j \rangle,$$

$$|z_j\rangle N_{\text{tot}} = \sum_{j=1}^{N_u} N_j$$



$$H_{\text{el.}} = \sum_{ij,\sigma} t_{ij}^{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{ijkl,\sigma\sigma'} t_{ijkl}^{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'}^{\dagger} c_{k\sigma} c_{l\sigma'},$$

$$S^2 = \sum_{i,j=1}^{N/2} c_{i,\uparrow} c_{j,\uparrow}^{\dagger} c_{i,\downarrow}^{\dagger} c_{j,\downarrow} + \frac{n_{\uparrow} - n_{\downarrow}}{2} + \frac{(n_{\uparrow} - n_{\downarrow})^2}{4}.$$



$$H = H_{\text{el.}} + M(s_0^2 - S^2)^2,$$

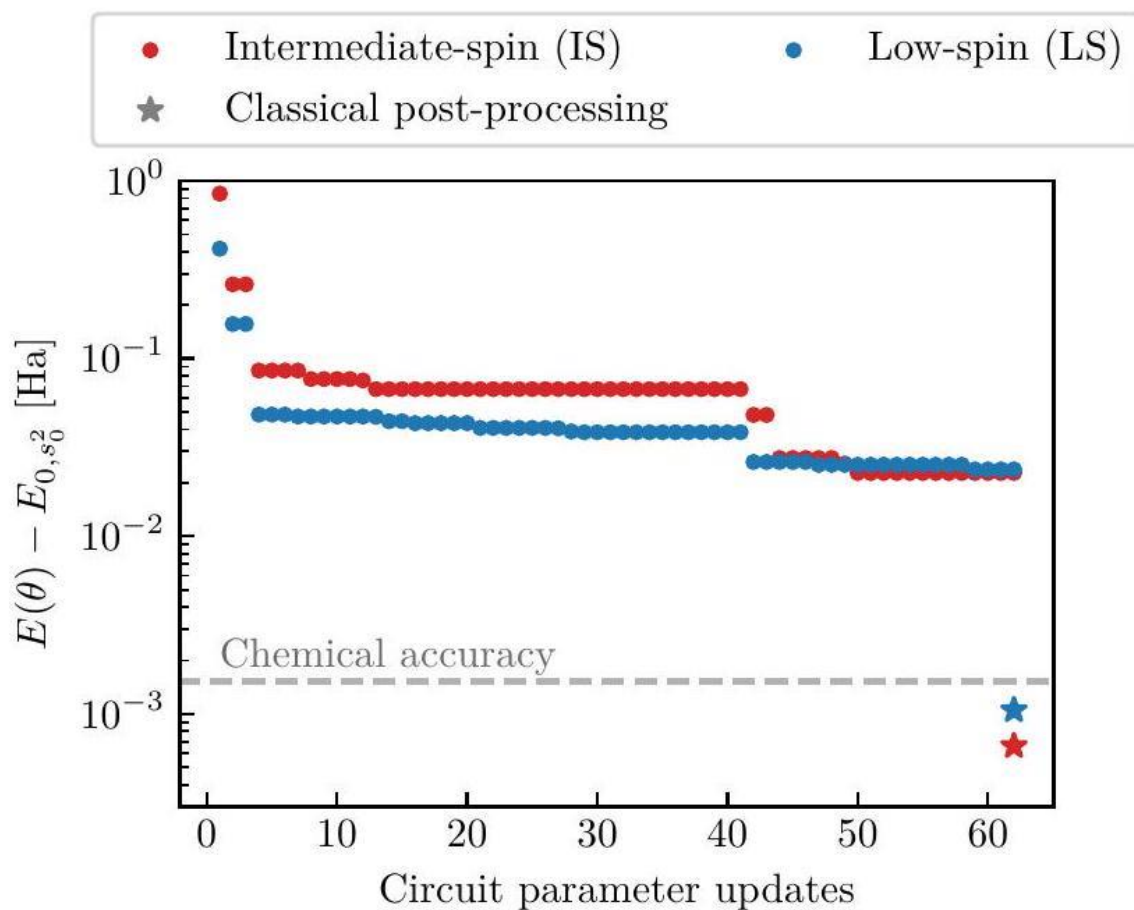
$$\sum_{i=1}^{N/2} \langle \psi_{\text{HF}} | Z_{i,\sigma} | \psi_{\text{HF}} \rangle = \sum_{i=1}^{N/2} \langle z_m | Z_{i,\sigma} | z_m \rangle,$$

$$H_{S_N^{(k)}} = P_{S_N^{(k)}} H P_{S_N^{(k)}}$$

$$P_{S_N^{(k)}} = \sum_{z_i^k \in S_N^{(k)}} |z_i^k\rangle \langle z_i^k| \{ |\psi_{\text{GS}}^k\rangle \}$$

$$\langle n_{i,\sigma} \rangle = \frac{1}{K} \sum_{k=1}^K \langle \psi_{\text{GS}}^k | n_{i,\sigma} | \psi_{\text{GS}}^k \rangle.$$

$$|0\rangle = |4^2\,S_{1/2}, m_J = -1/2\rangle \text{ and } |1\rangle = |3^2\text{D}_{5/2}, m_J = -1/2\rangle$$

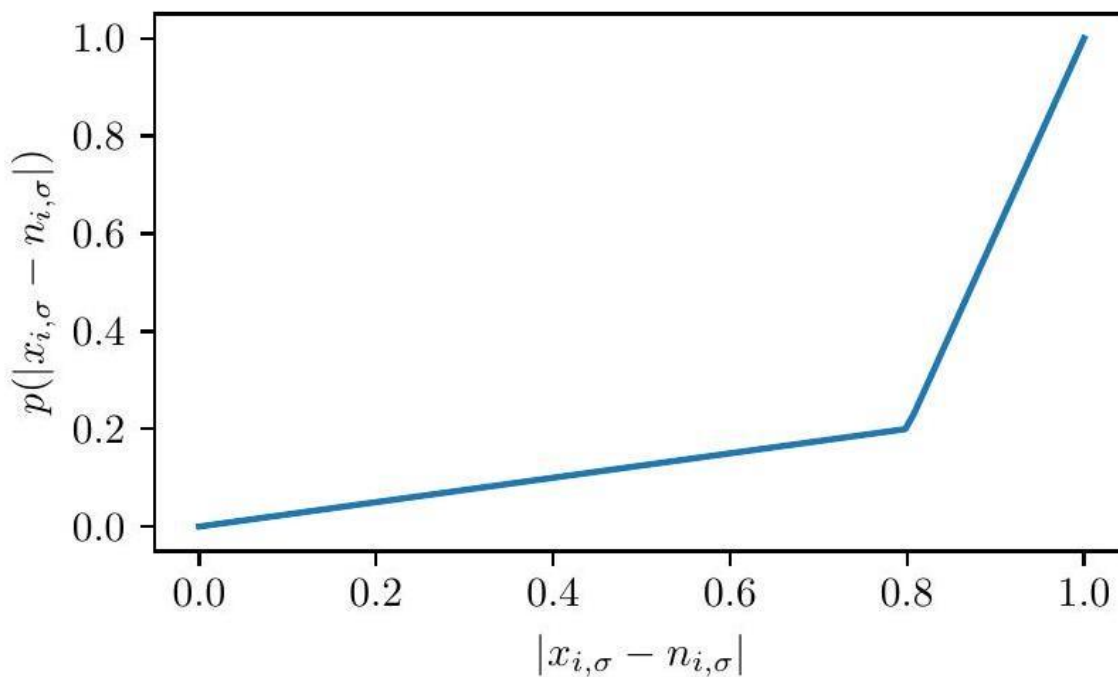


$$\Delta H = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$$

$$G(2\theta) = \begin{bmatrix} 1 & & & \\ & \cos \theta & \sin \theta & \\ & -\sin \theta & \cos \theta & \\ & & & 1 \end{bmatrix} Z^{\otimes N} \langle n_{i,\sigma} \rangle$$

$$p(|x_{i,\sigma} - n_{i,\sigma}|)$$

$$p(y) = \begin{cases} \delta \frac{y}{h}, & y \leq h \\ \delta + (1 - \delta) \frac{y - h}{1 - h}, & y > h \end{cases}$$



$$R(\theta,\phi)=\exp\left(-i\frac{\theta}{2}(X\cos\phi+Y\sin\phi)\right)$$

$$R_{XX}(-\pi/2)$$

$$E_j(\lambda)=\sum_{k=0}^{\infty}\lambda^kE_j^{(k)}$$

$$R_0=\Pi_0(E_0\mathbb{1}-H)^{-1}\Pi_0=\sum_{i=1}^{D-1}\frac{|\Phi_i\rangle\langle\Phi_i|}{E_0-E_i}$$

$$\text{with } \Pi_0 = (\mathbb{1} - |\Phi_0\rangle\langle\Phi_0|).$$

$$E^{(1)}=\langle V\rangle\equiv\langle\Phi_0|V|\Phi_0\rangle$$

$$E^{(2)}=\langle VR_0V\rangle$$

$$E^{(3)}=\langle VR_0VR_0V\rangle-\langle V\rangle\langle VR_0^2V\rangle$$

$$\tilde{E}_0=\langle\tilde{\Phi}_0|H|\tilde{\Phi}_0\rangle$$

$$P=|\tilde{\Phi}_0\rangle\langle\tilde{\Phi}_0|, Q=\mathbb{1}-P$$

$$H=H'+V' \text{ with } \\ H'=PHP+QHQ \text{ and } V'=PHQ+QHP.$$

$$|\tilde{\Phi}_0\rangle H' \propto V' + V$$

$$\sigma_i = \sigma_{i,1} \otimes \sigma_{i,2} \otimes \cdots \otimes \sigma_{i,d}$$

$$V=\sum_{i=1}^{L_V}v_i\sigma_i, H=\sum_{i=1}^{L_H}h_i\sigma_i, v_i, h_i\in\mathbb{R}$$

$$E^{(1)} = \sum_{i=1}^{L_V} v_i \langle \sigma_i \rangle$$

$$E^{(2)} = \langle VR_0V \rangle$$

$$\langle VR_0V \rangle (E_0 \mathbb{1} - H)^{-1} \langle \sigma_i U(t) \sigma_j \rangle$$

$$R=E_{D-1}-E_0$$

$$\Delta = E_1 - E_0$$

$$R_0 = \sum_{i=1}^{D-1} |\Phi_i\rangle\langle\Phi_i|\frac{1}{E_0-E}\Big|_{E=E_i} g_{\Delta,R}(E) - \frac{1}{E} \left[\Delta,R\right]$$

$$R_0=\sum_{i=0}^{D-1}g_{\Delta,R}(E_i-E_0)|\Phi_i\rangle\langle\Phi_i|,$$

$$g_{\Delta,R}(E)\colon [0,R+\Delta]\rightarrow \mathbb{R}$$

$$g_{\Delta,R}(E)(\,R+\Delta\,)$$

$$\sum_{n\in\mathbb{Z}}\beta_{\Delta,R,n}e^{-iEt_n}\text{ with }t_n\coloneqq\frac{2\pi n}{R+\Delta}$$

$$\text{and } \beta_{\Delta,R,n}\coloneqq\frac{1}{R+\Delta}\int_0^{R+\Delta}g_{\Delta,R}(E)e^{iEt_n}dE$$

$$R_0=\sum_{n\in\mathbb{Z}}\sum_{i=0}^{D-1}\beta_{\Delta,R,n}e^{-i(E_i-E_0)t_n}|\Phi_i\rangle\langle\Phi_i|$$

$$H,U(t)=e^{-iHt}$$

$$R_0=\sum_{n\in\mathbb{Z}}\beta_{\Delta,R,n}e^{iE_0t_n}U(t_n)$$

$$\begin{aligned} E^{(2)} &= \langle VR_0V \rangle \\ &= \sum_{n\in\mathbb{Z}} \beta_{\Delta,R,n} e^{-iE_0t_n} \langle VU(t_n)V \rangle \end{aligned}$$

$$\begin{aligned} R_{0,N} &:= \sum_{|n|\leq N} \beta_{\Delta,R,n} e^{iE_0t_n} U(t_n) \\ E_N^{(2)} &:= \langle VR_{0,N}V \rangle \\ &= \sum_{|n|\leq N} \beta_{\Delta,R,n} e^{iE_0t_n} \langle VU(t_n)V \rangle \end{aligned}$$

$$e^{iE_0t}\langle VU(t)V\rangle=\langle e^{iHt}Ve^{-iHt}V\rangle=\langle V(t)V\rangle$$

$$E_N^{(2)} = \sum_{|n|\leq N} \beta_{\Delta,R,n} e^{iE_0t_n} \sum_{i,j=1}^{L_V} v_i v_j \langle \sigma_i U(t_n) \sigma_j \rangle$$

$$|\beta_{\Delta,R,n}| \leq \frac{61R}{\Delta^2} \exp\left(-\sqrt{\frac{|n|\Delta}{256R}}\right)$$

$$\begin{array}{l} \left|E^{(2)}-E_N^{(2)}\right| \leq \frac{\epsilon}{2} \\ \text{if } N \geq \left\lceil \frac{2132R}{\Delta} \ln^2\left(\frac{5.3\cdot 10^4R\|v\|_1^2}{\Delta^3\epsilon}\right) \right\rceil, \end{array}$$

$$\|v\|_1=\sum_{i=1}^{L_V}|v_i|$$

$$V_U=\sum_{i=1}^L u_i U_i \langle \Phi_0|V_U|\Phi_0\rangle$$

$$\mathbb{P}[|X-\langle \Phi_0|V_U|\Phi_0\rangle|<\epsilon]\geq 1-\alpha$$

$$\mathcal{O}\left(\epsilon^{-1}\|u\|_{2/3}\ln\frac{L}{\alpha}\sqrt{\ln\frac{1}{\alpha}}\right)$$

$$\mathcal{O}\left(\epsilon^{-1}|u_i|^{2/3}\|u\|_{2/3}^{1/3}\ln\frac{L}{\alpha}\sqrt{\ln\frac{1}{\alpha}}\right)$$

$$\|u\|_{2/3}=\left(\sum_{i=1}^L|u_i|^{2/3}\right)^{3/2}$$

$$\tilde{\mathcal{O}}\left(\frac{\|h\|_1^{3/2}\|v\|_{2/3}^2}{\Delta^{7/2}\epsilon}\right)$$

$$\tilde{\mathcal{O}}\left(\frac{\|h\|_1^{3/2}\|v\|_{2/3}^2}{\Delta^{5/2}\epsilon}\right)$$

$$\|v\|_{2/3}=\left(\sum_{i=1}^{L_V}|v_i|^{2/3}\right)^{3/2}$$

$$K,\mathcal{I}=\{\phi_1,\ldots,\phi_K\}$$

$$\mathcal{H}_1(\mathcal{I})\Lambda^{N_{el}}(\mathcal{H}_1(\mathcal{I}))$$

$$H_{el}=\sum_{p,q\in\mathcal{I}}h_{pq}a_p^\dagger a_q+\frac{1}{2}\sum_{p,q,r,s\in\mathcal{I}}g_{pqrs}a_p^\dagger a_q^\dagger a_r a_s$$

$$h_{pq}=\int \overline{\phi_p}(\mathbf{x})\left(-\frac{\nabla^2}{2}-\sum_{I=1}^{N_{nuc}}\frac{Z_I}{|\mathbf{R}_I-\mathbf{x}|}\right)\phi_q(\mathbf{x})d\mathbf{x}$$

$$g_{pqrs}=\iint \frac{\overline{\phi_p}(\mathbf{x}_1)\overline{\phi_q}(\mathbf{x}_2)\phi_r(\mathbf{x}_2)\phi_s(\mathbf{x}_1)}{|\mathbf{x}_1-\mathbf{x}_2|}d\mathbf{x}_1d\mathbf{x}_2$$

$$F=\sum_{p\in\mathcal{I}}\epsilon_p a_p^\dagger a_p\binom{K}{N_{el}}$$

$$\mathcal{I}=\mathcal{I}_{\text{core}}\cup\mathcal{I}_{\text{act}}\cup\mathcal{I}_{\text{virt}}$$

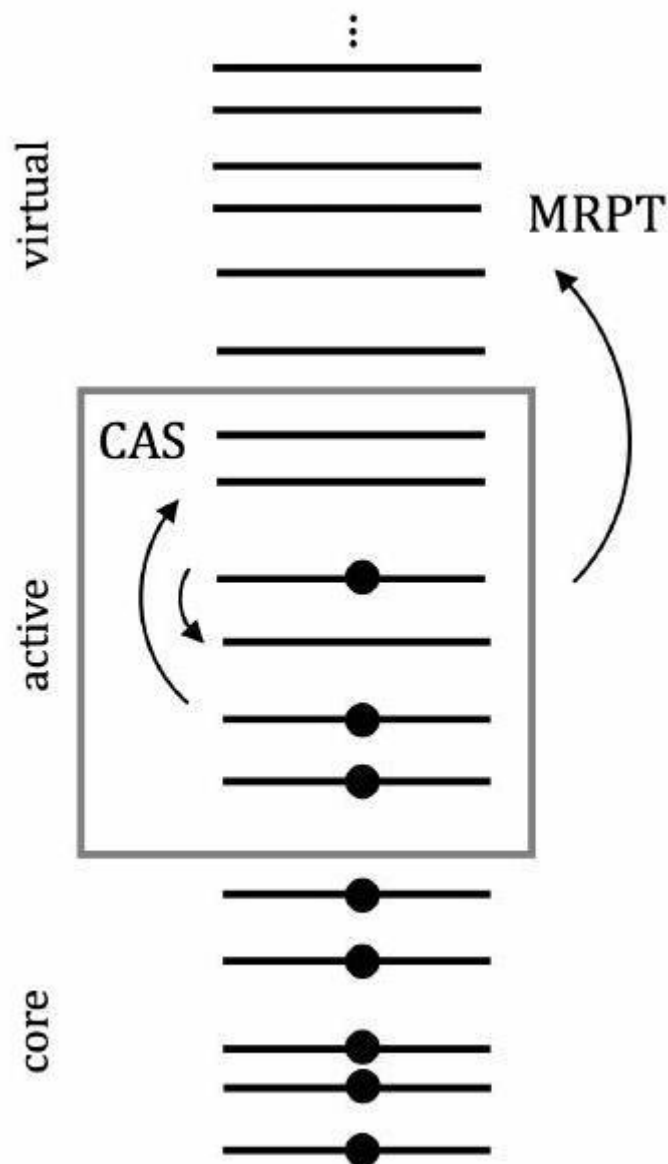
$$N_{el}^{act}=N_{el}-|\mathcal{I}_{\text{core}}|$$

$$\Lambda^{N_{el}^{act}}(\mathcal{H}_1(\mathcal{I}_{act}))$$

$$H_{CAS}=\sum_{a,b\in\mathcal{I}_{act}}h'_{ab}a_a^\dagger a_b+\frac{1}{2}\sum_{a,b,c,d\in\mathcal{I}_{act}}g_{abcd}a_a^\dagger a_b^\dagger a_c a_d$$

$$|\Phi_0^{CAS}\rangle E_0^{CAS} \Lambda^{N_{el}^{act}}(\mathcal{H}_1(\mathcal{I}_{act}))\binom{N_{el}^{act}}{k}$$

$$\Lambda^{N_{el}^{act}}(\mathcal{H}_1(\mathcal{I}_{act}\cup\mathcal{I}_{virt}))$$



$$H'_{el} = \sum_{p,q \in \mathcal{I}_{act} \cup \mathcal{I}_{virt}} h'_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s \in \mathcal{I}_{act} \cup \mathcal{I}_{virt}} g_{pqrs} a_p^\dagger a_q^\dagger a_r a_s + E_{core}.$$

$$H = H_{CAS} + F_{virt} + E_{core}$$

$$F_{virt} = \sum_{v \in \mathcal{I}_{virt}} \epsilon_v a_v^\dagger a_v$$

$$H_{CAS} |\Phi_0^{CAS}\rangle |\Phi_0\rangle = |\Phi_0^{CAS}\rangle \wedge |0 \dots 0\rangle$$

$$V = H'_{el} - H$$

$$V = \sum_{\substack{p,q \in \mathcal{I}_{act} \cup \mathcal{I}_{virt} \\ \{p,q\} \notin \mathcal{I}_{act}}} h'_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{\substack{p,q,r,s \in \mathcal{I}_{virt} \cup \mathcal{I}_{act} \\ \{p,q,r,s\} \notin \mathcal{I}_{act}}} g_{pqrs} a_p^\dagger a_q^\dagger a_r a_s - F_{virt}$$

$$\mathcal{O}(K^4) E^{\text{MRPT}(1)} E^{\text{MRPT}(2)} \mathcal{O}(K^8) \|v\|_{2/3}^2$$

$$V = H'_{el} - H \|v_{\text{diff}}\|_{2/3}^2 \|v\|_{2/3}^2$$

$$a_v|\Phi_0\rangle=0 \text{ if } a_v$$

$$\langle a_p^\dagger a_q \rangle \langle a_p^\dagger a_q^\dagger a_r a_s \rangle$$

$$E^{\mathrm{MRPT}(1)}=\langle V\rangle=0$$

$$E_N^{\mathrm{MRPT}(2)}=\sum_{|n|\leq N}\beta_{\Delta,R,n}e^{iE_0t}\langle VU(t_n)V\rangle$$

$$\begin{aligned}\langle VU(t_n)V\rangle&=\sum_{v,a,w,b}h'_{va}h'_{wb}\langle a_b^\dagger a_wU(t_n)a_v^\dagger a_a\rangle\\&+\frac{1}{2}\sum_{v,a,p,q,b,c}h'_{va}g_{pqbc}\langle a_c^\dagger a_b^\dagger a_q a_pU(t_n)a_v^\dagger a_a\rangle\\&+\frac{1}{2}\sum_{p,q,a,b,v,c}g_{pqab}h'_{vc}\langle a_c^\dagger a_vU(t_n)a_p^\dagger a_q^\dagger a_a a_b\rangle\\&+\frac{1}{4}\sum_{p,q,a,b,r,s,c,d}g_{pqab}g_{rs cd}\langle a_d^\dagger a_c^\dagger a_s a_rU(t_n)a_p^\dagger a_q^\dagger a_a a_b\rangle\\&=:T_1(t_n)+T_2(t_n)+T_3(t_n)+T_4(t_n)\end{aligned}$$

$$\begin{array}{l} v,w\in\mathcal{I}_{\mathrm{virt}},a,b,c,d\in\mathcal{I}_{\mathrm{act}}\\ p,q,r,s\in\mathcal{I}_{\mathrm{act}}\cup\mathcal{I}_{\mathrm{virt}},\{p,q\},\{r,s\}\not\subset\mathcal{I}_{\mathrm{act}}. \end{array}$$

$$n_v=a_v^\dagger a_v$$

$$[H,n_v] = [\epsilon_v n_v, n_v] = 0$$

$$\langle a_b^\dagger a_wU(t_n)a_v^\dagger a_a\rangle$$

$$T_1(t_n)=\sum_{\substack{v\in\mathcal{I}_{\mathrm{virt}}\\a,b\in\mathcal{I}_{\mathrm{act}}}}h'_{va}h'_{vb}\langle a_b^\dagger a_vU(t_n)a_v^\dagger a_a\rangle$$

$$a_p^\dagger(t)\equiv e^{iHt}a_p^\dagger e^{-iHt}$$

$$a_p(t)\equiv e^{iHt}a_p e^{-iHt}$$

$$a_v(t)=a_v e^{-i\epsilon_v t}$$

$$a_v^\dagger(t)=a_v^\dagger e^{i\epsilon_v t}$$

$$\begin{aligned}T_1(t_n)&=\sum_{\substack{v\in\mathcal{I}_{\mathrm{virt}}\\a,b\in\mathcal{I}_{\mathrm{act}}}}h'_{va}h'_{vb}\langle a_b^\dagger e^{-iHt_n}e^{iHt_n}a_v e^{-iHt_n}a_v^\dagger a_a\rangle\\&=\sum_{\substack{v\in\mathcal{I}_{\mathrm{virt}}\\a,b\in\mathcal{I}_{\mathrm{act}}}}h'_{va}h'_{vb}e^{-i\epsilon_v t_n}\langle a_b^\dagger e^{-iHt_n}a_v a_v^\dagger a_a\rangle\\&=\sum_{\substack{v\in\mathcal{I}_{\mathrm{virt}}\\a,b\in\mathcal{I}_{\mathrm{act}}}}h'_{va}h'_{vb}e^{-i(\epsilon_v+E_{\mathrm{core}})t_n}\langle a_b^\dagger e^{-iH_{\mathrm{CAS}}t_n}a_a\rangle\end{aligned}$$

$$a_v|\Phi_0\rangle=e^{-iHt_n}e^{-i(H_{\mathrm{CAS}}+E_{\mathrm{core}})t_n}$$



$$\begin{aligned}
T_1(t_n) &= \sum_{a,b \in \mathcal{J}_{act}} v_{a,b}(t_n) \langle a_b^\dagger e^{-iH_{CAS}t_n} a_a \rangle \\
T_2(t_n) &= \sum_{a,b,c,d \in \mathcal{J}_{act}} v_{abc,d}(t_n) \langle a_d^\dagger e^{-iH_{CAS}t_n} a_a^\dagger a_b a_c \rangle \\
T_3(t_n) &= \sum_{a,b,c,d \in \mathcal{J}_{act}} v_{bcd,a}(t_n) \langle a_d^\dagger a_c^\dagger a_b e^{-iH_{CAS}t_n} a_a \rangle \\
T_4(t_n) &= \sum_{a,b,c,d \in \mathcal{J}_{act}} v_{ab,cd}(t_n) \langle a_d^\dagger a_c^\dagger e^{-iH_{CAS}t_n} a_a a_b \rangle \\
&+ \sum_{a,b,c,d,e,f \in \mathcal{J}_{act}} v_{abc,def}(t_n) \langle a_f^\dagger a_e^\dagger a_d e^{-iH_{CAS}t_n} a_a^\dagger a_b a_c \rangle
\end{aligned}$$

$$\begin{aligned}
v_{a,b}(t) &= \sum_{v \in \mathcal{J}_{virt}} h'_{va} h'_{vb} e^{-i(\epsilon_v + E_{core})t} \\
v_{abc,d}(t) &= \sum_{v \in \mathcal{J}_{virt}} h'_{vd} g_{vabc} e^{-i(\epsilon_v + E_{core})t} \\
v_{ab,cd}(t) &= \frac{1}{2} \sum_{v \in \mathcal{J}_{virt}} g_{vwab} g_{vwcd} e^{-i(\epsilon_v + \epsilon_w + E_{core})t} \\
v_{abc,def}(t) &= \sum_{v \in \mathcal{J}_{virt}} g_{vabc} g_{vdef} e^{-i(\epsilon_v + E_{core})t}
\end{aligned}$$

$$\begin{aligned}
E_N^{\text{MRPT}(2)} &= \sum_{|n| \leq N} \beta_{\Delta,R,n} \sum_{i=1}^{L^{\text{MRPT}(2)}} v_{ni}^{\text{MRPT}(2)} \\
&\times \langle \sigma_{i,1} e^{-iH_{CAS}t_n} \sigma_{i,2} \rangle
\end{aligned}$$

$$\|v^{\text{MRPT}(2)}\beta\|_{2/3} = \left(\sum_{|n| \leq N} \sum_{i=1}^{L^{\text{MRPT}(2)}} |\beta_{\Delta,R,n} v_{ni}^{\text{MRPT}(2)}|^{2/3} \right)^{3/2}$$

$$\begin{aligned}
& \left(\sum_i |v_{ni}^{\text{MRPT}(2)}|^{2/3} \right)^{3/2} \\
& \leq \left(2^{2/3} \sum_{a,b \in \mathcal{I}_{act}} \left(\sum_{v \in \mathcal{I}_{virt}} |h'_{va} h'_{vb}| \right)^{2/3} \right. \\
& \quad + 2^{7/3} \sum_{a,b,c,d \in \mathcal{I}_{act}} \left(\sum_{v \in \mathcal{I}_{virt}} |h'_{va} g_{vbcd}| \right)^{2/3} \\
& \quad + 2^{2/3} \sum_{a,b,c,d \in \mathcal{I}_{act}} \left(\sum_{vw \in \mathcal{I}_{virt}} |g_{vwab} g_{vwcd}| \right)^{2/3} \\
& \quad \left. + 4 \sum_{a,b,c,d,e,f \in \mathcal{I}_{act}} \left(\sum_{v \in \mathcal{I}_{virt}} |g_{vabc} g_{vdef}| \right)^{2/3} \right)^{3/2} \\
& \equiv \|v^{\text{MRPT}(2)}\|_{2/3}.
\end{aligned}$$

$$\|v^{\text{MRPT}(2)}\beta\|_{2/3} \leq \|v^{\text{MRPT}(2)}\|_{2/3} \|\beta_{\Delta,R}\|_{2/3}$$

$$\|v^{\text{MRPT}(2)}\|_{2/3} \|v\|_{2/3}^2 L^{\text{MRPT}(2)} L_V^2$$

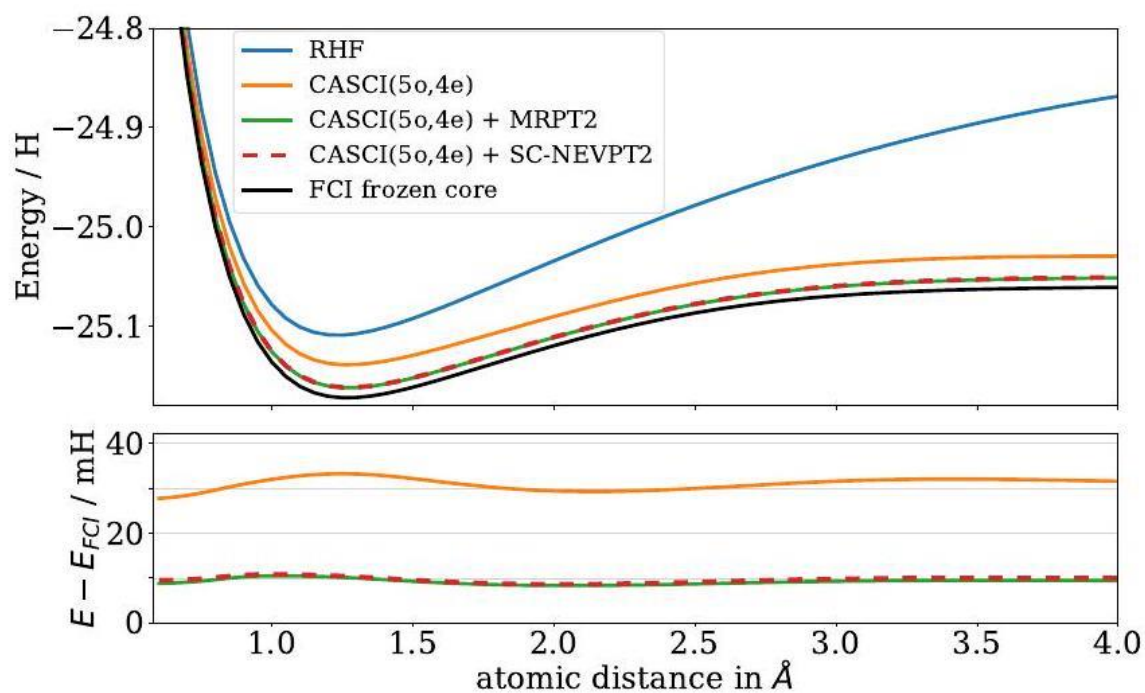
$$R_{CAS} + e^{-iH_{CAS}t} e^{i(E_0 - E_{\text{core}})t} = e^{iE_0^{CAS}t}$$

$$R_{CAS} + 2 \max_{v \in \mathcal{I}_{virt}} \epsilon_v$$

$$R_{CAS} \leq 2 \|h^{CAS}\|_1 \|h\|_1$$

$$\tilde{O}\left(\frac{\|h^{CAS}\|_1^{3/2} \|v^{\text{MRPT}(2)}\|_{2/3}}{\Delta^{7/2}\epsilon}\right),$$

$$\tilde{O}\left(\frac{\|h^{CAS}\|_1^{3/2} \|v^{\text{MRPT}(2)}\|_{2/3}}{\Delta^{5/2}\epsilon}\right) \|h^{CAS}\|_1 \|v^{\text{MRPT}(2)}\|_{2/3}$$



$$k_{\text{rate}} \propto \exp \{ -\Delta G_{TS} / (k_B T) \}$$

$$\Delta E_{TS} = E_{TS} - E_{\text{H}_2\text{OO}}$$

$$k_{\text{rate}} \propto \exp \{ -\Delta E_{TS} / (k_B T) \}$$

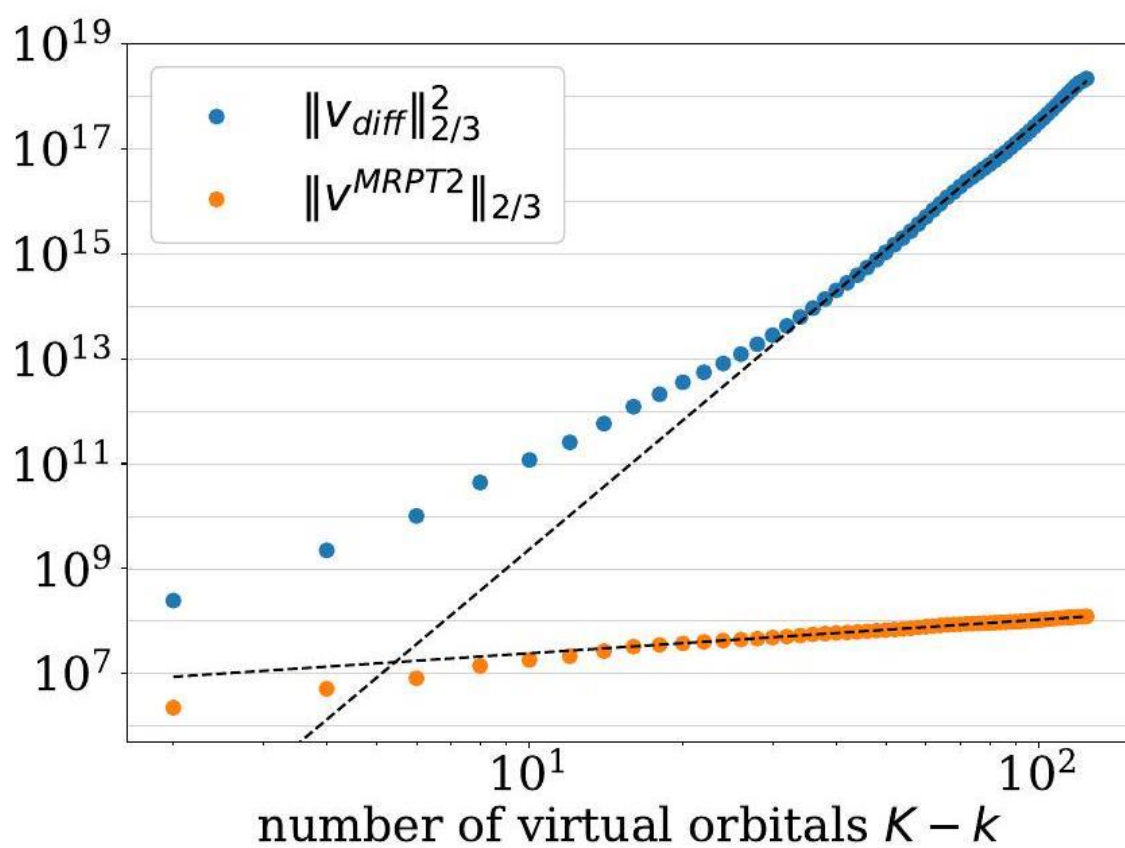
$$\|v^{\text{MRPT2}}\|_{2/3} \|v_{\text{diff}}\|_{2/3}^2$$

$$K - k = 122 \|v^{\text{MRPT2}}\|_{2/3} \|v_{\text{diff}}\|_{2/3}^2 \|v^{\text{MRPT2}}\|_{2/3} \|v_{\text{diff}}\|_{2/3}^2$$

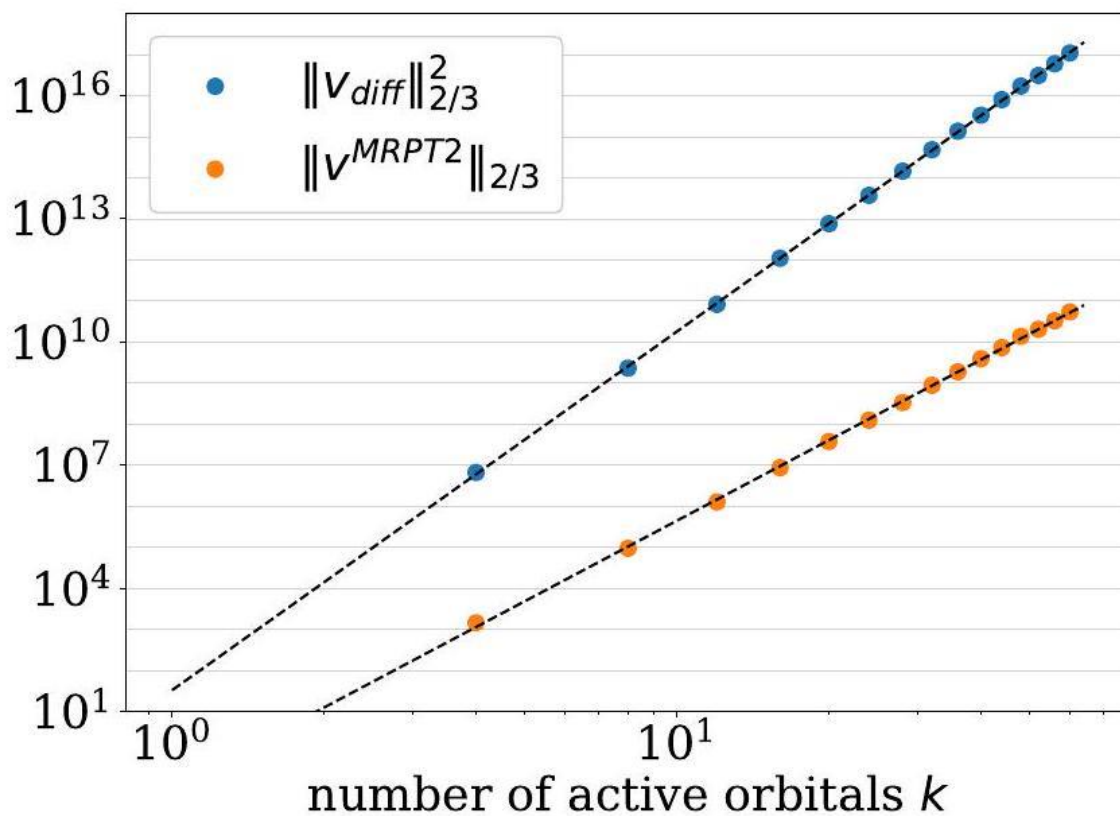
$$\|v_{\text{diff}}\|_{2/3}^2 \|v^{\text{MRPT2}}\|_{2/3}$$

$$\|v^{\text{MRPT2}}\|_{2/3} \|v_{\text{diff}}\|_{2/3}^2$$

$$\|v^{\text{MRPT2}}\|_{2/3}$$



$$\|v_{diff}\|_{2/3}^2 \|v^{MRPT2}\|_{2/3} \propto (K - k)^\beta$$



$$\|v_{diff}\|_{2/3}^2 \|v^{MRPT2}\|_{2/3} k/K = \text{const}$$

$$\|v^{\text{MRPT}(2)}\|_1\|\beta_{\Delta,R}\|_1$$

$$E_{int}=E_{AB}-E_A-E_B$$

$$\Lambda^N(\mathcal{H}_1)\mathcal{H}_{1,A}\mathcal{H}_{1,B}$$

$$\mathcal{H}_{AB}=\mathcal{H}_A\otimes\mathcal{H}_B=\Lambda^{N_A}(\mathcal{H}_{1,A})\otimes\Lambda^{N_B}(\mathcal{H}_{1,B})$$

$$a_\mu a_\mu^\dagger \mathcal{H}_A b_\nu, b_\nu^\dagger \mathcal{H}_B$$

$$\mathcal{I}_A=\{\phi_1^A,\ldots,\phi_{K_A}^A\} \text{ and } \mathcal{I}_B=\{\phi_1^B,\ldots,\phi_{K_B}^B\}$$

$$|\Phi_0^A\rangle \text{ and } |\Phi_0^B\rangle$$

$$\begin{aligned} H|\Phi_0\rangle &= (H_A\otimes\mathbb{1}+\mathbb{1}\otimes H_B)|\Phi_0^A\rangle\otimes|\Phi_0^B\rangle \\ &= (E_A+E_B)|\Phi_0\rangle E_{SRS}^{(k)} \end{aligned}$$

$$\mathcal{P}_1=-\sum_{ijkl}S_{il}S_{kj}a_i^\dagger a_jb_k^\dagger b_l$$

$$\text{where } S_{il}=\int \overline{\phi_i^A(\mathbf{x})}\phi_l^B(\mathbf{x})d\mathbf{x}$$

$$\phi_i^A(\mathbf{x}) \text{ and } \phi_l^B(\mathbf{x})$$

$$\begin{aligned} E_{SRS}^{(1)}(S^2) &= \langle V \rangle + \langle (\langle V \rangle - V) \mathcal{P}_1 \rangle \\ &=: E_{\text{pol}}^{(1)} + E_{\text{exch}}^{(1)} \end{aligned}$$

$$\begin{aligned} E_{SRS}^{(2)}(S^2) &= \langle VR_0V \rangle + \langle (\langle V \rangle - V) (\langle \mathcal{P}_1 \rangle - \mathcal{P}_1) R_0V \rangle \\ &=: E_{\text{pol}}^{(2)} + E_{\text{exch}}^{(2)}, \end{aligned}$$

$$\begin{aligned} V &= V_{elA-elB} + V_{elA-nucB} + V_{nucA-elB} - V_0 \\ &= \sum_{pqrs} g_{pqrs}^{AB} a_p^\dagger a_s b_q^\dagger b_r + \sum_{jk} h_{jk}^B a_k^\dagger a_j \\ &\quad + \sum_{lm} h_{lm}^A b_m^\dagger b_l - V_0 \end{aligned}$$

$$g_{pqrs}^{AB}=\iint\frac{\overline{\phi_p^A(\mathbf{x}_1)}\overline{\phi_q^B(\mathbf{x}_2)}\phi_r^B(\mathbf{x}_2)\phi_s^A(\mathbf{x}_1)}{|\mathbf{x}_1-\mathbf{x}_2|}d\mathbf{x}_1d\mathbf{x}_2$$

$$h_{jk}^B=-\sum_{i=1}^{N_{nuc}^B}\langle\phi_j|\frac{Z_i}{|\mathbf{r}-\mathbf{R}_{B_i}|}|\phi_k\rangle$$

$$h_{lm}^A=-\sum_{i=1}^{N_{nuc}^A}\langle\phi_l|\frac{Z_i}{|\mathbf{r}-\mathbf{R}_{A_i}|}|\phi_m\rangle$$

$$V_0=\sum_{i,j=1}^{N_{nuc}^A,N_{nuc}^B}\frac{Z_{A_i}Z_{B_j}}{\left|\mathbf{R}_{A_i}-\mathbf{R}_{B_j}\right|}$$

$$\langle V_{elA-nucB}\mathcal{P}_1R_0V_{elA-elB}\rangle$$

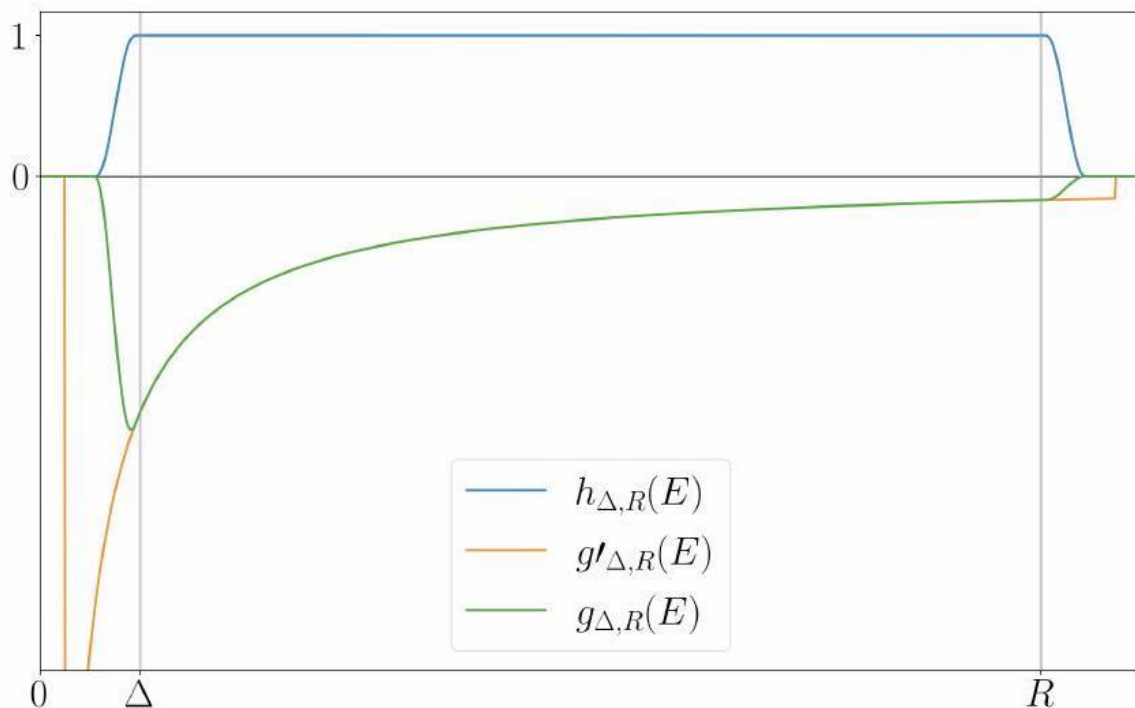
$$\begin{aligned}
& \langle V_{\text{elA-nucB}} \mathcal{P}_1 R_0 V_{\text{elA-elB}} \rangle \\
&= \sum_{\substack{ijkl \\ mn \\ pqrs}} S_{il} S_{kj} h_{mn}^B g_{pqrs}^{AB} \langle a_n^\dagger a_m a_i^\dagger a_j b_k^\dagger b_l R_0 a_p^\dagger a_s b_q^\dagger b_r \rangle \\
&= \sum_{\substack{n \in \mathbb{Z} \\ injkl \\ pqrs}} S_{il} S_{kj} h_{mn}^B g_{pqrs}^{AB} \beta_{\Delta,R,n} e^{iE_0 t_n} \\
&\times \langle a_n^\dagger a_m a_i^\dagger a_j b_k^\dagger b_l e^{-iH t_n} a_p^\dagger a_s b_q^\dagger b_r \rangle \\
&= \sum_{n \in \mathbb{Z}} \sum_{\substack{ijkl \\ mn}} S_{il} S_{kj} h_{mn}^B g_{pqrs}^{AB} \beta_{\Delta,R,n} e^{iE_0 t_n} \\
&\times \langle a_n^\dagger a_m a_i^\dagger a_j e^{-iH_A t_n} a_p^\dagger a_s \rangle_A \langle b_k^\dagger b_l e^{-iH_B t_n} b_q^\dagger b_r \rangle_B
\end{aligned}$$

$$\langle \dots \rangle_X = \langle \Phi_0^X | \dots | \Phi_0^X \rangle$$

$$\langle V_{\text{elA-nucB}} \mathcal{P}_1 R_0 V_{\text{elA-elB}} \rangle | \Phi_0^A \rangle, | \Phi_0^B \rangle$$

$$g'_{\Delta,R}(E)=-\frac{\mathbb{1}_{\left[\frac{\Delta}{4},R+\frac{\Delta}{4}\right]}}{E},$$

$$[a,b]\subset \mathbb{R} g_{\Delta,R}(E)h_{\Delta,R}$$



$$\eta(E)=\begin{cases} c_{\eta}e^{-(1-E)^{-1}}e^{-(1+E)^{-1}}, & |E|<1 \\ 0, & \text{else} \end{cases}$$

$$\int_{-1}^1 \eta(E) dE = 1$$

$$\frac{d^n}{dE^n}\eta \text{ at } E=1 \text{ and } E=-1$$

$$\eta_{\Delta}(E)=\frac{4}{\Delta}\eta\left(\frac{4E}{\Delta}\right)$$

$$\left[-\frac{\Delta}{4},\frac{\Delta}{4}\right]$$

$$h_{\Delta,R}(E)=\left(\mathbb{1}_{\left[\frac{3}{4}\Delta,R+\frac{\Delta}{4}\right]}*\eta_{\Delta}\right)(E)$$

$$E=\frac{\Delta}{2} \text{ and } E=R+\frac{\Delta}{2}$$

$$g_{\Delta,R}(E)=(g'_{\Delta,R}\cdot h_{\Delta,R})(E).$$

$$\beta_{\Delta,R,n}=\frac{1}{R+\Delta}\int_0^{R+\Delta}g_{\Delta,R}(E)e^{-iEt_n}dE$$

$$t_n=\frac{2\pi n}{R+\Delta},n\in\mathbb{Z}$$

$$|\beta_{\Delta,R,n}|\leq \frac{61R}{\Delta^2}2^{-\left(\frac{|n|\Delta}{256R}\right)^{1/2}}$$

$$\widehat{\mathcal{G}}_{\Delta,R}(t) \text{ of } g_{\Delta,R}(E)$$

$$\beta_{\Delta,R,n}=\frac{1}{R+\Delta}\widehat{\mathcal{G}}_{\Delta,R}(t_n)$$

$$\text{where } \widehat{\mathcal{G}}_{\Delta,R}(t)=\int_0^{R+\Delta}g_{\Delta,R}(E)e^{-iEt}dE$$

$$D^\ell \widehat{\mathcal{G}}_{\Delta,R}(t)=(-it)^\ell \widehat{\mathcal{G}}_{\Delta,R}(t)$$

$$|\beta_{\Delta,R,n}|=\frac{1}{R+\Delta}|\widehat{\mathcal{G}}_{\Delta,R}(t_n)|=\frac{1}{R+\Delta}\frac{|D^\ell \widehat{\mathcal{G}}_{\Delta,R}(t_n)|}{|t_n|^\ell}.$$

$$\left[\frac{\Delta}{2},R+\frac{\Delta}{2}\right]$$

$$|D^\ell \widehat{\mathcal{G}}_{\Delta,R}(t)|\leq \int_{\frac{\Delta}{2}}^{R+\frac{\Delta}{2}}|D^\ell g_{\Delta,R}(E)|dE=R\|D^\ell g_{\Delta,R}\|_\infty$$

$$|\beta_{\Delta,R,n}|\leq \frac{R}{R+\Delta}\frac{\|D^\ell g_{\Delta,R}\|_\infty}{|t_n|^\ell}\leq \frac{\|D^\ell g_{\Delta,R}\|_\infty}{|t_n|^\ell}$$

$$\|D^\ell g_{\Delta,R}\|_\infty=\sup_{E\in\left[\frac{\Delta}{2},R+\frac{\Delta}{2}\right]}|D^\ell(g'_{\Delta,R}\cdot h_{\Delta,R})(E)|$$

$$=\sup_{E\in\left[\frac{\Delta}{2},R+\frac{\Delta}{2}\right]}\left|\sum_{\ell'=0}^{\ell}\binom{\ell}{\ell'}(D^{\ell-\ell'}g'_{\Delta,R}(E))(D^{\ell'}h_{\Delta,R}(E))\right|$$

$$\leq\sup_{E\in\left[\frac{\Delta}{2},R+\frac{\Delta}{2}\right]}\sum_{\ell'=0}^{\ell}\binom{\ell}{\ell'}|D^{\ell-\ell'}g'_{\Delta,R}(E)||D^{\ell'}h_{\Delta,R}(E)|$$

$$\begin{aligned}
|D^{\ell'} h_{\Delta,R}(E)| &= \left| D^{\ell'} \left(\mathbb{1}_{\left[\frac{3}{4}\Delta, R+\frac{\Delta}{4}\right]} * \eta_{\Delta} \right) (E) \right| \\
&= \left| \left(\mathbb{1}_{\left[\frac{3}{4}\Delta, R+\frac{\Delta}{4}\right]} * D^{\ell'} \eta_{\Delta} \right) (E) \right| \\
&= \left| \int_{\frac{3}{4}\Delta}^{R+\frac{\Delta}{4}} D^{\ell'} \eta_{\Delta}(E-E') dE' \right| \\
&\leq R \|D^{\ell'} \eta_{\Delta}\|_{\infty}
\end{aligned}$$

$$\|D^{\ell'} \eta\|_{\infty} \leq c_{\eta} (16)^{\ell'} \ell'^{2\ell'}$$

$$\eta(E) \text{ and } \eta_{\Delta}(E)$$

$$D^{\ell'} \eta_{\Delta}(E) = \left(\frac{4}{\Delta}\right)^{\ell'+1} D^{\ell'} \eta\left(\frac{4E}{\Delta}\right)$$

$$|D^{\ell'} h_{\Delta,R}(E)| \leq \frac{4c_{\eta}R}{\Delta} \left(\frac{64}{\Delta}\right)^{\ell'} \ell'^{2\ell'}.$$

$$\left[\frac{\Delta}{2}, R + \frac{\Delta}{2}\right] g'_{\Delta,R}(E) - \frac{1}{E}$$

$$\begin{aligned}
&\sup_{E \in \left[\frac{\Delta}{2}, R+\frac{\Delta}{2}\right]} |D^{\ell-\ell'} g'_{\Delta,R}(E)| \\
&= \sup_{E \in \left[\frac{\Delta}{2}, R+\frac{\Delta}{2}\right]} \left| D^{\ell-\ell'} \frac{1}{E} \right| \\
&= (\ell - \ell')! \left(\frac{2}{\Delta}\right)^{\ell-\ell'+1}
\end{aligned}$$

$$\begin{aligned}
&\|D^{\ell} g_{\Delta,R}\|_{\infty} \\
&\leq \frac{4c_{\eta}R}{\Delta} \sum_{\ell'=0}^{\ell} \binom{\ell}{\ell'} (\ell - \ell')! \left(\frac{2}{\Delta}\right)^{\ell-\ell'+1} \left(\frac{64}{\Delta}\right)^{\ell'} \ell'^{2\ell'} \\
&= \frac{8c_{\eta}R2^{\ell}\ell!}{\Delta^{\ell+2}} \sum_{\ell'=0}^{\ell} (32)^{\ell'} \frac{\ell'^{2\ell'}}{\ell'!} \\
&\leq \frac{8c_{\eta}R2^{\ell}}{\Delta^{\ell+2}} (\ell+1)(32\ell^2)^{\ell} \\
&\leq \frac{8c_{\eta}R}{\Delta^2} \left(\frac{128\ell^2}{\Delta}\right)^{\ell}
\end{aligned}$$

$$\begin{aligned}
|\beta_{\Delta,R,n}| &\leq \frac{8c_{\eta}R}{\Delta^2} \left(\frac{128\ell^2}{\Delta|t_n|}\right)^{\ell} \\
&\leq \frac{8c_{\eta}R}{\Delta^2} \left(\frac{64R\ell^2}{\Delta|n|}\right)^{\ell}
\end{aligned}$$

$$\left(\frac{|n|\Delta}{256R}\right)^{1/2} \leq \ell \leq \left(\frac{|n|\Delta}{128R}\right)^{1/2}$$



$$|\beta_{\Delta,R,n}| \leq \frac{8c_\eta R}{\Delta^2} 2^{-\ell}$$

$$|\beta_{\Delta,R,n}| \leq \frac{8c_\eta R}{\Delta^2} 2^{-\left(\frac{|n|\Delta}{256R}\right)^{1/2}}$$

$$\left(\frac{|n|\Delta}{128R}\right)^{1/2} \text{ and } \left(\frac{|n|\Delta}{256R}\right)^{1/2}$$

$$\left(\frac{|n|\Delta}{128R}\right)^{1/2} - \left(\frac{|n|\Delta}{256R}\right)^{1/2} \geq 1$$

$$|n| \geq \frac{256R}{(\sqrt{2}-1)^2\Delta}$$

$$|n| \leq \frac{256\pi}{(\sqrt{2}-1)^2\Delta}$$

$$|\beta_{\Delta,R,n}| \leq \|g_{\Delta,R}\|_\infty = \frac{4}{\Delta}$$

$$|n| \leq \frac{256R}{(\sqrt{2}-1)^2\Delta}$$

$$\begin{aligned} |\beta_{\Delta,R,n}| &\leq \frac{4R}{\Delta^2} \\ &\leq \frac{4c_\eta R}{\Delta^2} 2^{-\frac{1}{\sqrt{2}-1}} \\ &\leq \frac{4c_\eta R}{\Delta^2} 2^{-\left(\frac{|n|\Delta}{256R}\right)^{1/2}} \end{aligned}$$

$$\left|E^{(2)} - E_N^{(2)}\right| g_{\Delta,R}$$

$$\tilde{N} = \tilde{N}(R, \Delta, \epsilon, \|v\|_1) \left|E^{(2)} - E_N^{(2)}\right|$$

$$\left|E^{(2)} - E_N^{(2)}\right| \leq \frac{\epsilon}{2} \text{ if } N \geq \tilde{N}$$

$$\tilde{N} \leq \left\lceil \frac{2132R}{\Delta} \ln^2 \left(\frac{5.3 \cdot 10^4 R^2 \|v\|_1^2}{\Delta^3 \epsilon} \right) \right\rceil$$

$$\left|E^{(2)} - E_N^{(2)}\right| = |\langle VR_0V \rangle - \langle VR_{0,N}V \rangle|$$

$$\begin{aligned} \left|E^{(2)} - E_N^{(2)}\right| &\leq \sum_{|n|>N} |\beta_{\Delta,R,n}| |\langle VU(t_n)V \rangle| \\ &\leq \sum_{|n|>N} |\beta_{\Delta,R,n}| \|V|\Phi_0\rangle\|_2 \|U(t_n)V|\Phi_0\rangle\|_2 \\ &= \|V|\Phi_0\rangle\|_2^2 \sum_{|n|>N} |\beta_{\Delta,R,n}| \\ &= \langle V^2 \rangle \sum_{|n|>N} |\beta_{\Delta,R,n}| \end{aligned}$$

$$\langle V^2 \rangle = \sum_{i,j=1}^{L_V} v_i v_j \langle \sigma_i \sigma_j \rangle \leq \|v\|_1^2$$

$$\left| E^{(2)} - E_N^{(2)} \right| \leq \|v\|_1^2 \sum_{|n|>N} |\beta_{\Delta,R,n}|$$

$$M_{\Delta,R} = \frac{61R}{\Delta^2} \text{ and } q_{\Delta,R} = \ln(2) \left(\frac{\Delta}{256R} \right)^{\frac{1}{2}}$$

$$|\beta_{\Delta,R,n}| \leq M_{\Delta,R} e^{-q_{\Delta,R}|n|^{1/2}}$$

$$\begin{aligned} \sum_{|n|>N} |\beta_{\Delta,R,n}| &\leq M_{\Delta,R} \sum_{|n|>N} e^{-q_{\Delta,R}|n|^{\frac{1}{2}}} \\ &\leq 2M_{\Delta,R} \int_N^{\infty} e^{-q_{\Delta,R}x^{\frac{1}{2}}} dx \\ &= \frac{4M_{\Delta,R}}{q_{\Delta,R}^2} \int_{q_{\Delta,R}N^{\frac{1}{2}}}^{\infty} ye^{-y} dy \\ &= \frac{4M_{\Delta,R}}{q_{\Delta,R}^2} \left(q_{\Delta,R}N^{\frac{1}{2}} + 1 \right) e^{-q_{\Delta,R}N^{\frac{1}{2}}} \\ &\leq \frac{8M_{\Delta,R}}{q_{\Delta,R}^2} e^{-\frac{q_{\Delta,R}}{2}N^{\frac{1}{2}}} \end{aligned}$$

$$\left| E^{(2)} - E_N^{(2)} \right| \leq \frac{8M_{\Delta,R}\|v\|_1^2}{q_{\Delta,R}^2} e^{-\frac{q_{\Delta,R}}{2}N^{\frac{1}{2}}}$$

$$\tilde{N} \equiv \left\lceil \frac{4}{q_{\Delta,R}^2} \ln^2 \left(\frac{16M_{\Delta,R}\|v\|_1^2}{q_{\Delta,R}^2 \epsilon} \right) \right\rceil$$

$$\left| E^{(2)} - E_N^{(2)} \right| \leq \frac{\epsilon}{2}$$

$$\tilde{N} \leq \left\lceil \frac{2132R}{\Delta} \ln^2 \left(\frac{5.3 \times 10^4 R^2 \|v\|_1^2}{\Delta^3 \epsilon} \right) \right\rceil$$

$$X=\langle \Phi_0|U|\Phi_0\rangle$$

$$\mathbb{P}[|X'-X|<\epsilon]\geq 1-\alpha$$

$$U_\psi|0\rangle=|\psi\rangle=\sqrt{a}|\psi'\rangle+\sqrt{1-a}|\psi'^\perp\rangle\\ \text{with } \langle\psi'^\perp|\psi'\rangle=0$$

$$a=|\langle\psi'\mid\psi\rangle|^2$$

$$\theta_a\in\left[0,\frac{\pi}{2}\right]\sin^2\left(\theta_a\right)=a$$

$$Q=-S_\psi S_{\psi'}$$

$$S_\psi = \mathbb{1} - 2|\psi\rangle\langle\psi|$$

$$S_{\psi'} = \mathbb{1} - 2|\psi'\rangle\langle\psi'|$$

$$S_\psi = U_\psi Z_0 U_\psi^\dagger \text{ where } Z_0 = \mathbb{1} - 2|0\rangle\langle 0|$$

$$Q^k|\psi\rangle$$

$$\mathbb{P}[|\psi'\rangle] = |\langle\psi'|Q^k|\psi\rangle|^2 = \sin^2\left((2k+1)\theta_a\right).$$

$$U_{\psi,flag}|0\rangle|0\rangle_{flag} = \sqrt{a}|\psi'\rangle|0\rangle_{flag} + \sqrt{a-1}|\psi'^\perp\rangle|1\rangle_{flag}$$

$$|\psi'\rangle|\psi'^\perp\rangle a\in[0,1]$$

$$\mathbb{P}\big[a\notin[a_l,a_u]\big]\leq\alpha, \text{ where } a_u-a_l<2\epsilon$$

$$|a-\hat{a}|<\epsilon 1-\alpha \mathcal{O}\left(\frac{1}{\epsilon}\ln\frac{1}{\alpha}\right)U_{\psi,flag}$$

$$U_{\psi'}|0\rangle=|\psi'\rangle$$

$$a=|\langle\psi'|V|\psi'\rangle|^2$$

$$|a-\hat{a}|<\epsilon$$

$$U_\psi=VU_{\psi'}$$

$$U_\psi|0\rangle=|\psi\rangle$$

$$a=|\langle\psi'\mid\psi\rangle|^2$$

$$Q^kU_{\psi,\text{flag}}|0\rangle|0\rangle_{\text{flag}}$$

$$\mathbb{P}[|0\rangle_{\text{flag}}] = \sin^2\left((2k+1)\theta_a\right).$$

$$U_{\psi'}U_{\psi}^\dagger Q^kU_{\psi}|0\rangle$$

$$\mathbb{P}[|0\rangle] = \left|\langle 0|U_{\psi'}^\dagger Q^kU_{\psi}|0\rangle\right|^2 = \sin^2\left((2k+1)\theta_a\right).$$

$$\hat{a} = |\langle\psi'|V|\psi'\rangle|^2 = |\langle\psi'\mid\psi\rangle|^2$$

$$|\hat{a}-a|<\epsilon$$

$$Q=-S_\psi S_{\psi'}=-U_\psi Z_0 U_\psi^\dagger U_{\psi'} Z_0 U_{\psi'}^\dagger$$

$$U_\psi^\dagger Q^k U_\psi |0\rangle$$

$$U_\psi,2k+1$$

$$U_\psi=VU_{\psi'}$$

$$X=re^{i\theta}=r\cos\left(\theta\right)+i r\sin\left(\theta\right), r\in\mathbb{R}_{\geq 0}, \theta\in\left[0,2\pi\right)$$

$$x_0 = |\langle \Phi_0 | U | \Phi_0 \rangle|^2 = r^2$$

$$x_1 = |\langle \Phi_0 | (+ | cU | \Phi_0) | + \rangle|^2 = \frac{1}{2} |1 + r e^{i\theta}|^2$$

$$x_2 = |\langle \Phi_0 | (+ | cU (\mathbb{1} \otimes e^{iZ\frac{\pi}{4}}) | \Phi_0) | + \rangle|^2 = \frac{1}{2} |1 - i r e^{i\theta}|^2$$

$$cU = \mathbb{1} \otimes |0\rangle\langle 0| + U \otimes |1\rangle\langle 1|$$

$$r = \sqrt{x_0}$$

$$\cos \theta = \frac{4x_1 - 1 - x_0}{2\sqrt{x_0}}$$

$$\sin \theta = -\frac{4x_2 - 1 - x_0}{2\sqrt{x_0}}$$

$$\begin{array}{ll} x_0: & V = U \qquad \qquad \qquad U_{\psi'} = U_0 \\ x_1: & V = cU \qquad \qquad \qquad U_{\psi'} = U_0 \otimes \mathbf{H} \\ x_2: & V = cU \left(\mathbb{1} \otimes e^{iZ\frac{\pi}{4}} \right) \quad U_{\psi'} = U_0 \otimes \mathbf{H} \end{array}$$

$$|x'_i-x_i|<\epsilon_i$$

$$X'=r'e^{i\theta'}$$

$$\begin{aligned} |X'-X| &= |r'e^{i\theta'}-re^{i\theta}| \\ &\leq |r'\cos\theta'-r\cos\theta|+|r'\sin\theta'-r\sin\theta| \\ &\leq |x'_0-x_0|+2|x'_1-x_1|+2|x'_2-x_2| \\ &\leq \epsilon_0+2\epsilon_1+2\epsilon_2 \end{aligned}$$

$$\epsilon_0=\epsilon_1=\epsilon_2=\epsilon/5$$

$$|X'-X|\leq \epsilon$$

$$\begin{aligned} &\mathbb{P}[|x'_i-x_i|<\epsilon_i\forall i\in\{0,1,2\}] \\ &\geq (1-\alpha_0)(1-\alpha_1)(1-\alpha_2) \\ &\geq 1-(\alpha_0+\alpha_1+\alpha_2) \end{aligned}$$

$$\alpha_0=\alpha_1=\alpha_2=\alpha/3$$

$$\begin{aligned} \mathbb{P}[|X'-X|\leq \epsilon] &= \mathbb{P}[|x'_i-x_i|<\epsilon_i\forall i\in\{0,1,2\}] \\ &\geq 1-\alpha \end{aligned}$$

$$V_U=\sum_{i=1}^L u_i U_i$$

$$X=\langle \Phi_0|V_U|\Phi_0\rangle$$

$$\mathbb{P}[|X'-X|<\epsilon]\geq 1-\alpha$$

$$\mathcal{O}\left(\epsilon^{-1}\|u\|_{2/3}\ln\frac{L}{\alpha}\sqrt{\ln\frac{1}{\alpha}}\right)\mathcal{O}\left(\epsilon^{-1}|u_i|^{2/3}\|u\|_{2/3}^{1/3}\ln\frac{L}{\alpha}\sqrt{\ln\frac{1}{\alpha}}\right)\|u\|_{2/3}=(\sum_{i=1}^L|u_i|^{2/3})^{3/2}$$

$$\sum_{i=1}^L u_i X'_i = X'.$$

$$X_i = \langle \Phi_0 | U_i | \Phi_0 \rangle$$

$$\mathbb{P}[|X'_i - X_i| < \epsilon_i] \geq 1 - \alpha'$$

$$(X_i - \epsilon_i, X_i + \epsilon_i) \mathbb{P}[|X'_i - X_i| < \epsilon_i, \forall 1 \leq i \leq L] = (1 - \alpha')^L \geq 1 - L\alpha'$$

$$(1+x)^r \geq 1+xr \text{ for } x \geq -1$$

$$\alpha' = \frac{\alpha}{2L} 1 - \frac{\alpha}{2} u_i (X'_i - X_i) |X'_i - X_i| \leq \epsilon_i |X' - X|$$

$$\begin{aligned} & \mathbb{P}[|X' - X| \geq \epsilon \text{ AND } |X'_i - X_i| \leq \epsilon_i \forall i] \\ &= \mathbb{P}\left(\left|\sum_{i=1}^L u_i (X'_i - X_i) \geq \epsilon\right| \text{ AND } |X'_i - X_i| \leq \epsilon_i \forall i\right) \\ &\leq \mathbb{P}\left(\sum_{i=1}^L |u_i| |X'_i - X_i| \geq \epsilon \text{ AND } |X'_i - X_i| \leq \epsilon_i \forall i\right) \\ &\leq \exp\left\{-\frac{\epsilon^2}{2\sum_i |u_i|^2 \epsilon_i^2}\right\} \leq \frac{\alpha}{2} \end{aligned}$$

$$|u_i||X'_i - X_i|$$

$$|X'_i - X_i| > \epsilon_i$$

$$\begin{aligned} \mathbb{P}[|X' - X| \geq \epsilon] &\leq \mathbb{P}[|X' - X| \geq \epsilon \text{ AND } |X'_i - X_i| \leq \epsilon_i \forall i] \\ &\quad + \mathbb{P}[|X'_i - X_i| > \epsilon_i \text{ for some } i] \\ &\leq \alpha, \end{aligned}$$

$$\epsilon^2 \geq 2\ln\left(\frac{2}{\alpha}\right) \sum_{i=1}^L |u_i|^2 \epsilon_i^2$$

$$\mathcal{L} = \sum_{i=1}^L \frac{c}{\epsilon_i} + \lambda \left(2\ln\left(\frac{2}{\alpha}\right) \sum_{i=1}^L |u_i|^2 \epsilon_i^2 - \epsilon^2 \right)$$

$$\frac{\partial \mathcal{L}}{\partial \epsilon_i} = \frac{\partial \mathcal{L}}{\partial \lambda}$$

$$\epsilon_i = \frac{\epsilon}{\sqrt{2\ln(2/\alpha)} |u_i|^{2/3} \|u\|_{2/3}^{1/3}},$$

$$\|u\|_{2/3} = \left(\sum_j |u_j|^{2/3} \right)^{3/2}$$

$$\mathcal{O}\left(\epsilon^{-1}|u_i|^{2/3}\|u\|_{2/3}^{1/3}\ln\frac{L}{\alpha}\sqrt{\ln\frac{1}{\alpha}}\right)$$

$$\mathcal{O}\left(\epsilon^{-1}\|u\|_{2/3}\ln\frac{L}{\alpha}\sqrt{\ln\frac{1}{\alpha}}\right)$$

$$\left|E^{(2)}-E_N^{(2)}\right|H=\sum_{i=1}^{L_H}h_i\sigma_i$$

$$V=\sum_{i=1}^{L_V}v_i\sigma_i$$

$$|\Phi_0\rangle E^{(2)}=\langle\Phi_0|VR_0V|\Phi_0\rangle$$

$$\begin{aligned} &\mathcal{O}\left(\frac{\|v\|_{2/3}^2\|h\|_1^{3/2}}{\Delta^{5/2}\epsilon}\ln^3\left(\frac{\|h\|_1^2\|v\|_1^2}{\Delta^3\epsilon}\right)\right)\\ &\times\ln\left(\frac{L_V^2\|h\|_1}{\alpha\Delta}\ln^2\left(\frac{\|h\|_1^2\|v\|_1^2}{\Delta^3\epsilon}\right)\right)\sqrt{\ln\frac{1}{\alpha}}\end{aligned}$$

$$\begin{aligned} &\mathcal{O}\left(\frac{\|v\|_{2/3}^2\|h\|_1^{3/2}}{\Delta^{7/2}\epsilon}\ln^5\left(\frac{\|h\|_1^2\|v\|_1^2}{\Delta^3\epsilon}\right)\right)\\ &\times\ln\left(\frac{L_V^2\|h\|_1}{\alpha\Delta}\ln^2\left(\frac{\|h\|_1^2\|v\|_1^2}{\Delta^3\epsilon}\right)\right)\sqrt{\ln\frac{1}{\alpha}}\end{aligned}$$

$$\left|E^{(2)}-E_N^{(2)}\right|X_N^{(2)}E_N^{(2)}$$

$$E^{(2)}=\sum_{n\in\mathbb{Z}}\beta_{\Delta,R,n}e^{iE_0t_n}\sum_{i,j=1}^{L_V}v_iv_j\langle\sigma_iU(t_n)\sigma_j\rangle$$

$$X_N^{(2)}=\sum_{|n|\leq N}\beta_{\Delta,R,n}e^{iE_0t_n}\sum_{i,j=1}^{L_V}v_iv_jX_{nij}$$

$$\langle\sigma_iU(t_n)\sigma_j\rangle$$

$$\left|E^{(2)}-E_N^{(2)}\right|\leq \frac{\epsilon}{2} \text{ if } N\geq \tilde{N}$$

$$\tilde{N}\leq \mathcal{O}\left(\frac{R}{\Delta}\ln^2\left(\frac{R^2\|v\|_1^2}{\Delta^3\epsilon}\right)\right)$$

$$\begin{aligned}
\left|X_{\tilde{N}}^{(2)} - E_{\tilde{N}}^{(2)}\right| &\leq \sum_{|n| \leq \tilde{N}} \sum_{i,j=1}^{L_V} |\beta_{\Delta,R,n} v_i v_j| \\
&\quad \times |X_{nij} - \langle \sigma_i U(t_n) \sigma_j \rangle| \\
\left|E^{(2)} - X_{\tilde{N}}^{(2)}\right| &\leq \left|E^{(2)} - E_{\tilde{N}}^{(2)}\right| + \left|E_{\tilde{N}}^{(2)} - X_{\tilde{N}}^{(2)}\right| \leq \epsilon \\
\|v^2 \beta_{\Delta,R}\|_{2/3} &\equiv \left(\sum_{|n| \leq \tilde{N}} \sum_{i,j=1}^{L_V} |\beta_{\Delta,R,n} v_i v_j|^{2/3} \right)^{3/2} \\
&= \|v\|_{2/3}^2 \left(\sum_{|n| \leq \tilde{N}} |\beta_{\Delta,R,n}|^{2/3} \right)^{3/2} \\
&= \mathcal{O} \left(\frac{\|v\|_{2/3}^2 R^{3/2}}{\Delta^{5/2}} \ln^3 \left(\frac{R^2 \|v\|_1^2}{\Delta^3 \epsilon} \right) \right)
\end{aligned}$$

$$\begin{aligned}
&\mathcal{O} \left(\frac{\|v^2 \beta_{\Delta,R}\|_{2/3}}{\epsilon} \ln \left(\frac{L_V^2 \tilde{N}}{\alpha} \right) \sqrt{\ln \frac{1}{\alpha}} \right) \\
&= \mathcal{O} \left(\frac{\|v\|_{2/3}^2 R^{3/2}}{\Delta^{5/2} \epsilon} \ln^3 \left(\frac{R^2 \|v\|_1^2}{\Delta^3 \epsilon} \right) \right. \\
&\quad \times \ln \left(\frac{L_V^2 R}{\alpha \Delta} \ln^2 \left(\frac{R^2 \|v\|_1^2}{\Delta^3 \epsilon} \right) \right) \left. \sqrt{\ln \frac{1}{\alpha}} \right)
\end{aligned}$$

$$t_{\tilde{N}} = \frac{2\pi \tilde{N}}{R + \Delta}$$

$$\begin{aligned}
&\mathcal{O} \left(\frac{\tilde{N} \|v^2 \beta_{\Delta,R}\|_{2/3}}{R \epsilon} \ln \left(\frac{L_V^2 \tilde{N}}{\alpha} \right) \sqrt{\ln \frac{1}{\alpha}} \right) \\
&= \mathcal{O} \left(\frac{\|v\|_{2/3}^2 R^{3/2}}{\Delta^{7/2} \epsilon} \ln^5 \left(\frac{R^2 \|v\|_1^2}{\Delta^3 \epsilon} \right) \right. \\
&\quad \times \ln \left(\frac{L_V^2 R}{\alpha \Delta} \ln^2 \left(\frac{R^2 \|v\|_1^2}{\Delta^3 \epsilon} \right) \right) \left. \sqrt{\ln \frac{1}{\alpha}} \right)
\end{aligned}$$

$$R = E_{D-1} - E_0$$

$$\begin{aligned}
R &\leq 2 \max_{i=0,\dots,D-1} |E_i| \\
&= 2 \sup_{\|\psi\|=1} \|H|\psi\rangle\|_2 \\
&\leq 2 \sup_{\|\psi\|=1} \sum_{i=1}^{L_H} |h_i| \|\sigma_i|\psi\rangle\|_2 \\
&\leq 2 \|h\|_1
\end{aligned}$$

$$\begin{aligned}
T_1(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b \in \mathcal{I}_{act}}} h'_{va} h'_{vb} \langle a_b^\dagger a_v U(t) a_v^\dagger a_a \rangle \\
T_2(t) &= \frac{1}{2} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} h'_{vd} g_{vabc} \langle a_d^\dagger a_v U(t) a_v^\dagger a_a^\dagger a_b a_c \rangle \\
&\quad + \frac{1}{2} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} h'_{vac} \frac{g_{avbc}}{g_{vac}} \langle a_d^\dagger a_v U(t) \frac{a_a^\dagger a_v^\dagger a_b a_c}{a_v^\dagger a_a^\dagger a_c a_b} \rangle \\
T_3(t) &= \frac{1}{2} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} h'_{va} g_{vbcd} \langle a_d^\dagger a_c^\dagger a_b a_v U(t) a_v^\dagger a_a \rangle \\
&\quad + \frac{1}{2} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} h'_{va} \frac{g_{bvcd}}{g_{vbd}} \langle \frac{a_d^\dagger a_c^\dagger a_v a_b}{a_c^\dagger a_d^\dagger a_b a_v} U(t) a_v^\dagger a_a \rangle \\
T_4(t) &= \frac{1}{4} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d, e, f \in \mathcal{I}_{act}}} g_{vabc} g_{vdef} \langle a_f^\dagger a_e^\dagger a_d a_v U(t) a_v^\dagger a_a^\dagger a_b a_c \rangle \\
&\quad + \frac{1}{4} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d, e, f \in \mathcal{I}_{act}}} g_{vabc} \frac{g_{dvef}}{g_{vdf}} \langle \frac{a_f^\dagger a_e^\dagger a_v a_d}{a_e^\dagger a_f^\dagger a_d a_v} U(t) a_v^\dagger a_a^\dagger a_b a_c \rangle \\
&\quad + \frac{1}{4} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d, e, f \in \mathcal{I}_{act}}} g_{vdef} \frac{g_{avbc}}{g_{vacb}} \langle a_f^\dagger a_e^\dagger a_d a_v U(t) \frac{a_a^\dagger a_v^\dagger a_b a_c}{a_v^\dagger a_a^\dagger a_c a_b} \rangle \\
&\quad + \frac{1}{4} \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d, e, f \in \mathcal{I}_{act}}} \frac{g_{vacb}}{g_{avbc}} \frac{g_{dvef}}{g_{vdf}} \langle \frac{a_f^\dagger a_e^\dagger a_v a_d}{a_e^\dagger a_f^\dagger a_d a_v} U(t) \frac{a_a^\dagger a_v^\dagger a_b a_c}{a_v^\dagger a_a^\dagger a_c a_b} \rangle \\
&\quad + \frac{1}{4} \sum_{\substack{v, w \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} g_{vwab} g_{vwcd} \langle a_d^\dagger a_c^\dagger a_w a_v U(t) a_v^\dagger a_w^\dagger a_a a_b \rangle \\
&\quad + \frac{1}{4} \sum_{\substack{v, w \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} g_{vwab} \frac{g_{wvcd}}{g_{vwcd}} \langle \frac{a_d^\dagger a_c^\dagger a_v a_w}{a_c^\dagger a_d^\dagger a_w a_v} U(t) a_v^\dagger a_w^\dagger a_a a_b \rangle
\end{aligned}$$

$$\begin{aligned}
T_1(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b \in \mathcal{I}_{act}}} h'_{va} h'_{vb} \langle a_b^\dagger a_v U(t) a_v^\dagger a_a \rangle \\
T_2(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} h'_{vd} g_{vabc} \langle a_d^\dagger a_v U(t) a_v^\dagger a_a^\dagger a_b a_c \rangle \\
T_3(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} h'_{va} g_{vbcd} \langle a_d^\dagger a_c^\dagger a_b a_v U(t) a_v^\dagger a_a \rangle \\
T_4(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d, e, f \in \mathcal{I}_{act}}} g_{vabc} g_{vdef} \langle a_f^\dagger a_e^\dagger a_d a_v U(t) a_v^\dagger a_a^\dagger a_b a_c \rangle \\
&+ \frac{1}{2} \sum_{\substack{v, w \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} g_{vwab} g_{vwcd} \langle a_d^\dagger a_c^\dagger a_w a_v U(t) a_v^\dagger a_w^\dagger a_a a_b \rangle.
\end{aligned}$$

$$a_v(t) \equiv e^{iHt} a_v e^{-iHt} = a_v e^{-i\epsilon_v t}$$

$$\begin{aligned}
T_1(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b \in \mathcal{I}_{act}}} h'_{va} h'_{vb} e^{-i(E_{core} + \epsilon_v)t} \langle a_b^\dagger e^{-iH_{CAST}t} a_a \rangle \\
T_2(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} g_{vabc} h'_{vd} e^{-i(E_{core} + \epsilon_v)t} \langle a_d^\dagger e^{-iH_{CAST}t} a_a^\dagger a_b a_c \rangle \\
T_3(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} h'_{va} g_{vbcd} e^{-i(E_{core} + \epsilon_v)t} \langle a_d^\dagger a_c^\dagger a_b e^{-iH_{CAST}t} a_a \rangle \\
T_4(t) &= \sum_{\substack{v \in \mathcal{I}_{virt} \\ a, b, c, d, e, f \in \mathcal{I}_{act}}} g_{vabc} g_{vdef} e^{-i(E_{core} + \epsilon_v)t} \langle a_f^\dagger a_e^\dagger a_d e^{-iH_{CAST}t} a_a^\dagger a_b a_c \rangle \\
&+ \frac{1}{2} \sum_{\substack{v, w \in \mathcal{I}_{virt} \\ a, b, c, d \in \mathcal{I}_{act}}} g_{vwab} g_{vwcd} e^{-i(E_{core} + \epsilon_v + \epsilon_w)t} \\
&\times \langle a_d^\dagger a_c^\dagger e^{-iH_{CAST}t} a_a a_b \rangle.
\end{aligned}$$

$$\begin{aligned}
v_{a,b}(t) &= \sum_{v \in \mathcal{I}_{virt}} h'_{va} h'_{vb} e^{-i(\epsilon_v + E_{core})t} \\
v_{abc,d}(t) &= \sum_{v \in \mathcal{I}_{virt}} h'_{vd} g_{vabc} e^{-i(\epsilon_v + E_{core})t} \\
v_{abc,def}(t) &= \sum_{v \in \mathcal{I}_{virt}} g_{vabc} g_{vdef} e^{-i(\epsilon_v + E_{core})t} \\
v_{ab,cd}(t) &= \frac{1}{2} \sum_{v, w \in \mathcal{I}_{virt}} g_{vwab} g_{vwcd} e^{-i(\epsilon_v + \epsilon_w + E_{core})t},
\end{aligned}$$

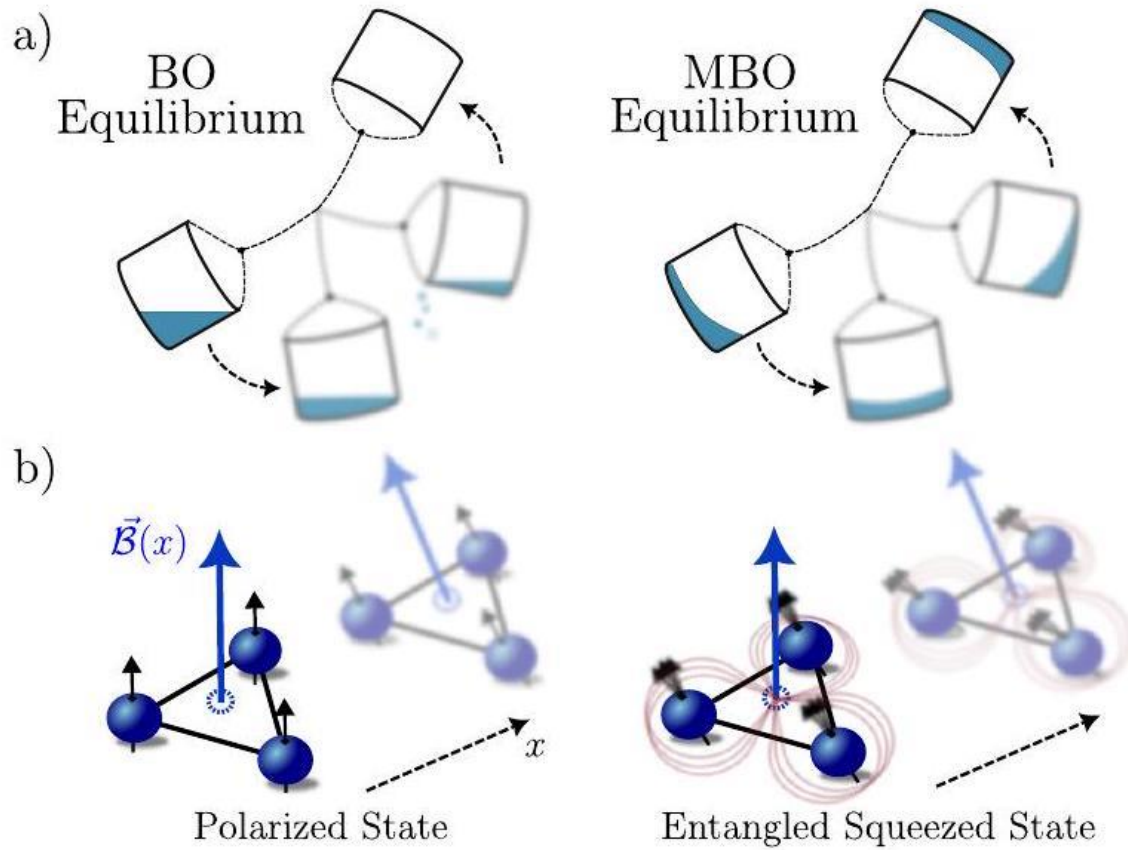
$$\|h\|_1 \|v\|_{2/3} V = H'_{el} - H$$



$$\begin{aligned}
H &= \sum_{a,b \in \mathcal{I}_{act}} h'_{ab} a_a^\dagger a_b + \frac{1}{2} \sum_{a,b,c,d \in \mathcal{I}_{act}} g_{abcd} a_a^\dagger a_b^\dagger a_c a_d \\
&+ \sum_{v \in \mathcal{I}_{virt}} \epsilon_v a_v^\dagger a_v + E_{core} \\
&\rightarrow \\
&\sum_{a,b \in \mathcal{I}_{act}} \sum_{i=1}^4 \frac{h'_{ab}}{4} \sigma_{abi} + \sum_{a,b,c,d \in \mathcal{I}_{act}} \sum_{i=1}^{16} \frac{g_{abcd}}{32} \sigma_{abcdi} \\
&+ \sum_{v \in \mathcal{I}_{virt}} \sum_{i=1}^4 \frac{\epsilon_v}{4} \sigma_{vi} + E_{core} \\
\|h\|_1 &\leq \sum_{a,b \in \mathcal{I}_{act}} |h'_{ab}| + \frac{1}{2} \sum_{a,b,c,d \in \mathcal{I}_{act}} |g_{abcd}| + \sum_{v \in \mathcal{I}_{virt}} |\epsilon_v| + |E_{core}|. \\
V &= \sum_{\substack{p,q \in \mathcal{I}_{act} \cup \mathcal{I}_{virt} \\ \{p,q\} \notin \mathcal{I}_{act}}} h'_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{\substack{p,q,r,s \in \mathcal{I}_{virt} \cup \mathcal{I}_{act} \\ \{p,q,r,s\} \notin \mathcal{I}_{act}}} g_{pqrs} a_p^\dagger a_q^\dagger a_r a_s - F_{virt} \\
&\rightarrow \\
&\sum_{\substack{p,q \in \mathcal{I}_{act} \cup \mathcal{I}_{virt} \\ \{p,q\} \notin \mathcal{I}_{act}}} \sum_{i=1}^4 \frac{h'_{pq}}{4} \sigma_{pqi} - \sum_{v \in \mathcal{I}_{virt}} \sum_{i=1}^4 \frac{\epsilon_v}{4} \sigma_{vi} \\
&+ \sum_{\substack{p,q,r,s \in \mathcal{I}_{virt} \cup \mathcal{I}_{act} \\ \{p,q,r,s\} \notin \mathcal{I}_{act}}} \sum_{i=1}^{16} \frac{g_{pqrs}}{32} \sigma_{pqrsi} \\
\|v\|_{2/3} &\leq 2 \left(\sum_{\substack{p,q \in \mathcal{I}_{act} \cup \mathcal{I}_{virt} \\ \{p,q\} \notin \mathcal{I}_{act}}} |h'_{pq}|^{2/3} + \sum_{v \in \mathcal{I}_{virt}} |\epsilon_v|^{2/3} \right. \\
&\quad \left. + \sum_{\substack{p,q,r,s \in \mathcal{I}_{virt} \cup \mathcal{I}_{act} \\ \{p,q,r,s\} \notin \mathcal{I}_{act}}} |g_{pqrs}|^{2/3} \right)^{3/2} \\
&\|h^{CAS}\|_1 \|v^{MRPT(2)}\|_{2/3} \|h\|_1 \\
\|h^{CAS}\|_1 &\leq \sum_{a,b \in \mathcal{I}_{act}} |h'_{ab}| + \frac{1}{2} \sum_{a,b,c,d \in \mathcal{I}_{act}} |g_{abcd}|. \\
&\|v^{MRPT(2)}\|_{2/3}
\end{aligned}$$

$$\begin{aligned}
\langle VU(t_n)V \rangle &= T_1(t_n) + T_2(t_n) + T_3(t_n) + T_4(t_n) \\
&= \frac{1}{4} \sum_{a,b \in \mathcal{I}_{act}} \sum_{ij=1}^2 v_{a,b}(t_n) \langle \sigma_{bj} e^{-iH_{CAS} t_n} \sigma_{ai} \rangle \\
&+ \frac{1}{16} \sum_{a,b,c,d \in \mathcal{I}_{act}} \sum_{i=1}^8 \sum_{j=1}^2 v_{abc,d}(t_n) \langle \sigma_{dj} e^{-iH_{CAS} t_n} \sigma_{abci} \rangle \\
&+ \frac{1}{16} \sum_{a,b,c,d \in \mathcal{I}_{act}} \sum_{i=1}^2 \sum_{j=1}^8 v_{bcd,a}(t_n) \langle \sigma_{bcdj} e^{-iH_{CAS} t_n} \sigma_{ai} \rangle \\
&+ \frac{1}{32} \sum_{a,b,c,d \in \mathcal{I}_{act}} \sum_{ij=1}^4 v_{ab,cd}(t_n) \langle \sigma_{cdj} e^{-iH_{CAS} t_n} \sigma_{abi} \rangle \\
&+ \frac{1}{64} \sum_{a,b,c,d,e,f \in \mathcal{I}_{act}} \sum_{ij=1}^8 v_{abc,def}(t_n) \langle \sigma_{defj} e^{-iH_{CAS} t_n} \sigma_{abci} \rangle, \\
&L^{\text{MRPT}(2)} \sum_{i=1} v_{ni}^{\text{MRPT}(2)} \langle \sigma_{i,1} e^{-iH_{CAS} t_n} \sigma_{i,2} \rangle \\
&\left(\sum_i |v_{ni}^{\text{MRPT}(2)}|^{2/3} \right)^{3/2} \\
&\leq \left(2^{2/3} \sum_{a,b \in \mathcal{I}_{act}} |v_{a,b}(t_n)|^{2/3} + 2^{7/3} \sum_{a,b,c,d \in \mathcal{I}_{act}} |v_{abc,d}(t_n)|^{2/3} \right. \\
&\quad \left. + 2^{2/3} \sum_{a,b,c,d \in \mathcal{I}_{act}} |v_{ab,cd}(t_n)|^{2/3} + 4 \sum_{a,b,c,d,e,f \in \mathcal{I}_{act}} |v_{abc,def}(t_n)|^{2/3} \right)^{3/2} \\
&\leq \left(2^{2/3} \sum_{a,b \in \mathcal{I}_{act}} \left(\sum_{v \in \mathcal{I}_{virt}} |h'_{va} h'_{vb}| \right)^{2/3} \right. \\
&\quad + 2^{7/3} \sum_{a,b,c,d \in \mathcal{I}_{act}} \left(\sum_{v \in \mathcal{I}_{virt}} |h'_{va} g_{vbcd}| \right)^{2/3} \\
&\quad + 2^{2/3} \sum_{a,b,c,d \in \mathcal{I}_{act}} \left(\sum_{vw \in \mathcal{I}_{virt}} |g_{vwab} g_{vwcd}| \right)^{2/3} \\
&\quad \left. + 4 \sum_{a,b,c,d,e,f \in \mathcal{I}_{act}} \left(\sum_{v \in \mathcal{I}_{virt}} |g_{vabc} g_{vdef}| \right)^{2/3} \right)^{3/2} \\
&\equiv \|v^{\text{MRPT}(2)}\|_{2/3}.
\end{aligned}$$

$$H(\hat{\sigma}, \hat{x}, \hat{q}) = \frac{\hat{q}^2}{2M} + V(\hat{x}) + H_{\text{int}}(\hat{\sigma}, \hat{x})$$



$$H_{\text{int}}(\hat{x}, \hat{\sigma}) = -\mu \vec{B}(\hat{x}) \cdot \hat{\sigma}.$$

$$\Omega(x, p) = \int_{-\infty}^{\infty} d\xi \langle x - \xi/2 | \hat{\Omega} | x + \xi/2 \rangle e^{i \frac{p\xi}{\hbar}}$$

$$f(\hat{x}) \leftrightarrow f(x)$$

$$g(\hat{q}) \leftrightarrow g(p)$$

$$(\hat{x}\hat{q} + \hat{q}\hat{x})/2 \leftrightarrow xp$$

$$\hat{\mathbf{H}}(x, p) = (p^2/(2M) + V(x))\hat{\mathbf{I}} + \hat{\mathbf{H}}_{\text{int}}(x) = (p^2/(2M) + V(x))\hat{\mathbf{I}} - \mu \vec{B}(x) \cdot \hat{\sigma}$$

$$\hat{\mathbf{H}}(x, p) |\psi_n^{\text{BO}}(x)\rangle$$

$$|\psi_n^{\text{BO}}(x)\rangle \mathbf{U}_{\text{BO}}(x) \hat{\mathbf{H}}_{\text{int}}(x) \vec{B}(x)$$

$$\mathcal{H}_n^{\text{BO}}(x, p) = \langle \psi_n^{\text{BO}}(x) | \hat{\mathbf{H}}(x, p) | \psi_n^{\text{BO}}(x) \rangle.$$

$$\dot{x} = \partial_p \mathcal{H}_n^{\text{BO}}, \dot{p} = -\partial_x \mathcal{H}_n^{\text{BO}}$$

$$\mathcal{H}_{\pm}^{\text{BO}}(x, p) = p^2/2M + V(x) \pm \mu B(x)$$

$$V_n^{\text{BO}}(x) \equiv \langle \psi_n^{\text{BO}}(x) | \hat{\mathbf{H}}_{\text{int}}(x) | \psi_n^{\text{BO}}(x) \rangle$$

$$\hat{U}_{\text{BO}} \equiv U_{\text{BO}}(\hat{x}) \hat{U}_{\text{BO}}^{\dagger} \hat{O} \hat{U}_{\text{BO}}$$

$$\hat{\mathbf{x}} \rightarrow \hat{\mathbf{x}}^M \equiv x\hat{\mathbf{I}}, \hat{\mathbf{q}} \rightarrow \hat{\mathbf{q}}^M \equiv p\hat{\mathbf{I}} - \hat{\mathbf{A}}_x(x),$$

$$\hat{\mathbf{A}}_x(x) = i\hbar(\partial_x \hat{\mathbf{U}}_{\text{BO}}) \hat{\mathbf{U}}_{\text{BO}}^\dagger \vec{\mathbf{B}}(x)$$

$$\hat{\mathbf{A}}_x(x) = -\frac{\hbar}{2}\theta'(x)\hat{\sigma}_x|\psi_n^{\text{BO}}(x)\rangle$$

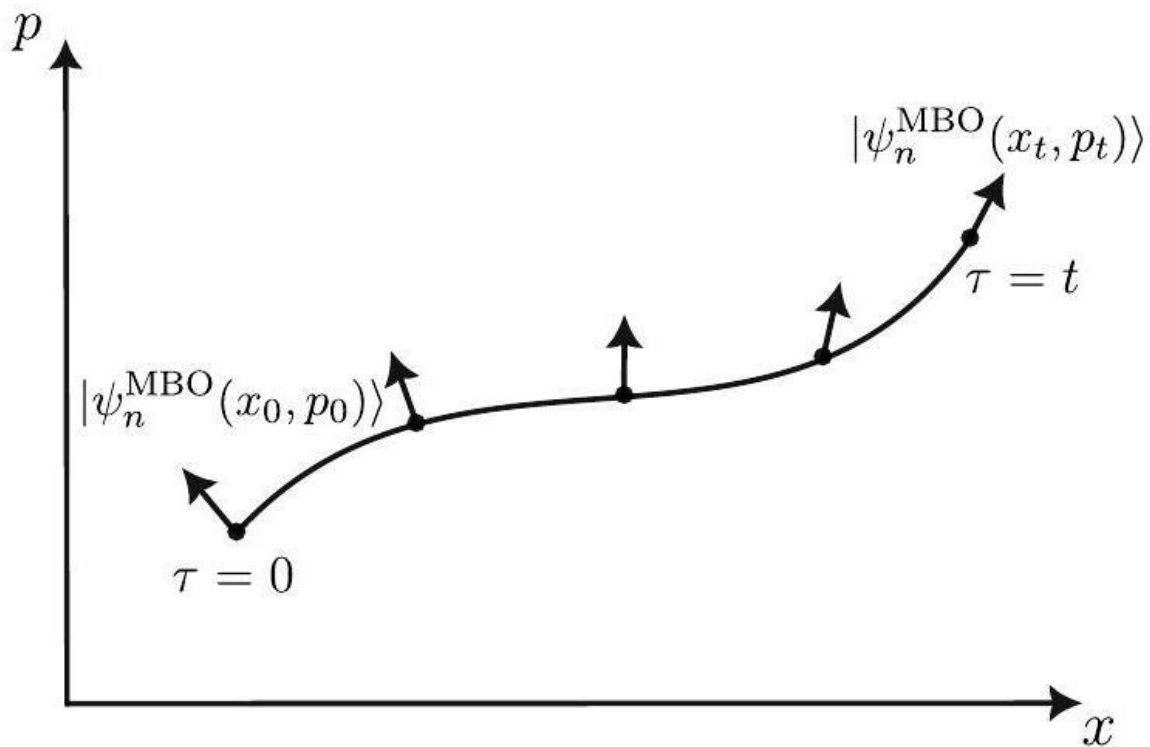
$$p \pm \hbar\theta'(x)/2$$

$$\hat{\mathbf{H}}^M(x,p) = \frac{(p - \hat{\mathbf{A}}_x(x))^2}{2M} + V(x) + \hat{\mathbf{H}}_{\text{int}}(x),$$

$$= \hat{\mathbf{H}}(x,p) - \frac{p\hat{\mathbf{A}}_x(x)}{M} + \frac{\hat{\mathbf{A}}_x^2(x)}{2M}.$$

$$\langle \psi_n^{\text{BO}}(x) | \hat{\mathbf{H}}^M(x,p) | \psi_n^{\text{BO}}(x) \rangle$$

$$\hat{\mathbf{H}}^M(x,p) | \psi_n^{\text{MBO}}(x,p) \rangle = \mathcal{H}_n^{\text{MBO}}(x,p) | \psi_n^{\text{MBO}}(x,p) \rangle.$$



$$\mathcal{H}_n^{\text{MBO}}(x,p) = \langle \psi_n^{\text{MBO}}(x,p) | \hat{\mathbf{H}}^M(x,p) | \psi_n^{\text{MBO}}(x,p) \rangle.$$

$$\hat{\Omega} = \Omega(\hat{x}, \hat{p}, t)$$

$$\frac{dx}{dt} = \frac{\partial \mathcal{H}_n^{\text{MBO}}(x,p)}{\partial p} = \langle \psi_n^{\text{MBO}} | \partial_p \hat{\mathbf{H}}^M | \psi_n^{\text{MBO}} \rangle$$

$$\frac{dp}{dt} = -\frac{\partial \mathcal{H}_n^{\text{MBO}}(x,p)}{\partial x} = -\langle \psi_n^{\text{MBO}} | \partial_x \hat{\mathbf{H}}^M | \psi_n^{\text{MBO}} \rangle.$$

$$(x_n(t), p_n(t))$$

$$\Omega_n^M(x,p) \equiv \langle \psi_n^{\text{MBO}}(x,p) | \hat{\Omega}^M(x,p) | \psi_n^{\text{MBO}}(x,p) \rangle$$

$$x = x_n(t)$$

$$p = p_n(t)$$

$$\langle \hat{\mathbf{q}}^{\text{M}}(t) \rangle = p_0(t) - A_x(t)$$

$$A_x(t) \equiv \langle \psi_0(t) | \hat{\mathbf{A}}_x(x_0(t)) | \psi_0(t) \rangle$$

$$|\psi_0(t)\rangle \equiv |\psi_0^{\text{MBO}}(x_0(t), p_0(t))\rangle$$

$$\left\langle (\hat{\mathbf{q}}^{\text{M}})^2(t) \right\rangle = [p_0(t) - A(t)]^2 + g_{xx}(t)$$

$$g_{xx}(t) = \langle \psi_0(t) | \hat{\mathbf{A}}_x^2(x_0(t)) | \psi_0(t) \rangle - A_x^2(t)$$

$$\Omega_n^{\text{M}}(t)\{x,p\} \equiv \{x_n(0), p_n(0)\} W_n^{\text{M}}(x,p)$$

$$\langle \hat{\Omega}(t) \rangle \approx \int \frac{dx \, dp}{2\pi\hbar} W_n^{\text{M}}(x,p) \Omega_n^{\text{M}}(t)$$

$$\Omega_n^{\text{M}}(t) = \Omega_n^{\text{M}}(x_n(t), p_n(t)) \hat{\Omega}^{\text{M}}(x,p) \hat{\Omega}_{mn}^{\text{M}}(x,p) \hat{\mathbf{H}}^{\text{M}}(x,p) \hat{\Omega}_{mn}^{\text{M}} \mathcal{H}_{mn}^{\text{MBO}}$$

$$\mathcal{H}_{mn}^{\text{MBO}}(x,p) \equiv \frac{\mathcal{H}_m^{\text{MBO}}(x,p) + \mathcal{H}_n^{\text{MBO}}(x,p)}{2}$$

$$\dot{x} = \partial_p \mathcal{H}_{mn}^{\text{MBO}}$$

$$\dot{p} = -\partial_x \mathcal{H}_{mn}^{\text{MBO}}$$

$$\hat{\Omega}_{mn}^{\text{M}}(t) = \text{e}^{i\Phi_{mn}(t)} \hat{\Omega}_{mn}^{\text{M}}(x_{mn}(t), p_{mn}(t)),$$

$$\Phi_{mn}(t) = \frac{1}{\hbar} \int_0^t \text{d}\tau [\mathcal{H}_m^{\text{MBO}}(x_{mn}(\tau), p_{mn}(\tau)) - \mathcal{H}_n^{\text{MBO}}(x_{mn}(\tau), p_{mn}(\tau))]$$

$$\mathcal{H}_{nn}^{\text{MBO}} = \mathcal{H}_n^{\text{MBO}}$$

$$\langle \hat{\Omega}(t) \rangle \approx \int \frac{dx \, dp}{2\pi\hbar} \text{Tr}\{\hat{\mathbf{W}}^{\text{M}}(x,p) \hat{\Omega}^{\text{M}}(t)\}$$

$$\vec{B}(x) = \mathcal{B}(x)(\cos \theta(x) \hat{z} + \sin \theta(x) \hat{y})$$

$$\hat{\mathbf{H}}^{\text{M}} = \frac{p^2}{2M} + \frac{\hbar^2(\theta'(x))^2}{8M} - \mu \vec{B}(x) \cdot \hat{\vec{\sigma}} + \frac{\hbar}{2M} p \theta'(x) \hat{\sigma}_{\perp},$$

$$\hat{\sigma}_{\perp} \equiv \hat{\sigma}_x$$

$$\mathcal{B}_{\text{eff}}(x,p) = \sqrt{\mathcal{B}(x)^2 + \frac{\hbar^2 p^2 (\theta'(x))^2}{4M^2 \mu^2}}$$

$$\phi(x,p) = \tan^{-1} \left(\frac{\hbar \theta'(x) p}{2M \mu \mathcal{B}(x)} \right)$$

$$\mathcal{B}(x) = \mathcal{B}$$



$$\theta(x)=\theta_0(1+\mathrm{erf}(x/d))$$

$$|\psi_-^{\rm MBO}\rangle=\cos\left(\phi/2\right)|\psi_-^{\rm BO}\rangle-\sin\left(\phi/2\right)|\psi_+^{\rm BO}\rangle$$

$$\mathcal{H}^{\rm MBO}_{\mp}(x,p)=\frac{p^2}{2M}+\frac{\hbar^2(\theta'(x))^2}{2M}\mp\mu\mathcal{B}_{\rm eff}(x,p).$$

$$\mathcal{H}^{\rm MBO}_-(x,p)|\tan\left(\phi(x,p)\right)|\ll \mathcal{B}_{\rm eff}\left(x,p\right)$$

$$M\rightarrow M+\kappa(x), \text{ with } \kappa(x)=\frac{(\hbar\theta'(x))^2}{4\mu\mathcal{B}(x)}$$

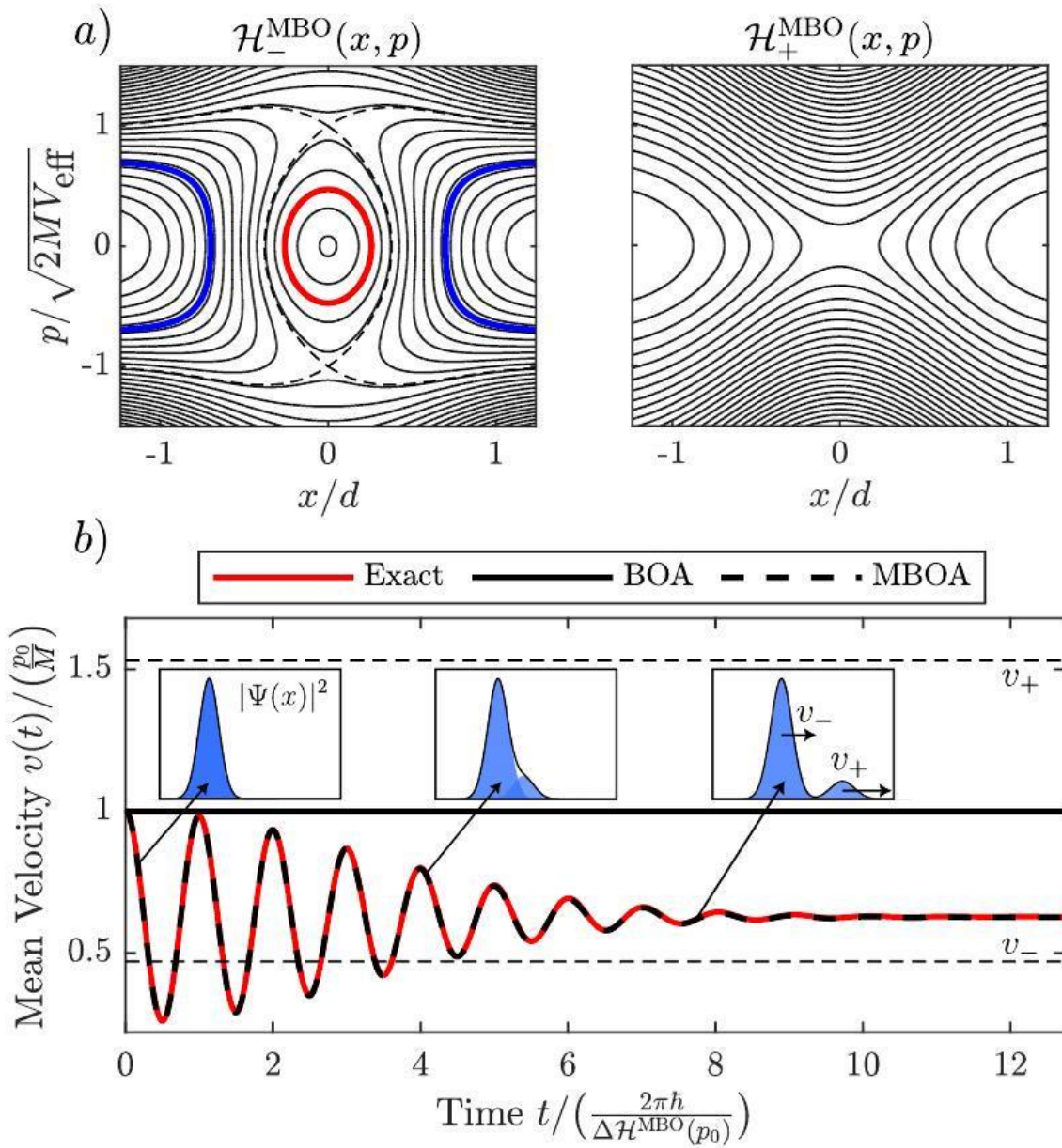
$$M\dot{x}=M\langle\partial_p\hat{\mathbf{H}}^{\rm M}\rangle=p-\langle\hat{\mathbf{A}}_x(x)\rangle=\langle\hat{\mathbf{q}}^{\rm M}\rangle$$

$$A(x,p)\equiv\langle\hat{\mathbf{A}}_x\rangle$$

$$\dot{p}=-\langle\partial_x\hat{\mathbf{H}}^{\rm M}\rangle$$

$$\dot{x}_{\pm}=\left.\langle\partial_p\hat{\mathbf{H}}^{\rm M}\rangle_{\pm}\right|_{p=p_0}=\frac{p_0}{M}\pm\frac{\hbar\theta'}{2M}\sin\phi(p_0)$$

$$\hat{\mathbf{q}}^{\rm M}_{mn}(t)\,\hbar\omega=\Delta\mathcal{H}^{\rm MBO}(p_0)=\mathcal{H}^{\rm MBO}_+(p_0)-\mathcal{H}^{\rm MBO}_-(p_0)$$



$$\hat{H} = \frac{\hat{p}^2}{2M} - \sum_{i=1}^N \mu \vec{B}(\hat{x}) \cdot \hat{\sigma}_i.$$

$$\hat{\mathbf{A}}_x(x) = -\hbar\theta'(x)\hat{\mathbf{S}}_x$$

$$\hat{\mathbf{S}}_x = \sum_{i=1}^N \hat{\sigma}_x^i/2$$

$$\hat{\mathbf{H}}^{\mathbf{M}} = \frac{p^2}{2M} - 2\mu\vec{B}(x) \cdot \hat{\mathbf{S}} + \frac{p\hbar\theta'(x)}{M}\hat{\mathbf{S}}_{\perp} + \frac{(\hbar\theta'(x))^2}{2M}\hat{\mathbf{S}}_{\perp}^2,$$

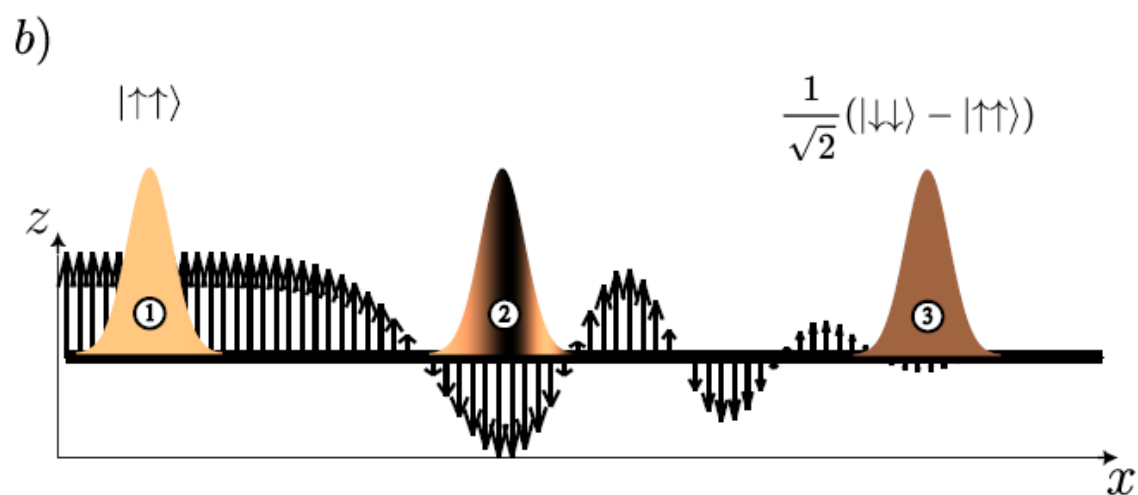
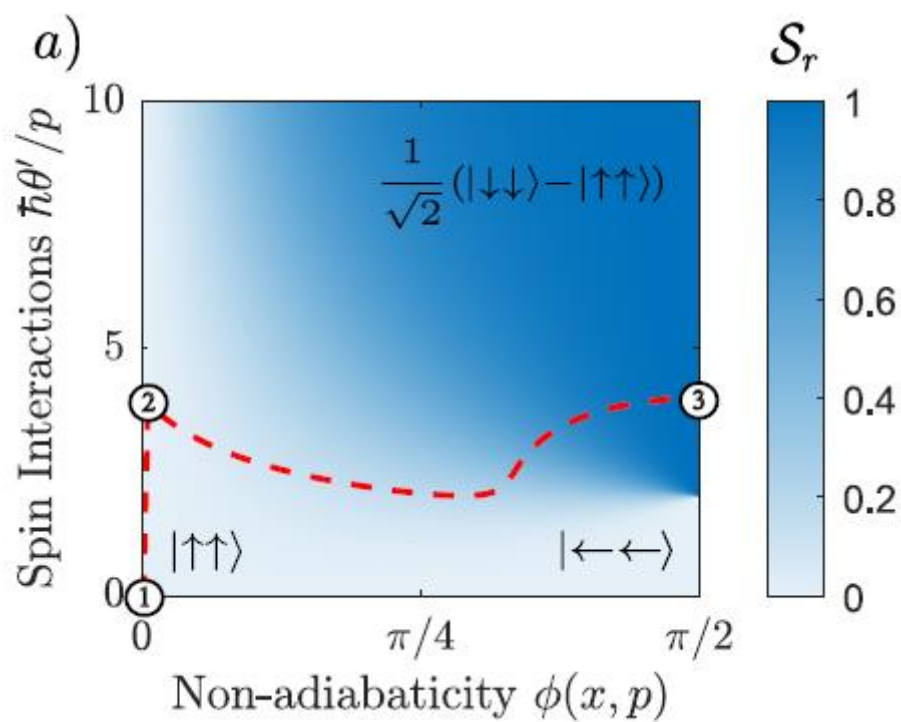
$$\phi=\tan^{-1}\left(\hbar\theta'p/2M\mu B\right)\text{ and }\hbar\theta'/p$$

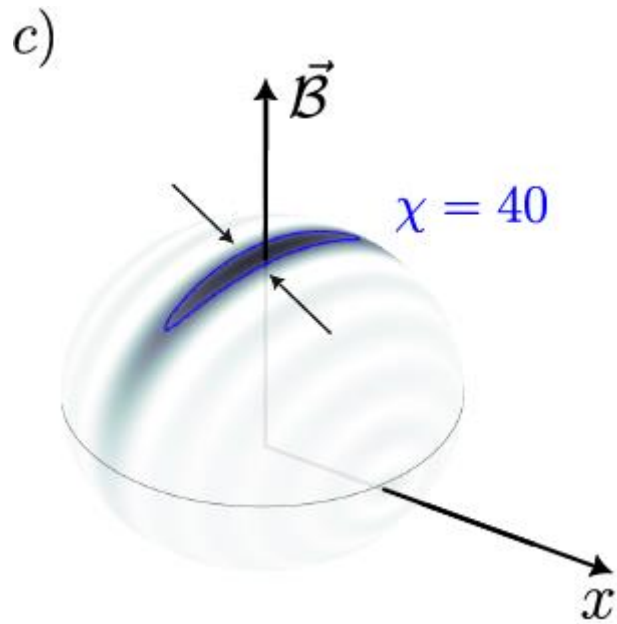
$$\mathcal{S}_r=-\text{Tr}(\rho_r\log_2\,\rho_r)$$

$$\hbar\theta'/p>2$$

$$\phi \rightarrow \pi/2$$

$$S_x = \frac{1}{\sqrt{2}}(|\downarrow\downarrow\rangle - |\uparrow\uparrow\rangle)$$





$$\chi \equiv \frac{N(\hbar\theta')^2}{4m\mu B}$$

$$\frac{\Delta\hat{S}_x}{\Delta\hat{S}_y} = \frac{1}{\sqrt{1+\chi}},$$

$$\Delta\hat{S}_i = \sqrt{\langle\hat{S}_i^2\rangle - \langle\hat{S}_i\rangle^2}$$

$$\Delta\hat{S}_x\Delta\hat{S}_y = N/4$$

$$\Delta\hat{S}_x/N \sim 1/N$$

$$\vec{\xi} = (\xi_1, \dots, \xi_N)$$

$$\vec{\eta} = (\eta_1, \dots, \eta_N)$$

$$H(\vec{\xi},\vec{\eta},x,q)=\frac{q^2}{2M}+V(x)+H_{\rm int}(\vec{\xi},\vec{\eta},x)$$

$$V(x)=kx^2/2$$

$$H_{\rm int}(\vec{\xi},\vec{\eta},x)=\frac{|\vec{\eta}|^2}{2m}+U_0\sum_{i=1}^N\left(\Theta(-\xi_i)+\Theta(\xi_i-x)\right),$$

$$\frac{|\vec{\eta}|^2}{2m}=E_0^{\rm fast}$$

$$x_*=\sqrt{2E_0^{\rm fast}/k}$$

$$\mathbf{H}_{\rm int}(x)\equiv H_{\rm int}(\vec{\xi},\vec{\eta},x)$$

$$\rho(x)=\delta(E^{\rm fast}(x)-\mathbf{H}_{\rm int}(x))$$

$$S(x,E^{\rm fast})=\ln \Omega(x,E^{\rm fast})$$

$$\Omega(x,E^{\rm fast})=\int \mathrm{d}\vec{\xi}\,\mathrm{d}\vec{\eta}\delta(E^{\rm fast}-\mathbf{H}_{\rm int}(x))$$

$$S=N/2\ln\left(x^2E^{\rm fast}(x)\right)+\mathrm{const}$$

$$\mathcal{H}^{\rm BO}(x,p)=\frac{p^2}{2M}+\frac{1}{2}kx^2+E_0^{\rm fast}\left(\frac{x_0}{x}\right)^2,$$

$$V^{\rm BO}(x)=E_0^{\rm fast}(x_0/x)^2$$

$$\hbar^2\pi^2n^2/(2mx^2)$$

$$\vec{\xi}'(x)=\frac{\vec{\xi}}{x},\qquad \vec{\eta}'(x)=x\vec{\eta}$$

$$\mathbf{q}=p-\mathbf{A}_x(x)=p-\sum_{i=1}^NA_x^{(i)}(\xi_i,\eta_i,x)$$

$$\mathrm{d}\xi'_i/\mathrm{d}x=\left\{A_x^{(i)}(\xi'_i,\eta'_i,x),\xi'_i\right\}$$

$$\mathrm{d}\eta'_i/\mathrm{d}x=\left\{A_x^{(i)}(\xi'_i,\eta'_i,x),\eta'_i\right\}$$

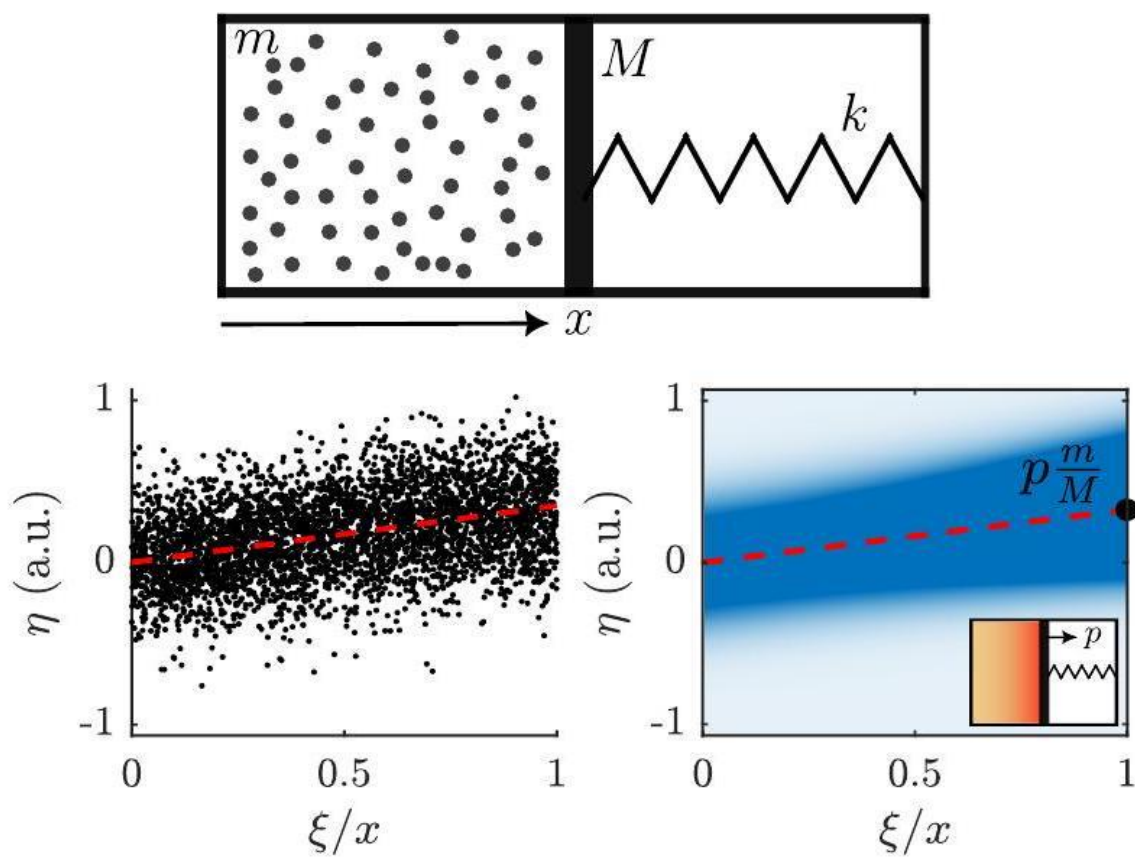
$$\mathbf{A}_x(x)=\vec{\xi}\cdot\vec{\eta}/x=\vec{\xi}'(x)\cdot\vec{\eta}'(x)/x$$

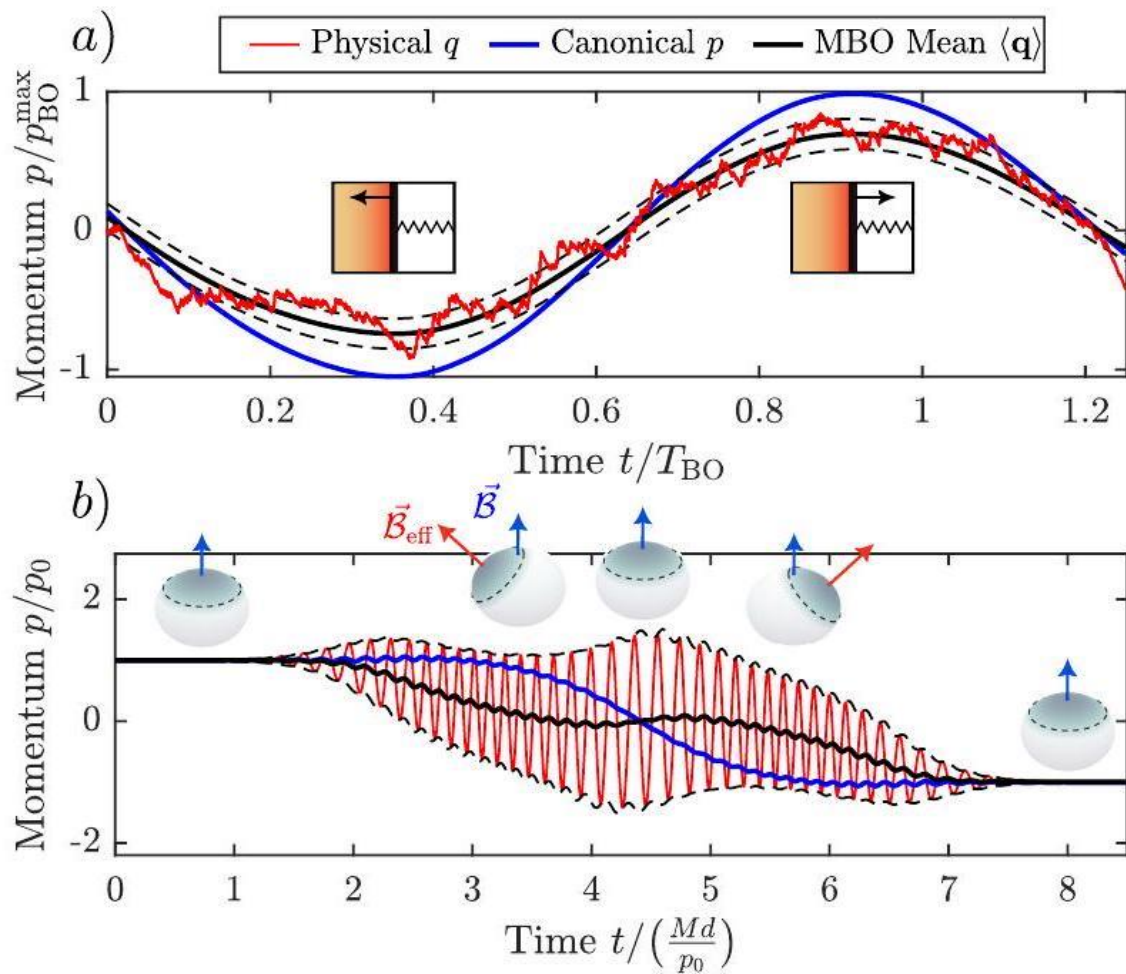
$$\mathbf{q}=p-\mathbf{A}_x(x)$$

$$\mathbf{H}^{\rm M}(x,p)=\frac{(p-\mathbf{A}_x(x))^2}{2M}+\frac{1}{2}kx^2$$

$$+\frac{|\vec{\eta}|^2}{2m}+U_0\sum_{i=1}^N\left(\Theta(-\xi_i)+\Theta(\xi_i-x)\right),$$

$$\mathcal{H}^{\rm MBO}(x,p)=\frac{p^2}{2(M+\kappa)}+\frac{1}{2}kx^2+E_0^{\rm fast}\left(\frac{x_0}{x}\right)^2$$





$$\sigma_{\mathbf{q}}^2(x,p) = \langle \psi_n^{\text{MBO}} | \hat{A}_x^2 | \psi_n^{\text{MBO}} \rangle_c \equiv g_n^{\text{M}}(x,p)$$

$$g_n^{\text{M}} \equiv \langle \hat{A}_x^2 \rangle - \langle \hat{A}_x \rangle^2$$

$$\langle \mathbf{q} \rangle = p / \left(1 + \frac{\kappa}{M} \right)$$

$$\mathbf{q}_{\pm} = \langle \mathbf{q} \rangle \pm \sigma_{\mathbf{q}}$$

$$\sigma_{\mathbf{q}}^2 = \frac{E^{\text{fast}}}{N} \frac{2\kappa}{1 + \kappa/M}$$

$$K \equiv \frac{\langle \mathbf{q}^2 \rangle}{2M} = \frac{\langle \mathbf{q} \rangle^2}{2M} + \frac{g_n^{\text{M}}(x,p)}{2M}.$$

$$p = q - \hbar \theta'(x) S_x$$

$$\langle \mathbf{q} \rangle = p - \frac{\hbar \theta'}{2} \sin \phi$$

$$\hat{\Omega} = \Omega(\hat{x}, \hat{q})$$

$$\langle \hat{\Omega}(t) \rangle = \text{Tr} \left\{ \hat{\rho} e^{\frac{i}{\hbar} t \hat{H}} \hat{\Omega} e^{-\frac{i}{\hbar} t \hat{H}} \right\}$$

$$e^{-i\hat{H}t/\hbar}=\lim_{N\rightarrow\infty}\left(1-\frac{i\Delta t}{\hbar}\hat{H}\right)^N$$

$$\Delta t=t/N$$

$$\mathbb{H}=\mathbb{H}^C\otimes\mathbb{H}^Q$$

$$\hat{I}=\sum_m\int\mathrm{d}x|x,m\rangle\langle x,m|$$

$$\langle x,m|\hat{H}|y,n\rangle=\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi\hbar}e^{\frac{i}{\hbar}p(x-y)}\hat{\mathbf{H}}_{mn}\left(\frac{x+y}{2},p\right)$$

$$\hat{\mathbf{H}}_{mn}(x,p)=\int_{-\infty}^{\infty}\mathrm{d}\xi e^{\frac{i}{\hbar}p\xi}\left\langle x-\frac{\xi}{2},m\left|\hat{H}\right|x+\frac{\xi}{2},n\right\rangle.$$

$$\langle x_N^b,m_N|e^{-\frac{i}{\hbar}t\hat{H}}|x_0^b,m_0\rangle=\int\;D[x^b(\tau)]D[p^b(\tau)]$$

$$e^{\frac{i}{\hbar}\int_0^tp^b(\tau)\dot{x}^b(\tau)\mathrm{d}\tau}\left[\mathcal{T}_t\mathrm{exp}\left\{-\frac{i}{\hbar}\int_0^t\mathrm{d}\tau\hat{\mathbf{H}}(x^b(\tau),p^b(\tau))\right\}\right]_{m_Nm_0}$$

$$\langle x_0^f,m_0|e^{\frac{i}{\hbar}t\hat{H}}|x_N^f,m_N\rangle=\int\;D[x^f(\tau)]D[p^f(\tau)]$$

$$e^{-\frac{i}{\hbar}\int_0^tp^f(\tau)\dot{x}^f(\tau)\mathrm{d}\tau}\left[\mathcal{T}_t\mathrm{exp}\left\{-\frac{i}{\hbar}\int_0^t\mathrm{d}\tau\hat{\mathbf{H}}(x^f(\tau),p^f(\tau))\right\}\right]_{m_0m_N}^\dagger$$

$$x=\frac{x^f+x^b}{2}~p=\frac{p^f+p^b}{2}~\delta x=x^f-x^b~\delta p=p^f-p^b$$

$$\langle \hat{\Omega}(t) \rangle = \int \; D[x]D[p]D[\delta x]D[\delta p]e^{\frac{i}{\hbar}\int_0^t\; \mathrm{d}\tau(\delta x(\tau)\dot{p}(\tau)-\delta p(\tau)\dot{x}(\tau))}$$

$$\mathrm{Tr}\left\{\hat{\mathbf{W}}(x(0),p(0))\left[\mathcal{T}_te^{-\frac{i}{\hbar}\int_0^t\mathrm{d}\tau\hat{\mathbf{H}}\left(x(\tau)+\frac{\delta x(\tau)}{2},p(\tau)+\frac{\delta p(\tau)}{2}\right)}\right]^\dagger\right.\\ \left.\hat{\mathbf{\Omega}}(x(t),p(t))\left[\mathcal{T}_te^{-\frac{i}{\hbar}\int_0^t\mathrm{d}\tau\hat{\mathbf{H}}\left(x(\tau)-\frac{\delta x(\tau)}{2},p(\tau)-\frac{\delta p(\tau)}{2}\right)}\right]\right\}$$

$$\hat{\mathcal{O}}_U'\equiv\hat{U}^\dagger\hat{\mathcal{O}}\hat{U}$$

$$\hat{U}=e^{-\frac{i}{\hbar}\hat{G}}$$

$$\hat{\mathbf{O}}_U'(x,p)=\hat{U}^\dagger(x,p)\star\hat{\mathbf{O}}(x,p)\star\hat{U}(x,p)$$

$$(f\star g)(x,p)=f(x,p)e^{\frac{i\hbar}{2}\Lambda}g(x,p)$$

$$\Lambda=(\overline{\boldsymbol{\sigma}}_x\vec{\partial}_p-\overline{\boldsymbol{\sigma}}_p\vec{\partial}_x)$$

$$\begin{array}{c}
\delta\hat{\mathbf{K}}(\bar{x}_1^f, p_1^f) \delta\hat{\mathbf{K}}(\bar{x}_2^f, p_2^f) \cdot \cdot \cdot \delta\hat{\mathbf{K}}(\bar{x}_{N-1}^f, p_{N-1}^f) \delta\hat{\mathbf{K}}(\bar{x}_N^f, p_N^f) \\
\leftarrow \quad 0 \quad \hat{\mathbf{W}}(x_0, p_0) \xrightarrow{e^{\frac{i}{\hbar}(\delta x_0(p_1-p_0)-\delta p_1(x_1-x_0))}} \cdot \cdot \cdot e^{\frac{i}{\hbar}(\delta x_N(p_{N+1}-p_N)-\delta p_N(x_N-x_{N-1}))} \hat{\mathbf{\Omega}}(x_N, p_{N+1}) \quad t \rightarrow \tau
\end{array}$$

$$\delta\hat{\mathbf{K}}^\dagger(\bar{x}_1^b, p_1^b) \delta\hat{\mathbf{K}}^\dagger(\bar{x}_2^b, p_2^b) \cdot \cdot \cdot \delta\hat{\mathbf{K}}^\dagger(\bar{x}_{N-1}^b, p_{N-1}^b) \delta\hat{\mathbf{K}}^\dagger(\bar{x}_N^b, p_N^b)$$

$$\delta\hat{\mathbf{K}}(x,p)=\left(1+\frac{i\Delta t}{\hbar}\hat{\mathbf{H}}(x,p)\right)$$

$$\bar{x}_i=(x_i+x_{i-1})/2$$

$$\hat{\mathbf{O}}_U(x,p)=\hat{\mathbf{U}}(x,p)\hat{\mathbf{O}}_U'(x,p)\hat{\mathbf{U}}^\dagger(x,p),$$

$$\hat{\mathbf{U}}(x,p)\equiv e^{-\frac{i}{\hbar}\hat{\mathbf{G}}(x,p)}$$

$$\hat{\mathbf{H}}\rightarrow\hat{\mathbf{H}}_U',\hat{\mathbf{\Omega}}\rightarrow\hat{\mathbf{\Omega}}_U'$$

$$\hat{\mathcal{U}}^\dagger\star\hat{\mathcal{U}}=\hat{\mathbf{I}}$$

$$\hat{\mathbf{U}}^\dagger\hat{\mathbf{U}}=\hat{\mathbf{I}}$$

$$\hat{U}\equiv U_{\rm BO}(\hat{x})$$

$$\hat{\mathbf{H}}(x,p)\hat{\mathbf{H}}_{U_{\rm BO}}(x,p)\equiv\hat{\mathbf{H}}^{\rm M}(x,p)$$

$$\hat{\mathbf{H}}_U'=\hat{\mathcal{U}}_{\rm BO}^\dagger\star\hat{\mathbf{H}}\star\hat{\mathcal{U}}_{\rm BO}\approx\hat{\mathbf{U}}_{\rm BO}^\dagger\hat{\mathbf{H}}\hat{\mathbf{U}}_{\rm BO}.$$

$$\hat{\mathbf{O}}_{U_{\rm BO}}(x,p)\rightarrow\hat{\mathbf{O}}(x,p)$$

$$\hat{\mathbf{H}}_U'=\hat{\mathcal{U}}_{\rm MBO}^\dagger\star\hat{\mathbf{H}}_{U_{\rm BO}}'\star\hat{\mathcal{U}}_{\rm MBO}\approx\hat{\mathbf{U}}_{\rm MBO}^\dagger\hat{\mathbf{H}}_{U_{\rm BO}}'\hat{\mathbf{U}}_{\rm MBO}.$$

$$\begin{array}{l}
\langle\hat{\Omega}(t)\rangle=\sum_{m,n}\int D[x(\tau)]D[p(\tau)]D[\delta x(\tau)]D[\delta p(\tau)]\\
e^{\frac{i}{\hbar}\int\mathrm{d}\tau\left(p\delta x-\dot{x}\delta p+\mathcal{H}_m^{\rm MBO}\left(x+\frac{\delta x}{2},p+\frac{\delta p}{2}\right)-\mathcal{H}_n^{\rm MBO}\left(x-\frac{\delta x}{2},p-\frac{\delta p}{2}\right)\right)}\\
\hat{\mathbf{W}}_{nm}^{\rm M}(x(0),p(0))\hat{\Omega}_{mn}^{\rm M}(x(t),p(t))
\end{array}$$

$$\dot{x}=\frac{\partial\mathcal{H}_{mn}^{\rm MBO}}{\partial p},\dot{p}=-\frac{\partial\mathcal{H}_{mn}^{\rm MBO}}{\partial x}.$$

$$\mathcal{H}_{mn}^{\rm MBO}(x,p)\equiv\frac{\mathcal{H}_m^{\rm MBO}(x,p)+\mathcal{H}_n^{\rm MBO}(x,p)}{2}.$$

$$\begin{array}{l}
\Phi_{mn}(t)=\frac{1}{\hbar}\int_0^t\mathrm{d}\tau[\mathcal{H}_m^{\rm MBO}(x_{mn}(\tau),p_{mn}(\tau))\\
-\mathcal{H}_n^{\rm MBO}(x_{mn}(\tau),p_{mn}(\tau))]
\end{array}$$

$$\boldsymbol{\Omega}_{mn}^{\rm M}(t)=\mathrm{e}^{i\Phi_{mn}(t)}\boldsymbol{\Omega}_{mn}^{\rm M}(x_{mn}(t),p_{mn}(t)).$$

$$\langle\hat{\Omega}(t)\rangle\approx\int\frac{\mathrm{d}x\,\mathrm{d}p}{2\pi\hbar}\mathrm{Tr}\{\hat{\mathbf{W}}^{\rm M}(x,p)\hat{\Omega}^{\rm M}(t)\},$$

$$\hat{U}(\lambda) \equiv e^{-\frac{i}{\hbar}\lambda\hat{G}}$$

$$\hat{\mathcal{U}}(x,p;\lambda) \equiv \hat{\mathcal{U}}(\lambda)$$

$$\hat{\mathbf{U}}(x,p;\lambda) \equiv \hat{\mathbf{U}}(\lambda) \equiv e^{-\frac{i}{\hbar}\lambda\hat{\mathbf{G}}(x,p)}$$

$$\hat{\mathcal{U}}(\lambda) \neq \hat{\mathbf{U}}(\lambda)$$

$$\hat{\mathcal{U}}^\dagger(\lambda) \star \hat{\mathcal{U}}(\lambda) = \hat{\mathbf{I}}$$

$$\hat{\mathbf{U}}^\dagger(\lambda)\hat{\mathbf{U}}(\lambda) = \hat{\mathbf{I}}$$

$$\hat{U}(\lambda=1) \equiv \hat{U}, \hat{\mathcal{U}}(\lambda=1) \equiv \hat{\mathcal{U}}$$

$$\hat{\mathbf{U}}(\lambda=1) \equiv \hat{\mathbf{U}}$$

$$\hat{\mathbf{Q}}'(\lambda) \equiv \hat{\mathbf{U}}^\dagger(\lambda)\hat{\mathbf{Q}}\hat{\mathbf{U}}(\lambda).$$

$$\hat{\mathbf{Q}}'(\lambda=1) \equiv \hat{\mathbf{Q}}'$$

$$\mathbb{H}^Q \otimes \mathbb{H}^C \hat{U}(\lambda)$$

$$\hat{\mathcal{O}}'_U(\lambda) \equiv \hat{U}^\dagger(\lambda)\hat{\mathcal{O}}\hat{U}(\lambda).$$

$$\hat{\mathcal{O}}'_U(\lambda) = \hat{\mathcal{U}}^\dagger(\lambda) \star \hat{\mathcal{O}} \star \hat{\mathcal{U}}(\lambda) \equiv \hat{\mathbf{U}}^\dagger(\lambda)\hat{\mathcal{O}}_U(\lambda)\hat{\mathbf{U}}(\lambda)$$

$$\hat{\mathcal{O}}_U(x,p;\lambda) = \hat{\mathbf{U}}(x,p;\lambda)\hat{\mathcal{O}}'_U(x,p;\lambda)\hat{\mathbf{U}}^\dagger(x,p;\lambda)$$

$$\hat{U} = \hat{U}_{\text{BO}}$$

$$\hat{\mathbf{O}}_{U_{\text{BO}}} \equiv \hat{\mathbf{O}}^{\text{M}}$$

$$\hat{\mathbf{A}}_x(\lambda) \equiv (i\hbar\partial_x\hat{\mathbf{U}}_{\text{BO}}(\lambda))\hat{\mathbf{U}}_{\text{BO}}^\dagger(\lambda)$$

$$\hat{\mathbf{B}}'_x(\lambda) \equiv (i\hbar\partial_x\hat{\mathbf{U}}_{\text{MBO}}(\lambda))\hat{\mathbf{U}}_{\text{MBO}}^\dagger(\lambda)$$

$$\hat{\mathbf{B}}'_p(\lambda) \equiv (i\hbar\partial_p\hat{\mathbf{U}}_{\text{MBO}}(\lambda))\hat{\mathbf{U}}_{\text{MBO}}^\dagger(\lambda)$$

$$\hat{\mathbf{A}}_x(x;\lambda=1) \equiv \hat{\mathbf{A}}_x(x)$$

$$\hat{\mathbf{B}}'_{x,p}(x,p;\lambda=1) \equiv \hat{\mathbf{B}}'_{x,p}(x,p)$$

$$\hat{\mathbf{B}}_{x,p} = \hat{\mathbf{U}}_{\text{BO}}\hat{\mathbf{B}}'_{x,p}\hat{\mathbf{U}}_{\text{BO}}^\dagger$$

$$[\hat{\mathbf{F}}'_x, \hat{\mathbf{H}}'_{U_{\text{BO}}}] = 0, \quad \hat{\mathbf{F}}'_x = \partial_x \hat{\mathbf{H}}'_{U_{\text{BO}}} + \frac{i}{\hbar} [\hat{\mathbf{B}}'_x, \hat{\mathbf{H}}'_{U_{\text{BO}}}]$$

$$[\hat{\mathbf{F}}'_p, \hat{\mathbf{H}}'_{U_{\text{BO}}}] = 0, \quad \hat{\mathbf{F}}'_p = \partial_p \hat{\mathbf{H}}'_{U_{\text{BO}}} + \frac{i}{\hbar} [\hat{\mathbf{B}}'_p, \hat{\mathbf{H}}'_{U_{\text{BO}}}]$$

$$\partial_x \hat{\mathbf{H}}'_{U_{\text{BO}}} = \hat{\mathbf{U}}_{\text{BO}}^\dagger \left(\partial_x \hat{\mathbf{H}}_{U_{\text{BO}}} + \frac{i}{\hbar} [\hat{\mathbf{A}}_x, \hat{\mathbf{H}}_{U_{\text{BO}}}] \right) \hat{\mathbf{U}}_{\text{BO}}$$

$$\hat{\mathbf{F}}_x = \partial_x \hat{\mathbf{H}}_{U_{\text{BO}}} + \frac{i}{\hbar} [\hat{\mathbf{A}}_x + \hat{\mathbf{B}}_x, \hat{\mathbf{H}}_{U_{\text{BO}}}],$$

$$\hat{\mathbf{F}}_p = \partial_p \hat{\mathbf{H}}_{U_{\text{BO}}} + \frac{i}{\hbar} [\hat{\mathbf{B}}_p, \hat{\mathbf{H}}_{U_{\text{BO}}}].$$

$\hat{\Omega}$	Operator in $\mathbb{H}^Q \otimes \mathbb{H}^C$.
$\hat{\Omega}$	Partial Weyl symbol in $\mathbb{H}^Q$
$\hat{U}$	Unitary transformation $\hat{U}(\lambda) \equiv e^{-\frac{i}{\hbar}\lambda\hat{G}}$
$\hat{\mathbf{G}}$	Generating function
$\hat{\mathcal{U}}$	Weyl symbol of $\hat{U}(\lambda)$
$\hat{\mathbf{U}}$	$\hat{\mathbf{U}}(x, p; \lambda) \equiv e^{-\frac{i}{\hbar}\lambda\hat{\mathbf{G}}(x, p)}$
$\hat{\mathbf{A}}_x$	BO AGP $\hat{\mathbf{A}}_x \equiv (i\hbar\partial_x \hat{\mathbf{U}}_{\text{BO}}(\lambda))\hat{\mathbf{U}}_{\text{BO}}^\dagger(\lambda)$
$\hat{\mathbf{B}}'_{x,p}$	MBO AGPs $\hat{\mathbf{B}}'_{x,p}(\lambda) \equiv (i\hbar\partial_{x,p} \hat{\mathbf{U}}_{\text{MBO}}(\lambda))\hat{\mathbf{U}}_{\text{MBO}}^\dagger(\lambda)$
$\hat{\mathbf{F}}_{x,p}$	Generalized forces

$$\hat{\mathcal{O}}'_U(\lambda) = \hat{U}^\dagger(\lambda) \hat{\mathcal{O}} \hat{U}(\lambda) = e^{\frac{i}{\hbar}\lambda\hat{G}} \hat{\mathcal{O}} e^{-\frac{i}{\hbar}\lambda\hat{G}}.$$

$$\hat{\mathcal{O}}'_U(\lambda = 1) \equiv \hat{\mathcal{O}}'_U$$

$$\hat{\mathcal{O}}'_U(\lambda = 0) = \hat{\mathcal{O}}$$

$$\frac{d\hat{\mathcal{O}}'_U(\lambda)}{d\lambda} = \frac{i}{\hbar} (\hat{\mathbf{G}} \star \hat{\mathcal{O}}'_U(\lambda) - \hat{\mathcal{O}}'_U(\lambda) \star \hat{\mathbf{G}}).$$

$$\frac{d\hat{\mathcal{O}}'_U(\lambda)}{d\lambda} = \frac{1}{i\hbar} [\hat{\mathcal{O}}'_U(\lambda), \hat{\mathbf{G}}] + \{\hat{\mathcal{O}}'_U(\lambda), \hat{\mathbf{G}}\}_{\text{SPB}} + \mathcal{O}(\hbar),$$

$$\{\hat{\mathbf{A}}, \hat{\mathbf{B}}\}_{\text{SPB}} \equiv \frac{1}{2} \left(\frac{\partial \hat{\mathbf{A}}}{\partial x} \frac{\partial \hat{\mathbf{B}}}{\partial p} + \frac{\partial \hat{\mathbf{B}}}{\partial p} \frac{\partial \hat{\mathbf{A}}}{\partial x} - \frac{\partial \hat{\mathbf{A}}}{\partial p} \frac{\partial \hat{\mathbf{B}}}{\partial x} - \frac{\partial \hat{\mathbf{B}}}{\partial x} \frac{\partial \hat{\mathbf{A}}}{\partial p} \right).$$

$$\hat{\mathcal{O}}'_U(\lambda) = e^{\frac{i}{\hbar}\lambda\hat{G}} (\hat{\mathcal{O}} + \int_0^\lambda d\lambda' e^{-\frac{i}{\hbar}\lambda'\hat{G}} (\{\hat{\mathcal{O}}'_U(\lambda'), \hat{\mathbf{G}}\}_{\text{SPB}}) e^{\frac{i}{\hbar}\lambda'\hat{G}}) e^{-\frac{i}{\hbar}\lambda\hat{G}}$$

$$(\hat{\mathcal{O}}'_U)^{(0)}(\lambda) = e^{\frac{i}{\hbar}\lambda\hat{G}} \hat{\mathcal{O}} e^{-\frac{i}{\hbar}\lambda\hat{G}}$$

$$(\hat{\mathcal{O}}'_U)^{(1)}(\lambda) (\hat{\mathcal{O}}'_U)^{(n)}(\lambda)$$

$$(\hat{\mathcal{O}}'_U)^{(n)}(\lambda) = e^{\frac{i}{\hbar}\lambda\hat{G}} (\hat{\mathcal{O}} + \int_0^\lambda d\lambda' e^{-\frac{i}{\hbar}\lambda'\hat{G}} (\{(\hat{\mathcal{O}}'_U)^{(n-1)}(\lambda'), \hat{\mathbf{G}}\}_{\text{SPB}}) e^{\frac{i}{\hbar}\lambda'\hat{G}}) e^{-\frac{i}{\hbar}\lambda\hat{G}}$$

$$\hat{\mathbf{O}}'_U(\lambda) = e^{\frac{i}{\hbar}\lambda\hat{\mathbf{G}}} \left(\mathcal{T}_\lambda \exp \left\{ \int_0^\lambda d\lambda' \mathcal{L}(\lambda', \hat{\mathbf{G}}) \right\} \hat{\mathbf{O}} \right) e^{-\frac{i}{\hbar}\lambda\hat{\mathbf{G}}}$$

$$\begin{aligned} \mathcal{L}(\lambda, \hat{\mathbf{G}}) \hat{\mathbf{O}} &= e^{-\frac{i}{\hbar}\lambda\hat{\mathbf{G}}} \left(\left\{ e^{\frac{i}{\hbar}\lambda\hat{\mathbf{G}}} \hat{\mathbf{O}} e^{-\frac{i}{\hbar}\lambda\hat{\mathbf{G}}}, \hat{\mathbf{G}} \right\}_{\text{SPB}} \right) e^{\frac{i}{\hbar}\lambda\hat{\mathbf{G}}} \\ &\equiv e^{-\frac{i}{\hbar}\lambda\hat{\mathbf{G}}} \left(\{ \hat{\mathbf{O}}'(\lambda), \hat{\mathbf{G}} \}_{\text{SPB}} \right) e^{\frac{i}{\hbar}\lambda\hat{\mathbf{G}}} \end{aligned}$$

$$\hat{\mathbf{O}}'_U(\lambda = 0) = \hat{\mathbf{O}}$$

$$\hat{\mathbf{U}}(x, p; \lambda = 1) \equiv \hat{\mathbf{U}}(x, p)$$

$$\hat{\mathbf{O}}'_U(x, p) = \hat{\mathbf{U}}^\dagger(x, p) \hat{\mathbf{O}}_U(x, p) \hat{\mathbf{U}}(x, p),$$

$$\hat{\mathbf{O}}_U \equiv \mathcal{T}_\lambda \exp \left\{ \int_0^1 d\lambda \mathcal{L}(\lambda, \hat{\mathbf{G}}) \right\} \hat{\mathbf{O}}.$$

$$\hat{U} = U_{\text{BO}}(\hat{x}) \equiv e^{-\frac{i}{\hbar}\hat{\mathbf{G}}_{\text{BO}}}$$

$$\hat{\mathbf{O}}'_{U_{\text{BO}}} = \hat{U}_{\text{BO}}^\dagger \star \hat{\mathbf{O}} \star \hat{U}_{\text{BO}} = \hat{\mathbf{U}}_{\text{BO}}^\dagger \hat{\mathbf{O}}_{U_{\text{BO}}} \hat{\mathbf{U}}_{\text{BO}}.$$

$$\hat{\mathbf{O}}_{U_{\text{BO}}} \equiv \hat{\mathbf{O}}^{\text{M}}$$

$$\hat{U}_{\text{BO}}^\dagger \star \hat{\mathbf{x}} \star \hat{U}_{\text{BO}} = \hat{\mathbf{U}}_{\text{BO}}^\dagger \hat{\mathbf{x}} \hat{\mathbf{U}}_{\text{BO}} = \hat{\mathbf{x}}, \text{ resulting in } \hat{\mathbf{x}}^{\text{M}} = \hat{\mathbf{x}}$$

$$\begin{aligned} (\hat{\mathbf{q}}^{\text{M}})' &= \hat{\mathbf{U}}_{\text{BO}}^\dagger \left(1 + \frac{i\hbar}{2} \Lambda \right) \hat{\mathbf{q}} \left(1 + \frac{i\hbar}{2} \Lambda \right) \hat{\mathbf{U}}_{\text{BO}}, \\ &= \hat{\mathbf{q}} + (i\hbar \partial_x \hat{\mathbf{U}}_{\text{BO}}^\dagger) \hat{\mathbf{U}}_{\text{BO}}, \end{aligned}$$

$$(\partial_x \hat{\mathbf{U}}_{\text{BO}}^\dagger) \hat{\mathbf{U}}_{\text{BO}} = -\hat{\mathbf{U}}_{\text{BO}}^\dagger (\partial_x \hat{\mathbf{U}}_{\text{BO}}) \text{ and } \hat{\mathbf{q}}' = \hat{\mathbf{q}}$$

$$\hat{\mathbf{q}}^{\text{M}} = \hat{\mathbf{U}}_{\text{BO}} (\hat{\mathbf{q}}^{\text{M}})' \hat{\mathbf{U}}_{\text{BO}}^\dagger = \hat{\mathbf{q}} - (i\hbar \partial_x \hat{\mathbf{U}}_{\text{BO}}) \hat{\mathbf{U}}_{\text{BO}}^\dagger = \hat{\mathbf{q}} - \hat{\mathbf{A}}_x$$

$$(\hat{\mathbf{q}}^2)'_{U_{\text{BO}}} = \hat{\mathbf{q}}'_{U_{\text{BO}}} \star \hat{\mathbf{q}}'_{U_{\text{BO}}} = (\hat{\mathbf{q}}'_{U_{\text{BO}}})^2$$

$$\hat{\mathbf{q}}'_{U_{\text{BO}}} \Lambda \hat{\mathbf{q}}'_{U_{\text{BO}}} = 0$$

$$(\hat{\mathbf{q}}^2)^{\text{M}} = (\hat{\mathbf{q}}^{\text{M}})^2 = (\hat{\mathbf{q}} - \hat{\mathbf{A}}_x)^2$$

$$\mathcal{L}(\lambda, \hat{\mathbf{G}}_{\text{BO}}) \hat{\mathbf{x}} = 0$$

$$\begin{aligned} \mathcal{L}(\lambda_1, \hat{\mathbf{G}}_{\text{BO}}) \hat{\mathbf{q}} &= e^{-\frac{i}{\hbar}\lambda_1 \hat{\mathbf{G}}_{\text{BO}}} \left(\{ p \hat{\mathbf{I}}, \hat{\mathbf{G}}_{\text{BO}} \}_{\text{SPB}} \right) e^{\frac{i}{\hbar}\lambda_1 \hat{\mathbf{G}}_{\text{BO}}} \\ &= -e^{-\frac{i}{\hbar}\lambda_1 \hat{\mathbf{G}}_{\text{BO}}} \partial_x \hat{\mathbf{G}}_{\text{BO}} e^{\frac{i}{\hbar}\lambda_1 \hat{\mathbf{G}}_{\text{BO}}} \end{aligned}$$

$$\mathcal{L}(\lambda_2, \hat{\mathbf{G}}_{\text{BO}}) \mathcal{L}(\lambda_1, \hat{\mathbf{G}}_{\text{BO}}) \hat{\mathbf{q}} = 0$$

$$\hat{\mathbf{q}}^{\text{M}} = \hat{\mathbf{q}} - \int_0^1 d\lambda_1 e^{-\frac{i}{\hbar}\lambda_1 \hat{\mathbf{G}}_{\text{BO}}} \partial_x \hat{\mathbf{G}}_{\text{BO}} e^{\frac{i}{\hbar}\lambda_1 \hat{\mathbf{G}}_{\text{BO}}} = \hat{\mathbf{q}} - \hat{\mathbf{A}}_x,$$

$$\partial_\lambda \hat{\mathbf{A}}_x(\lambda) = e^{-\frac{i}{\hbar}\lambda \hat{\mathbf{G}}_{\text{BO}}} \partial_x \hat{\mathbf{G}}_{\text{BO}} e^{\frac{i}{\hbar}\lambda \hat{\mathbf{G}}_{\text{BO}}}.$$



$$\begin{aligned}
(\hat{\mathbf{q}}^2)^{\text{M}} &= \hat{\mathbf{q}}^2 - 2p \int_0^1 d\lambda_1 \frac{\partial}{\partial \lambda_1} (\hat{\mathbf{A}}_x(\lambda_1)) + \\
&\frac{1}{2} \int_0^1 \int_0^1 d\lambda_2 d\lambda_1 \left[\frac{\partial}{\partial \lambda_1} (\hat{\mathbf{A}}_x(\lambda_1)), \frac{\partial}{\partial \lambda_2} (\hat{\mathbf{A}}_x(\lambda_2)) \right]_+ \\
(\hat{\mathbf{q}}^2)^{\text{M}} &= \hat{\mathbf{q}}^2 - 2p \hat{\mathbf{A}}_x + \hat{\mathbf{A}}_x^2 = (\hat{\mathbf{q}} - \hat{\mathbf{A}}_x)^2 \\
\hat{\mathbf{x}}^{(0)}(\lambda) &= x \hat{\mathbf{I}} \\
\{\hat{\mathbf{x}}^{(0)}, \hat{\mathbf{G}}_{\text{BO}}\}_{\text{SPB}} &= 0 \\
\hat{\mathbf{x}}^{\text{M}} &= \hat{\mathbf{U}}_{\text{BO}} \hat{\mathbf{x}}^{(0)}(\lambda = 1) \hat{\mathbf{U}}_{\text{BO}}^\dagger = x \hat{\mathbf{I}} \\
\hat{\mathbf{q}}^{(0)}(\lambda) &= p \hat{\mathbf{I}} \\
\hat{\mathbf{q}}^{(1)}(\lambda) &= e^{\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} (p \hat{\mathbf{I}} - \hat{\mathbf{A}}_x(\lambda)) e^{-\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} \\
\{\hat{\mathbf{q}}^{(0)}, \hat{\mathbf{G}}_{\text{BO}}\}_{\text{SPB}} &= -\partial_x \hat{\mathbf{G}}_{\text{BO}} \\
\{\hat{\mathbf{q}}^{(1)}(\lambda), \hat{\mathbf{G}}_{\text{BO}}\}_{\text{SPB}} &= -\partial_x \hat{\mathbf{G}}_{\text{BO}} \\
\hat{\mathbf{q}}^{(2)}(\lambda) &= \hat{\mathbf{q}}^{(1)}(\lambda) \\
\hat{\mathbf{q}}^{\text{M}} &= \hat{\mathbf{U}}_{\text{BO}} \hat{\mathbf{q}}^{(1)}(\lambda = 1) \hat{\mathbf{U}}_{\text{BO}}^\dagger = p \hat{\mathbf{I}} - \hat{\mathbf{A}}_x(\lambda = 1) \\
(\hat{\mathbf{q}}^2)^{\text{M}}: (\hat{\mathbf{q}}^2)^{(0)}(\lambda) &= p^2 \hat{\mathbf{I}} \\
\{(\hat{\mathbf{q}}^2)^{(0)}, \hat{\mathbf{G}}_{\text{BO}}\}_{\text{SPB}} &= -2p \partial_x \hat{\mathbf{G}}_{\text{BO}} \\
(\hat{\mathbf{q}}^2)^{(1)}(\lambda) &= e^{\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} (p^2 \hat{\mathbf{I}} - 2p \hat{\mathbf{A}}_x(\lambda)) e^{-\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} \\
\{(\hat{\mathbf{q}}^2)^{(1)}, \hat{\mathbf{G}}_{\text{BO}}\}_{\text{SPB}} &= -2p \partial_x \hat{\mathbf{G}}_{\text{BO}} + \left[e^{\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} \hat{\mathbf{A}}_x(\lambda) e^{-\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}}, \partial_x \hat{\mathbf{G}}_{\text{BO}} \right]_+ \\
(\hat{\mathbf{q}}^2)^{(2)}(\lambda) &= e^{\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} \left(p^2 \hat{\mathbf{I}} - 2p \hat{\mathbf{A}}_x(\lambda) + \int_0^\lambda d\lambda' \left[\hat{\mathbf{A}}_x(\lambda'), \frac{\partial}{\partial \lambda'} (\hat{\mathbf{A}}_x(\lambda')) \right]_+ \right) e^{-\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} \\
&= e^{\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} (p^2 \hat{\mathbf{I}} - 2p \hat{\mathbf{A}}_x(\lambda) + \hat{\mathbf{A}}_x^2(\lambda)) e^{-\frac{i}{\hbar} \lambda \hat{\mathbf{G}}_{\text{BO}}} \\
\partial_\lambda \hat{\mathbf{A}}_x^2(\lambda) &= [\hat{\mathbf{A}}_x(\lambda), \partial_\lambda \hat{\mathbf{A}}_x(\lambda)]_+ \\
\hat{\mathbf{q}}^{(3)} &= \hat{\mathbf{q}}^{(2)} \\
(\hat{\mathbf{q}}^2)^{\text{M}} &= \hat{\mathbf{U}}_{\text{BO}} ((\hat{\mathbf{q}}^2)^{(2)}(\lambda = 1)) \hat{\mathbf{U}}_{\text{BO}}^\dagger = (p \hat{\mathbf{I}} - \hat{\mathbf{A}}_x)^2 \\
\hat{U} &= \hat{U}_{\text{BO}} \hat{U}_{\text{MBO}} = e^{-\frac{i}{\hbar} \hat{G}_{\text{BO}}} e^{-\frac{i}{\hbar} \hat{G}_{\text{MBO}}} \\
\hat{U}_{\text{MBO}}^\dagger (\hat{U}_{\text{BO}}^\dagger \hat{\mathbf{H}}_{U_{\text{BO}}} \hat{U}_{\text{BO}}) \hat{U}_{\text{MBO}} &\equiv \hat{U}_{\text{MBO}}^\dagger \hat{\mathbf{H}}'_{U_{\text{BO}}} \hat{U}_{\text{MBO}} \\
\hat{\mathcal{O}}'_U &= \hat{\mathcal{U}}_{\text{MBO}}^\dagger \star \hat{\mathcal{O}}'_{U_{\text{BO}}} \star \hat{\mathcal{U}}_{\text{MBO}} \approx \hat{U}_{\text{MBO}}^\dagger \hat{\mathcal{O}}'_{U_{\text{BO}}} \hat{U}_{\text{MBO}}.
\end{aligned}$$

$$\hat{\mathbf{O}}'_U = \hat{\mathcal{U}}_{\text{MBO}}^\dagger \star \hat{\mathbf{O}}'_{U_{\text{BO}}} \star \hat{\mathcal{U}}_{\text{MBO}} \approx \hat{\mathbf{U}}_{\text{MBO}}^\dagger \hat{\mathbf{O}}'_{U_{\text{BO}}} \hat{\mathbf{U}}_{\text{MBO}} \\ + \hat{\mathbf{U}}_{\text{MBO}}^\dagger \left(\int_0^1 d\lambda \mathcal{L}(\lambda, \hat{\mathbf{G}}_{\text{MBO}}) \hat{\mathbf{O}}'_{U_{\text{BO}}} \right) \hat{\mathbf{U}}_{\text{MBO}} + \mathcal{O}(\mathcal{L}^2)$$

$$\hat{\mathbf{G}} \equiv \hat{\mathbf{G}}_{\text{MBO}}$$

$$\int_0^1 d\lambda \mathcal{L}(\lambda, \hat{\mathbf{G}}) \hat{\mathbf{O}}'_{U_{\text{BO}}} = \\ \frac{1}{2} \int_0^1 d\lambda e^{-\frac{i}{\hbar} \lambda \hat{\mathbf{G}}} \left[\partial_x \left(e^{\frac{i}{\hbar} \lambda \hat{\mathbf{G}}} \hat{\mathbf{O}}'_{U_{\text{BO}}} e^{-\frac{i}{\hbar} \lambda \hat{\mathbf{G}}} \right), \partial_p \hat{\mathbf{G}} \right]_+ e^{\frac{i}{\hbar} \lambda \hat{\mathbf{G}}} \\ -(x \leftrightarrow p)$$

$$\int_0^1 d\lambda \mathcal{L}(\lambda, \hat{\mathbf{G}}) \hat{\mathbf{O}}'_{U_{\text{BO}}} = \frac{1}{2} \int_0^1 d\lambda \left[\partial_x \hat{\mathbf{O}}'_{U_{\text{BO}}} + \right. \\ \left. \frac{i}{\hbar} [\hat{\mathbf{B}}'_x(\lambda), \hat{\mathbf{O}}'_{U_{\text{BO}}}], \partial_\lambda \hat{\mathbf{B}}'_p(\lambda) \right]_+ - (x \leftrightarrow p)$$

$$\int_0^1 d\lambda \mathcal{L}(\lambda, \hat{\mathbf{G}}) \hat{\mathbf{O}}'_{U_{\text{BO}}} \approx \frac{1}{2} [\partial_x \hat{\mathbf{O}}'_{U_{\text{BO}}}, \hat{\mathbf{B}}'_p]_+ - (x \leftrightarrow p),$$

$$\hat{\mathbf{B}}'_x \equiv \hat{\mathbf{B}}'_x(\lambda = 1)$$

$$\hat{\mathbf{B}}'_p \equiv \hat{\mathbf{B}}'_p(\lambda = 1)$$

$$\hat{\mathbf{H}}^{\text{SA}} \approx \hat{\mathbf{H}}^{\text{M}} + \\ \frac{1}{2} \left[\partial_x \hat{\mathbf{H}}^{\text{M}} + \frac{i}{\hbar} [\hat{\mathbf{A}}_x, \hat{\mathbf{H}}^{\text{M}}], \hat{\mathbf{B}}_p \right]_+ - \frac{1}{2} [\partial_p \hat{\mathbf{H}}^{\text{M}}, \hat{\mathbf{B}}_x]_+,$$

$$\hat{\mathbf{q}}^{\text{SA}} \approx p \hat{\mathbf{I}} - \hat{\mathbf{A}}_x - \hat{\mathbf{B}}_x - \frac{1}{2} [\partial_x \hat{\mathbf{A}}_x, \hat{\mathbf{B}}_p]_+$$

$$\hat{\mathbf{x}}^{\text{SA}} \approx x \hat{\mathbf{I}} + \hat{\mathbf{B}}_p$$

$$\vec{B}(x) = B(x)(\cos \theta(x) \hat{z} + \sin \theta(x) \hat{y})$$

$$\hat{\mathbf{G}}_{\text{BO}}(x) = -\frac{\hbar \theta(x)}{2} \hat{\sigma}_x, \hat{\mathbf{G}}_{\text{MBO}}(x, p) = -\frac{\hbar \phi(x, p)}{2} \hat{\sigma}_y,$$

$$\phi(x, p) = \tan^{-1} \left(\frac{\hbar \theta'(x) p}{2 M \mu B(x)} \right)$$

$$\mathcal{H}_{\pm}^{\text{MBO}} = \frac{p^2}{2M} + \frac{(\hbar \theta'(x))^2}{8M} \pm \sqrt{(\mu B(x))^2 + \left(\frac{\hbar \theta'(x) p}{2M} \right)^2}$$

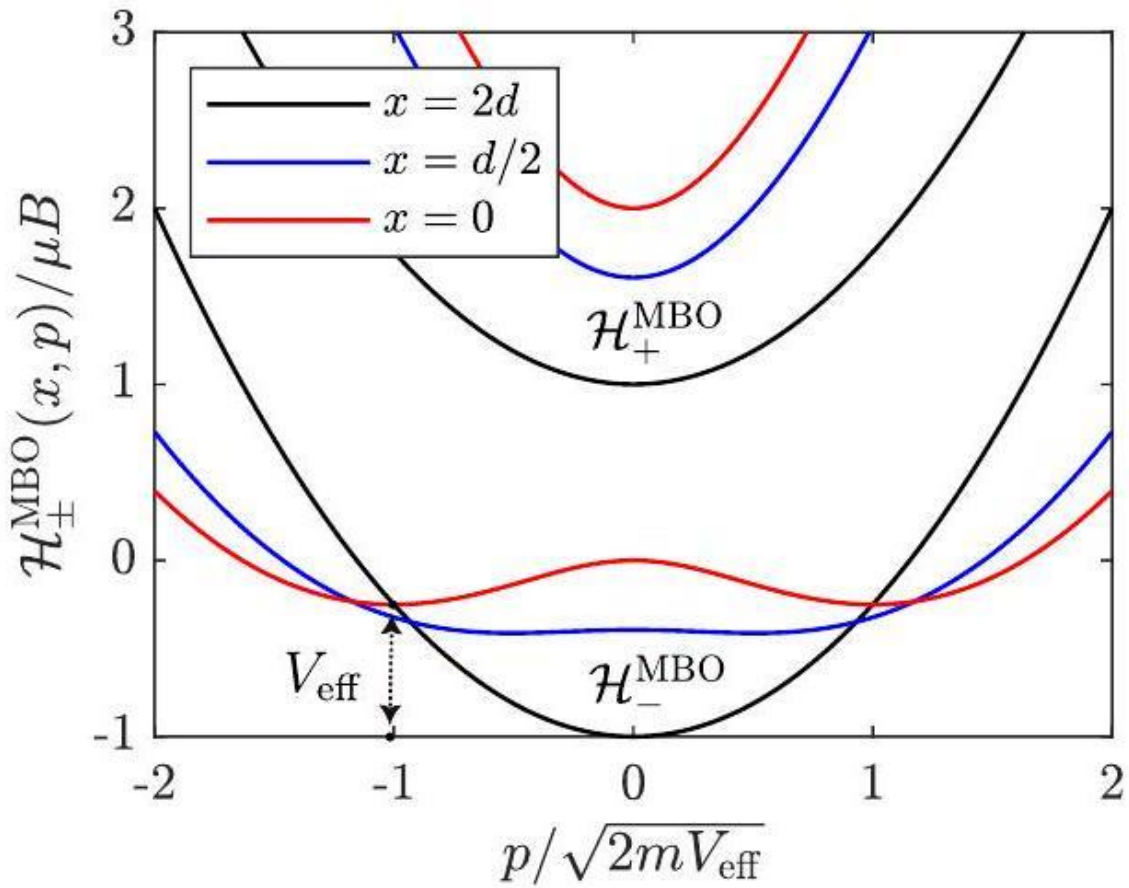
$$\theta(x) = \theta_0(1 + \text{erf}(x/d))$$

$$\theta'(x) = 2\theta_0/(\sqrt{\pi}d)\exp[-x^2/d^2]$$



$$\zeta = \frac{\hbar^2 \theta_0^2}{\pi M \mu B d^2}$$

$$\varepsilon_{\min} = \begin{cases} \mu B \left(\frac{\zeta}{2} - 1 \right), & \zeta < 1 \\ -\frac{\mu B}{2\zeta}, & \zeta > 1 \end{cases}$$



$$|\Psi(t=0)\rangle \propto \int dx e^{-(x-x_0)^2/4\sigma_x^2} e^{\frac{i}{\hbar} p_0 x} |x\rangle \otimes |\psi^{\text{BO}}(x)\rangle.$$

$$\dot{x}=\langle\partial_p\hat{\mathbf{H}}^{\mathbf{M}}\rangle$$

$$\dot{p}=-\langle\partial_x\hat{\mathbf{H}}^{\mathbf{M}}\rangle$$

$$\langle\partial_p\hat{\mathbf{H}}^{\mathbf{M}}\rangle_{\text{BO}}=\frac{p}{M}$$

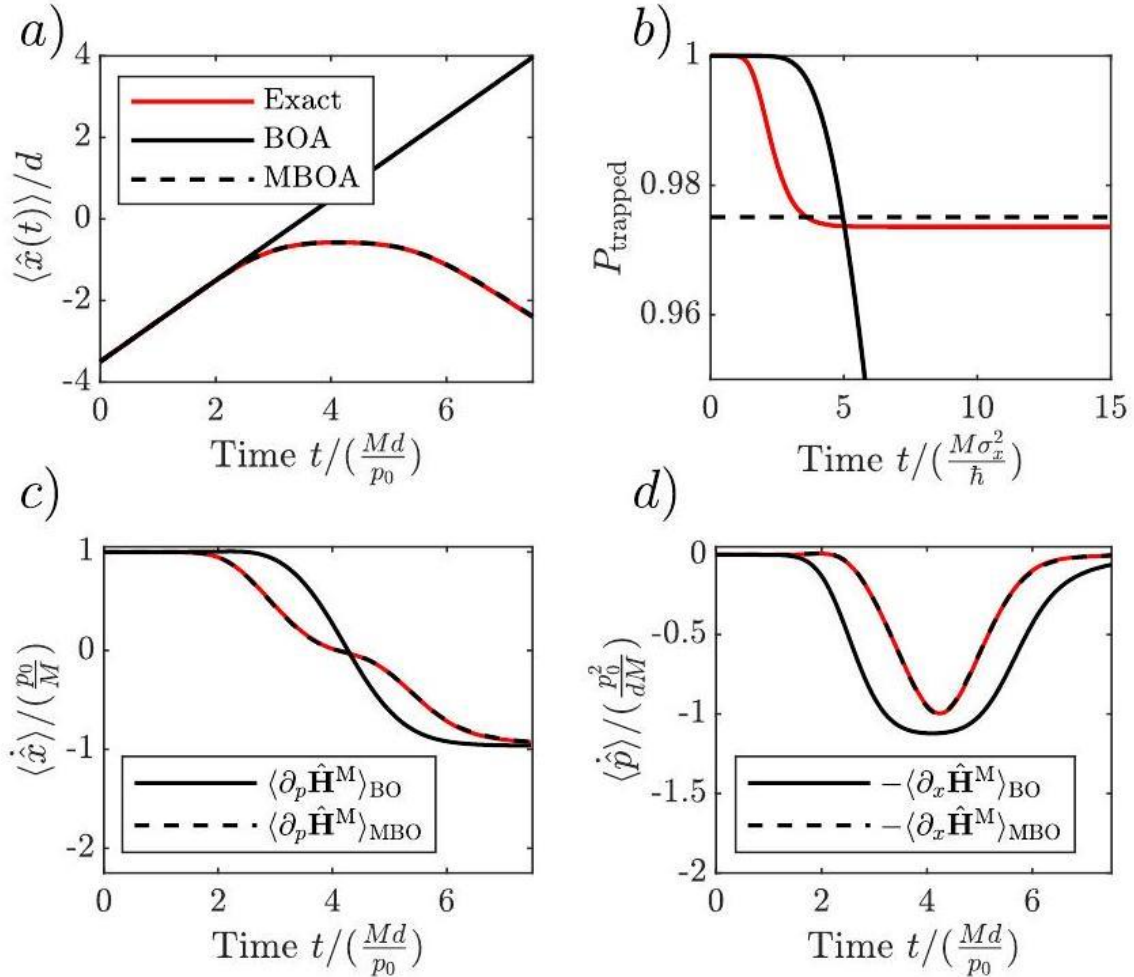
$$\langle\partial_p\hat{\mathbf{H}}^{\mathbf{M}}\rangle_{\text{MBO}}=\frac{p}{M}-\frac{\hbar\theta'(x)}{2M}\sin\phi(x,p)$$

$$\hat{\mathbf{W}}^{\mathbf{M}}(x,p)=W(x,p)\begin{pmatrix}\cos^2\left(\frac{\phi(x,p)}{2}\right)&\frac{\sin\phi(x,p)}{2}\\\frac{\sin\phi(x,p)}{2}&\sin^2\left(\frac{\phi(x,p)}{2}\right)\end{pmatrix},$$

$$W(x, p) = 2 \exp \left(-\frac{(x - x_0)^2}{2\sigma_x^2} - \frac{2\sigma_x^2(p - p_0)^2}{\hbar^2} \right)$$

$$P_{\text{trapped}} \approx \int \frac{dx dp}{2\pi\hbar} W(x, p) \cos^2 \left(\frac{\phi(x, p)}{2} \right).$$

$$x \in (-d/2, d/2), \text{ with } P_{\text{trapped}} = \int_{-d/2}^{d/2} dx |\Psi(x)|^2$$



$$x \in (-d/2, d/2)$$

$$d\langle \hat{x} \rangle / dt \partial_p \hat{\mathbf{H}}^M$$

$$p_0 = (1/\sqrt{2\pi})\hbar\theta_0/d$$

$$\sigma_x = d/4$$

$$x_0 = p_0 = 0 \text{ and } \sigma_x = d/10$$

$$\mathcal{H}_{mn}^{\text{MBO}} = \frac{\mathcal{H}_m^{\text{MBO}} + \mathcal{H}_n^{\text{MBO}}}{2},$$

$$\begin{aligned}\dot{x}_{--}(\tau) &\equiv \dot{x}_{-}(\tau) = \frac{p}{M} - \frac{\hbar\theta'}{2M} \sin \phi(p), \\ \dot{p}_{--}(\tau) &\equiv \dot{p}_{-}(\tau) = 0, \\ \dot{x}_{++}(\tau) &\equiv \dot{x}_{+}(\tau) = \frac{p}{M} + \frac{\hbar\theta'}{2M} \sin \phi(p), \\ \dot{p}_{++}(\tau) &\equiv \dot{p}_{+}(\tau) = 0,\end{aligned}$$

$$\dot{x}_{-+}(\tau) = \dot{x}_{+-}(\tau) = \frac{p}{M}, \dot{p}_{-+}(\tau) = \dot{p}_{+-}(\tau) = 0.$$

$$\Phi_{+-}(t) = \frac{2t}{\hbar} \sqrt{(\mu B)^2 + \left(\frac{\hbar\theta' p}{2M}\right)^2} \equiv \frac{t\Delta\mathcal{H}(p)}{\hbar},$$

$$\Phi_{-+}(t) = -\Phi_{+-}(t)$$

$$\Delta\mathcal{H}(p) = \mathcal{H}_+^{\text{MBO}}(p) - \mathcal{H}_-^{\text{MBO}}(p)$$

$$\hat{\mathbf{q}}^{\text{M}} = p\hat{\mathbf{I}} - \hat{\mathbf{A}}_x$$

$$\hat{\mathbf{q}}^{\text{M}}(t) = \begin{pmatrix} p - \frac{\hbar\theta'}{2} \sin \phi(p) & e^{\frac{it\Delta\mathcal{H}(p)}{\hbar}} \frac{\hbar\theta'}{2} \cos \phi(p) \\ e^{\frac{it\Delta\mathcal{H}(p)}{\hbar}} \frac{\hbar\theta'}{2} \cos \phi(p) & p + \frac{\hbar\theta'}{2} \sin \phi(p) \end{pmatrix}.$$

$$\langle \hat{q}(t) \rangle \approx p_0 +$$

$$\frac{\hbar\theta'}{4} \int \frac{dx \, dp}{2\pi\hbar} W(x,p) \sin(2\phi(p)) \left(\cos\left(\frac{t}{\hbar}\Delta\mathcal{H}(p)\right) - 1 \right)$$

$$\lim_{t\rightarrow\infty} \langle \hat{q}(t) \rangle \approx p_0 - \frac{\hbar\theta'}{4} \sin(2\phi(p_0)) \sim \cos(t\Delta\mathcal{H}/\hbar) \langle \sin(2\phi(p)) \rangle \approx \sin(2\phi(p_0))$$

$$\hat{\mathbf{B}}_x' = (i\hbar\partial_x\hat{\mathbf{U}}_{\text{MBO}})\hat{\mathbf{U}}_{\text{MBO}}^\dagger = -\frac{\hbar\partial_x\phi(x,p)}{2}\hat{\sigma}_y,$$

$$\hat{\mathbf{B}}_p' = (i\hbar\partial_p\hat{\mathbf{U}}_{\text{MBO}})\hat{\mathbf{U}}_{\text{MBO}}^\dagger = -\frac{\hbar\partial_p\phi(x,p)}{2}\hat{\sigma}_y.$$

$$\mathcal{B}(x) = \mathcal{B}$$

$$\theta'(x) = \theta'$$

$$\hat{\mathbf{H}}^{\text{SA}}, \hat{\mathbf{x}}^{\text{SA}}$$

$$\partial_x \hat{\mathbf{A}}_x = \hat{\mathbf{B}}_x = 0$$

$$\hat{\mathbf{H}}^{\text{SA}} = \hat{\mathbf{H}}^{\text{M}}, \hat{\mathbf{q}}^{\text{SA}} = \hat{\mathbf{q}}^{\text{M}}, \hat{\mathbf{x}}^{\text{SA}} = \hat{\mathbf{x}}^{\text{M}} + \hat{\mathbf{B}}_p = x\hat{\mathbf{I}} + \hat{\mathbf{B}}_p.$$

$$\hat{\mathbf{H}}^{\text{SA}} = \hat{\mathbf{H}}^{\text{M}}$$

$$\hat{\mathbf{x}}^{\text{SA}}(t) = \begin{pmatrix} x + \left(\frac{p}{M} - \frac{\hbar\theta'}{2M} \sin \phi\right)t & ie^{\frac{it\Delta\mathcal{H}}{\hbar}} \frac{\hbar\phi'}{2} \\ -ie^{\frac{it\Delta\mathcal{H}}{\hbar}} \frac{\hbar\phi'}{2} & x + \left(\frac{p}{M} + \frac{\hbar\theta'}{2M} \sin \phi\right)t \end{pmatrix}$$

$$\hat{\mathbf{q}}^{\text{SA}}(t) = \begin{pmatrix} p - \frac{\hbar\theta'}{2}\sin\phi & e^{-\frac{it\Delta\mathcal{H}}{\hbar}}\frac{\hbar\theta'}{2}\cos\phi \\ e^{\frac{it\Delta\mathcal{H}}{\hbar}}\frac{\hbar\theta'}{2}\cos\phi & p + \frac{\hbar\theta'}{2}\sin\phi \end{pmatrix}.$$

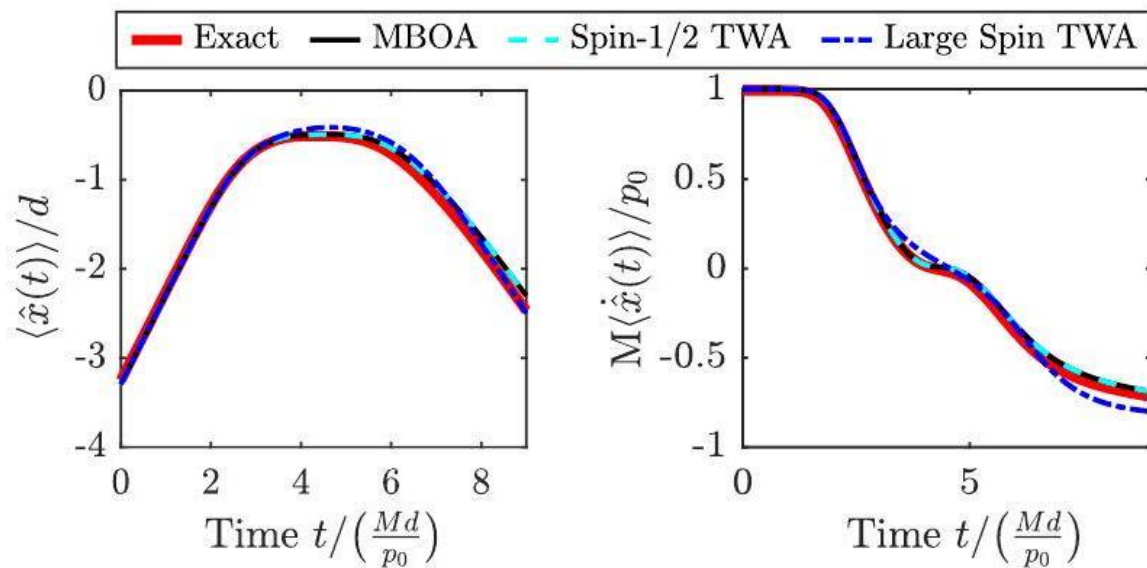
$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{\hat{q}(t)}{M}.$$

$$\mathrm{d}\hat{\mathbf{x}}^{\text{SA}}/\mathrm{d}t = \hat{\mathbf{q}}^{\text{SA}}/M$$

$$\mathcal{B}(x) = \mathcal{B}$$

$$\theta(x) = \theta_0(1 + \text{erf}(x/d))$$

$$p_0 = \hbar\theta_0/(\sqrt{2\pi}d)\sigma_x = d/4$$



$$\hat{H}=\hat{q}^2/2M-\mu\vec{B}(\hat{x})\cdot\hat{\vec{S}}/S$$

$$\dot{x}=\frac{\partial H}{\partial q},\dot{q}=-\frac{\partial H}{\partial x},\hbar\dot{\vec{S}}=-\vec{S}\times\frac{\partial H}{\partial \vec{S}},$$

$$H(x,q,\vec{S})=q^2/2M-\mu\vec{B}(x)\cdot(\vec{S}/S)$$

$$|\vec{S}|=\sqrt{S(S+1)}$$

$$p=q-\hbar S_x\theta'(x),\vec{S}'(x)=R(\theta(x))\vec{S}$$

$$H_{S\rightarrow\infty}^{\text{M}}(x,p,\vec{S}')=\frac{(p+\hbar S'_x\theta'(x))^2}{2M}-\mu\mathcal{B}(x)\frac{S'_z}{S}$$

$$H_{S=1/2}^{\text{M}}(x,p,\vec{S}')=\frac{p^2}{2M}+\frac{(\hbar\theta'(x))^2}{8M}-\mu\mathcal{B}(x)\frac{S'_z}{S}+\frac{\hbar S'_x\theta'(x)p}{M}$$

$$(x(0),p(0))=(x_0,p_0)$$

$$\vec{S}(0)=\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$$

$$\{\vec{S}(0)\} = \left(\pm \frac{1}{2}, \pm \frac{1}{2}, \frac{1}{2}\right)$$

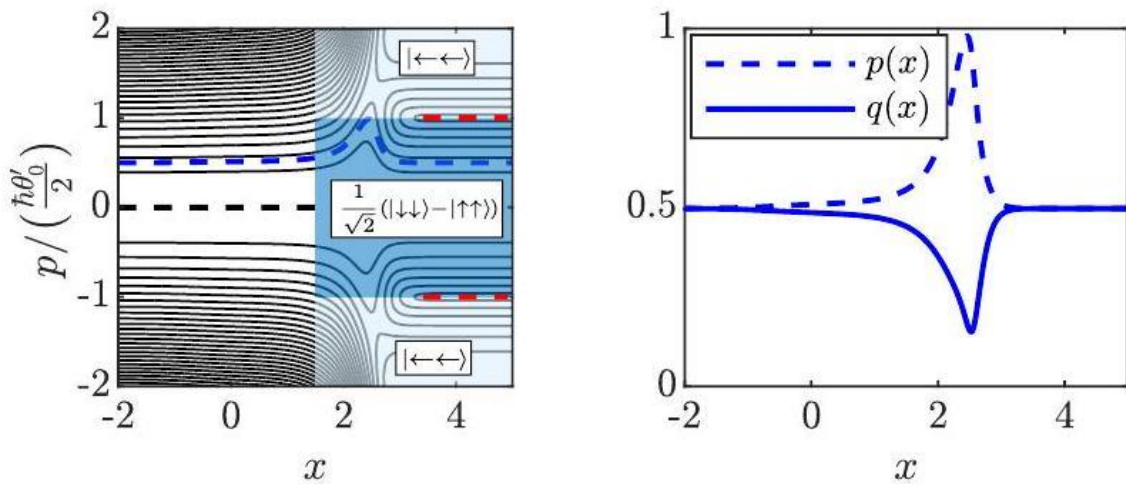
$$W(x,p) = 2\exp\left(-\frac{(x-x_0)^2}{2\sigma_x^2} - \frac{2\sigma_x^2(p-p_0)^2}{\hbar^2}\right)H_{S=1/2}^{\text{M}}H_{S\rightarrow\infty}^{\text{M}}$$

$$\zeta=\frac{(\hbar\theta'_0)^2}{4M\mu\mathcal{B}_0}\ll 1$$

$$\mathcal{B}(x)=\frac{\mathcal{B}_0}{2}\left(1+\mathrm{erf}\left(\frac{x_B^0-x}{d_B}\right)\right)$$

$$\theta'(x)=\frac{\theta'_0}{2}\left(1+\mathrm{erf}\left(\frac{x-x_{\theta'}^0}{d_{\theta'}}\right)\right)$$

$$V(x)=\sqrt{(2\mu\mathcal{B}(x))^2+\left(\frac{(\hbar\theta'(x))^2}{4M}\right)^2}-\frac{(\hbar\theta'(x))^2}{4M}},$$



$$\hat{\mathbf{A}}_x(x)=-\hbar\theta'(x)\hat{\mathbf{S}}_x$$

$$\hat{\mathbf{S}}_x=\sum_{i=1}^N\hat{\sigma}_x^i/2$$

$$(\hat{\mathbf{H}}^{\text{M}})'=\frac{p^2}{2M}-2\mu\mathcal{B}\hat{\mathbf{S}}_z+\frac{p\hbar\theta'}{M}\hat{\mathbf{S}}_x+\frac{(\hbar\theta')^2}{2M}\hat{\mathbf{S}}_x^2.$$

$$\hat{\mathbf{S}}_z=\sum_{i=1}^N\hat{\sigma}_z^i/2$$

$$|p|\ll N|\hbar\theta'|$$

$$(\hat{\mathbf{H}}^{\text{M}})'\cong \frac{p^2}{2M}-2\mu\mathcal{B}\left(\hat{\mathbf{S}}_z-\frac{\chi}{N}\hat{\mathbf{S}}_x^2\right)$$

$$\chi=N(\hbar\theta')^2/4M\mu\mathcal{B}$$

$$\hat{\mathbf{S}}_+ \cong \sqrt{N}a, \hat{\mathbf{S}}_- \cong \sqrt{N}a^\dagger, \hat{\mathbf{S}}_z = \frac{N}{2} - a^\dagger a.$$

$$(\hat{\mathbf{H}}^{\mathbf{M}})' \cong \frac{p^2}{2M} - \mu BN + 2\mu B \left(a^\dagger a + \frac{\chi}{4} (a + a^\dagger)^2 \right)$$

$$\hat{\mathbf{U}}_{\text{MBO}} = \exp \frac{r}{2} (a^2 - a^{\dagger 2}), r = \frac{1}{4} \ln (1 + \chi),$$

$$\hat{\mathbf{U}}_{\text{MBO}}^\dagger (\hat{\mathbf{H}}^{\mathbf{M}})' \hat{\mathbf{U}}_{\text{MBO}} = \frac{p^2}{2M} - \mu BN + 2\mu B \sqrt{1 + \chi} a^\dagger a + \mu B (\sqrt{1 + \chi} - 1).$$

$$|\psi_0^{\text{MBO}}\rangle = \hat{\mathbf{U}}_{\text{MBO}} |0\rangle$$

$$\Delta \hat{\mathbf{S}}_x^2 = \frac{N}{4} \langle \psi_0^{\text{MBO}} | (a + a^\dagger)^2 | \psi_0^{\text{MBO}} \rangle = \frac{N}{4} \frac{1}{\sqrt{1 + \chi}}$$

$$\Delta \hat{\mathbf{S}}_y^2 = -\frac{N}{4} \langle \psi_0^{\text{MBO}} | (a - a^\dagger)^2 | \psi_0^{\text{MBO}} \rangle = \frac{N}{4} \sqrt{1 + \chi}$$

$$\Delta \hat{\mathbf{S}}_y = \frac{\sqrt{N}}{2} (1 + \chi)^{1/4}$$

$$\Delta \hat{\mathbf{S}}_y \sim N/2 = S$$

$$V(x)=kx^2/2$$

$$\boldsymbol{\rho}(x,p)=\delta(E(x,p)-\mathbf{H}(x,p))$$

$$S(x,p,E)=\ln \, \Omega(x,p,E)$$

$$\Omega(x,p,E)=\int \, \mathrm{d}\vec{\xi} \, \mathrm{d}\vec{\eta} \delta(E-\mathbf{H}(x,p))$$

$$S(x,E)=\frac{N}{2}\ln\left[2\pi m E^{\text{fast}}x^2\right]-\ln\left[(N/2)!\right],$$

$$E^{\text{fast}}\equiv E-\frac{p^2}{2M}-\frac{1}{2}kx^2$$

$$x^2E^{\text{fast}}(x)=\text{const.}$$

$$\mathcal{H}^{\text{BO}}(x,p)=\frac{1}{\Omega(x,p,E)}\int \, \mathrm{d}\vec{\xi} \, \mathrm{d}\vec{\eta} \delta(E(x,p)-\mathbf{H}(x,p))\mathbf{H}(x,p),$$

$$=\frac{p^2}{2m}+\frac{1}{2}kx^2+E_0^{\text{fast}}\left(\frac{x_0^2}{x^2}\right),$$

$$\boldsymbol{\rho}_{\beta}(x,p)=\frac{1}{Z_{\beta}(x,p)}e^{-\beta(x,p)\mathbf{H}(x,p)}$$

$$S_{\beta}(x,p,\beta)=\beta E_{\beta}(x,p)+\ln \, Z_{\beta}(x,p)$$

$$S_{\beta}(x,p,\beta)=N\ln\left(x\sqrt{\frac{2\pi m}{\beta}}\right)+\frac{N}{2}$$

$$\frac{x^2}{\beta(x,q)} = \text{const}$$

$$\begin{aligned}\mathcal{H}^{\text{BO}}(x,p) &= \frac{1}{Z_\beta(x,p)} \int \mathrm{d}\vec{\xi} \, \mathrm{d}\vec{\eta} e^{-\beta(x,p)\mathbf{H}(x,p)} \mathbf{H}(x,p), \\ &= \frac{p^2}{2m} + \frac{1}{2} kx^2 + \frac{N}{2\beta_0} \left(\frac{x_0^2}{x^2} \right).\end{aligned}$$

$$E_0^{\text{fast}} = N/(2\beta_0)$$

$$\mathbf{q} = p - \mathbf{A}_x(x)$$

$$\rho^{\mathbf{M}}(x,p) = \frac{1}{Z_\beta^{\mathbf{M}}(x,p)} e^{-\beta^{\mathbf{M}}(x,p)\mathbf{H}^{\mathbf{M}}(x,p)}$$

$$\begin{aligned}\mathbf{H}^{\mathbf{M}}(x,p) &= \frac{(p-\mathbf{A}_x(x))^2}{2M} + \frac{1}{2} kx^2 + \frac{|\vec{\eta}|^2}{2m} \\ + U_0 \sum_{i=1}^N & \left(\Theta(-\xi_i) + \Theta(\xi_i-x) \right), \mathbf{A}_x(x) = \frac{\vec{\xi} \cdot \vec{\eta}}{x}\end{aligned}$$

$$\mathbf{H}^{\mathbf{M}}(x,p) = \frac{p^2}{2M} + \frac{1}{2} kx^2 + \frac{\vec{\eta}^T \cdot \hat{\mu}^{-1}(\vec{\xi}) \cdot \vec{\eta}}{2} + \vec{b}(\vec{\xi})^T \cdot \vec{\eta}$$

$$\hat{\mu}^{-1}(\vec{\xi}) = \frac{1}{m} \hat{1} + \frac{\vec{\xi} \cdot \vec{\xi}^T}{Mx^2}$$

$$\vec{b}(\vec{\xi}) = -\frac{p}{M} \frac{\vec{\xi}}{x}$$

$$\hat{\mu}^{-1}(\vec{\xi})1/m + |\vec{\xi}|^2/(x^2M)$$

$$\begin{aligned}Z_\beta^{\mathbf{M}}(x,p) &= \int \mathrm{d}\vec{\xi} \, \mathrm{d}\vec{\eta} e^{-\beta^{\mathbf{M}}\mathbf{H}^{\mathbf{M}}(x,p)} \\ &= x^N \left(\frac{2\pi m}{\beta^{\mathbf{M}}} \right)^{N/2} e^{-\frac{\beta^{\mathbf{M}} kx^2}{2}} \int_0^1 \mathrm{d}\vec{\xi} \frac{e^{-\frac{\beta^{\mathbf{M}} p^2}{2M} \frac{1}{1+\frac{m}{M}|\vec{\xi}|^2}}}{\sqrt{1+\frac{m}{M}|\vec{\xi}|^2}}\end{aligned}$$

$$\int_0^1 \mathrm{d}\vec{\xi} f(|\vec{\xi}|^2) = \int_{-\infty}^\infty \mathrm{d}u f(uN) P(u)$$

$$P(u) = \int_0^1 \mathrm{d}\vec{\xi} \delta(u-|\vec{\xi}|^2/N), f(uN) = \frac{e^{-\frac{\beta^{\mathbf{M}} p^2}{2M} \frac{1}{1+\frac{mN}{M}u}}}{\sqrt{1+\frac{mN}{M}u}}$$

$$\lim_{N\rightarrow\infty} P(u) = \delta(u-1/3),$$

$$\lim_{N \rightarrow \infty} \int_0^1 d\vec{\xi} f(|\vec{\xi}|^2) = \int_{-\infty}^{\infty} du f(uN) \delta(u - 1/3) \\ = f(N/3)$$

$$Z_{\beta}^M(x,p) \stackrel{N \rightarrow \infty}{=} x^N \left(\frac{2\pi m}{\beta^M} \right)^{N/2} \frac{e^{-\beta^M \left(\frac{p^2}{2(M+\kappa)} + \frac{\kappa x^2}{2} \right)}}{\sqrt{\frac{1+\kappa}{M}}}$$

$$\kappa = \frac{mN}{3}$$

$$E_{\beta}^M(x,p) = \int d\vec{\xi} d\vec{\eta} \frac{e^{-\beta^M \mathbf{H}^M(x,p)}}{Z_{\beta}^M(x,p)} \mathbf{H}^M(x,p) \\ = \frac{p^2}{2M} \frac{\int d\vec{\xi} e^{-\frac{\beta^M p^2}{2M}} \frac{1}{1 + \frac{m}{M} |\vec{\xi}|^2} \left(1 + \frac{m}{M} |\vec{\xi}|^2\right)^{-3/2}}{\int d\vec{\xi} e^{-\frac{\beta^M p^2}{2M}} \frac{1}{1 + \frac{m}{M} |\vec{\xi}|^2} \left(1 + \frac{m}{M} |\vec{\xi}|^2\right)^{-1/2}} + \frac{1}{2} \kappa x^2 + \frac{N}{2\beta^M} \\ \stackrel{N \rightarrow \infty}{=} \frac{p^2}{2(M+\kappa)} + \frac{1}{2} \kappa x^2 + \frac{N}{2\beta^M}$$

$$S_{\beta}^M(x,p) = N \ln \left(x \sqrt{\frac{2\pi m}{\beta^M(x,p)}} \right) + \frac{N}{2} - \frac{1}{2} \ln \left(1 + \frac{\kappa}{M} \right).$$

$$\beta_0^M = \frac{\beta_0}{\left(1 + \frac{\kappa}{M}\right)^{\frac{1}{N}}}$$

$$\beta_0^M \approx \beta_0 (1 - m/(3M))$$

$$\beta_0^M \approx \beta_0 (1 - \ln(\kappa/M)/N)$$

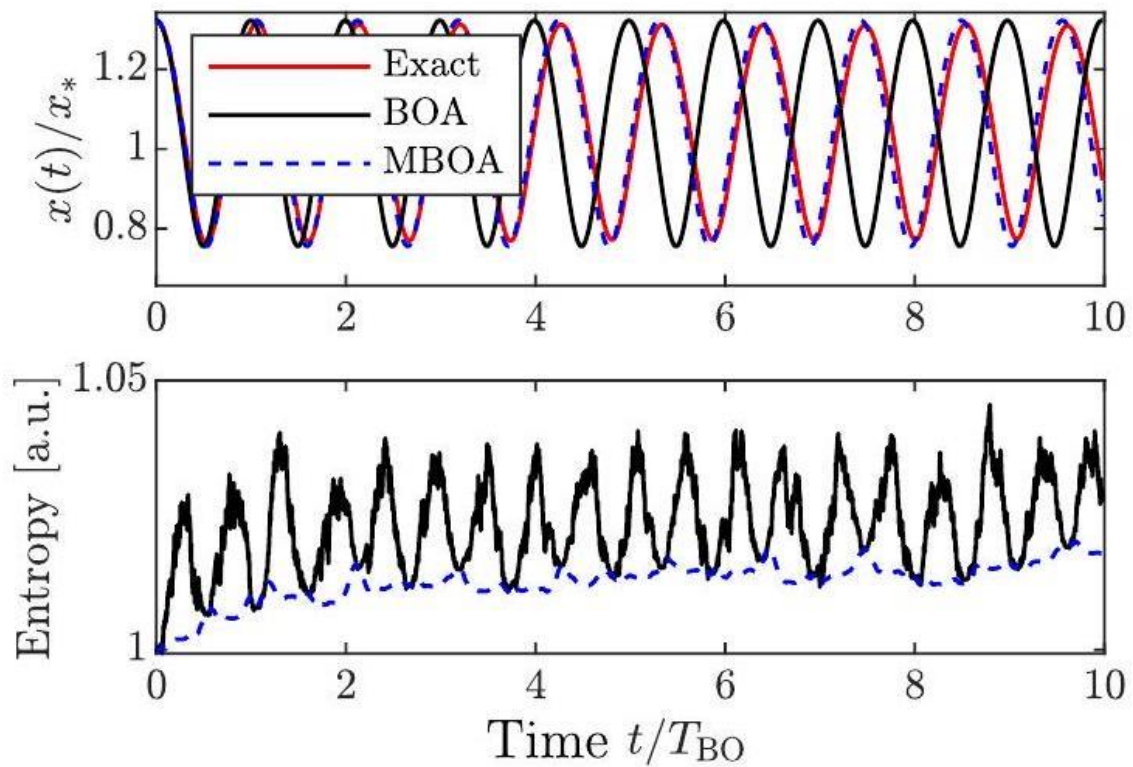
$$E_0^{\text{fast}} = \int d\vec{\xi} d\vec{\eta} \frac{e^{-\beta_0^M \mathbf{H}^M(x,0)} |\vec{\eta}|^2}{Z_{\beta}^M(x,0)} \frac{1}{2m} \\ \stackrel{N \rightarrow \infty}{=} \frac{N}{2\beta_0^M} \left(1 - \frac{1}{N} \frac{\kappa}{M+\kappa} \right)$$

$$\beta_0^M = \beta_0 \left(1 - \frac{1}{N} \frac{\kappa}{M+\kappa} \right).$$

$$\mathcal{H}^{\text{MBO}}(x,p) = \frac{p^2}{2(M+\kappa)} + \frac{1}{2} \kappa x^2 + \frac{N}{2\beta_0^M} \left(\frac{x_0^2}{x^2} \right) \\ \approx \frac{p^2}{2(M+\kappa)} + \frac{1}{2} \kappa x^2 + \frac{N}{2\beta_0} \left(\frac{x_0^2}{x^2} \right) \left(1 + \frac{1}{N} \frac{\kappa}{\kappa+M} \right)$$

$$\mathbf{H}_i^M = \frac{\eta_i^2}{2m} - \frac{p\eta_i}{M} \frac{\xi_i}{x} + U_0(\Theta(-\xi_i) + \Theta(\xi_i - x)),$$

$$\boldsymbol{\rho}_i = e^{-\beta^M \mathbf{H}_i^M} / Z_i^M$$



$$\kappa/M \equiv Nm/(3M) = 2/15$$

$$x(t=0) = 1.75x_*(\beta_0) = 1.75\sqrt{N/(k\beta_0)}$$

$$x_* = \sqrt{1.75}x_*(\beta_0)$$

$$\langle \eta_i \rangle = p \frac{m \xi_i}{M x}.$$

$$\begin{aligned} \langle \mathbf{q} \rangle &= \left\langle p - \frac{\vec{\xi} \cdot \vec{\eta}}{x} \right\rangle = p - \frac{1}{Z_{\beta}^M} \int d\vec{\xi} d\vec{\eta} \frac{\vec{\xi} \cdot \vec{\eta}}{x} e^{-\beta^M \mathbf{H}^M} \\ &= p \left(1 - \int d\vec{\xi} \frac{\frac{m}{M} |\vec{\xi}|^2}{1 + \frac{m}{M} |\vec{\xi}|^2} \right) \stackrel{N \rightarrow \infty}{=} \frac{p}{1 + \frac{\kappa}{M}} \end{aligned}$$

$$p = q + \vec{\xi} \cdot \vec{\eta}/x$$

$$\kappa/M = mN/3M = 5/12$$

$$x(t=0) = 1.25x_*(\beta_0) = 1.25\sqrt{N/(k\beta_0)}p_{\text{BO}}^{\text{max}}$$

$$\sigma_{\mathbf{q}}^2 = \langle \mathbf{q}^2 \rangle - \langle \mathbf{q} \rangle^2 = \langle \mathbf{A}_x^2 \rangle - \langle \mathbf{A}_x \rangle^2 \stackrel{N \rightarrow \infty}{=} \frac{\kappa M}{\kappa + M} \frac{1}{\beta^M}$$

$$S(x,q) = \ln \Omega(x,q), S^M(x,p) = \ln \Omega^M(x,p),$$

$$\Omega(x, q, E) = \int d\vec{\xi} d\vec{\eta} \delta(E - H(\vec{\xi}, \vec{\eta}, x, q)),$$

$$\stackrel{N \rightarrow \infty}{=} \frac{(2\pi m x^2)^{\frac{N}{2}}}{(N/2)!} \left(E - \frac{q^2}{2M} - \frac{1}{2} k x^2 \right)^{\frac{N}{2}}$$

$$\Omega^M(x, p, E) = \int \frac{d\vec{\xi} d\vec{\eta}}{\delta} (E - H^M(\vec{\xi}, \vec{\eta}, x, p)),$$

$$\stackrel{N \rightarrow \infty}{=} \frac{(2\pi m x^2)^{\frac{N}{2}}}{(N/2)! \sqrt{1 + \frac{\kappa}{M}}} \left(E - \frac{p^2}{2(M + \kappa)} - \frac{1}{2} k x^2 \right)^{\frac{N}{2}}$$

$$H(\xi, \eta, x, p) = \frac{q^2}{2M} + \frac{\eta^2}{2m} + \frac{1}{2} k x^2 + U_0(\Theta(-\xi) + \Theta(\xi - x)).$$

$$\mathcal{S}(x, p, E) = \int d\xi d\eta \Theta(E - \mathbf{H}(x, p))$$

$$\begin{aligned} \mathcal{S}(x, p, E) &= \int d\xi d\eta \Theta(E - \mathbf{H}(x, p)) \\ &= 2x\sqrt{2mE^{\text{fast}}} \end{aligned}$$

$$E^{\text{fast}} = E - \frac{p^2}{2M} - \frac{1}{2} k x^2$$

$$x^2 E^{\text{fast}}(x) = \text{const}$$

$$E_n^{\text{fast}}(x) = \frac{\pi^2 n^2}{2m x^2}$$

$$x^2 E^{\text{fast}}(x) = \text{const}$$

$$\mathcal{S}^M(x, p, E) = \int d\xi d\eta \Theta(E - \mathbf{H}^M(x, p))$$

$$\begin{aligned} \eta(\xi) &= \frac{p \frac{m\xi}{Mx}}{1 + \frac{m\xi^2}{Mx^2}} \pm \sqrt{\frac{2m}{1 + \frac{m\xi^2}{Mx^2}} \left(E - \frac{p^2}{2M \left(1 + \frac{m\xi^2}{Mx^2} \right)} - \frac{1}{2} k x^2 \right)}, \left\langle \frac{p\xi\eta(\xi)}{Mx} \right\rangle \approx \frac{p^2}{M} \int_0^x d\xi \frac{m\xi^2}{Mx^2} = \frac{p^2}{M} \frac{m}{3M} \\ &\approx \frac{p \frac{m\xi}{Mx}}{1 + \frac{m\xi^2}{Mx^2}} \pm \sqrt{\frac{2mE}{1 + \frac{m\xi^2}{Mx^2}} \left\langle \frac{\xi^2 \eta^2(\xi)}{2Mx^2} \right\rangle} \approx \frac{m}{M} E \int_0^x d\xi \frac{\xi^2}{x^2} = E \frac{m}{3M} \end{aligned}$$

$$\eta(\xi) \approx p \frac{m\xi}{Mx} \pm \sqrt{2mE} \left(1 - \frac{m\xi^2}{2Mx^2} \right) + \mathcal{O}\left(\frac{m^2}{M^2}\right)$$



$$\begin{aligned}\mathcal{S}^{\text{M}}(x,p,E) &\approx 2\sqrt{2mE} \int_0^x \left(1 - \frac{m}{2M} \frac{\xi^2}{x^2}\right) \\ &= 2x\sqrt{2Em} \left(1 - \frac{m}{6M}\right)\end{aligned}$$

$$\begin{aligned}\mathcal{H}^{\text{MBO}} &= \frac{p^2}{2M} \left(1 - \frac{m}{6M}\right) + \frac{1}{2} kx^2 + E_0 \left(\frac{x_0}{x}\right)^2 \\ &\approx \frac{p^2}{2\left(M + \frac{m}{3}\right)} + \frac{1}{2} kx^2 + E_0 \left(\frac{x_0}{x}\right)^2\end{aligned}$$

$$p=|\boldsymbol{p}|\sim mv$$

$$E\sim mv^2$$

$$\begin{aligned}L_{\text{pNRQED}} = &-\frac{1}{4}\int d^3x F_{\mu\nu}(x)F^{\mu\nu}(x) + \int d^3x \{\psi^\dagger(t,\boldsymbol{x})[i\partial_t - h_e(t,\boldsymbol{x})]\psi(t,\boldsymbol{x}) + N^\dagger(t,\boldsymbol{x})[i\partial_t - h_{Ze}(t,\boldsymbol{x})]N(t,\boldsymbol{x})\} \\ &- \int d^3x d^3y [\psi^\dagger(t,\boldsymbol{x})\psi(t,\boldsymbol{x})V_{Ze}(\boldsymbol{x}-\boldsymbol{y},\boldsymbol{\sigma}) + N^\dagger(t,\boldsymbol{x})N(t,\boldsymbol{x})V_{ZZ}(\boldsymbol{x}-\boldsymbol{y})]N^\dagger(t,\boldsymbol{y})N(t,\boldsymbol{y})\end{aligned}$$

$$F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$$

$$h_e(t,\boldsymbol{x})=eA_0(t,\boldsymbol{x})-\frac{\boldsymbol{D}_{-e}^2(t,\boldsymbol{x})}{2m}-\frac{\boldsymbol{D}_{-e}^4(t,\boldsymbol{x})}{8m^3}$$

$$h_{Ze}(t,\boldsymbol{x})=-ZeA_0(t,\boldsymbol{x})-\frac{\boldsymbol{D}_{Ze}^2(t,\boldsymbol{x})}{2M}$$

$$i\boldsymbol{D}_q(t,\boldsymbol{x})=i\nabla_x-q\boldsymbol{A}(t,\boldsymbol{x})$$

$$V_{Ze}(\boldsymbol{x},\sigma)=V_{Ze}^{\text{LO}}(\boldsymbol{x})+V_{Ze}^{\text{NLO}}(\boldsymbol{x},\sigma_e)$$

$$V_{Ze}^{\text{LO}}(\boldsymbol{x})=-\frac{Z\alpha}{|\boldsymbol{x}|}$$

$$V_{Ze}^{\text{NLO}}(\boldsymbol{x},\sigma_e)=V_{Ze}^{\text{ct}}(\boldsymbol{x})+V_{Ze}^{\text{SO}}(\boldsymbol{x},\sigma_e),$$

$$V_{Ze}^{\text{ct}}(\boldsymbol{x})=-\frac{Z\alpha}{m^2}\Big(-\frac{c_D}{8}+4d_2\Big)4\pi\delta(\boldsymbol{x}),$$

$$V_{Ze}^{\text{SO}}(\boldsymbol{x},\sigma_e)=-ic_S\frac{Z\alpha}{4m^2}\boldsymbol{\sigma}_e\cdot\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|^3}\times\nabla_x\right),$$

$$c_D=1+\frac{\alpha}{\pi}\left(\frac{8}{3}\log\frac{m}{\mu}\right), c_S=1+\frac{\alpha}{\pi}, d_2=\frac{\alpha}{60\pi}.$$

$$V_{ZZ}(\boldsymbol{x})=\frac{Z^2\alpha}{|\boldsymbol{x}|}$$

$$\begin{aligned}|\varphi(t)\rangle = &\int d^3x d^3y_1 d^3y_2 \varphi(t,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2) \\ &\times \psi^\dagger(t,\boldsymbol{x})N^\dagger(t,\boldsymbol{y}_1)N^\dagger(t,\boldsymbol{y}_2)|\text{US}\rangle\end{aligned}$$

$$\begin{aligned}L_{\text{PNRQED}} = &-\frac{1}{4}\int d^3x F_{\mu\nu}(x)F^{\mu\nu}(x) + \int d^3x d^3y_1 d^3y_2 \varphi^\dagger(t,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2)[i\partial_t - h_e(t,\boldsymbol{x}) - h_{Ze}(t,\boldsymbol{y}_1) - h_{Ze}(t,\boldsymbol{y}_2) \\ &- V_{Ze}(\boldsymbol{x}-\boldsymbol{y}_1,\boldsymbol{\sigma}) - V_{Ze}(\boldsymbol{x}-\boldsymbol{y}_2,\boldsymbol{\sigma}) - V_{ZZ}(\boldsymbol{y}_1-\boldsymbol{y}_2)]\varphi(t,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2)\end{aligned}$$

$$\mathbf{R} = \frac{m\mathbf{x} + M(\mathbf{y}_1 + \mathbf{y}_2)}{m + 2M}.$$

$$z = x - \frac{y_1 + y_2}{2},$$

$$\mathbf{r} = \mathbf{y}_1 - \mathbf{y}_2$$

$$\varphi(\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2,t)=U_{-e}(\boldsymbol{x},\boldsymbol{R},t)U_{+Ze}(\boldsymbol{y}_1,\boldsymbol{R},t)U_{+Ze}(\boldsymbol{y}_2,\boldsymbol{R},t)\\ \times S(t,\boldsymbol{x},\boldsymbol{y}_1,\boldsymbol{y}_2,t),$$

$$U_q(\boldsymbol{x},\boldsymbol{R},t)=e^{iq\int_x^Rdx'\cdot\boldsymbol{A}(\boldsymbol{x}',t)}$$

$$A_0(t,\boldsymbol{R})\rightarrow A_0(t,\boldsymbol{R})-\partial_t\theta(t,\boldsymbol{R})$$

$$\boldsymbol{A}(t,\boldsymbol{R})\rightarrow \boldsymbol{A}(t,\boldsymbol{R})+\nabla_R\theta(t,\boldsymbol{R})$$

$$S(t,\boldsymbol{R},\boldsymbol{r},z)\rightarrow e^{-ie_{\rm tot}\theta(t,\boldsymbol{R})}S(t,\boldsymbol{R},\boldsymbol{r},z)$$

$$e_{\rm tot}=-e(1-2Z),$$

$$L_{\rm pNRQED} = -\frac{1}{4}\int d^3x F_{\mu\nu}(x)F^{\mu\nu}(x) + \int d^3R d^3r d^3z S^\dagger(t,\boldsymbol{R},\boldsymbol{r},\boldsymbol{z}) \left[i\partial_t + \frac{\nabla_R^2}{2M_{\rm tot}} + e_{\rm tot}A_0(t,\boldsymbol{R}) + e_{\rm eff}\boldsymbol{z}\cdot\boldsymbol{E}(t,\boldsymbol{R}) \right. \\ \left. - h_0(\boldsymbol{r},\boldsymbol{z}) + \frac{\nabla_r^2}{M} - V_{ZZ}^{\rm LO}(\boldsymbol{r}) + \frac{\nabla_z^2}{4M} + \frac{\nabla_z^4}{8m^3} - V_{Ze}^{\rm NLO}(\boldsymbol{z}+\boldsymbol{r}/2,\boldsymbol{\sigma}) - V_{Ze}^{\rm NLO}(\boldsymbol{z}-\boldsymbol{r}/2,\boldsymbol{\sigma}) \right] S(t,\boldsymbol{R},\boldsymbol{r},\boldsymbol{z})$$

$$h_0(\boldsymbol{r},\boldsymbol{z})=-\frac{\nabla_z^2}{2m}+V_{Ze}^{\rm LO}(\boldsymbol{z}+\boldsymbol{r}/2)+V_{Ze}^{\rm LO}(\boldsymbol{z}-\boldsymbol{r}/2),$$

$$M_{\rm tot}=m+2M,$$

$$\boldsymbol{E}(t,\boldsymbol{R})=-\partial_t\boldsymbol{A}(t,\boldsymbol{R})-\nabla_R A_0(t,\boldsymbol{R})$$

$$e_{\rm eff}=2e\frac{M+Zm}{m+2M}=e+\mathcal{O}(\alpha^2).$$

$$\nabla_r\sim (M/m)^{1/4}m\alpha\sim m\alpha^{5/8}$$

$$-\nabla_r^2/M\sim m\alpha^2\sqrt{m/M}\sim m\alpha^{11/4}$$

$$h_0(\boldsymbol{r},\boldsymbol{z})+V_{ZZ}^{\rm LO}(\boldsymbol{r})\mathcal{O}(m\alpha^2)$$

$$-\nabla_r^2/M\mathcal{O}(m\alpha^{11/4})$$

$$V_{ZZ}^{\rm LO}(\boldsymbol{r})h_0(\boldsymbol{r},\boldsymbol{z})$$

$$\nabla_z^2/4M$$

$$\mathcal{O}(m\alpha^{7/2})\nabla_z^4/8m^3+V_{Ze}^{\rm NLO}$$

$$\mathcal{O}(m\alpha^4)\mathcal{O}(m\alpha^5)$$

$$h_0(\boldsymbol{r},\boldsymbol{z})+\nabla_r^2/M+V_{ZZ}^{\rm LO}(\boldsymbol{r})+\cdots$$

$$S(t,\boldsymbol{r},\boldsymbol{z})=\sum_{\kappa}\Psi_{\kappa}(t,\boldsymbol{r})\phi_{\kappa}(\boldsymbol{r};\boldsymbol{z})$$



$$\phi_{\kappa}(\mathbf{r};\mathbf{z})=\langle\mathbf{z}\mid\mathbf{r},\kappa\rangle$$

$$h_0(\mathbf{r},\mathbf{z})\phi_{\kappa}(\mathbf{r};\mathbf{z})=V_{\kappa}^{\text{light}}(\mathbf{r})\phi_{\kappa}(\mathbf{r};\mathbf{z})$$

$$\int d^3z\phi_{\kappa}^*(\mathbf{r};\mathbf{z})\phi_{\kappa'}(\mathbf{r};\mathbf{z})=\delta_{\kappa\kappa'}$$

$$\kappa=\,^1\Sigma_g^+$$

$$L_{\text{BOEFT}}=-\frac{1}{4}\int d^3xF_{\mu\nu}(x)F^{\mu\nu}(x)\\ +\int d^3r\sum_{\kappa\kappa'}\Psi_{\kappa}^{\dagger}(t,\mathbf{r})\left\{\left[i\partial_t+e_{\text{tot}}A_0(t,\mathbf{0})-H_{\kappa}^{(0)}(\mathbf{r})-\delta E_{\kappa}(\mathbf{r})\right]\delta_{\kappa\kappa'}-C_{\kappa\kappa'}^{\text{nad}}(\mathbf{r})\right\}\Psi_{\kappa'}(t,\mathbf{r})$$

$$H_{\kappa}^{(0)}(\mathbf{r})=-\frac{\nabla_r^2}{M}+V_{ZZ}^{\text{LO}}(\mathbf{r})+V_{\kappa}^{\text{light}}(\mathbf{r})$$

$$\delta E_{\kappa}(\mathbf{r})=\delta^{\text{rec}}E_{\kappa}(\mathbf{r})+\delta^{\text{rec},2}E_{\kappa}(\mathbf{r})+\delta^{\text{NLO}}E_{\kappa}(\mathbf{r})+\delta^{\text{US}}E_{\kappa}(\mathbf{r})$$

$$H_{\kappa}^{(0)}m\alpha^2\sqrt{m/M}\sim m\alpha^{11/4}$$

$$\delta^{\text{rec}}E_{\kappa}(\mathbf{r})=\int d^3z\phi_{\kappa}^*(\mathbf{r};\mathbf{z})\left(-\frac{\nabla_z^2}{4M}\right)\phi_{\kappa}(\mathbf{r};\mathbf{z})=\langle\mathbf{r},\kappa|(-\nabla_z^2)/(4M)|\mathbf{r},\kappa\rangle$$

$$m\alpha^2m/M\sim m\alpha^{7/2}$$

$$\delta^{\text{rec},2}E_{\kappa}(\mathbf{r})=\sum_{\bar{\kappa}\neq\kappa}\frac{|\langle\mathbf{r},\kappa|(-\nabla_z^2)/(4M)|\mathbf{r},\bar{\kappa}\rangle|^2}{V_{\kappa}^{\text{light}}(\mathbf{r})-V_{\bar{\kappa}}^{\text{light}}(\mathbf{r})}$$

$$m\alpha^2(m/M)^2\sim m\alpha^5$$

$$\delta^{\text{NLO}}E_{\kappa}(\mathbf{r})=\int d^3z\phi_{\kappa}^*(\mathbf{r};\mathbf{z})\left[V_{Ze}^{\text{NLO}}(\mathbf{z}+\mathbf{r}/2,\sigma)+V_{Ze}^{\text{NLO}}(\mathbf{z}-\mathbf{r}/2,\sigma)-\frac{\nabla_z^4}{8m^3}\right]\phi_{\kappa}(\mathbf{r};\mathbf{z})$$

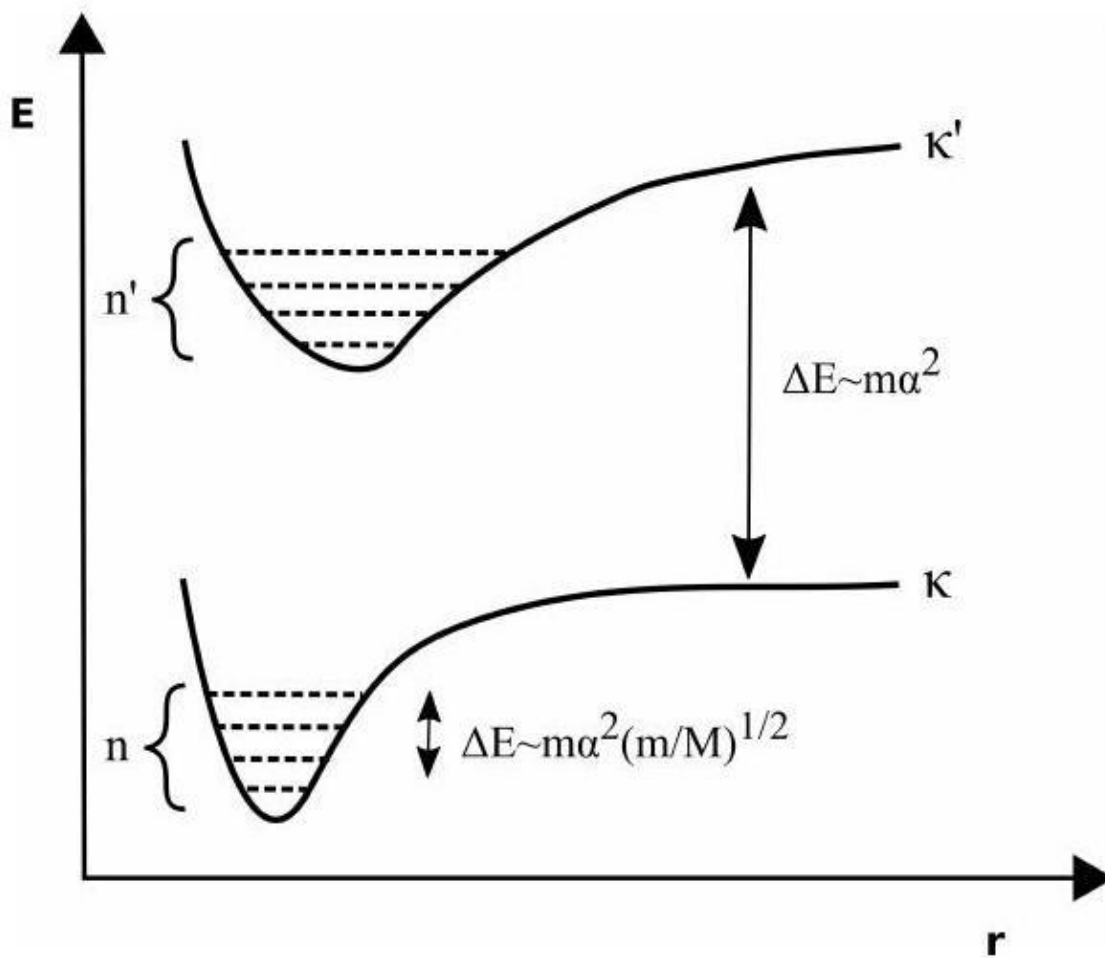
$$\delta^{\text{US}}E_{\kappa}(\mathbf{r})=-\frac{e^2}{6\pi^2}\left\{-\frac{Ze^2}{2m^2}\left[\log\left(\frac{\mu}{m}\right)+\frac{5}{6}-\log(2)\right]\rho_{\kappa}(\mathbf{r})\right.\\ \left.+\sum_{\bar{\kappa}\neq\kappa}|\langle\mathbf{r},\kappa|\mathbf{v}_z|\mathbf{r},\bar{\kappa}\rangle|^2\left(V_{\kappa}^{\text{light}}(\mathbf{r})-V_{\bar{\kappa}}^{\text{light}}(\mathbf{r})\right)\log\left(\frac{m}{|V_{\kappa}^{\text{light}}(\mathbf{r})-V_{\bar{\kappa}}^{\text{light}}(\mathbf{r})|}\right)\right\},$$

$$\mathbf{v}_z=-i\nabla_z/m,\langle\mathbf{r},\kappa|\mathbf{v}_z|\mathbf{r},\bar{\kappa}\rangle$$

$$\langle\mathbf{r},\kappa|\mathbf{v}_z|\mathbf{r},\bar{\kappa}\rangle=\int d^3z\phi_{\kappa}^*(\mathbf{r};\mathbf{z})\mathbf{v}_z\phi_{\bar{\kappa}}(\mathbf{r};\mathbf{z})$$

$$\rho_{\kappa}(\mathbf{r})=|\phi_{\kappa}(\mathbf{r};\mathbf{z}=\mathbf{r}/2)|^2+|\phi_{\kappa}(\mathbf{r};\mathbf{z}=-\mathbf{r}/2)|^2.$$

$$C_{\kappa\kappa'}^{\text{nad}}(\mathbf{r})=\int d^3z\phi_{\kappa}^*(\mathbf{r};\mathbf{z})[-\nabla_r^2/M,\phi_{\kappa'}(\mathbf{r};\mathbf{z})]\\ =\int d^3z\phi_{\kappa}^*(\mathbf{r};\mathbf{z})\left(-\frac{\nabla_r^2}{M}\phi_{\kappa'}(\mathbf{r};\mathbf{z})\right)+\frac{2}{M}\int d^3z\phi_{\kappa}^*(\mathbf{r};\mathbf{z})(-i\nabla_r\phi_{\kappa'}(\mathbf{r};\mathbf{z}))(-i\nabla_r)$$



$$-\nabla_r^2/M \ll m\alpha^2$$

$$V(\mathbf{r}) = V_{ZZ}^{\text{LO}}(\mathbf{r}) + V_0^{\text{light}}(\mathbf{r})$$

$$V(\mathbf{r}) \approx \frac{1}{2}K_0(\mathbf{r} - \mathbf{r}_0)^2, \text{ where } K_0 = \nabla_{r_0}^2 V(\mathbf{r}_0).$$

$$E_0 = 3 \sqrt{\frac{K_0}{2M}}$$

$$\nabla_{r_0} V(\mathbf{r}_0) = \nabla_{r_0} \left(\frac{\alpha Z^2}{r_0} + V_0^{\text{light}}(\mathbf{r}_0) \right) = 0.$$

$$r_0 \sim \frac{1}{m\alpha}$$

$$K_0 = \nabla_{r_0}^2 V(\mathbf{r}_0) \sim m^3 \alpha^4$$

$$E_0 \sim \left(\frac{m^3 \alpha^4}{M} \right)^{1/2} = m\alpha^2 \sqrt{\frac{m}{M}}$$

$$m\alpha^2 \sqrt{m/M}$$

$$2\langle\Psi_0|\frac{\nabla_r^2}{M}|\Psi_0\rangle=E_0$$

$$\frac{\nabla_r^2}{M}\sim m\alpha^2\sqrt{\frac{m}{M}}$$

$$\sqrt{m/M}\sim\alpha^{3/4}\approx0.025$$

$$\nabla_r\sim m\alpha\left(\frac{M}{m}\right)^{1/4}$$

$$w\sim\alpha\left(\frac{m}{M}\right)^{3/4}$$

$$\nabla_r=(\partial_r,\partial_\theta/r,\partial_\phi/(r\sin\theta))$$

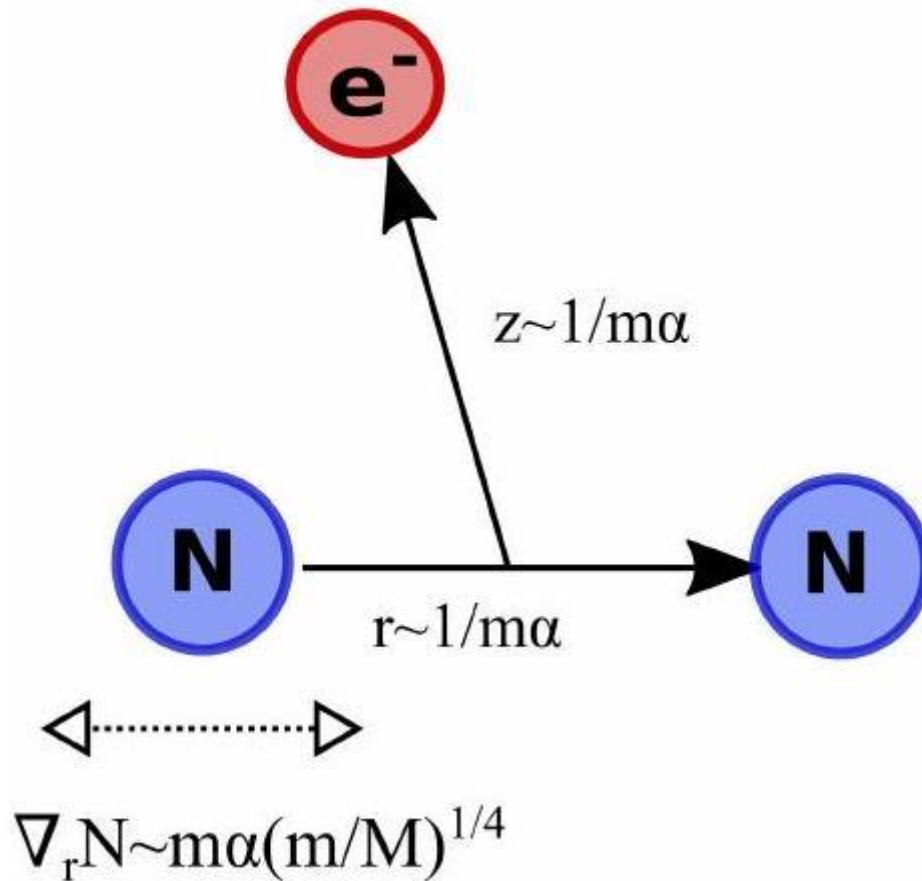
$$r\sim r_0\sim 1/(m\alpha)$$

$$-2/(Mr)\partial/\partial r\sim m\alpha^2(m/M)^{3/4}$$

$$L^2/(Mr^2)m\alpha^2(m/M)$$

$$\nabla_z\sim 1/z\sim m\alpha$$

$$E_{\text{heavy}} \sim m\alpha^2 (m/M)^{1/2} \quad E_{\text{light}} \sim m\alpha^2$$



$$\mathcal{O}(m\alpha^2(m/M)^{3/4})$$

$$\mathcal{O}(m\alpha^2(m/M))$$

$$i\partial_t \Psi_\kappa(t, \mathbf{r}) = H_\kappa^{(0)}(\mathbf{r}) \Psi_\kappa(t, \mathbf{r})$$

$$i\partial_t \Psi_\kappa(t, \mathbf{r}) = \left[H_\kappa^{(0)}(\mathbf{r}) + C_{\kappa\kappa}^{\text{nad}}(\mathbf{r}) \right] \Psi_\kappa(t, \mathbf{r})$$

$$\Psi_{\kappa n}^{(0)}(\mathbf{r}) = \langle \mathbf{r} | \kappa n \rangle^{(0)}$$

$$E_{\kappa n} = E_{\kappa n}^{(0)} + E_{\kappa n}^{(1)} + E_{\kappa n}^{(2)} + \dots$$

$$E_{\kappa n}^{(1)} = {}^{(0)}\langle \kappa n | C_{\kappa\kappa}^{\text{nad}} | \kappa n \rangle^{(0)},$$

$${}^{(0)}\langle \kappa n | O | \bar{\kappa} \bar{n} \rangle^{(0)} = \int d^3r \Psi_{\kappa n}^{(0)*}(\mathbf{r}) O(\mathbf{r}) \Psi_{\bar{\kappa} \bar{n}}^{(0)}(\mathbf{r})$$

$$m\alpha^2(m/M)^{3/4} \sim m\alpha^{25/8}$$

$$m\alpha^2(m/M)^{3/2} \sim m\alpha^{17/4}$$

$$E_{\kappa n}^{\text{mix}} = \sum_{\bar{\kappa} \neq k, \bar{n}} \frac{|\langle {}^{(0)}\kappa n | C_{\kappa \bar{\kappa}}^{\text{nad}} | \bar{\kappa} \bar{n} \rangle^{(0)}|^2}{E_{\kappa n} - E_{\bar{\kappa} \bar{n}}}.$$

$$(m/M)^{1/4} \sim \alpha^{3/8}$$

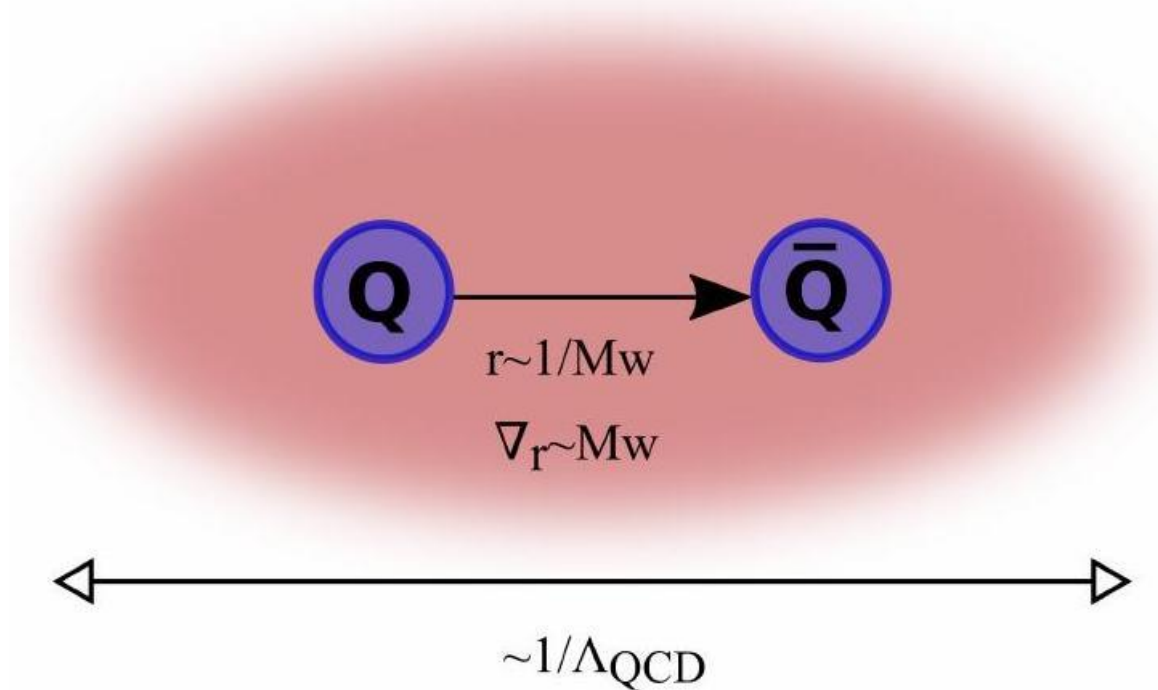
$$m\alpha^2(m/M) \sim m\alpha^{7/2}$$

$$m\alpha^2(m/M)^2 \sim m\alpha^5$$

$$Mw^2 \ll \Lambda_{\text{QCD}}$$

$$Mw \gg \Lambda_{\text{QCD}} \gg Mw^2$$

$$E_{\text{heavy}} \sim Mw^2 \qquad E_{\text{light}} \sim \Lambda_{\text{QCD}}$$



$$\begin{aligned} L_{\text{pNRQCD}} = & \int d^3R \left\{ -\frac{1}{4} G_{\mu\nu}^a G^{\mu\nu a} + \sum_{i=1}^{n_f} \bar{q}_i i \not{p}_q \right. \\ & + \int d^3r \left(\text{Tr} [S^\dagger (i\partial_0 - h_s) S + O^\dagger (iD_0 - h_o) O] \right. \\ & \quad + g \text{Tr} [O^\dagger \mathbf{r} \cdot \mathbf{E} S + S^\dagger \mathbf{r} \cdot \mathbf{E} O] \\ & \quad \left. \left. + \frac{g}{2} \text{Tr} [O^\dagger \mathbf{r} \cdot \mathbf{E} O + O^\dagger O \mathbf{r} \cdot \mathbf{E}] \right) \right\} \end{aligned}$$

$$G^{\mu\nu a} = \bar{G}^{\mu\nu a}(\mathbf{R},t), q_i = q_i(\mathbf{R},t) \; iD_0O = i\partial_0O - g[A_0(\mathbf{R},t),O]$$

$$h_s = -\frac{\nabla_r^2}{M} + V_s(r),$$

$$h_o = -\frac{\nabla_r^2}{M} + V_o(r),$$

$$V_s(r)=-4\alpha_s/(3r)+\cdots$$

$$V_o(r)=\alpha_s/(6r)+\cdots$$

$$h_0(\boldsymbol{R})=\frac{1}{2}(\boldsymbol{E}^a\boldsymbol{E}^a+\boldsymbol{B}^a\boldsymbol{B}^a)-\sum_{f=1}^{n_f}\bar{q}_fi\boldsymbol{D}\cdot\boldsymbol{\gamma}q_f$$

$$h_0(\boldsymbol{R})G_{\kappa}^{ia}(\boldsymbol{R})|\text{US}\rangle=\Lambda_{\kappa}G_{\kappa}^{ia}(\boldsymbol{R})|\text{US}\rangle,$$

$$\kappa=\{J^{P_C},f\}$$

$$|\kappa\rangle=O^{a\dagger}(\boldsymbol{r},\boldsymbol{R})G_{\kappa}^{ia}(\boldsymbol{R})|\text{US}\rangle,$$

$$\int \, d^3rd^3R \sum_{i\kappa} \, |\kappa\rangle \Psi_{\kappa}^i(t,\boldsymbol{r},\boldsymbol{R})$$

$$L_{\rm BOEFT}=\int \, d^3R d^3r \sum_{\kappa} \, \Psi_{\kappa}^{i\dagger}(t,\boldsymbol{r},\boldsymbol{R})\big[(i\partial_t-h_o-\Lambda_{\kappa})\delta^{ij} \\ -\sum_{\lambda} \, P_{\kappa\lambda}^i b_{\kappa\lambda} r^2 P_{\kappa\lambda}^{j\dagger}+\cdots\big] \Psi_{\kappa}^j(t,\boldsymbol{r},\boldsymbol{R})$$

$$P_{10}^l=\hat{r}^l\\ P_{1\pm 1}^l=(\hat{\theta}^l\pm i\hat{\phi}^l)/\sqrt{2}$$

$$\hat{r}=(\sin{(\theta)}\cos{(\phi)},\sin{(\theta)}\sin{(\phi)},\cos{(\theta)})^T,\\ \hat{\theta}=(\cos{(\theta)}\cos{(\phi)},\cos{(\theta)}\sin{(\phi)},-\sin{(\theta)})^T,\\ \hat{\phi}=(-\sin{(\phi)},\cos{(\phi)},0)^T$$

$$P_{\kappa\lambda}^ib_{\kappa\lambda}r^2P_{\kappa\lambda}^{j\dagger}$$

$$b_{\kappa\lambda}=b_{\kappa-\lambda}=b_{\kappa\Lambda}$$

$$V_{\kappa\lambda}=V_o(r)+\Lambda_{\kappa}+b_{\kappa\lambda}r^2$$

$$\Psi_{\kappa\lambda}=P_{\kappa\lambda}^{i\dagger}\Psi_{\kappa}^i$$

$$\Psi_{\kappa}^i=\sum_{\lambda}P_{\kappa\lambda}^i\Psi_{\kappa\lambda}$$

$$L_{\rm BOEFT}=\int \, d^3R d^3r \sum_{\kappa\lambda\lambda'} \, \Psi_{\kappa\lambda}^{\dagger}(t,\boldsymbol{r},\boldsymbol{R})\{[i\partial_t-V_o(r)-\Lambda_{\kappa} \\ -b_{\kappa\lambda}r^2+\cdots]\delta_{\lambda\lambda'}+P_{\kappa\lambda}^{i\dagger}\frac{\nabla_r^2}{M}P_{\kappa\lambda'}^i\}\Psi_{\kappa\lambda'}(t,\boldsymbol{r},\boldsymbol{R})$$

$$P_{\kappa\lambda}^{i\dagger}\frac{\nabla_r^2}{M}P_{\kappa\lambda'}^i=\frac{\nabla_r^2}{M}+C_{\kappa\lambda\lambda'}^{\rm nad},$$

$$C_{\kappa\lambda\lambda'}^{\rm nad}=P_{\kappa\lambda}^{i\dagger}\left[\frac{\nabla_r^2}{M},P_{\kappa\lambda'}^i\right]$$

$$C_{\kappa\lambda\lambda'}^{\rm nad}P_{\kappa\lambda'}^i[{\bf L}^2/(Mr^2),P_{\kappa\lambda'}^i]M_W^2$$

$$i\partial_t\Psi_{\kappa\lambda}(t,\boldsymbol{r},\boldsymbol{R})=\left[\left(-\frac{\nabla_r^2}{M}+V_o(r)+\Lambda_{\kappa}+b_{\kappa\lambda}r^2\right)\delta_{\lambda\lambda'}\right.\\ \left.-\sum_{\lambda'}C_{\kappa\lambda\lambda'}^{\rm nad}\right]\Psi_{\kappa\lambda'}(t,\boldsymbol{r},\boldsymbol{R})$$

$$M_N=2M+\varepsilon_N$$

$$m\alpha^2\sqrt{m/M}$$

$$m/M\sim\alpha^{3/2}\mathcal{O}(m\alpha^5)$$

$$L_{\Psi-A}=\int\,d^3r\sum_{\kappa\kappa'}\Psi_{\kappa}^{\dagger}(t,\boldsymbol{r})[e_{\rm tot}A_0(t,\boldsymbol{0})\delta_{\kappa\kappa'}\\ +e\boldsymbol{E}(t,\boldsymbol{0})\cdot\langle\boldsymbol{r},\kappa|\boldsymbol{z}|\boldsymbol{r},\kappa'\rangle]\Psi_{\kappa'}(t,\boldsymbol{r}),$$

$$e_{\rm eff}=e+\mathcal{O}(\alpha^2)$$

$$e_{\rm eff}\langle\boldsymbol{r},\kappa|\boldsymbol{z}|\boldsymbol{r},\kappa'\rangle$$

$$\langle\boldsymbol{r},\kappa|\boldsymbol{z}|\boldsymbol{r},\kappa'\rangle=\int\,d^3z\phi_{\kappa}^*(\boldsymbol{r};\boldsymbol{z})\boldsymbol{z}\phi_{\kappa}(\boldsymbol{r};\boldsymbol{z})$$

$$i\Pi_{\kappa}(t,\boldsymbol{r},t',\boldsymbol{r}')=\langle\text{US}|T[\Psi_{\kappa}(t,\boldsymbol{r})\Psi_{\kappa}^{\dagger}(t',\boldsymbol{r}')]| \text{US}\rangle\\ =\int_{-\infty}^{+\infty}\frac{dE}{2\pi}e^{-iE(t-t')}i\Pi_{\kappa}(E,\boldsymbol{r},\boldsymbol{r}')$$

$$i\Pi_{\kappa}(E,\boldsymbol{r},\boldsymbol{r}')=i\Pi_{\kappa}^{(0)}(E,\boldsymbol{r},\boldsymbol{r}')\\ +\int\,d^3\bar{\boldsymbol{r}}i\Pi_{\kappa}^{(0)}(E,\boldsymbol{r},\bar{\boldsymbol{r}})\left[-e^2\sum_{\bar{\kappa}}\langle\bar{\boldsymbol{r}},\kappa|\boldsymbol{z}^i|\bar{\boldsymbol{r}},\bar{\kappa}\rangle I^{ij}(E-H_{\bar{\kappa}}^{(0)}(\bar{\boldsymbol{r}}))\langle\bar{\boldsymbol{r}},\bar{\kappa}|\boldsymbol{z}^i|\bar{\boldsymbol{r}},\kappa\rangle\right]i\Pi_{\kappa}^{(0)}(E,\bar{\boldsymbol{r}},\boldsymbol{r}')$$

$$\Pi_{\kappa}^{(0)}(E,\boldsymbol{r},\boldsymbol{r}')H_{\kappa}^{(0)}(\boldsymbol{r})$$

$$\Pi_{\kappa}^{(0)}(E,\boldsymbol{r},\boldsymbol{r}')=\Pi_{\kappa}^{(0)}(E,\boldsymbol{r})\delta^3(\boldsymbol{r}-\boldsymbol{r}'),$$

$$\Pi_{\kappa}^{(0)}(E,\boldsymbol{r})=\frac{1}{E-H_{\kappa}^{(0)}(\boldsymbol{r})+i\eta}$$

$$I^{ij}(E)=\int\,\frac{d^4k}{(2\pi)^4}\frac{i}{k^2}\boldsymbol{k}^2\left(\delta^{ij}-\frac{k^ik^j}{\boldsymbol{k}^2}\right)\frac{i}{E-k^0+i\eta}$$

$$(\Pi_{\kappa}(E,\boldsymbol{r},\boldsymbol{r}')=\Pi_{\kappa}(E,\boldsymbol{r})\delta^3(\boldsymbol{r}-\boldsymbol{r}'))$$

$$i\Pi_{\kappa}(E,\boldsymbol{r})=i\Pi_{\kappa}^{(0)}(E,\boldsymbol{r})\\ +i\Pi_{\kappa}^{(0)}(E,\boldsymbol{r})[-i\Sigma_{\kappa}(E,\boldsymbol{r})]i\Pi_{\kappa}^{(0)}(E,\boldsymbol{r})$$



$$\Sigma_{\kappa}(E, \mathbf{r}) = -ie^2 \sum_{\bar{\kappa}} \langle \mathbf{r}, \kappa | z^i | \mathbf{r}, \bar{\kappa} \rangle \\ \times I^{ij} \left(E - H_{\bar{\kappa}}^{(0)}(\mathbf{r}) \right) \langle \mathbf{r}, \kappa | z^j | \mathbf{r}, \bar{\kappa} \rangle.$$

$$\Sigma_{\kappa} \left(H_{\kappa}^{(0)}(\mathbf{r}), \mathbf{r} \right) = -ie^2 \sum_{\bar{\kappa}} \langle \mathbf{r}, \kappa | z^i | \mathbf{r}, \bar{\kappa} \rangle \\ \times I^{ij} \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - V_{\bar{\kappa}}^{\text{light}}(\mathbf{r}) \right) \langle \mathbf{r}, \kappa | z^j | \mathbf{r}, \bar{\kappa} \rangle.$$

$$I^{ij}(E) = -iE^3 \frac{\delta^{ij}}{6\pi^2} \left[\frac{1}{\epsilon} + \frac{1}{2} \log(4\pi) - \frac{\gamma_E}{2} \right. \\ \left. + \log \left(\frac{\mu}{-E - i\eta} \right) + \frac{5}{6} - \log(2) \right].$$

$$\Sigma_{\kappa}^{\text{div}} \left(H_{\kappa}^{(0)}(\mathbf{r}), \mathbf{r} \right) = -e^2 \frac{\delta^{ij}}{6\pi^2} \frac{1}{\epsilon} \sum_{\bar{\kappa}} \langle \mathbf{r}, \kappa | z^i | \mathbf{r}, \bar{\kappa} \rangle \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - V_{\bar{\kappa}}^{\text{light}}(\mathbf{r}) \right)^3 \langle \mathbf{r}, \bar{\kappa} | z^j | \mathbf{r}, \kappa \rangle \\ = -e^2 \frac{\delta^{ij}}{6\pi^2} \frac{1}{\epsilon} \sum_{\bar{\kappa}} \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - V_{\bar{\kappa}}^{\text{light}}(\mathbf{r}) \right) \langle \mathbf{r}, \kappa | z^i \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - h_0(\mathbf{r}; \mathbf{z}) \right) | \mathbf{r}, \bar{\kappa} \rangle \langle \mathbf{r}, \bar{\kappa} | \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - h_0(\mathbf{r}; \mathbf{z}) \right) z^j | \mathbf{r}, \kappa \rangle.$$

$$\langle \mathbf{r}, \kappa | z^i \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - h_0(\mathbf{r}; \mathbf{z}) \right) | \mathbf{r}, \bar{\kappa} \rangle \\ = \langle \mathbf{r}, \kappa | [h_0(\mathbf{r}, \mathbf{z}), z^i] | \mathbf{r}, \bar{\kappa} \rangle = -i \langle \mathbf{r}, \kappa | v_z^i | \mathbf{r}, \bar{\kappa} \rangle$$

$$v_z^i = -i \nabla_z^i / m$$

$$\Sigma_{\kappa}^{\text{div}} \left(H_{\kappa}^{(0)}(\mathbf{r}), \mathbf{r} \right)$$

$$\Sigma_{\kappa}^{\text{div}} \left(H_{\kappa}^{(0)}(\mathbf{r}), \mathbf{r} \right) = -e^2 \frac{\delta^{ij}}{6\pi^2} \frac{1}{\epsilon} \sum_{\bar{\kappa}} \langle \mathbf{r}, \kappa | v_z^i | \mathbf{r}, \bar{\kappa} \rangle \\ \times \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - V_{\bar{\kappa}}^{\text{light}}(\mathbf{r}) \right) \langle \mathbf{r}, \bar{\kappa} | v_z^j | \mathbf{r}, \kappa \rangle \\ = -e^2 \frac{1}{6\pi^2} \frac{1}{\epsilon} \frac{1}{2} \langle \mathbf{r}, \kappa | \left[v_z^i, [v_z^i, h_0(\mathbf{r}, \mathbf{z})] \right] | \mathbf{r}, \kappa \rangle$$

$$V_{Ze}^{LO}(\mathbf{z} \pm \mathbf{r}/2) h_0(\mathbf{r}, \mathbf{z})$$

$$\left[v_z^i, [v_z^i, h_0] \right] = -\frac{1}{m^2} \left[\nabla_z^i, [\nabla_z^i, h_0] \right] \\ = -\frac{Ze^2}{m^2} [\delta^3(\mathbf{z} - \mathbf{r}/2) + \delta^3(\mathbf{z} + \mathbf{r}/2)]$$

$$1/\epsilon + 1/2 \log(4\pi) - \gamma_E/2 I^{ij}(E)$$

$$\Sigma_{\kappa} \left(H_{\kappa}^{(0)}(\mathbf{r}), \mathbf{r} \right) = \\ -\frac{e^2}{6\pi^2} \left\{ -\frac{Ze^2}{2m^2} \left[\log \left(\frac{\mu}{m} \right) + \frac{5}{6} - \log(2) \right] \rho_{\kappa}(\mathbf{r}) \right. \\ \left. + \sum_{\bar{\kappa}} \left| \langle \mathbf{r}, \kappa | \mathbf{v}_z | \mathbf{r}, \bar{\kappa} \rangle \right|^2 \left(V_{\kappa}^{\text{light}}(\mathbf{r}) - V_{\bar{\kappa}}^{\text{light}}(\mathbf{r}) \right) \right. \\ \left. \times \log \left(\frac{m}{-V_{\kappa}^{\text{light}}(\mathbf{r}) + V_{\bar{\kappa}}^{\text{light}}(\mathbf{r}) - i\eta} \right) \right\}$$

$$\rho_{\kappa}(\boldsymbol{r})=|\phi_{\kappa}(\boldsymbol{r};\boldsymbol{z}=\boldsymbol{r}/2)|^2+|\phi_{\kappa}(\boldsymbol{r};\boldsymbol{z}=-\boldsymbol{r}/2)|^2.$$

$$V_{\bar{\kappa}}^{\rm light}(\boldsymbol{r})=V_{\kappa}^{\rm light}(\boldsymbol{r})$$

$$V_{\kappa}^{\rm light}(\boldsymbol{r})>V_{\bar{\kappa}}^{\rm light}(\boldsymbol{r})$$

$$\Sigma_{\kappa}\left(H_{\kappa}^{(0)}(\boldsymbol{r}),\boldsymbol{r}\right)$$

$$\begin{aligned}\delta E_{\kappa}^{\rm US}(\boldsymbol{r}) = & -\frac{e^2}{6\pi^2}\bigg\{-\frac{Ze^2}{2m^2}\Big[\log\left(\frac{\mu}{m}\right)+\frac{5}{6}-\log(2)\Big]\rho_{\kappa}(\boldsymbol{r}) \\ & +\sum_{\bar{\kappa}}\left|\langle\boldsymbol{r},\kappa|\boldsymbol{v}_z|\boldsymbol{r},\bar{\kappa}\rangle\right|^2\left(V_{\kappa}^{\rm light}(\boldsymbol{r})-V_{\bar{\kappa}}^{\rm light}(\boldsymbol{r})\right) \\ & \times\log\left(\frac{m}{\left|V_{\kappa}^{\rm light}(\boldsymbol{r})-V_{\bar{\kappa}}^{\rm light}(\boldsymbol{r})\right|}\right)\bigg\}\end{aligned}$$

$$\Psi(\boldsymbol{R},q,t)=\underbrace{\psi(q,t)}_{\text{nuclear}}\underbrace{\Phi(\boldsymbol{R},q,t)}_{\text{electronic}},$$

$$r(q,t)\!:=\!\frac{\nabla_q|\psi(q,t)|}{|\psi(q,t)|}$$

$$\hat{H}=-\frac{1}{2M}\nabla_q^2+\hat{H}^{BO}+\hat{V}^{ext}(\boldsymbol{R},q,t),$$

$$\hat{H}^{BO}\!:=\!-\frac{1}{2}\nabla_R^2\!-\!\frac{1}{\sqrt{x^2+y^2+(z+q/2)^2}}\!-\!\frac{1}{\sqrt{x^2+y^2+(z-q/2)^2}}\!+\!\frac{1}{q}.$$

$$\boldsymbol{E}(t) = \big(0,0,\varepsilon e^{-\alpha(t-t_0)^2}\sin{(\omega t)}\big),$$

$$\hat{V}^{ext}(\boldsymbol{R},q,t)=\boldsymbol{E}(t)\cdot\boldsymbol{R}=\varepsilon ze^{-\alpha(t-t_0)^2}\sin{(\omega t)}.$$

$$\Psi(\boldsymbol{R},q,t)=\psi(q,t)\Phi(\boldsymbol{R},q,t)$$

$$\langle \Phi \mid \Phi \rangle_R = 1 \text{ for all } q \text{ and } t$$

$$\hat{K}_q\psi+V_d(q,t)\psi=\imath\frac{\partial\psi}{\partial t}$$

$$\hat{H}^{BO}\Phi+(\hat{D}^{(2)}+\hat{D}^{(1)})\Phi+\hat{V}^{ext}\Phi-V_d(q,t)\Phi=\imath\frac{\partial\Phi}{\partial t}$$

$$V_d(q,t)\!:=\!V_r(q,t)+\imath V_i(q,t)$$

$$\hat{D}^{(1)}:=-\frac{\nabla_q\psi}{\psi}\frac{\nabla_q}{M}$$

$$\hat{D}^{(2)}:=-\frac{\nabla_q^2}{2M}$$

$$\begin{aligned}r_{\psi}(q,t)&:=\Re(\psi^{-1}\nabla_q\psi)=\frac{\nabla_q|\psi|}{|\psi|}\\ p_{\psi}(q,t)&:=\Im(\psi^{-1}\nabla_q\psi)=\nabla_q(\arg\psi)\end{aligned}$$

$$r_{\Phi}(\mathbf{R}, q, t) := \Re(\Phi^{-1} \nabla_q \Phi) = \frac{\nabla_q |\Phi|}{|\Phi|}$$

$$p_{\Phi}(\mathbf{R}, q, t) := \Im(\Phi^{-1} \nabla_q \Phi) = \nabla_q (\arg \Phi)$$

$$\overline{p_{\Phi}} := \langle \Phi | p_{\Phi} | \Phi \rangle_{\mathbf{R}},$$

$$V_i(q,t)=-\frac{1}{M}(2r_{\psi}+\nabla_q)\overline{p_{\Phi}}$$

$$\nabla_q V_r(q,t)=\langle \Phi | \nabla_q (\hat{H}_{BO} + \hat{V}^{ext}) | \Phi \rangle_{\mathbf{R}} + (4r_{\psi} + 2\nabla_q) \langle \Phi | \hat{D}^{(2)} | \Phi \rangle_{\mathbf{R}}$$

$$V_i=\Im(\langle \Phi | \hat{H}_{el} | \Phi \rangle_{\mathbf{R}})$$

$$\hat{H}_{el}=\hat{H}_{BO}+\hat{D}^{(1)}+\hat{D}^{(2)}+\hat{V}^{ext}$$

$$V_r=\Re(\langle \Phi | \hat{H}_{el} | \Phi \rangle_{\mathbf{R}})$$

$$\psi(q,t)\colon=|\psi(q,t)|e^{iS(q,t)}$$

$$p(q,t)=\nabla_q s(q,t)$$

$$p_t=p(q,t)|_{q=q_t}$$

$$\frac{dq_t}{dt}=\frac{p_t}{M}$$

$$\frac{d}{dt}:=\frac{\partial}{\partial t}+\frac{p_t}{M}\nabla_q$$

$$\frac{dp_t}{dt}=-\nabla_q(V+U)|_{q=q_t}$$

$$\frac{ds_t}{dt}=\frac{p_t^2}{2M}-(V+U)|_{q=q_t}$$

$$\frac{d\rho_t}{dt}=-\frac{\rho_t}{M}(\nabla_q p)|_{q=q_t}$$

$$\rho_t=|\psi(q_t)|^2$$

$$U(q,t)\colon=-\frac{\hbar^2}{2M}\frac{\nabla_q^2|\psi|}{|\psi|}.$$

$$w_t\colon=w(q_t)=|\psi(q_t)|^2dq_t,$$

$$w_t=w_0=w,$$

$$\langle \hat{O} \rangle_t = \int O(q) |\psi(q,t)|^2 dq \approx \sum_{i=1}^{N_{traj}} O\left(q_t^{(i)}\right) w^{(i)}$$

$$\Phi(\mathbf{R},q,t)\colon=\sum_{\mu=1}^{N_{bas}}C_{\mu}(q,t)\phi_{\mu}(\mathbf{R},q).$$

$$p_t\colon=p_{\psi}+\overline{p_{\Phi}},$$

$$\frac{dp_\psi}{dt} = -\nabla_q(V_r+U)\big|_{q=q_t} + \frac{\overline{p_\phi}}{M}\nabla_q p_\psi.$$

$$U(q,t)\colon=-\frac{r_\psi^2+\nabla_q r_\psi}{2M}$$

$$\frac{d\boldsymbol{C}(q,t)}{dt}=-\imath\boldsymbol{S}^{-1}\boldsymbol{H}_D\boldsymbol{C}+\frac{p_t}{M}\nabla_q\boldsymbol{C}$$

$$\mathbf{H}_D = \mathbf{H}^{BO} + \mathbf{V}^{ext} - \frac{\nabla_q \psi}{\psi} \frac{1}{M} \left(\mathbf{D}^{(1)} + \mathbf{S} \nabla_q \right) - \frac{1}{2M} \left(\mathbf{D}^{(2)} + \mathbf{S} \nabla_q^2 + 2 \mathbf{D}^{(1)} \nabla_q \right) - \mathbf{S} V_d$$

$$\begin{aligned} S_{\mu\nu} &= \langle \phi_\mu \mid \phi_\lambda \rangle_{\boldsymbol{R}}, \\ H_{\mu\nu}^{BO} &= \langle \phi_\mu \mid \hat{H}^{BO} \phi_\lambda \rangle_{\boldsymbol{R}}, \\ V_{\mu\nu}^{ext} &= \langle \phi_\mu \mid \hat{V}^{ext} \phi_\lambda \rangle_{\boldsymbol{R}}, \\ D_{\mu\nu}^{(1)} &= \langle \phi_\mu \mid \nabla_q \phi_\lambda \rangle_{\boldsymbol{R}}, \\ D_{\mu\nu}^{(2)} &= \langle \phi_\mu \mid \nabla_q^2 \phi_\lambda \rangle_{\boldsymbol{R}}. \end{aligned}$$

$$\boldsymbol{f} = (f_1(q), f_2(q), \ldots, f_N(q))$$

$$\tilde{F}(q) = \sum_{k=1}^N b_k f_k(q) = \boldsymbol{f} \cdot \boldsymbol{b}$$

$$I = \langle \psi(q) | (F(q) - \tilde{F}(q))^2 | \psi(q) \rangle \approx \sum_i^{N_{\text{traj}}} \left(F\left(q_t^{(i)}\right) - \tilde{F}\left(q_t^{(i)}\right) \right)^2 w^{(i)}$$

$$\Omega b = d$$

$$\begin{aligned}\Omega_{kk'} &= \sum_i^{N_{\text{traj}}} f_k\left(q_t^{(i)}\right) f_{k'}\left(q_t^{(i)}\right) w^{(i)} \\ d_k &= \sum_i^{N_{\text{traj}}} F\left(q_t^{(i)}\right) f_k\left(q_t^{(i)}\right) w^{(i)}\end{aligned}$$

$$V_d\text{ (Eq. (9)) is } \boldsymbol{f}^{V_d} = \{1, e^{-11q/20}, e^{-11q/10}, 1/q\}$$

$$\mathcal{G} = \sum_{i=1}^{N_{\text{traj}}} \left(\left(q_t^{(i)} \right)^2 + \left(p_t^{(i)} \right)^2 + \sum_{\mu=1}^{N_{\text{bas}}} \left| C_{i\mu} \right|^2 \right).$$

$$\psi^{-1}\nabla_q\psi=r_\psi+\imath p_\psi$$

$$\overline{p_\Phi} \colon = -\imath \langle \Phi \nabla_q \Phi \rangle,$$

$$d_k = -\frac{1}{2} \langle \psi | \nabla_q f_k | \psi \rangle_q = -\frac{1}{2} \sum_i^{N_{traj}} w^{(i)} \nabla_q f_k \bigg|_{q=q_t^{(i)}}$$

$$\psi(q,0)=\left(\frac{\alpha_{coh}}{\pi}\right)^{1/4}\exp\left(-\frac{\alpha_{coh}}{2}(q-\langle q\rangle_0)^2\right)$$

$$V^{Erf}=\langle \Phi | \hat{H}^{BO} + \hat{V}^{ext} | \Phi \rangle_R,$$

$$F(q)\!:=\!Ae^{-\alpha q}+F_{\rm atomic} \text{ if } q>q_{cut},$$

$$E(q)\!:=\!aq^2+E_0$$

$$C(q)\!:=\!aq^2+bq+C_0(q)$$

$$g_\lambda\!:=\!\frac{1}{2}\phi_\lambda^{(1)}+\frac{1}{2}\phi_\lambda^{(2)},$$

$$u_\lambda\!:=\!\frac{1}{\sqrt{2\sigma q}}\phi_\lambda^{(1)}-\frac{1}{\sqrt{2\sigma q}}\phi_\lambda^{(2)},$$

$$\left\langle \phi_\lambda^{(1)} \mid \phi_\lambda^{(2)} \right\rangle_R = 1 - s_\lambda q^2$$

$$H=\frac{\mathbf{p}^2}{2M}+U_0(\mathbf{x})\hat{c}_H^\dagger\hat{c}_H+U_a(\mathbf{x})(1-\hat{c}_H^\dagger\hat{c}_H)+\sum_n\epsilon_n\hat{c}_n^\dagger\hat{c}_n+\sum_n g(\mathbf{x})(V_n\hat{c}_n^\dagger\hat{c}_H+V_n^*\hat{c}_H^\dagger\hat{c}_n),$$

$$\Gamma(\epsilon)=2\pi\sum_n|V_n|^2\delta(\epsilon-\epsilon_n)$$

$$H_e(\mathbf{x})=U_a(\mathbf{x})+[U_0(\mathbf{x})-U_a(\mathbf{x})]\hat{c}_H^\dagger\hat{c}_H+\sum_n\epsilon_n\hat{c}_n^\dagger\hat{c}_n+\sum_n\left(V_n(\mathbf{x})\hat{c}_n^\dagger\hat{c}_H+V_n^*(\mathbf{x})\hat{c}_H^\dagger\hat{c}_n\right)$$

$$V_n(\mathbf{x})=g(\mathbf{x})V_n$$

$$\Gamma(\epsilon,\mathbf{x})=g^2(\mathbf{x})\Gamma(\epsilon)$$

$$G^r(\epsilon,\mathbf{x})=[\epsilon-\epsilon_H-\Sigma^r(\epsilon,\mathbf{x})]^{-1}$$

$$\Sigma^r(\epsilon,\mathbf{x})=\int\frac{d\epsilon'}{2\pi}\frac{\Gamma(\epsilon',\mathbf{x})}{\epsilon-\epsilon'+i0^+}$$

$$\epsilon_H=U_0(\mathbf{x})-U_a(\mathbf{x})\Sigma^r(\epsilon,\mathbf{x})$$

$$\langle n_H \rangle (\mathbf{x}) = \langle \hat{c}_H^\dagger \hat{c}_H \rangle$$

$$\langle H_{\rm int} \rangle (\mathbf{x}) = \left\langle \sum_n \left(V_n(\mathbf{x}) \hat{c}_n^\dagger \hat{c}_H + V_n^*(\mathbf{x}) \hat{c}_H^\dagger \hat{c}_n \right) \right\rangle$$

$$\langle n_H \rangle (\mathbf{x})\!=\!-\frac{1}{\pi}\int_{-\infty}^{\infty}d\epsilon f(\epsilon)\mathrm{Im}[G^r(\epsilon,\mathbf{x})]$$

$$\langle H_{\rm int} \rangle (\mathbf{x})=-\frac{2}{\pi}\int_{-\infty}^{\infty}d\epsilon f(\epsilon)\mathrm{Im}[G^r(\epsilon,\mathbf{x})\Sigma^r(\epsilon,\mathbf{x})]$$

$$f(\epsilon) = \left[1 + e^{\beta(\epsilon - \mu)}\right]^{-1}$$

$$\beta=1/k_BT$$

$$\mathcal{G}(\mathbf{x})=-k_BT\ln\,\Xi(\mathbf{x}),\Xi(\mathbf{x})=\mathrm{Tr}e^{-\beta(H_e(\mathbf{x})-\mu\hat{N})}$$

$$\mathcal{G}(\mathbf{x})=U_a(\mathbf{x})-U_a(\mathbf{x}_{\mathrm{ref}})+\int_{\mathbf{x}_{\mathrm{ref}}}^{\mathbf{x}}d\mathbf{x}'\left\{\frac{\partial[U_0(\mathbf{x}')-U_a(\mathbf{x}')]}{\partial\mathbf{x}'}\langle n_H\rangle(\mathbf{x}')+\frac{1}{g(\mathbf{x}')}\frac{\partial g(\mathbf{x}')}{\partial\mathbf{x}'}\langle H_{\mathrm{int}}\rangle(\mathbf{x}')\right\}$$

$$E_{\mathrm{adia}}\left(\mathbf{x}\right)\equiv\mathcal{G}(\mathbf{x})|_{T=0}$$

$$\mathcal{C}^{\sigma}(t)=\int_{-\infty}^{+\infty}\frac{d\epsilon}{2\pi}e^{\sigma i\epsilon t}\Gamma(\epsilon)f^{\sigma}(\epsilon)\simeq\sum_{k=1}^Kd_k^{\sigma}e^{-\nu_k^{\sigma}t}$$

$$f^{\sigma}(\epsilon) = \left[1 + e^{\sigma \beta (\epsilon - \mu)}\right]^{-1}$$

$$\hat{\rho}_{\mathbf{J}} \in \mathcal{F}_e \otimes \mathcal{F}_e^* \otimes \mathcal{H}_x \otimes \mathcal{H}_x^* \otimes \mathcal{F}_{\text{eff}}$$

$$\frac{\partial}{\partial t}\hat{\rho}_{\mathbf{J}}(t)=-i[H_{\text{mol}},\hat{\rho}_{\mathbf{J}}]-\gamma_{\mathbf{J}}\hat{\rho}_{\mathbf{J}}-i\sum_{m=1}^{\Omega}(-1)^{\Omega-m}\mathcal{C}_{j_m}\hat{\rho}_{\mathbf{J}\bar{m}}-i\sum_{j\Omega+1}\mathcal{A}_{j\Omega+1}\hat{\rho}_{\mathbf{J}^+},$$

$$\gamma_{\mathbf{J}}=\sum_{(k,\sigma)\in\mathbf{J}}\nu_k^{\sigma}\cdot\mathbf{J}^+$$

$$H_{\text{mol}}=\frac{\mathbf{p}^2}{2M}+U_0(\mathbf{x})\hat{c}_H^\dagger\hat{c}_H+U_a(\mathbf{x})(1-\hat{c}_H^\dagger\hat{c}_H)$$

$$\begin{aligned} \mathcal{C}_j\hat{\rho}_{\mathbf{J}} &= g(\mathbf{x})d_j\hat{c}_j\hat{\rho}_{\mathbf{J}} - (-1)^{\Omega}d_j^*\hat{\rho}_{\mathbf{J}}\hat{c}_jg(\mathbf{x}) \\ \mathcal{A}_j\hat{\rho}_{\mathbf{J}} &= g(\mathbf{x})\hat{c}_j\hat{\rho}_{\mathbf{J}} + (-1)^{\Omega}\hat{\rho}_{\mathbf{J}}\hat{c}_jg(\mathbf{x}) \end{aligned}$$

$$\hat{\rho}_{\mathbf{J}} \approx \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} A_1(n_1,\alpha_1) A_2(\alpha_1,n_2,\alpha_2) \cdots A_d(\alpha_{d-1},n_d)$$

$$\Gamma(\epsilon)=\frac{\eta\gamma^2}{(\epsilon-\epsilon_0)^2+\gamma^2}\Big[1-\frac{1}{1+e^{(\epsilon-E_B/2)/\delta}}\frac{1}{1+e^{-(\epsilon+E_B/2)/\delta}}\Big]$$

$$U_0(x)=A_0\big(e^{2C_0(x-x_0)}-2e^{C_0(x-x_0)}\big)$$

$$U_a(x)=A_1\big(e^{2C_1(x-x_1)}-2e^{C_1(x-x_1)}\big)+B_1+\frac{1}{(x-D_1)^4}$$

$$g(x)=\frac{2}{1+e^{-c_g(x-x_g)}},$$

$$\rho_{ii}(k)=\frac{1}{2\pi}\int\,dx\int\,dx'e^{-ik(x-x')}\rho_{ii}(x,x')$$

$$\rho_{ii}(x,x')\equiv\langle i|\langle x|\hat{\rho}|x'\rangle|i\rangle.$$

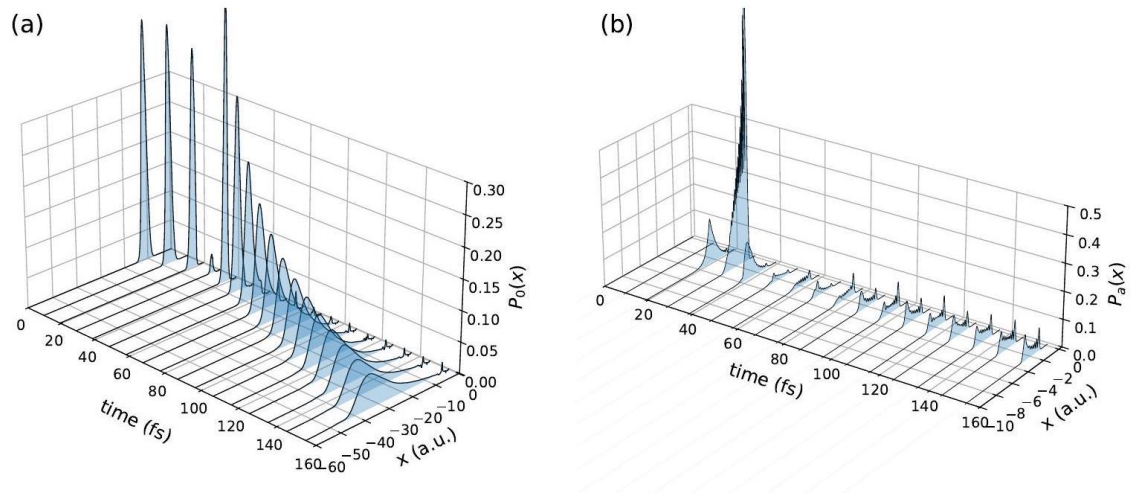
$$P_i(E)=\rho_{ii}(k)\frac{dk}{dE}=\frac{\rho_{ii}(k)}{\hbar}\sqrt{\frac{M}{2E}}$$

$$E\rightarrow 0,\sqrt{1/E}$$

$$\hat{\rho}^{\mathfrak{p}\mathfrak{j}}=\mathcal{P}\hat{\rho}\mathcal{P}$$



$$\mathcal{P} = I - \sum_{E_i < 0} |\psi_i\rangle\langle\psi_i|$$



$$i\partial_t\psi_t(x) = \varepsilon^{-2}\left(-\Delta + 2\mathrm{Re}\int_{\mathbb{R}^3}\frac{e^{-ikx}}{\sqrt{|k|}}\varphi_t(k)\mathrm{d}k\right)\psi_t(x)$$

$$i\partial_t\varphi_t(k) = |k|\varphi_t(k) + \int_{\mathbb{R}^3}\frac{e^{-ikx}}{\sqrt{|k|}}|\psi_t(x)|^2\,\mathrm{d}x$$

$$i\partial_t\varphi_t(k) = |k|\varphi_t(k) + \int_{\mathbb{R}^3}\frac{e^{-ikx}}{\sqrt{|k|}}|\psi_{\varphi_t}(x)|^2\,\mathrm{d}x$$

$$\mathcal{H}=L^2(\mathbb{R}^3_x)\otimes\mathcal{F}$$

$$\mathcal{F}\colon=\Gamma_{\mathrm{sym}}\left(L^2(\mathbb{R}^3_k)\right)$$

$$[a_k,a_\ell^*]=\delta(k-\ell)\text{ and }[a_k,a_\ell]=[a_k^*,a_\ell^*]=0$$

$$p^2\colon=-\Delta, H_f\colon=\int_{\mathbb{R}^3}\omega(k)a_k^*a_k\mathrm{d}k, \omega(k)\colon=|k|$$

$$p^2+\varepsilon\int_{\mathbb{R}^3}(\mathbf{G}(x,k)a_k^*+\overline{\mathbf{G}(x,k)}a_k)\mathrm{d}k+\varepsilon^2H_f$$

$$L^2(\mathbb{R}^3_x)\otimes\mathcal{F}$$

$$\mathbf{G}(x,k)\colon=e^{-ikx}\omega(k)^{-1/2}$$

$$\omega^{-1}G\not\in L^2(\mathbb{R}^3_k)$$

$$\mathbf{G}_\Lambda(x,k)\colon=\mathbf{G}(x,k)\mathbf{1}_{|k|\leqslant\Lambda}$$

$$p^2+\varepsilon\int_{\mathbb{R}^3}(\mathbf{G}_\Lambda(x,k)a_k^*+\overline{\mathbf{G}_\Lambda(x,k)}a_k)\mathrm{d}k+\varepsilon^2H_f$$

$$Q(H^\varepsilon_\Lambda)=Q(p^2+H_f)\text{ for all }\Lambda\in(0,\infty).$$

$$\exp\left(-itH^\varepsilon_\Lambda\right)\exp\left(-it4\pi\varepsilon^2\ln\Lambda\right)\overset{\Lambda\rightarrow\infty}{\longrightarrow}\exp\left(-itH^\varepsilon\right)$$

$$\varepsilon^{-1}\varphi\in L^2(\mathbb{R}_k^3)$$

$$\mathcal{E}(\psi,\varphi)=\int\mathrm{d}x|\nabla\psi(x)|^2+\int\mathrm{d}k\omega(k)|\varphi(k)|^2+\iint\mathrm{d}k\mathrm{d}x|\psi(x)|^2\frac{2\mathrm{Re}(e^{-ikx}\varphi(k))}{\sqrt{\omega(k)}}$$

$$(\psi_t,\varphi_t)\in L^2(\mathbb{R}_x^3)\times L^2(\mathbb{R}_k^3)$$

$$\begin{cases} i\partial_t\psi_t=h_{\varphi_t}\psi_t\\ i\varepsilon^{-2}\partial_t\varphi_t=\omega\varphi_t+\sigma(\psi_t) \end{cases}$$

$$h_{\varphi_t}=p^2+V_{\varphi_t} \text{ with } V_{\varphi_t}(x)=2\mathrm{Re}\langle\varphi_t,\mathbf{G}(x,\cdot)\rangle$$

$$\sigma(\psi_t)(k)=\langle\psi_t,\mathbf{G}(\cdot,k)\psi_t\rangle$$

$$i\partial_t\varphi_t=\omega\varphi_t+\sigma(\psi_{\varphi_t})$$

$$\begin{aligned} H^r(\mathbb{R}_x^3) &:= \left\{ \psi \in L^2(\mathbb{R}_x^3) \colon \left\| (1-\Delta)^{r/2} \psi \right\|_{L^2} < \infty \right\}, \quad r \in \mathbb{R}, \\ \mathfrak{h}_s &:= \left\{ \varphi \in L^2(\mathbb{R}_k^3) \colon \left\| \omega^s \varphi \right\|_{L^2} < \infty \right\}, \quad s \in \mathbb{R}. \end{aligned}$$

$$e(\varphi)\!:=\!\inf\sigma(h_\varphi)<0$$

$$\Delta(\varphi)=\inf\{|e(\varphi)-\lambda| \colon \lambda\in\sigma(h_\varphi)\setminus\{e(\varphi)\}\},$$

$$\varphi_t=e^{-i\omega t}\varphi_0-i\int_0^te^{-i\omega(t-s)}\sigma(\psi_{\varphi_s})\mathrm{d}s$$

$$\varphi\in\mathcal{C}\left((-T_-,T_+);\mathfrak{h}_{1/2}\right)\cap\mathcal{C}^1\left((-T_-,T_+);\mathfrak{h}_{-1/2}\right).$$

$$\inf_{t\in J}\Delta\left(\varphi_t\right)>0$$

$$\varphi_0\in\mathfrak{h}_0\cap\mathfrak{h}_{1/2}$$

$$\varphi\in\mathcal{C}\big((-T_-,T_+);\mathfrak{h}_0\big)$$

$$\liminf_{t\rightarrow T_+}\Delta\left(\varphi_t\right)=0$$

$$\Delta\left(\varphi_t\right)\varphi_t\mapsto\psi_{\varphi_t}$$

$$\mathcal{E}_{\mathrm{field}}\left(u\right)\!:=\!e(u)+\left\| u\right\| _{\mathfrak{h}_{1/2}}^2.$$

$$\mathcal{M}\!:=\!\{T_y\varphi_*\colon y\in\mathbb{R}^3\},(T_yu)(k)\!:=\!e^{-iky}u(k),$$

$$\mathrm{dist}_{\mathfrak{h}_{1/2}}(u,\mathcal{M})\!:=\!\inf_{y\in\mathbb{R}^3}\left\| u-T_y\varphi_*\right\|_{\mathfrak{h}_{1/2}}.$$

$$\mathrm{dist}_{\mathfrak{h}_{1/2}}(\varphi_0,\mathcal{M})\leqslant\eta$$

$$\inf_{t\in\mathbb{R}}\Delta\left(\varphi_t\right)>0.$$



$$\exp\left(i\varepsilon^{-2}\int_0^te(\varphi_{\varepsilon^{-2}s})\mathrm{d}s\right)\psi_{\varepsilon^{-2}t}^{\varepsilon}\underset{\varepsilon\rightarrow 0}{\longrightarrow}\psi_{\varphi_t}\text{ and }\varphi_{\varepsilon^{-2}t}^{\varepsilon}\underset{\varepsilon\rightarrow 0}{\longrightarrow}\varphi_t$$

$$e(\varphi_s^{\varepsilon}):=\inf\sigma(h_{\varphi_s^{\varepsilon}})$$

$$R_{\varphi_t} \coloneqq Q_{\varphi_t} \left(h_{\varphi_t} - e(\varphi_t) \right)^{-1} Q_{\varphi_t}, Q_{\varphi_t} = 1 - P_{\varphi_t}, P_{\varphi_t} = |\psi_{\varphi_t}\rangle \langle \psi_{\varphi_t}|,$$

$$\mathbb{H}_\Lambda(t)=H_f-\iint\,\mathrm{d}k\,\mathrm{d}\ell\langle\psi_{\varphi_t},\mathbf{G}_\Lambda(\cdot,k)R_{\varphi_t}\mathbf{G}_\Lambda(\cdot,\ell),\psi_{\varphi_t}\rangle(a_k^*+a_{-k})(a_\ell^*+a_{-\ell})$$

$$H_f=\mathrm{d}\Gamma(\omega)L^2(\mathbb{R}_x^3)$$

$$\varphi_0\in\mathfrak{h}_{1/2}\text{ with }e(\varphi_0)<0$$

$$\Psi\in D\left(H_f^{1/2}\right)$$

$$\Psi\in C([-T,T],\mathcal{F})\cap L^\infty\left([-T,T],D\left(H_f^{1/2}\right)\right)$$

$$\begin{cases} i\partial_t\Psi(t) \,=\, \mathbb{H}_\Lambda(t)\Psi(t) \\ \Psi(0) \,=\, \Psi \end{cases}$$

$$D\left(\left(1+H_f\right)^{-1/2}\right)$$

$$\mathbb{U}(t)\coloneqq s-\lim_{\Lambda\rightarrow\infty}\mathbb{U}_\Lambda(t)\exp\left(-it4\pi\ln\Lambda\right)$$

$$\Psi^\varepsilon(\varphi_0)=\psi_{\varphi_0}\otimes W(\varepsilon^{-1}\varphi_0)\Omega$$

$$\psi_{\varphi_0}\geqslant h_{\varphi_0}=p^2+V_{\varphi_0}\Omega=(1,\boldsymbol{0})$$

$$W(f)\coloneqq\exp\left(a^*(f)-a(f)\right)$$

$$h_{\varphi_0}=p^2+V_{\varphi_0}$$

$$\varphi_0\in\mathfrak{h}_0\cap\mathfrak{h}_{1/2}\text{ with }e(\varphi_0)<0$$

$$h_{\varphi_t}=p^2+V_{\varphi_t}$$

$$\mu(t)=\int_0^t\left(\mathrm{Im}\langle\varphi_s,\partial_s\varphi_s\rangle+\|\omega^{1/2}\varphi_s\|_{L^2}^2+e(\varphi_s)\right)\mathrm{d}s$$

$$\left\|\exp\left(-i\varepsilon^{-2}tH^\varepsilon+i\varepsilon^{-2}\mu(t)\right)(\psi_{\varphi_0}\otimes W(\varepsilon^{-1}\varphi_0)\Omega)-\psi_{\varphi_t}\otimes W(\varepsilon^{-1}\varphi_t)\mathbb{U}(t)\Omega\right\|\leqslant C\varepsilon^{\frac{1}{10}\ln\frac{1}{\varepsilon}}$$

$$\gamma_{\text{particle}}^\varepsilon(t)\coloneqq\mathrm{Tr}_{\mathcal{F}}\big(e^{-i\varepsilon^{-2}tH^\varepsilon}|\Psi^\varepsilon(\varphi_0)\rangle\langle\Psi^\varepsilon(\varphi_0)|e^{i\varepsilon^{-2}tH^\varepsilon}\big)$$

$$\varphi_0\in\mathfrak{h}_0\cap\mathfrak{h}_{1/2}$$

$$h_{\varphi_t}=p^2+V_{\varphi_t}$$

$$\left|\mathrm{Tr}_{L^2}|\gamma_{\text{particle}}^\varepsilon(t)-|\psi_{\varphi_t}\rangle\langle\psi_{\varphi_t}|\right|\leqslant C\varepsilon^{\frac{1}{10}\ln\frac{1}{\varepsilon}}$$

$$U_K^\varepsilon:=\exp\left(\varepsilon\int\mathrm{d}k(\mathbf{B}_K(x,k)a_k^*-\overline{\mathbf{B}_K(x,k)}a_k)\mathrm{d}k\right)$$

$$\boldsymbol{B}_K(x,k)\colon=\frac{\boldsymbol{G}(x,k)}{k^2}\,\mathbf{1}_{|k|\geqslant K}$$

$$\Psi_K^\varepsilon(\varphi_0)\colon=W(\varepsilon^{-1}\varphi_0)(U_K^\varepsilon)^*(\psi_{\varphi_0}\otimes\Omega).$$

$$\Psi_K^\varepsilon(\varphi_0)$$

$$\|\Psi_K^\varepsilon(\varphi_0)-\Psi^\varepsilon(\varphi_0)\|\leqslant C\varepsilon K^{-1}$$

$$\|(U_K^\varepsilon - \mathbf{1})\Psi\| \leqslant C\varepsilon \|B_K\|_{L^2} \|(N+1)^{1/2}\Psi\|,$$

$$\Psi\in D(N^{1/2})$$

$$\|B_K\|_{L^2}\leqslant CK^{-1}$$

$$N\colon=\int_{\mathbb{R}^3}a_k^*a_k\,\mathrm{d}k$$

$$\gamma_{\mathrm{field}}^\varepsilon(t)(k,\ell)\colon=\varepsilon^2\langle e^{-i\varepsilon^{-2}tH^\varepsilon}\Psi_K^\varepsilon(\varphi_0),a_k^*a_\ell e^{-i\varepsilon^{-2}tH^\varepsilon}\Psi_K^\varepsilon(\varphi_0)\rangle$$

$$\lim_{\varepsilon\rightarrow 0}\mathrm{Tr}_{L^2}\big(\gamma_{\mathrm{field}}^\varepsilon(0)\big)=\|\varphi_0\|_{L^2}^2$$

$$\varphi_0\in\mathfrak{h}_0\cap\mathfrak{h}_{1/2}\text{with }e(\varphi_0)<0$$

$$\left\|N^{1/2}W(\varepsilon^{-1}\varphi_t)^*e^{-i\varepsilon^{-2}tH^\varepsilon}\Psi_K^\varepsilon(\varphi_0)\right\|^2\leqslant C\varepsilon^{-29/15}\ln\frac{1}{\varepsilon}$$

$$\mathrm{Tr}_{L^2}|\gamma_{\mathrm{field}}^\varepsilon(t)-|\varphi_t\rangle\langle\varphi_t||\leqslant C\varepsilon^{1/15}\ln\frac{1}{\varepsilon}$$

$$e^{-i\varepsilon^{-2}tH^\varepsilon}\Psi_K^\varepsilon(\varphi_0)W(\varepsilon^{-1}\varphi_t)\Omega\mathcal{O}(\varepsilon^{-2})|\varphi_t\rangle\langle\varphi_t|$$

$$t=\mathcal{O}(\varepsilon^{-2})$$

$$t=\mathcal{O}(\alpha^2)$$

$$\mathbb{H}_\Lambda(t)=\mathbb{H}_{\mathcal{D},K,\Lambda}(t)-4\pi\ln\Lambda\mathbb{H}_{\mathcal{D},K,\Lambda}(t)$$

$$(a^*(\mathbf{f})\Psi)(x)\colon=\left(\int_{\mathbb{R}^3}\mathbf{f}(x,k)a_k^*\mathrm{d}k\right)\Psi(x), (a(\mathbf{f})\Psi)(x)\colon=\left(\int_{\mathbb{R}^3}\overline{\mathbf{f}(x,k)}a_k\mathrm{d}k\right)\Psi(x)$$

$$\mathbf{f}\colon\mathbb{R}_x^3\times\mathbb{R}_k^3\rightarrow\mathbb{C}$$

$$\omega^{-1/2}\mathbf{f}(x,\cdot)\in L^2(\mathbb{R}_k^3)$$

$$\mathbf{f}(x,k)=e^{-ikx}f(k)$$

$$f\colon\mathbb{R}_k^3\rightarrow\mathbb{C}$$

$$\phi(\mathbf{f})\colon=a^*(\mathbf{f})+a(\mathbf{f})$$

$$\begin{aligned} G_K(x,k) &= e^{-ikx} G_K(k) \quad \text{with} \quad G_K(k) = \omega(k)^{-1/2} \mathbf{1}_{|k| \leq K} \\ B_K(x,k) &= e^{-ikx} B_K(k) \quad \text{with} \quad B_K(k) = \frac{G(k)}{|k|^2} \mathbf{1}_{|k| \geq K} \end{aligned}$$

$$\boldsymbol{B}_{K,\Lambda}(x,k) := e^{-ikx} B_{K,\Lambda}(k), B_{K,\Lambda}(k) := B_K(k) \mathbf{1}_{|k| \leq \Lambda}$$

$$N_K := \int \mathbf{1}_{|k| \geq K} a_k^* a_k \, dk, H_{f,K} := \int \mathbf{1}_{|k| \geq K} \omega(k) a_k^* a_k \, dk$$

$$\langle A \rangle := (1+A^*A)^{1/2},$$

$$X\lesssim Y$$

$$p\colon=-i\nabla_x, \omega(k)\colon=|k|,$$

$$\begin{aligned} H^r &:= \left\{ \psi \in L^2(\mathbb{R}_x^3) \colon \left\| (1+p^2)^{r/2} \psi \right\|_{L^2} < \infty \right\}, r \in \mathbb{R}, \\ \mathfrak{h}_s &:= \left\{ \varphi \in L^2(\mathbb{R}_k^3) \colon \left\| \omega^s \varphi \right\|_{L^2} < \infty \right\}, s \in \mathbb{R}. \end{aligned}$$

$$\hat{f}(k) \mathop{:}= \int_{\mathbb{R}^3} e^{-ikx} f(x) \mathrm{d} x, f(x) = (2\pi)^{-3} \int_{\mathbb{R}^3} e^{ikx} \hat{f}(k) \mathrm{d} k$$

$$\mathbf{f}(x,k)=e^{-ikx}f(k) \text{ with } f\colon \mathbb{R}^3\rightarrow \mathbb{R}$$

$$\mathrm{supp}(f)\subseteq \{|k|\geqslant K\} \text{ for } K\geqslant 0$$

$$\begin{aligned} \|a(\mathbf{f})\Psi\| &\leq \|f\|_{L^2}\left\|N_K^{\frac{1}{2}}\Psi\right\|, \|a(\mathbf{f})\Psi\| \leq \left\|\omega^{-\frac{1}{2}}f\right\|_{L^2}\left\|H_{f,K}^{\frac{1}{2}}\Psi\right\| \\ \|a^*(\mathbf{f})\Psi\| &\leq \|f\|_{L^2}\left\|\left\langle N_K^{\frac{1}{2}}\right\rangle\Psi\right\|, \|a^*(\mathbf{f})\Psi\| \leq \max\left\{\|f\|_{L^2},\left\|\omega^{-\frac{1}{2}}f\right\|_{L^2}\right\}\left\|\left\langle H_{f,K}^{\frac{1}{2}}\right\rangle\Psi\right\| \end{aligned}$$

$$\Psi \in L^2(\mathbb{R}_x^3) \otimes \mathcal{F}$$

$$\mathbf{g}(x,k)=e^{-ikx}g(k) \text{ with } g\colon \mathbb{R}^3\rightarrow \mathbb{R}$$

$$\mathrm{supp}(g)\subseteq \{|k|\geqslant \Lambda\} \text{ for } \Lambda\geqslant K$$

$$\|a(\mathbf{f})a(\mathbf{g})\Psi\| \leq \left\|\omega^{-\frac{1}{4}}f\right\|_{L^2}\left\|\omega^{-\frac{1}{4}}g\right\|_{L^2}\left\|\left\langle N_K^{\frac{1}{2}}\right\rangle H_{f,K}^{\frac{1}{2}}\Psi\right\|.$$

$$\mathbf{f}(x,k)=e^{-ikx}f(k) \text{ with } f\colon \mathbb{R}^3\rightarrow \mathbb{R}$$

$$\|a(\mathbf{f})\Psi\|^2 \leqslant \mathcal{C}_{s,r}(f) \| \langle |p|^r \rangle \mathrm{d}\Gamma(\omega^s)^{\frac{1}{2}} \Psi \|^2 \text{ with } \mathcal{C}_{s,r}(f) = \sup_{h \in \mathbb{R}^3} \int \mathrm{d}k \frac{|f(k)|^2}{\omega(k)^s (1+|h-k|^{2r})}$$

$$\Psi \in L^2(\mathbb{R}_x^3) \otimes \mathcal{F}$$

$$\mathrm{d}\Gamma(\omega^s)=\int\,\,\omega(k)^sa_k^*a_kdk$$

$$\mathcal{C}_{s,r}(f) \leqslant \int \mathrm{d}k \frac{|f(k)|^2}{|k|^s (1+|k|^{2r})}$$



$$f_s = \omega^{-\frac{s}{2}} f$$

$$\begin{aligned} \|a(\mathbf{f})\Psi\|^2 &= \int dk \, d\ell \left\langle e^{ikx} \overline{f_s(k)} \omega^{\frac{s}{2}}(k) a_k \Psi, \frac{\langle |p-k|^r \rangle}{\langle |p-\ell|^r \rangle} \overline{\langle |p-\ell|^r \rangle} e^{i\ell x} \overline{f_s(\ell)} \omega^{\frac{s}{2}}(\ell) a_\ell \Psi \right\rangle \\ &\leq \int dk \, d\ell \left\| \frac{1}{\langle |p-k|^r \rangle} f_s(k) \langle |p-\ell|^r \rangle e^{i\ell x} \omega^{\frac{s}{2}}(\ell) a_\ell \Psi \right\|^2 \\ &= \int d\ell \omega^s(\ell) \langle |p-\ell|^r \rangle e^{i\ell x} a_\ell \Psi, \int dk \frac{|f_s(k)|^2}{\langle |p-k|^r \rangle^2} \langle |p-\ell|^r \rangle e^{i\ell x} a_\ell \Psi \\ &\leq \left\| \int dk \frac{|f_s(k)|^2}{\langle |p-k|^r \rangle^2} \right\| \|\langle |p|^r \rangle d\Gamma(\omega^s)^{\frac{1}{2}} \Psi\|^2 \end{aligned}$$

$$\langle |p-\ell|^r \rangle e^{i\ell x} = e^{i\ell x} \langle |p|^r \rangle \psi \in L^2(\mathbb{R}^3)$$

$$\left\| \int dk \frac{|f_s(k)|^2}{\langle |p-k|^r \rangle^2} \psi \right\| = \left[\int dp \left| \int dk \frac{|f_s(k)|^2}{\langle |p-k|^r \rangle^2} \hat{\psi}(p) \right|^2 \right]^{\frac{1}{2}} \leq \sup_{p \in \mathbb{R}^3} \int dk \frac{|f_s(k)|^2}{1+|p-k|^{2r}}.$$

$$\begin{aligned} \|\omega^{-s} G_K\|_{L^2} &\lesssim K^{1-s} \\ \|\mathbf{1}_{|k|\geq 2} |k|^{-1} G_K\|_{L^2} &\lesssim \sqrt{\ln K} \\ \|\omega^{s-1} k B_K\|_{L^2} &\lesssim K^{s-1} \end{aligned}$$

$$\begin{aligned} \mathcal{C}_{0,1}(G_K) &\lesssim \ln K, \mathcal{C}_{0,r}(kB_K) \lesssim K^{-3r/2} \\ \mathcal{C}_{1,1}(G_K) &\lesssim 1, \mathcal{C}_{1,1}(\omega kB_K) \lesssim K^{-3/4} \\ \mathcal{C}_{s,1}(\omega G_K) &\lesssim K^{2-s}, \mathcal{C}_{0,2}(\omega kB_K) \lesssim K^{-1} \end{aligned}$$

$$\begin{aligned} \mathcal{C}_{0,r}(kB_K) &= \sup_{h \in \mathbb{R}^3} \int \frac{\mathbf{1}(|k| \geq K)}{|k|^3 (1+|k-h|^{2r})} dk \\ &\leq K^{-\frac{3}{2}r} \sup_{h \in \mathbb{R}^3} \int \frac{\mathbf{1}(|k| \geq K)}{|k|^{3-\frac{3}{2}r} (1+|k-h|^{2r})} dk \lesssim K^{-\frac{3}{2}r} \end{aligned}$$

$$\Psi \in L^2(\mathbb{R}^3_x) \otimes \mathcal{F}$$

$$\|a(\mathbf{G}_K)\Psi\| \lesssim \min \left\{ (\ln K)^{\frac{1}{2}} \left\| \langle p \rangle N^{\frac{1}{2}} \Psi \right\|, \left\| \langle p \rangle H_f^{\frac{1}{2}} \Psi \right\|, K^{\frac{1}{2}} \left\| H_f^{\frac{1}{2}} \Psi \right\| \right\},$$

$$\|a(\omega \mathbf{G}_K)\Psi\| \lesssim \min \left\{ K \left\| \langle p \rangle N^{\frac{1}{2}} \Psi \right\|, K^{\frac{1}{2}} \left\| \langle p \rangle H_f^{\frac{1}{2}} \Psi \right\| \right\},$$

$$\|a(k \mathbf{B}_K)\Psi\| \lesssim \min \left\{ K^{-\frac{3}{4}} \left\| \langle p \rangle N^{\frac{1}{2}} \Psi \right\|, K^{-\frac{1}{2}} \left\| H_f^{\frac{1}{2}} \Psi \right\| \right\},$$

$$\|a(\omega k \mathbf{B}_K)\Psi\| \lesssim \min \left\{ K^{-\frac{3}{8}} \left\| \langle p \rangle H_f^{\frac{1}{2}} \Psi \right\|, K^{-\frac{1}{2}} \left\| \langle p^2 \rangle N^{\frac{1}{2}} \Psi \right\| \right\}.$$

$$|\langle \Psi, a(k \mathbf{B}_K) a(k \mathbf{B}_\Lambda) \Phi \rangle| \lesssim (K\Lambda)^{-\frac{1}{4}} \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Psi \right\| \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Phi \right\|$$

$$\|a(k \mathbf{B}_K) a(k \mathbf{B}_\Lambda) \Psi\| \lesssim (K\Lambda)^{-\frac{3}{8}} \|\langle p \rangle N \Psi\|$$

$$|\langle \Psi, a(k\mathbf{B}_K)a(k\mathbf{B}_\Lambda)\Phi \rangle| = \left| \left\langle \Psi, a(k\mathbf{B}_K)a(k\mathbf{B}_\Lambda) \left\langle N_K^{\frac{1}{2}} \right\rangle^{-1} \Phi \right\rangle \right|$$

$$= \left| \left\langle (N_K + 3)^{\frac{1}{2}} \Psi, a(k\mathbf{B}_K)a(k\mathbf{B}_\Lambda) \left\langle N_K^{\frac{1}{2}} \right\rangle^{-1} \Phi \right\rangle \right|$$

$$\lesssim \left\| \left\langle N_K^{\frac{1}{2}} \right\rangle \Psi \right\| \left\| a(k\mathbf{B}_K)a(k\mathbf{B}_\Lambda) \left\langle N_K^{\frac{1}{2}} \right\rangle^{-1} \Phi \right\|$$

$$\lesssim \left\| \omega^{-\frac{1}{4}} k B_K \right\|_{L^2} \left\| \omega^{-\frac{1}{4}} k B_\Lambda \right\|_{L^2} \left\| \left\langle N_K^{\frac{1}{2}} \right\rangle \Psi \right\| \left\| H_{f,K}^{\frac{1}{2}} \Phi \right\|$$

$$\lesssim (K\Lambda)^{-\frac{1}{4}} \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Phi \right\| \left\| H_f^{\frac{1}{2}} \Psi \right\|$$

$$\|a(k\mathbf{B}_K)a(k\mathbf{B}_\Lambda)\Psi\|^2 \leq \mathcal{C}_{0,\frac{1}{2}}(kB_K) \left\| \langle |p|^{\frac{1}{2}} \rangle a(k\mathbf{B}_\Lambda) N^{\frac{1}{2}} \Psi \right\|^2$$

$$\left\| \langle |p|^{\frac{1}{2}} \rangle a(k\mathbf{B}_\Lambda) N^{\frac{1}{2}} \Psi \right\|^2 \leq 2 \left\| a \left(\langle |k|^{\frac{1}{2}} \rangle k B_\Lambda \right) N^{\frac{1}{2}} \Psi \right\|^2 + 2 \left\| a(k\mathbf{B}_\Lambda) \langle |p|^{\frac{1}{2}} \rangle N^{\frac{1}{2}} \Psi \right\|^2$$

$$\leq 2\mathcal{C}_{0,1} \left(|k|^{\frac{3}{2}} B_\Lambda \right) \|\langle p \rangle N \Psi\|^2 + 2\mathcal{C}_{0,\frac{1}{2}}(kB_\Lambda) \left\| \langle |p|^{\frac{1}{2}} \rangle^2 N \Psi \right\|^2.$$

$$\langle |p|^{1/2} \rangle^2 \lesssim \langle p \rangle$$

$$\mathcal{C}_{0,1}(|k|^{3/2}B_\Lambda) = \mathcal{C}_{1,1}(\omega k B_\Lambda)$$

$$\omega(k) = |k|$$

$$A_K := \phi(\mathbf{G}_K) + 2a^*(k\mathbf{B}_K) \cdot p + 2p \cdot a(k\mathbf{B}_K)$$

$$D_K := 2a^*(k\mathbf{B}_K)a(k\mathbf{B}_K) + a^*(k\mathbf{B}_K)^2 + a(k\mathbf{B}_K)^2 + 4\pi \ln K$$

$$|\langle \Psi, A_K R A_K \Psi \rangle| \lesssim K^2 (\|\langle p \rangle R \langle p \rangle\| + \|R\|) \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \langle p \rangle \Psi \right\|^2,$$

$$|\langle \Psi, [N, A_K] R A_K \Psi \rangle| \lesssim K^2 (\|\langle p \rangle R \langle p \rangle\| + \|R\|) \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \langle p \rangle \Psi \right\|^2,$$

$$|\langle \Psi, D_K \Psi \rangle| \lesssim K^{-\frac{1}{2}} \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Psi \right\|^2 + \ln K \|\Psi\|^2,$$

$$|\langle \Psi, [N, D_K] \Psi \rangle| \lesssim K^{-\frac{1}{2}} \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Psi \right\|^2.$$

$$|\langle \Psi, A_K R A_K \Psi \rangle| \lesssim \ln K (\| \langle p \rangle R \langle p \rangle \| + \| R \|) \left\| \left\langle N^{\frac{1}{2}} \right\rangle \langle p \rangle \Psi \right\|^2,$$

$$|\langle \Psi, [N, A_K] R A_K \Psi \rangle| \lesssim \ln K (\| \langle p \rangle R \langle p \rangle \| + \| R \|) \left\| \left\langle N^{\frac{1}{2}} \right\rangle \langle p \rangle \Psi \right\|^2,$$

$$|\langle \Psi, D_K \Psi \rangle| \lesssim \ln K \left\| \left\langle N^{\frac{1}{2}} \right\rangle \langle p \rangle \Psi \right\|^2,$$

$$|\langle \Psi, [N, D_K] \Psi \rangle| \lesssim K^{-\frac{1}{2}} \left\| \left\langle N^{\frac{1}{2}} \right\rangle \langle p \rangle \Psi \right\|^2.$$

$$|\langle \Psi, \phi(\mathbf{G}_K) R \phi(\mathbf{G}_K) \Psi \rangle| \lesssim K^2 \| R \| \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Psi \right\|^2,$$

$$|\langle \Psi, (a^*(k\mathbf{B}_K) \cdot p) R (p \cdot a(k\mathbf{B}_K)) \Psi \rangle| \lesssim K^{-1} \| \langle p \rangle R \langle p \rangle \| \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Psi \right\|^2.$$

$$\begin{aligned} \langle \Psi, (p \cdot a(k\mathbf{B}_K)) R (a^*(k\mathbf{B}_K) \cdot p) \Psi \rangle &= \left\langle (N_K + 2)^{\frac{1}{2}} \Psi, (p \cdot a(k\mathbf{B}_K)) \left\langle N_K^{\frac{1}{2}} \right\rangle^{-1} R (a^*(k\mathbf{B}_K) \cdot p) \Psi \right\rangle \\ &\lesssim \left\| p \left\langle N_K^{\frac{1}{2}} \right\rangle \Psi \right\| \left\| a(k\mathbf{B}_K) \left\langle N_K^{\frac{1}{2}} \right\rangle^{-1} R (a^*(k\mathbf{B}_K) \cdot p) \Psi \right\| \\ &\lesssim \mathcal{C}_{0,1}(kB_K)^{\frac{1}{2}} \left\| p \left\langle N_K^{\frac{1}{2}} \right\rangle \Psi \right\| \| R a^*(k\mathbf{B}_K) \cdot p \Psi \| \\ &\lesssim K^{-\frac{1}{2}} \left\| R^{\frac{1}{2}} \right\| \left\| \langle p \rangle \left\langle N_K^{\frac{1}{2}} \right\rangle \Psi \right\| \left\| R^{\frac{1}{2}} a^*(k\mathbf{B}_K) \cdot p \Psi \right\| \end{aligned}$$

$$\langle \Psi, (p \cdot a(k\mathbf{B}_K)) R (a^*(k\mathbf{B}_K) \cdot p) \Psi \rangle \leq K^{-1} \| R \| \left\| \langle p \rangle \left\langle H_f^{\frac{1}{2}} \right\rangle \Psi \right\|^2.$$

$$|\langle \Psi, a^*(\mathbf{G}_K) R a(\mathbf{G}_K) \Psi \rangle| \lesssim \mathcal{C}_{0,1}(G_K) \| R \| \left\| \langle p \rangle \left\langle N^{\frac{1}{2}} \right\rangle \Psi \right\|^2 \leq \ln K \| R \| \left\| \langle p \rangle \left\langle N^{\frac{1}{2}} \right\rangle \Psi \right\|^2$$

$$\begin{aligned} |\langle \Psi, a(\mathbf{G}_K) R a^*(\mathbf{G}_K) \Psi \rangle| &= \left\langle (N + 2)^{\frac{1}{2}} \Psi, a(\mathbf{G}_K) \left\langle N^{\frac{1}{2}} \right\rangle^{-1} R \left\langle N^{\frac{1}{2}} \right\rangle^{-1} a^*(\mathbf{G}_K) (N + 2)^{\frac{1}{2}} \Psi \right\rangle \\ &\lesssim \left\| a(\mathbf{G}_K) \left\langle N^{\frac{1}{2}} \right\rangle^{-1} R^{\frac{1}{2}} \right\|^2 \left\| \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \Psi \right\|^2 \\ &\lesssim \ln K \left\| \langle p \rangle R^{\frac{1}{2}} \right\|^2 \left\| \left\langle N^{\frac{1}{2}} \right\rangle \Psi \right\|^2 \end{aligned}$$

$$\begin{aligned}
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-1} (A_K - \phi(\mathbf{G}_K)) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-1} \right\| \lesssim K^{-\frac{3}{4}} \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-1} A_K \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-1} \right\| \lesssim (\ln K)^{\frac{1}{2}} \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-2} [H_f, A_K] \langle p \rangle^{-2} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-1} \right\| \lesssim K \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-1} (D_K - 4\pi \ln K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-2} \right\| \lesssim K^{-\frac{3}{4}} \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-1} D_K \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-2} \right\| \lesssim \ln K
\end{aligned}$$

$$L^2(\mathbb{R}_x^3) \otimes \mathcal{F}$$

$$\begin{aligned}
A_K - \phi(\mathbf{G}_K) &= 2p \cdot a(k\mathbf{B}_K) + 2a^*(k\mathbf{B}_K) \cdot p \left\langle N^{\frac{1}{2}} \right\rangle^m \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-1} (p \cdot a(k\mathbf{B}_K)) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-1} \right\| \lesssim \left\| a(k\mathbf{B}_K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \lesssim K^{-3/4} \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-m-1} (a^*(k\mathbf{B}_K) \cdot p) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \lesssim \left\| \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \langle p \rangle^{-1} (a^*(k\mathbf{B}_K) \cdot p) \langle p \rangle^{-1} \right\| \\
& \lesssim \left\| a(k\mathbf{B}_K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \\
& \lesssim K^{-3/4}
\end{aligned}$$

$$[H_f, A_K] = a^*(\omega \mathbf{G}_K) - a(\omega \mathbf{G}_K) + 2a^*(\omega k \mathbf{B}_K) \cdot p - 2p \cdot a(\omega k \mathbf{B}_K)$$

$$\begin{aligned}
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-2} a(\omega \mathbf{G}_K) \langle p \rangle^{-2} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-1} \right\| \lesssim K \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-2} (p \cdot a(\omega k \mathbf{B}_K)) \langle p \rangle^{-2} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-2} \right\| \leq \left\| a(\omega k \mathbf{B}_K) \langle p \rangle^{-2} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \lesssim K^{-\frac{1}{2}} \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-1} a^*(k\mathbf{B}_K) a(k\mathbf{B}_K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-2} \right\| = \left\| \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \langle p \rangle^{-1} a^*(k\mathbf{B}_K) a(k\mathbf{B}_K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \\
& \lesssim \left\| a(k\mathbf{B}_K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\|^2 \\
& \lesssim K^{-3/2} \\
& \left\| \left\langle N^{\frac{1}{2}} \right\rangle^m \langle p \rangle^{-1} a(k\mathbf{B}_K)^2 \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-m-2} \right\| \lesssim \left\| a(k\mathbf{B}_K)^2 \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-2} \right\| \lesssim K^{-\frac{3}{4}}
\end{aligned}$$

$$\begin{aligned}
\|V_\varphi \psi\|_{L^2} &\leq C \|\varphi\|_{\mathfrak{h}_{1/2}} \|\psi\|_{H^1} \forall \varphi \in \mathfrak{h}_{1/2}, \\
\|V_\varphi \psi\|_{L^2} &\leq C \|\varphi\|_{\mathfrak{h}_{-s}} \|\psi\|_{H^2} \forall \varphi \in \mathfrak{h}_{-s}, \psi \in H^1, \\
|\langle \psi, V_\varphi \psi \rangle| &\leq C \|\varphi\|_{\mathfrak{h}_{-1/2}} \|\psi\|_{H^1}^2 \forall \varphi \in \mathfrak{h}_{-1/2}, \psi \in H^1, \\
|\langle \psi, V_\varphi \psi \rangle| &\leq C \|\varphi\|_{\mathfrak{h}_{1/2}} (\delta^{-1} \|\psi\|_{L^2}^2 + \delta \|\psi\|_{H^1}^2) \forall \varphi \in \mathfrak{h}_{1/2}, \psi \in H^1,
\end{aligned}$$

$$\begin{aligned}
\|V_\varphi\psi\|_{L^2} &\leq C\|\varphi\|_{\mathfrak{h}_{1/2}}\|\psi\|_{H^1} & \forall \varphi \in \mathfrak{h}_{1/2}, \quad \psi \in H^1, \\
\|V_\varphi\psi\|_{L^2} &\leq C\|\varphi\|_{\mathfrak{h}_{-s}}\|\psi\|_{H^2} & \forall \varphi \in \mathfrak{h}_{-s}, \quad \psi \in H^2, \quad s \in [0, \frac{3}{4}], \\
|\langle \psi, V_\varphi\psi \rangle| &\leq C\|\varphi\|_{\mathfrak{h}_{-1/2}}\|\psi\|_{H^1}^2 & \forall \varphi \in \mathfrak{h}_{-1/2}, \quad \psi \in H^1, \\
|\langle \psi, V_\varphi\psi \rangle| &\leq C\|\varphi\|_{\mathfrak{h}_{1/2}}(\delta^{-1}\|\psi\|_{L^2}^2 + \delta\|\psi\|_{H^1}^2) & \forall \varphi \in \mathfrak{h}_{1/2}, \quad \psi \in H^1, \quad \delta > 0.
\end{aligned}$$

$$\|\psi\|_{H^1}^2 \leq C\left(1 + \|\varphi\|_{\mathfrak{h}_{1/2}}^2\right)\|\psi\|_{L^2}^2 + C\langle \psi, (p^2 + V_\varphi)\psi \rangle.$$

$$\begin{aligned}
\left\| \int dk \omega(k)^{-1/2} e^{ikx} \varphi(k) \psi \right\|^2 &= \int dk d\ell \omega^{-\frac{1}{2}}(k) \varphi(k) \omega^{-\frac{1}{2}}(\ell) \varphi(\ell) \langle e^{ikx} \psi, e^{i\ell x} \psi \rangle \\
&\leq \left\| \int dk \frac{1}{\omega^{s+1}(k) \langle |p-k|^r \rangle^2} \right\| \|\omega^{s/2} \varphi\|_2^2 \|\langle |p|^r \rangle \psi\|^2 \\
&\leq \mathcal{C}_{s,r}(\omega^{-1/2}) \|\varphi\|_{\mathfrak{h}_{s/2}}^2 \|\psi\|_{H^r}^2
\end{aligned}$$

$$\mathcal{C}_{1,1}(\omega^{-1/2}) \lesssim 1$$

$$\mathcal{C}_{-s,2}(\omega^{-1/2}) \lesssim 1 \text{ for } s \in \left[0, \frac{3}{4}\right]$$

$$|\langle \psi, V_\varphi \psi \rangle| \leq 2 \int dk \omega^{-1/2}(k) |\varphi(k)| |\widehat{|\psi|^2}(k)| \leq C \|\varphi\|_{\mathfrak{h}_{-1/2}} \|\psi\|_{L^4}^2$$

$$\|\psi\|_{L^4} \lesssim \|\psi\|_{H^1}$$

$$\varphi = \varphi_K + \varphi_{>K} \text{ with } \varphi_K(k) := \mathbf{1}_{|k| \leq K} \varphi(k)$$

$$\begin{aligned}
|\langle \psi, V_{\varphi_K} \psi \rangle| &\leq \|\psi\|_{L^2}^2 \int_{|k| \leq K} dk \omega(k)^{-1/2} |\varphi(k)| \leq CK \|\varphi\|_{\mathfrak{h}_{1/2}} \|\psi\|_{L^2}^2 \\
|\langle \psi, (V_\varphi - V_{\varphi_K}) \psi \rangle| &\leq 2K^{-1} \int_{|k| \geq K} dk \omega(k)^{1/2} |\varphi(k)| |\widehat{|\psi|^2}(k)| \leq 2K^{-1} \|\varphi\|_{\mathfrak{h}_{1/2}} \|\psi\|_{L^4}^2
\end{aligned}$$

$$|\langle \psi, V_\varphi \psi \rangle| \leq C(K\|\psi\|_{L^2}^2 + K^{-1}\|\psi\|_{H^1}^2)\|\varphi\|_{\mathfrak{h}_{1/2}}$$

$$\|\sigma(\psi)\|_{\mathfrak{h}_s} \leq C\|\psi\|_{H^1}^2$$

$$\|\sigma(\psi) - \sigma(\phi)\|_{\mathfrak{h}_{-s}} \leq C(\|\psi\|_{H^1} + \|\phi\|_{H^1})\|\psi - \phi\|_{L^2}, s \in [0, 1/2]$$

$$\|\sigma(\psi) - \sigma(\phi)\|_{\mathfrak{h}_{1/2}} \leq C(\|\psi\|_{H^1} + \|\phi\|_{H^1})\|\psi - \phi\|_{H^1}$$

$$\sigma(\psi)(k) = \omega(k)^{-1/2} \widehat{|\psi|^2}(k)$$

$$\|\sigma(\psi)\|_{\mathfrak{h}_s}^2 = \int_{|k| \leq 1} \frac{|\widehat{|\psi|^2}(k)|^2}{|k|^{1+2s}} dk + \int_{|k| > 1} \frac{|\widehat{|\psi|^2}(k)|^2}{|k|^{1+2s}} dk =: I_1 + I_2$$

$$I_1 \leq \|\psi\|_{L^2}^4 \int_{|k| \leq 1} |k|^{-1-2s} dk \lesssim 1 \text{ for } s \in \left[-\frac{1}{2}, \frac{1}{2}\right]$$

$$I_2 \leq \int_{\mathbb{R}^3} |\widehat{|\psi|^2}(k)|^2 dk = \|\psi\|_{L^4}^4 \lesssim \|\psi\|_{H^1}^4$$

$$\rho := |\psi|^2 - |\phi|^2$$



$$\|\sigma(\psi) - \sigma(\phi)\|_{\mathfrak{h}_{-s}}^2 = \int \frac{|\hat{\rho}(k)|^2}{|k|^{1+2s}} dk = c_s \iint \frac{\rho(x)\rho(y)}{|x-y|^{2-2s}} dx dy$$

$$d=3, \lambda=2-2s, s\in\left[0,\frac{1}{2}\right]$$

$$p=q=p_s\colon=\frac{3}{2+s}\in\left[\frac{6}{5},\frac{3}{2}\right]$$

$$\|\sigma(\psi)-\sigma(\phi)\|_{\mathfrak{h}_{-s}}^2\leqslant C_s\|\rho\|_{L^{p_s}}^2$$

$$\rho=|\psi|^2-|\phi|^2=(\psi-\phi)\bar{\psi}+(\overline{\psi-\phi})\phi$$

$$q_s\frac{1}{p_s}=\frac{1}{2}+\frac{1}{q_s}q_s=\frac{6}{1+2s}\in H^1\hookrightarrow L^{q_s}$$

$$\|\rho\|_{L^{p_s}}\leqslant\|\psi-\phi\|_{L^2}(\|\psi\|_{L^{q_s}}+\|\phi\|_{L^{q_s}})\leqslant C\|\psi-\phi\|_{L^2}(\|\psi\|_{H^1}+\|\phi\|_{H^1})$$

$$\|\sigma(\psi)-\sigma(\phi)\|_{\mathfrak{h}_{1/2}}=\||\psi|^2-|\phi|^2\|_{L^2}$$

$$\||\psi|^2-|\phi|^2\|_{L^2}\leqslant\|\psi-\phi\|_{L^6}(\|\psi\|_{L^3}+\|\phi\|_{L^3})$$

$$H^1(\mathbb{R}^3)\hookrightarrow L^6(\mathbb{R}^3)$$

$$\|\psi-\phi\|_{L^6}\leqslant C\|\nabla(\psi-\phi)\|_{L^2}\leqslant C\|\psi-\phi\|_{H^1}$$

$$\|\psi\|_{L^3}\leqslant C\|\psi\|_{H^1}^{1/2}$$

$$\|\sigma(\psi)-\sigma(\phi)\|_{\mathfrak{h}_{1/2}}=\||\psi|^2-|\phi|^2\|_{L^2}\leqslant C\|\psi-\phi\|_{H^1}(\|\psi\|_{H^1}+\|\phi\|_{H^1}).$$

$$H^\varepsilon=(U_K^\varepsilon)^*H_{\mathcal{D},K}^\varepsilon U_K^\varepsilon$$

$$\begin{aligned} H_{\mathcal{D},K}^\varepsilon &= p^2 + \varepsilon \big(\phi(\mathbf{G}_K) + 2a^*(k\mathbf{B}_K) \cdot p + 2p \cdot a(k\mathbf{B}_K) \big) \\ &+ \varepsilon^2 \big(H_f + 2a^*(k\mathbf{B}_K)a(k\mathbf{B}_K) + a^*(k\mathbf{B}_K)a^*(k\mathbf{B}_K) + a(k\mathbf{B}_K)a(k\mathbf{B}_K) + 4\pi \ln K \big) \\ &- \varepsilon^3 \phi(\omega\mathbf{B}_K) + \varepsilon^4 \left\| \omega^{\frac{1}{2}} B_K \right\|_{L^2}^2 \end{aligned}$$

$$Q(H_{\mathcal{D},K}^\varepsilon)=Q(p^2+H_f)$$

$$\begin{aligned} &\pm\left(H_{\mathcal{D},K}^\varepsilon-(p^2+\varepsilon^2H_f)\right)\leqslant\frac{1}{2}(p^2+\varepsilon^2H_f)+CK\\ &\pm\left(H_{\mathcal{D},K}^\varepsilon-(p^2+\varepsilon^2H_f)\right)\leqslant\frac{1}{2}(p^2+\varepsilon^2H_f)+C\varepsilon^2(\ln K)(N+1) \end{aligned}$$

$$|\langle \Psi, \varepsilon a(\boldsymbol{G}_K) \Psi \rangle| \leqslant CK^{1/2} \|\Psi\| \left\| \varepsilon H_f^{1/2} \Psi \right\|.$$

$$|\langle \Psi, \varepsilon a(\boldsymbol{G}_K) \Psi \rangle| = \left| \left\langle \langle N^{1/2} \rangle \Psi, \varepsilon a(\boldsymbol{G}_K) N^{-1/2} \Psi \right\rangle \right| \leqslant C \varepsilon (\ln K)^{1/2} \left\| \langle N^{1/2} \rangle \Psi \right\| \|\langle p \rangle \Psi\|.$$

$$\mathcal{H}_{\mathcal{D},K,\varphi}^\varepsilon=e^{-ig_{K,\varphi}(x)}W(\varepsilon^{-1}\varphi)^*H_{\mathcal{D},K}^\varepsilon W(\varepsilon^{-1}\varphi)e^{ig_{K,\varphi}(x)}$$

$$g_{K,\varphi}(x)=2\mathrm{Im}\langle\varphi,\mathbf{B}(\cdot,k)\rangle e^{-ig_{K,\varphi}(x)}$$

$$W(\varepsilon^{-1}\varphi)^*H_{\mathcal{D},K}^\varepsilon W(\varepsilon^{-1}\varphi)=\mathfrak{h}_0+\varepsilon\mathfrak{h}_1+\varepsilon^2\mathfrak{h}_2-\varepsilon^3\phi(\omega\mathbf{B}_K)+\varepsilon^4\left\|\omega^{\frac{1}{2}}B_K\right\|_{L^2}^2$$

$$\mathfrak{h}_0=p^2+2\mathrm{Re}\langle\varphi,\mathbf{G}_K\rangle+2\langle\varphi,k\mathbf{B}_K\rangle\cdot p+2p\cdot\langle k\mathbf{B}_K,\varphi\rangle+4|\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle|^2+\left\|\omega^{\frac{1}{2}}\varphi\right\|_{L^2}^2,$$

$$\mathfrak{h}_1=\phi(\mathbf{G}_K+\omega\varphi)+2a^*(k\mathbf{B}_K)\cdot p+2p\cdot a(k\mathbf{B}_K)+4\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle\cdot\phi(k\mathbf{B}_K),$$

$$\mathfrak{h}_2=H_f+2a^*(k\mathbf{B}_K)a(k\mathbf{B}_K)+a^*(k\mathbf{B}_K)^2+a(k\mathbf{B}_K)^2+4\pi\ln K-2\mathrm{Re}\langle\mathbf{B}_K,\omega\varphi\rangle.$$

$$\begin{aligned}\mathcal{H}_{\mathcal{D},K,\varphi}^\varepsilon=&h_\varphi+\left\|\omega^{\frac{1}{2}}\varphi\right\|_{L^2}^2+\varepsilon(A_K+\phi(\omega\varphi))+\varepsilon^2(H_f+D_K-2\mathrm{Re}\langle\omega\varphi,\mathbf{B}_K\rangle)\\&-\varepsilon^3\phi(\omega\mathbf{B}_K)+\varepsilon^4\left\|\omega^{\frac{1}{2}}B_K\right\|_{L^2}^2\end{aligned}$$

$$e^{-ig_{K,\varphi}(x)}pe^{ig_{K,\varphi}(x)}=p-2\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle,$$

$$e^{-ig_{K,\varphi}(x)}\mathfrak{h}_0e^{ig_{K,\varphi}(x)}=(p-2\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle)^2+2\mathrm{Re}\langle\varphi,\mathbf{G}_K\rangle+2\langle\varphi,k\mathbf{B}_K\rangle\cdot(p-2\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle)$$

$$+(p-2\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle)\cdot\langle k\mathbf{B}_K,\varphi\rangle+4|\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle|^2+\left\|\omega^{\frac{1}{2}}\varphi\right\|_{L^2}^2$$

$$=p^2+2\mathrm{Re}\langle\varphi,\mathbf{G}_K\rangle+2\mathrm{Im}\langle\varphi,k\mathbf{B}_K\rangle\cdot p+2p\cdot\mathrm{Im}\langle k\mathbf{B}_K,\varphi\rangle+\left\|\omega^{\frac{1}{2}}u\right\|_{L^2}^2$$

$$=p^2+2\mathrm{Re}\langle\varphi,\mathbf{G}_K\rangle+2\mathrm{Re}\langle\varphi,k^2\mathbf{B}_K\rangle+\left\|\omega^{\frac{1}{2}}\varphi\right\|_{L^2}^2$$

$$p\cdot\mathrm{Im}\langle\varphi,k\mathbf{B}_K\rangle=-\mathrm{Im}\langle k\mathbf{B}_K,\varphi\rangle\cdot p+\mathrm{Re}\langle\varphi,k^2\mathbf{B}_K\rangle$$

$$e^{-ig_{K,\varphi}(x)}\mathfrak{h}_1e^{ig_{K,\varphi}(x)}$$

$$=\phi(\mathbf{G}_K+\omega\varphi)+2a^*(k\mathbf{B}_K)\cdot(p-2\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle)+2(p-2\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle)\cdot a(k\mathbf{B}_K)\\+4\mathrm{Re}\langle\varphi,k\mathbf{B}_K\rangle\cdot\phi(k\mathbf{B}_K)$$

$$=\phi(\mathbf{G}_K+\omega\varphi)+2a^*(k\mathbf{B}_K)\cdot p+2p\cdot a(k\mathbf{B}_K)$$

$$e(\varphi)=\inf\sigma(h_\varphi)$$

$$\Delta\left(\varphi\right)=\inf\{|e(\varphi)-\lambda|:\lambda\in\sigma\left(h_\varphi\right)\setminus\{e(\varphi)\}\}$$

$$\varphi\in C([-T,T];\mathfrak{h}_{1/2})$$

$$\varphi_t=e^{-i\omega t}\varphi_0-i\int_0^te^{-i\omega(t-s)}\sigma(\psi_{\varphi_s})\mathrm{d}s$$

$$\sigma(\psi_{\varphi_s})=\widehat{\omega^{-1/2}|\psi_{\varphi_s}|^2}$$

$$B_r(\varphi)\!:=\!\left\{u\in\mathfrak{h}_{1/2}\!:\!\|u-\varphi\|_{\mathfrak{h}_{1/2}}\leqslant r\right\}.$$

$$\Delta\left(u\right)\geqslant\frac{1}{2}\Delta\left(\varphi\right)>0$$

$$|e(\varphi)-e(u)|+|\lambda_1(\varphi)-\lambda_1(u)|\leqslant Cr$$

$$\varphi\xi\in\mathfrak{h}_{1/2}\text{ and all }\psi\in H^1\text{ with }\|\psi\|_{L^2}=1$$

$$|\langle\psi,(h_\varphi-h_\xi)\psi\rangle|\leqslant C\|\varphi-\xi\|_{\mathfrak{h}_{1/2}}\|\psi\|_{H^1}^2$$

$$e(u) = \inf \sigma(h_u)$$

$$e(u) \leq \langle \psi_\varphi, h_u \psi_\varphi \rangle \leq e(\varphi) + C \|\varphi - u\|_{\mathfrak{h}_{1/2}} \|\psi_\varphi\|_{H^1}^2 \leq e(\varphi) + Cr$$

$$|e(\varphi) - e(u)| \leq Cr$$

$$\|\psi_u\|_{H^1}^2 \leq C \left(1 + \|u\|_{\mathfrak{h}_{1/2}}^2 + e(u)\right) \leq C \left(1 + \|\varphi\|_{\mathfrak{h}_{1/2}}^2\right) \leq C$$

$$\lambda_1(u) := \inf(\sigma(h_u) \setminus \{e(u)\})$$

$$\lambda_1(u) = \sup_{\text{codim}(V)=1} \inf_{\psi \in V} \{\langle \psi, h_u \psi \rangle : \|\psi\|_{L^2} = 1\}$$

$$V = \{\psi_\varphi\}^\perp$$

$$\lambda_1(u) \geq \inf_{\substack{\psi \in H^1, \|\psi\|=1 \\ \psi \perp \psi_\varphi}} \langle \psi, h_u \psi \rangle \geq \inf_{\substack{\psi \in H^1, \|\psi\|=1 \\ \psi \perp \psi_\varphi}} (\langle \psi, h_\varphi \psi \rangle - Cr \|\psi\|_{H^1}^2)$$

$$\|\varphi\|_{\mathfrak{h}_{1/2}} \leq C$$

$$\|\psi\|_{H^1}^2 \leq C(1 + \langle \psi, h_\varphi \psi \rangle)$$

$$\lambda_1(u) \geq (1 - Cr) \inf_{\substack{\psi \in H^1, \|\psi\|=1 \\ \psi \perp \psi_\varphi}} \langle \psi, h_\varphi \psi \rangle - Cr = (1 - Cr) \lambda_1(\varphi) - Cr$$

$$\Delta(u) = \lambda_1(u) - e(u)$$

$$\Delta(u) \geq \Delta(\varphi) - Cr.$$

$$\Delta(u) \geq \frac{1}{2} \Delta(\varphi) > 0 \text{ for all } u \in B_r(\varphi) \text{ with } 0 < r \leq r_0$$

$$\lambda_1(\varphi) \geq (1 - Cr) \lambda_1(u) - Cr$$

$$|\lambda_1(u) - \lambda_1(\varphi)| \leq Cr$$

$$\|\psi_u - \psi_\xi\|_{H^1} \leq \frac{C}{\Delta(\varphi)^{1/2}} (\|\psi_u\|_{H^1} + \|\psi_\xi\|_{H^1}) \|u - \xi\|_{\mathfrak{h}_{1/2}}$$

$$\|\psi_u - \psi_\xi\|_{L^2} \leq \frac{C}{\Delta(\varphi)^{1/2}} (\|\psi_u\|_{H^2} + \|\psi_\xi\|_{H^2}) \|u - \xi\|_{\mathfrak{h}_{-1/2}}$$

$$\text{for all } u, \xi \in B_r(\varphi) \cap \mathfrak{h}_{-1/2} \text{ with } 0 < r \leq r_0$$

$$\psi_u - \psi_\xi \in H^1 \text{ and } u - \xi \in \mathfrak{h}_{1/2}$$

$$\|\psi_u - \psi_\xi\|_{H^1}^2 \leq C \left((1 + \|u - \xi\|_{\mathfrak{h}_{1/2}}^2) \|\psi_u - \psi_\xi\|_{L^2}^2 + \langle \psi_u - \psi_\xi, h_{u-\xi}(\psi_u - \psi_\xi) \rangle \right).$$

$$\|\psi_u - \psi_\xi\|_{L^2}^2 \leq 2 \|Q_u \psi_\xi\|_{L^2}^2$$

$$Q_u = \mathbf{1} - |\psi_u\rangle\langle\psi_u|$$

$$\|Q_u \psi_\xi\|_{L^2}^2 \leq \frac{1}{\Delta(u)} \langle \psi_\xi, (h_u - e(u)) \psi_\xi \rangle \leq \frac{2}{\Delta(\varphi)} \langle \psi_\xi, (h_u - e(u)) \psi_\xi \rangle$$



$$\begin{aligned}\langle \psi_\xi, (h_u - e(u))\psi_\xi \rangle &= \langle \psi_\xi - \psi_u, h_u \psi_\xi \rangle - \langle \psi_\xi - \psi_u, \psi_\xi \rangle \langle \psi_u, h_u \psi_u \rangle \\ &= e(\xi) \langle \psi_\xi - \psi_u, \psi_\xi \rangle + \langle \psi_\xi - \psi_u, V_{u-\xi} \psi_\xi \rangle \\ &\quad - \langle \psi_\xi - \psi_u, \psi_\xi \rangle (\langle \psi_u, h_\xi \psi_u \rangle + \langle \psi_u, V_{u-\xi} \psi_u \rangle),\end{aligned}$$

$$h_u = h_\xi + V_{u-\xi}$$

$$e(\xi) \leq \langle \psi_u, h_\xi \psi_u \rangle$$

$$\langle \psi_\xi - \psi_u, \psi_\xi \rangle \geq 0$$

$$\begin{aligned}\langle \psi_\xi, (h_u - e(u))\psi_\xi \rangle &\leq \|\psi_\xi - \psi_u\|_{L^2} \left(\|V_{u-\xi} \psi_\xi\|_{L^2} + \|V_{u-\xi} \psi_u\|_{L^2} \right) \\ &\leq C \|\psi_\xi - \psi_u\|_{L^2} \left(\|\psi_\xi\|_{H^1} + \|\psi_u\|_{H^1} \right) \|u - \xi\|_{\mathfrak{h}_{1/2}} \\ &\leq \frac{1}{10} \|\psi_\xi - \psi_u\|_{L^2}^2 + C \left(\|\psi_u\|_{H^1} + \|\psi_\xi\|_{H^1} \right)^2 \|u - \xi\|_{\mathfrak{h}_{1/2}}^2,\end{aligned}$$

$$\|\psi_u - \psi_\xi\|_{L^2}^2 \leq C \Delta(\varphi)^{-1} \left(\|\psi_u\|_{H^1} + \|\psi_\xi\|_{H^1} \right)^2 \|u - \xi\|_{\mathfrak{h}_{1/2}}^2.$$

$$h_{u-\xi} = h_u - V_\xi$$

$$\begin{aligned}\langle \psi_u - \psi_\xi, h_{u-\xi}(\psi_u - \psi_\xi) \rangle &= \langle \psi_u - \psi_\xi, h_u \psi_u - \psi_\xi \rangle - \langle \psi_u - \psi_\xi, V_\xi(\psi_u - \psi_\xi) \rangle \\ &\leq \langle \psi_\xi, (h_u - e(u))\psi_\xi \rangle - \langle \psi_u - \psi_\xi, V_\xi(\psi_u - \psi_\xi) \rangle\end{aligned}$$

$$(h_u - e(u))\psi_u = \|\xi\|_{\mathfrak{h}_{1/2}} \leq C$$

$$|\langle \psi_u - \psi_\xi, V_\xi(\psi_u - \psi_\xi) \rangle| \leq C \|\psi_u - \psi_\xi\|_{L^2} \|\psi_u - \psi_\xi\|_{H^1}$$

$$\|\psi_u - \psi_\xi\|_{L^2} \leq C \Delta(\varphi)^{-1} \left(\|V_{u-\xi} \psi_\xi\|_{L^2} + \|V_{u-\xi} \psi_u\|_{L^2} \right)$$

$$\Delta(\varphi_0) > \Delta(u) > u \in B_r(\varphi_0) u \in B_r(\varphi_0) \psi_u \geq h_u$$

$$\begin{aligned}\|\psi_u\|_{H^1} &\leq C \left(1 + \|u\|_{\mathfrak{h}_{1/2}} \right) \leq \lambda \|\varphi_0\|_{\mathfrak{h}_{1/2}} \\ X_T &:= C([-T, T]; B_r(\varphi_0))\end{aligned}$$

$$(\mathcal{T}u)(t) := e^{-it\omega} \varphi_0 - i \int_0^t e^{i(s-t)\omega} \sigma(\psi_{u_s}) ds, |t| \leq T$$

$$\|\mathcal{T}u(t) - \varphi_0\|_{\mathfrak{h}_{1/2}} \leq \|(e^{-it\omega} - 1)\varphi_0\|_{\mathfrak{h}_{1/2}} + T \sup_{|s| \leq T} \|\sigma(\psi_{u_s})\|_{\mathfrak{h}_{1/2}}$$

$$\lim_{t \rightarrow 0} \|(e^{-it\omega} - 1)\varphi_0\|_{\mathfrak{h}_{1/2}} = 0$$

$$\|\sigma(\psi_{u_s})\|_{\mathfrak{h}_{1/2}} \leq C \|\psi_{u_s}\|_{H^1}^2 \leq C \lambda^2$$

$$\mathcal{T}(X_T) \subseteq X_T$$

$$\begin{aligned}\|\mathcal{T}u(t) - \mathcal{T}\xi(t)\|_{\mathfrak{h}_{1/2}} &\leq \int_0^{|t|} \|\sigma(\psi_{u_s}) - \sigma(\psi_{\xi_s})\|_{\mathfrak{h}_{1/2}} ds \leq C |t| \lambda \sup_{|s| \leq T} \|\psi_{u_s} - \psi_{\xi_s}\|_{H^1} \\ &\leq CD |t| \lambda^2 \sup_{|s| \leq T} \|u_s - \xi_s\|_{\mathfrak{h}_{1/2}}\end{aligned}$$



$$\|\mathcal{T}u - \mathcal{T}\xi\|_{X_T} \leq TCD\lambda^2 \|u - \xi\|_{X_T}$$

$$\Delta\left(\varphi_t\right)\geqslant\Delta\left(\varphi_0\right)/2$$

$$\xi\in\mathcal{C}([-T,T];\mathfrak{h}_{1/2})$$

$$\xi_0=\varphi_0e(\xi_t)<\|\psi_{\xi_s}\|_{H^1}^2\leqslant C\left(1+\|\xi_s\|_{\mathfrak{h}_{1/2}}^2\right)$$

$$\|\xi_t-\varphi_0\|_{\mathfrak{h}_{1/2}}\leqslant\|(e^{-it\omega}-1)\varphi_0\|_{\mathfrak{h}_{1/2}}+CT\sup_{|s|\leqslant T}C\left(1+\|\xi_s\|_{\mathfrak{h}_{1/2}}^2\right)$$

$$t\mapsto\|\xi_t\|_{\mathfrak{h}_{1/2}}$$

$$\xi\in\mathcal{C}([-T,T];B_r(\varphi_0))$$

$$\xi=\varphi\text{ on }[-T,T]$$

$$g(t)\colon=\sigma(\psi_{\varphi_t})$$

$$t\mapsto g(t)\mathfrak{h}_{-1/2}v(t)\colon=e^{i\omega t}\varphi_t$$

$$v(t)=\varphi_0-i\int_0^te^{i\omega s}g(s)\mathrm{d}s$$

$$g\in\mathcal{C}([-T,T];\mathfrak{h}_{-1/2})$$

$$\partial_tv(t)=-ie^{i\omega t}g(t)\mathfrak{h}_{-1/2}$$

$$\varphi_t=e^{-i\omega t}v(t)\in C^1([-T,T];\mathfrak{h}_{-1/2})$$

$$\|\varphi_t\|_{L^2}\leqslant\|\varphi_0\|_{L^2}+\int_0^{|t|}\|\sigma(\psi_{\varphi_s})\|_{L^2}\,\mathrm{d}s$$

$$\sup_{|s|\leqslant T}\|\sigma(\psi_{\varphi_s})\|_{L^2}\leqslant C\sup_{|t|\leqslant T}\|\varphi_t\|_{L^2}\leqslant C(T)t, t_0\in[-T,T]$$

$$\|\varphi_t-\varphi_{t_0}\|_{L^2}\leqslant\|(e^{-i\omega(t-t_0)}-1)\varphi_{t_0}\|_{L^2}+\int_{t_0}^t\|\sigma(\psi_{\varphi_s})\|_{L^2}\,\mathrm{d}s$$

$$\varphi\in\mathcal{C}([-T,T];L^2)$$

$$\frac{d}{dt}\mathcal{E}_{\mathrm{field}}\left(\varphi_t\right)=\left\langle \psi_{\varphi_t},V_{i\omega\varphi_t}\psi_{\varphi_t}\right\rangle +2\mathrm{Re}\left\langle \dot{\varphi}_t,\omega\varphi_t\right\rangle =0$$

$$\dot{\varphi}_t=-i\left(\omega\varphi_t+\sigma(\psi_{\varphi_t})\right)$$

$$2\mathrm{Re}\langle\dot{\varphi}_t,\omega\varphi_t\rangle=-2\mathrm{Im}\langle\sigma(\psi_{\varphi_t}),\omega\varphi_t\rangle=-\langle\psi_{\varphi_t},V_{i\omega\varphi_t}\psi_{\varphi_t}\rangle$$

$$(1-\alpha)\|\varphi_t\|_{\mathfrak{h}_{1/2}}^2\leqslant\mathcal{E}_{\mathrm{field}}\left(\varphi_0\right)+C_0,\forall t\in I,$$

$$\sup_{t\in I}\|\varphi_t\|_{\mathfrak{h}_{1/2}}<\infty$$

$$J \subset \liminf_{t \in J} \Delta(\varphi_t) > u \mapsto \psi_u \{ \varphi_t : t \in J \} u \mapsto \sigma(\psi_u) \mathfrak{h}_{1/2}$$

$$\liminf_{t \uparrow T_+} \Delta(\varphi_t) = 0 \text{ resp. } \liminf_{t \downarrow -T_-} \Delta(\varphi_t) = 0$$

$$R_{\varphi_t}=Q_{\varphi_t}\left(h_{\varphi_t}-e(\varphi_t)\right)^{-1}Q_{\varphi_t},$$

$$\|R_{\varphi_t}\|+\left\|\langle p\rangle R_{\varphi_t}^{1/2}\right\|+\left\|\langle p^2\rangle R_{\varphi_t}\right\|+\left\|\psi_{\varphi_t}\right\|_{H^2}\leqslant C.$$

$$t\mapsto \psi_{\varphi_t} \text{ is in } C((-T,T);H^1)\cap C^1((-T,T);L^2)$$

$$\partial_t\psi_{\varphi_t}=R_{\varphi_t}V_{i\omega_{\varphi_t}}\psi_{\varphi_t}$$

$$\|\dot{\psi}_{\varphi_t}\|_{L^2}+\|\dot{\sigma}(\psi_{\varphi_t})\|_{L^2}+\|\dot{R}_{\varphi_t}\|+\|\langle p\rangle \dot{R}_{\varphi_t}\langle p\rangle\|\leqslant C$$

$$L^2(\mathbb{R}^3)\dot{f}(t) \mathop{:=} \partial_t f(t)$$

$$\|R_{\varphi_t}\|\lesssim 1$$

$$\inf_{|t|\leqslant T}\Delta(\varphi_t)>0$$

$$p^2=h_{\varphi_t}-V_{\varphi_t} \text{ and } h_{\varphi_t}R_{\varphi_t}=Q_{\varphi_t}+e(\varphi_t)R_{\varphi_t}$$

$$R_{\varphi_t}^{1/2}\langle p\rangle^2R_{\varphi_t}^{1/2}=R_{\varphi_t}^{1/2}(1+p^2)R_{\varphi_t}^{1/2}=R_{\varphi_t}(1+e(\varphi_t))+Q_{\varphi_t}-R_{\varphi_t}^{1/2}V_{\varphi_t}R_{\varphi_t}^{1/2},$$

$$\left\|\langle p\rangle R_{\varphi_t}^{1/2}\right\|^2\lesssim 1+\left\|R_{\varphi_t}^{1/2}\right\|\left\|\langle p\rangle R_{\varphi_t}^{1/2}\right\|$$

$$|e(\varphi_t)|\lesssim 1$$

$$\langle p^2\rangle R_{\varphi_t}=R_{\varphi_t}(1+e(\varphi_t))+Q_{\varphi_t}-V_{\varphi_t}R_{\varphi_t}$$

$$\|\langle p^2\rangle R_{\varphi_t}\|\lesssim 1+\|V_{\varphi_t}R_{\varphi_t}\|\lesssim 1+\|\langle p\rangle R_{\varphi_t}\|\lesssim 1$$

$$\|\psi_{\varphi_t}\|_{H^2}^2\leqslant 1+\|p^2\psi_{\varphi_t}\|_{L^2}^2\leqslant 1+|e(\varphi_t)|+\|V_{\varphi_t}\psi_{\varphi_t}\|_{L^2}^2\leqslant 1+\|\psi_{\varphi_t}\|_{H^1}^2$$

$$\|\psi_{\varphi_t}\|_{H^1}\lesssim 1$$

$$\langle \psi_{\varphi_t}, \partial_t \psi_{\varphi_t} \rangle = 2 \mathrm{Re} \langle \psi_{\varphi_t}, \partial_t \psi_{\varphi_t} \rangle = \partial_t \|\psi_{\varphi_t}\|^2 = 0$$

$$\left(h_{\varphi_t}-e(\varphi_t)\right)\psi_{\varphi_t}=0$$

$$(\partial_t h_{\varphi_t})\psi_{\varphi_t}+\left(h_{\varphi_t}-e(\varphi_t)\right)\partial_t\psi_{\varphi_t}-\dot{e}(\varphi_t)\psi_{\varphi_t}=0$$

$$\dot{e}(\varphi_t)=\langle \psi_{\varphi_t},(\partial_t h_{\varphi_t})\psi_{\varphi_t}\rangle$$

$$Q_{\varphi_t}\left(h_{\varphi_t}-e(\varphi_t)\right)Q_{\varphi_t}\partial_t\psi_{\varphi_t}=-Q_{\varphi_t}(\partial_th_{\varphi_t})\psi_{\varphi_t}.$$

$$\partial_t\psi_{\varphi_t}=-R_{\varphi_t}(\partial_th_{\varphi_t})\psi_{\varphi_t}$$

$$h_{\varphi} = p^2 + V_{\varphi}$$

$$\partial_t h_{\varphi_t} = V_{\partial_t \varphi_t}$$

$$\partial_t \varphi_t = -i\omega \varphi_t - i\sigma(\psi_{\varphi_t})$$

$$\partial_t h_{\varphi_t} = -V_{i\omega \varphi_t} - V_{i\sigma(\psi_{\varphi_t})}$$

$$\overline{\sigma(\psi_{\varphi_t})(k)} = \sigma(\psi_{\varphi_t})(-k)V_{i\sigma(\psi_{\varphi_t})} = \partial_t \psi_{\varphi_t} = R_{\varphi_t} V_{i\omega \varphi_t} \psi_{\varphi_t} \|\dot{\psi}_{\varphi_t}\|_{L^2}$$

$$\dot{\sigma}(\psi_{\varphi_t})(k) = \langle R_{\varphi_t} V_{i\omega \varphi_t} \psi_{\varphi_t}, \mathbf{G}(\cdot, k) \psi_{\varphi_t} \rangle + \langle \psi_{\varphi_t}, \mathbf{G}(\cdot, k) R_{\varphi_t} V_{i\omega \varphi_t} \psi_{\varphi_t} \rangle.$$

$$|\langle R_{\varphi_t} V_{i\omega \varphi_t} \psi_{\varphi_t}, \mathbf{G}(\cdot, k) \psi_{\varphi_t} \rangle| \lesssim \|R_{\varphi_t} V_{i\omega \varphi_t} \psi_{\varphi_t}\|_{H^1} \|\psi_{\varphi_t}\|_{H^1} \lesssim 1$$

$$\dot{Q}_{\varphi_t} = -\dot{P}_{\varphi_t} = P_{\varphi_t} V_{i\omega \varphi_t} R_{\varphi_t} - R_{\varphi_t} V_{i\omega \varphi_t} P_{\varphi_t}$$

$$P_{\varphi_t} = |\psi_{\varphi_t}\rangle \langle \psi_{\varphi_t}|$$

$$\dot{R}_{\varphi_t} = P_{\varphi_t} V_{i\omega \varphi_t} R_{\varphi_t}^2 - R_{\varphi_t}^2 V_{i\omega \varphi_t} P_{\varphi_t} - R_{\varphi_t} \left(\dot{h}_{\varphi_t} - \dot{e}(\varphi_t) \right) R_{\varphi_t}.$$

$$\|\dot{R}_{\varphi_t}\| + \|\langle p \rangle \dot{R}_{\varphi_t} \langle p \rangle\| \leqslant C$$

$$\langle p \rangle^{-1} \left(\dot{h}_{\varphi_t} - \dot{e}(\varphi_t) \right) \langle p \rangle^{-1} = \langle p \rangle^{-1} (V_{i\omega \varphi_t} - \langle \psi_{\varphi_t}, V_{i\omega \varphi_t} \psi_{\varphi_t} \rangle) \langle p \rangle^{-1} \lesssim 1$$

$$\mathbb{H}_{\Lambda}(t) = H_f - \langle \psi_{\varphi_t} \phi(\mathbf{G}_{\Lambda}) R_{\varphi_t} \phi(\mathbf{G}_{\Lambda}) \psi_{\varphi_t} \rangle$$

$$\mathbb{H}_{\Lambda}(t)\mathbb{H}_{\mathcal{D},K,\Lambda}(t)-4\pi\ln\Lambda$$

$$\mathbf{B}_{K,\Lambda}(x,k) = \mathbf{B}_K(x,k) \mathbf{1}_{|k| \leqslant \Lambda} = \frac{e^{-ikx}}{|k|^{3/2}} \mathbf{1}_{K \leqslant |k| \leqslant \Lambda}$$

$$\mathbb{H}_{\mathcal{D},K,\Lambda}(t) = H_f + \langle \psi_{\varphi_t}, (D_{K,\Lambda} + 2\mathrm{Re}\langle \sigma(\psi_{\varphi_t}), \mathbf{B}_{K,\Lambda} \rangle - A_{K,\Lambda} R_{\varphi_t} A_{K,\Lambda}) \psi_{\varphi_t} \rangle_{L^2}$$

$$A_{K,\Lambda} = \phi(\mathbf{G}_K) + 2p \cdot a(k\mathbf{B}_{K,\Lambda}) + 2a^*(\mathbf{k}B_{K,\Lambda}) \cdot p$$

$$D_{K,\Lambda} = 2a^*(k\mathbf{B}_{K,\Lambda})a(k\mathbf{B}_{K,\Lambda}) + a^*(k\mathbf{B}_{K,\Lambda})^2 + a(k\mathbf{B}_{K,\Lambda})^2 + 4\pi\ln K$$

$$A_{K,\infty} = A_K \text{ and } D_{K,\infty} = D_K$$

$$\pm \mathbb{H}_{\Lambda}(t) \leqslant C\Lambda^2 H_f + C \text{ for all } 1 < \Lambda < \infty$$

$$\pm \mathbb{H}_{\mathcal{D},K,\Lambda}(t) \leqslant CK^2 H_f + C \ln K \text{ for all } 2 \leqslant K < \Lambda \leqslant \infty$$

$$\mathbb{H}_{\mathcal{D},K,\Lambda}(t) = \mathbb{H}_{\Lambda}(t) + 4\pi\ln\Lambda \text{ for all } 2 \leqslant K < \Lambda < \infty$$

$$|\langle \Psi, (\mathbb{H}_{\mathcal{D},K,\infty}(t) - \mathbb{H}_{\mathcal{D},K,\Lambda}(t)) \Phi \rangle| \leqslant \frac{CK^{1/2}}{\Lambda^{1/4}} (\langle \Psi, H_f \Psi \rangle + \langle \Phi, H_f \Phi \rangle + 1)$$

$$\mathbb{H}_{\mathcal{D},K}(t) \coloneqq \mathbb{H}_{\mathcal{D},K,\infty}(t)$$

$$\|R_{\varphi_t}\| \lesssim 1$$

$$\|\langle p \rangle P_{\varphi_t}\| \lesssim 1$$

$$\|\langle p \rangle R_{\varphi_t} \langle p \rangle\| \lesssim 1$$

$$\underline{h:=h_{\varphi_t}e:=e(\varphi_t), R:=R_{\varphi_t}(h-e)R=Q=1-P=|\psi\rangle\langle\psi|}$$

$$\phi^-(f)\!:=\!a^*(f)-a(f)$$

$$2a^*(k\mathbf{B})a(k\mathbf{B})+a^*(k\mathbf{B})a^*(k\mathbf{B})+a(k\mathbf{B})a(k\mathbf{B})=\phi(k\mathbf{B})^2-\|k\mathbf{B}\|_{L^2}^2\phi(k\mathbf{B})=-[p,\phi^-(\mathbf{B})]$$

$$[[p^2,\phi^-(\mathbf{B})],\phi^-(\mathbf{B})]=2([p,\phi^-(\mathbf{B})])^2-p[\phi(k\mathbf{B}),\phi^-(\mathbf{B})]-[\phi(k\mathbf{B}),\phi^-(\mathbf{B})]p$$

$$[\phi(k\mathbf{B}),\phi^-(\mathbf{B})]=2\mathrm{Re}\langle\mathbf{B},k\mathbf{B}\rangle=0$$

$$[p,\phi^-(\mathbf{B})]=\phi(k\mathbf{B})$$

$$\phi(k\mathbf{B})^2=\frac{1}{2}[[h-e,\phi^-(\mathbf{B})],\phi^-(\mathbf{B})]$$

$$\psi\in L^2(\mathbb{R}^3_x)$$

$$\langle \psi, \phi(k\mathbf{B})^2 \psi \rangle = - \langle \psi, \phi^-(\mathbf{B})(h-e)\phi^-(\mathbf{B}) \psi \rangle.$$

$$2p\cdot a(k\mathbf{B})+2a^*(k\mathbf{B})\cdot p=-[h-e,\phi^-(\mathbf{B})]-\phi(k^2\mathbf{B})$$

$$\mathbf{G}_K-k^2\mathbf{B}=\mathbf{G}_K-k^2\mathbf{B}_{K,\Lambda}=\mathbf{G}_\Lambda \text{ and } P(h-e)=0$$

$$\begin{aligned} PA_{K,\Lambda}Q &= P\phi(\mathbf{G}_\Lambda)Q + P\phi^-(\mathbf{B})(h-e)Q \\ QA_{K,\Lambda}P &= Q\phi(\mathbf{G}_\Lambda)P - Q(h-e)\phi^-(\mathbf{B})P \end{aligned}$$

$$R=Q(h-e)^{-1}Q$$

$$\begin{aligned} \langle \psi, A_{K,\Lambda}RA_{K,\Lambda}\psi \rangle &= \langle \psi, \phi(\mathbf{G}_\Lambda)R\phi(\mathbf{G}_\Lambda)\psi \rangle + \langle \psi, \phi^-(\mathbf{B})Q\phi(\mathbf{G}_\Lambda)\psi \rangle \\ &\quad - \langle \psi, \phi(\mathbf{G}_\Lambda)Q\phi^-(\mathbf{B})\psi \rangle - \langle \psi, \phi^-(\mathbf{B})(h-e)\phi^-(\mathbf{B})\psi \rangle. \end{aligned}$$

$$\begin{aligned} &\langle \psi, \phi^-(\mathbf{B})Q\phi(\mathbf{G}_\Lambda)\psi \rangle - \langle \psi, \phi(\mathbf{G}_\Lambda)Q\phi^-(\mathbf{B})\psi \rangle \\ &= \langle \psi, [\phi^-(\mathbf{B}), \phi(\mathbf{G}_\Lambda)]\psi \rangle - \langle \psi, \phi^-(\mathbf{B})P\phi(\mathbf{G}_\Lambda)\psi \rangle + \langle \psi, \phi(\mathbf{G}_\Lambda)P\phi^-(\mathbf{B})\psi \rangle \\ &= -2\mathrm{Re}\langle \mathbf{B}, \mathbf{G}_\Lambda \rangle + 2\mathrm{Re}\langle \langle \psi, \mathbf{G}_\Lambda \psi \rangle, \langle \psi, \mathbf{B} \psi \rangle \rangle \\ &= -2\mathrm{Re}\langle \mathbf{B}, \mathbf{G} \rangle + 2\mathrm{Re}\langle \sigma(\psi), \langle \psi, \mathbf{B} \psi \rangle \rangle \end{aligned}$$

$$\mathbb{H}_{\mathcal{D},K,\Lambda}(t)=\mathbb{H}_{\Lambda}(t)+4\pi\ln K-\|k\mathbf{B}\|_{L^2}^2+2\mathrm{Re}\langle\mathbf{B},\mathbf{G}\rangle=\mathbb{H}_{\Lambda}(t)+4\pi\ln\Lambda,$$

$$\langle \mathbf{B}, 2\mathbf{G}-k^2\mathbf{B} \rangle = \langle \mathbf{B}, \mathbf{G} \rangle = \langle \mathbf{B}_{K,\Lambda}, \mathbf{G} \rangle = 4\pi\ln\Lambda-4\pi\ln K$$

$$\mathbf{B}_K-\mathbf{B}_{K,\Lambda}=\mathbf{B}_\Lambda$$

$$\mathbb{H}_{\mathcal{D},K,\infty}(t)-\mathbb{H}_{\mathcal{D},K,\Lambda}(t)=\langle \psi_{\varphi_t},(D_K-D_{K,\Lambda}+2\mathrm{Re}\langle \sigma(\psi_{\varphi_t}),\mathbf{B}_\Lambda \rangle)\psi_{\varphi_t} \rangle$$

$$+\big(\langle \psi_{\varphi_t},(A_{K,\Lambda}-A_K)R_{\varphi_t}A_K\psi_{\varphi_t} \rangle+\text{H.c.}\big),$$

$$A_K-A_{K,\Lambda}=2a^*(k\mathbf{B}_\Lambda)\cdot p+2p\cdot a(k\mathbf{B}_\Lambda)$$

$$\langle \psi_{\varphi_t}, A_{K,\Lambda}R_{\varphi_t}A_{K,\Lambda}\psi_{\varphi_t} \rangle \leqslant CK^2(H_f+1)$$



$$\begin{aligned} & \frac{1}{4} \langle \psi_{\varphi_t}, (A_K - A_{K,\Lambda}) R_{\varphi_t} (A_K - A_{K,\Lambda}) \psi_{\varphi_t} \rangle \\ & \leq \langle \psi_{\varphi_t}, (a^*(k\mathbf{B}_\Lambda) \cdot p) R_{\varphi_t} (p \cdot a(k\mathbf{B}_\Lambda)) \psi_{\varphi_t} \rangle + \langle \psi_{\varphi_t}, (p \cdot a(k\mathbf{B}_\Lambda)) R_{\varphi_t} (a^*(k\mathbf{B}_\Lambda) \cdot p) \psi_{\varphi_t} \rangle \\ & \leq C\Lambda^{-1}(H_f + 1) \end{aligned}$$

$$\Psi, \Phi \in D\left(H_f^{1/2}\right)$$

$$|\langle \Psi, (6.18 \text{ b}) \Phi \rangle| \lesssim CK\Lambda^{-\frac{1}{2}}(\langle \Psi, T\Psi \rangle + \langle \Phi, T\Phi \rangle + 1)$$

$$\mathbf{B}_K-\mathbf{B}_{K,\Lambda}=\mathbf{B}_\Lambda$$

$$\begin{aligned} D_K-D_{K,\Lambda} &= 2a^*(k\mathbf{B}_K)a(k\mathbf{B}_\Lambda)+2a^*(k\mathbf{B}_\Lambda)a(k\mathbf{B}_{K,\Lambda}) \\ &\quad + (a^*(k\mathbf{B}_K)a^*(k\mathbf{B}_\Lambda)+a^*(k\mathbf{B}_\Lambda)a^*(k\mathbf{B}_{K,\Lambda})+\text{H.c.}) \end{aligned}$$

$$\Psi, \Phi \in D\left(H_f^{1/2}\right)$$

$$|\langle \Psi, (D_K - D_{K,\Lambda}) \Phi \rangle| \lesssim C(K\Lambda)^{-\frac{1}{4}}(\langle \Psi, H_f \Psi \rangle + \langle \Phi, H_f \Phi \rangle + 1)$$

$$\|\sigma(\psi_{\varphi_t})\|_{L^2} \lesssim \|B_\Lambda\|_{L^2} \lesssim \Lambda^{-1}$$

$$\mathbb{H}_{\mathcal{D},K,\Lambda}(t)\varphi_0\in\mathfrak{h}_{1/2}e(\varphi_0)<T,C,K_0>$$

$$\begin{aligned} \frac{2}{3}H_f-C\ln K(N+1) &\leq \mathbb{H}_{\mathcal{D},K,\Lambda}(t) \leq \frac{3}{2}H_f+C\ln K \\ \pm \partial_t \mathbb{H}_{\mathcal{D},K,\Lambda}(t) &\leq CK^2(H_f+1) \\ \pm i[\mathbb{H}_{\mathcal{D},K,\Lambda}(t),N] &\leq CK^2(H_f+1) \end{aligned}$$

$$|t|\leq TK_0\leq K<\Lambda\leq\infty-A_{K,\Lambda}R_{\varphi_t}A_{K,\Lambda}\pm D_K\leq\frac{1}{4}H_f+C\ln K$$

$$|2\mathrm{Re}\langle\sigma(\psi_{\varphi_t}),B_{K,\Lambda}\rangle|\lesssim\|B_K\|_{L^2}\lesssim K^{-1}$$

$$D_{K,\Lambda}+2\mathrm{Re}\langle\sigma(\psi_{\varphi_t}),\mathbf{B}_{K,\Lambda}\rangle-A_{K,\Lambda}R_{\varphi_t}A_{K,\Lambda}\gtrsim\ln K(N+1)$$

$$\begin{aligned} \partial_t \mathbb{H}_{\mathcal{D},K,\Lambda}(t) &= 2\mathrm{Re}\langle \dot{\psi}_{\varphi_t}, (D_{K,\Lambda} + 2\mathrm{Re}\langle \sigma(\psi_{\varphi_t}), \mathbf{B}_{K,\Lambda} \rangle - A_{K,\Lambda} R_{\varphi_t} A_{K,\Lambda}) \psi_{\varphi_t} \rangle \\ &\quad + \langle \psi_{\varphi_t}, (2\mathrm{Re}\langle \dot{\sigma}(\psi_{\varphi_t}), \mathbf{B}_{K,\Lambda} \rangle - A_{K,\Lambda} \dot{R}_{\varphi_t} A_{K,\Lambda}) \psi_{\varphi_t} \rangle \end{aligned}$$

$$\langle \Psi, \langle \dot{\psi}_{\varphi_t}, A_{K,\Lambda} R_{\varphi_t} A_{K,\Lambda} \psi_{\varphi_t} \rangle \Psi \rangle = \langle \dot{\psi}_{\varphi_t} \otimes \Phi, (A_{K,\Lambda} R_{\varphi_t} A_{K,\Lambda}) \psi_{\varphi_t} \otimes \Phi \rangle$$

$$\begin{aligned} 2\mid & \langle \dot{\psi}_{\varphi_t} \otimes \Phi, (A_{K,\Lambda} R_{\varphi_t} A_{K,\Lambda}) \psi_{\varphi_t} \otimes \Phi \rangle \\ & \leq \mid \langle \dot{\psi}_{\varphi_t} \otimes \Phi, (A_{K,\Lambda} R_{\varphi_t} A_{K,\Lambda}) \dot{\psi}_{\varphi_t} \otimes \Phi \rangle \mid + \mid \langle \psi_{\varphi_t} \otimes \Phi, (A_{K,\Lambda} R_{\varphi_t} A_{K,\Lambda}) \psi_{\varphi_t} \otimes \Phi \rangle \mid \\ & \leq CK^2(\|\langle p \rangle R_{\varphi_t} \langle p \rangle\| + \|R_{\varphi_t}\|) \Big(\|\langle p \rangle \dot{\psi}_{\varphi_t}\|_{L^2}^2 + \|\langle p \rangle \psi_{\varphi_t}\|_{L^2}^2 \Big) \Big\| \left\langle H_f^{1/2} \right\rangle \Phi \Big\|^2 \\ & \leq CK^2 \left\| \left\langle H_f^{\frac{1}{2}} \right\rangle \Phi \right\|^2 \end{aligned}$$

$$\|\langle p \rangle \dot{\psi}_{\varphi_t}\|_{L^2}=\|\langle p \rangle R_{\varphi_t}V_{i\omega\varphi_t}\psi_{\varphi_t}\|_{L^2}\leq C$$

$$\|F^{-1/2}D_KF^{-1/2}\|\lesssim 1$$

$$F=K^{-1/2}(1+H_f)+\ln K$$

$$|\langle \Psi,D_K\Phi\rangle|\lesssim \langle \Psi,F\Psi\rangle+\langle \Phi,F\Phi\rangle \text{ for all } \Psi,\Phi\in D\left(H_f^{1/2}\right)$$

$$\begin{aligned}\langle \Psi, [\mathbb{H}_{\mathcal{D},\Lambda,K}(t),N]\Psi\rangle=&\langle \psi_{\varphi_t}\otimes \Psi, [D_{K,\Lambda},N]\psi_{\varphi_t}\otimes \Psi\rangle\\&-2\mathrm{Re}\langle \psi_{\varphi_t}\otimes \Psi, [A_{K,\Lambda},N]R_{\varphi_t}A_{K,\Lambda}\psi_{\varphi_t}\otimes \Psi\rangle\end{aligned}$$

$$\mathbb{U}_{K,\Lambda}(t)\,\mathbb{H}_{\mathcal{D},K,\Lambda}(t)\mathbb{U}_{K,\Lambda}(t)\stackrel{\Lambda\rightarrow\infty}{\rightarrow}\mathbb{U}_{K,\infty}(t)e(\varphi_0)<\mathbb{H}_{\mathcal{D},K,\Lambda}(t)$$

$$K_0\leqslant K<\Lambda\leqslant\infty\text{ and }\Psi\in D\left(H_f^{1/2}\right)\subset\mathcal{F}$$

$$\Psi\in C([-T,T],\mathcal{F})\cap L^\infty\left([-T,T],D\left(H_f^{1/2}\right)\right)$$

$$\begin{cases} i\partial_t\Psi(t) \,=\, \mathbb{H}_{\mathcal{D},K,\Lambda}(t)\Psi(t) \\ \Psi(0) \,=\, \Psi \end{cases}$$

$$D\left((1+H_f)^{-1/2}\right)\Psi\mapsto \Psi(t)\mathbb{U}_{K,\Lambda}(t)$$

$$\langle \mathbb{U}_{K,\Lambda}(t)\Psi,H_f\mathbb{U}_{K,\Lambda}(t)\Psi\rangle\leqslant C_K\langle \Psi,(H_f+1)\Psi\rangle$$

$$\Lambda\in (K,\infty], |t|\leqslant T$$

$$s-\lim_{\Lambda\rightarrow\infty}\mathbb{U}_{K,\Lambda}(t)=\mathbb{U}_{K,\infty}(t)$$

$$K\geqslant K_0, |t|\leqslant T t\mapsto \mathbb{U}_{K,\infty}(t)\mathbb{U}_{\Lambda}(t)$$

$$\mathbb{U}_{\Lambda}(t)=\mathbb{U}_{K,\Lambda}(t)\mathrm{exp}\left(it4\pi\mathrm{ln}\,\Lambda\right).$$

$$\mathbb{U}_{\Lambda}(t)\mathrm{exp}\left(-it4\pi\mathrm{ln}\,\Lambda\right)\stackrel{\Lambda\rightarrow\infty}{\rightarrow}\mathbb{U}_{K,\infty}(t)=:\mathbb{U}(t)$$

$$\Psi\in D\left(H_f^{1/2}\right)$$

$$\|(\mathbb{U}_{K,\Lambda}(t)-\mathbb{U}_{K,\infty}(t))\Psi\|^2=2\mathrm{Re}\int_0^t\langle \mathbb{U}_{K,\Lambda}(s)\Psi,(\mathbb{H}_{\mathcal{D},K,\Lambda}(s)-\mathbb{H}_{\mathcal{D},K,\infty}(s))\mathbb{U}_{K,\infty}(s)\Psi\rangle\mathrm{d}s$$

$$\begin{aligned}&\leqslant \frac{C_KK^{\frac{1}{2}}}{\Lambda^{1/4}}\int_0^t\big(\langle \mathbb{U}_{K,\Lambda}(s)\Psi,H_f\mathbb{U}_{K,\Lambda}(s)\Psi\rangle+\langle \mathbb{U}_{K,\infty}(s)\Psi,H_f\mathbb{U}_{K,\infty}(s)\Psi\rangle+1\big)\mathrm{d}s\\&\leqslant C_K|t|K^{\frac{1}{2}}\Lambda^{-\frac{1}{4}}\end{aligned}$$

$$D\left(H_f^{1/2}\right)\subseteq\mathcal{F}$$

$$\mathbb{U}_{K,\Lambda}(t)\stackrel{\Lambda\rightarrow\infty}{\rightarrow}\mathbb{U}_{K,\infty}(t)$$

$$\mathbb{U}(t)^*(N+1)^m\mathbb{U}(t)\leqslant C_m(N+1)^m$$

$$\mathbb{U}(t)=\mathbb{U}_{K,\infty}(t)$$

$$i\partial_t\left\| (N+1)^{\frac{1}{2}}\mathbb{U}(t)\Psi\right\|^2\leqslant |\langle \mathbb{U}(t)\Psi, [\mathbb{H}_{\mathcal{D},K,\infty}(t),N]\mathbb{U}(t)\Psi\rangle|\leqslant C\left\| (N+1)^{\frac{1}{2}}\mathbb{U}(t)\Psi\right\|^2,$$

$$\tilde{\delta}(t) := e^{i\varepsilon^{-2}\mu(t)}W(\varepsilon^{-1}\varphi_t)^*e^{-it\varepsilon^{-2}H^\varepsilon}W(\varepsilon^{-1}\varphi_0)\psi_{\varphi_0}\otimes\Omega - \psi_{\varphi_t}\otimes\mathbb{U}(t)\Omega$$

$$e^{-it\varepsilon^{-2}H^\varepsilon}\mathbb{U}(t)(\varphi_t,\psi_{\varphi_t})\varphi_0\in\mathfrak{h}_{1/2}e(\varphi_0)$$

$$\mu(t)=\int_0^t\left(\operatorname{Im}\langle\varphi_s,\partial_s\varphi_s\rangle+\|\omega^{1/2}\varphi_s\|_{L^2}^2+e(\varphi_s)\right)\mathrm{d}s$$

$$i\partial_t\mathbb{U}(t)\Omega=\mathbb{H}_{\mathcal{D},K,\infty}(t)\mathbb{U}(t)\Omega, i\partial_t\varphi_t=\omega\varphi_t+\sigma(\psi_{\varphi_t}), \partial_t\psi_{\varphi_t}=R_{\varphi_t}V_{i\omega\varphi_t}\psi_{\varphi_t}$$

$$\mathbb{H}_{\mathcal{D},K,\infty}(t)\left(h_{\varphi_t}-e(\varphi_t)\right)\psi_{\varphi_t}$$

$$\delta(t) \mathop{:=} \xi_K(t) - \psi_{\varphi_t} \otimes \mathbb{U}(t) \Omega$$

$$\xi_K(t) \mathop{:=} e^{i\varepsilon^{-2}\mu(t)}U_K^\varepsilon W(\varepsilon^{-1}\varphi_t)^*e^{-it\varepsilon^{-2}H^\varepsilon}W(\varepsilon^{-1}\varphi_0)(U_K^\varepsilon)^*\psi_{\varphi_0}\otimes\Omega$$

$$U_K^\varepsilon=\exp\big(\varepsilon a^*(\boldsymbol{B}_K)-\varepsilon a(\boldsymbol{B}_K)\big), \boldsymbol{B}_K(x,k)=\frac{\boldsymbol{G}(x,k)}{k^2}\mathbf{1}_{\{|k|\geqslant K\}}$$

$$\|(U_K^\varepsilon-\mathbf{1})\Psi\|\lesssim \varepsilon\|B_K\|_{L^2}\|(N+1)^{1/2}\Psi\|\text{ for all }\Psi\in D(N^{1/2}),$$

$$\|B_K\|_{L^2}\lesssim K^{-1}$$

$$\|(U_K^\varepsilon)^*\delta(t)-\tilde{\delta}(t)\|\leqslant \|((U_K^\varepsilon)^*-\mathbf{1})\psi_{\varphi_0}\otimes\Omega\|+\|((U_K^\varepsilon)^*-\mathbf{1})\psi_{\varphi_t}\otimes\mathbb{U}(t)\Omega\|\lesssim \varepsilon K^{-1}$$

$$\|\tilde{\delta}(t)\|\lesssim \|\delta(t)\|+\varepsilon K^{-1}$$

$$K=\varepsilon^{-4/5}\delta(t)$$

$$U_K^\varepsilon W(\varepsilon^{-1}\varphi_t)^*=W(\varepsilon^{-1}\varphi_t)^*U_K^\varepsilon e^{-ig_{K,\varphi_t}(x)}$$

$$g_{K,\varphi_t}(x)=2\mathrm{Im}\langle\varphi_t,\boldsymbol{B}_K(x,\cdot)\rangle,$$

$$U_K^\varepsilon H^\varepsilon (U_K^\varepsilon)^* = H_{\mathcal{D},K}^\varepsilon$$

$$\xi_K(t)=e^{i\varepsilon^{-2}\mu(t)}e^{-ig_{K,\varphi_t}(x)}W(\varepsilon^{-1}\varphi_t)^*e^{-it\varepsilon^{-2}H_{\mathcal{D},K}^\varepsilon}W(\varepsilon^{-1}\varphi_0)e^{ig_{K,\varphi_0}(x)}\psi_{\varphi_0}\otimes\Omega$$

$$\left\| \left(p^2 + \varepsilon^2 H_f \right)^{1/2} \xi_K(t) \right\| \leqslant CK^{\frac{1}{2}}$$

$$\begin{aligned}&\left\| \left(p^2 + \varepsilon^2 H_f \right)^{1/2} \xi_K(t) \right\| \\&= \left\| \left(p^2 + \varepsilon^2 H_f \right)^{1/2} e^{-ig_{K,\varphi_t}(x)} W(\varepsilon^{-1}\varphi_t)^* e^{-it\varepsilon^{-2}H_{\mathcal{D},K}} W(\varepsilon^{-1}\varphi_0) e^{ig_{K,\varphi_0}(x)} \psi_{\varphi_0} \otimes \Omega \right\| \\&\lesssim \left\| \left(p^2 + \varepsilon^2 H_f + 1 \right)^{1/2} e^{-it\varepsilon^{-2}H_{\mathcal{D},K}^\varepsilon} W(\varepsilon^{-1}\varphi_0) e^{ig_{K,\varphi_0}(x)} \psi_{\varphi_0} \otimes \Omega \right\|\end{aligned}$$

$$\begin{aligned}e^{ig_{K,\varphi_t}(x)}p^2e^{-ig_{K,\varphi_t}(x)}&=p^2+p\cdot(\nabla g_{K,\varphi_t})(x)+(\nabla g_{K,\varphi_t})(x)\cdot p+|(\nabla g_{K,\varphi_t})(x)|^2\\&\leqslant 2p^2+2|(\nabla g_{K,\varphi_t})(x)|^2\end{aligned}$$

$$W(\varepsilon^{-1}\varphi_t)\varepsilon^2H_fW(\varepsilon^{-1}\varphi_t)^*=\varepsilon^2H_f+\varepsilon\phi(\omega\varphi_t)+\|\varphi_t\|_{\mathfrak{h}_{1/2}}^2\leqslant 2\varepsilon^2H_f+2\|\varphi_t\|_{\mathfrak{h}_{1/2}}^2$$

$$\|\varphi_t\|_{\mathfrak{h}_{1/2}}^2\lesssim 1$$

$$|(\nabla g_{K,\varphi_t})(x)|=2|\langle\varphi_t,k\mathbf{B}(x,\cdot)\rangle|\leqslant\|\varphi_t\|_{\mathfrak{h}_{1/2}}\|\omega^{1/2}B_K\|_{L^2}\lesssim 1$$

$$\begin{aligned}
\|(p^2 + \varepsilon^2 H_f)^{1/2} \xi_K(t)\| &\lesssim \|(H_{\mathcal{D},K}^\varepsilon + K)^{1/2} W(\varepsilon^{-1} \varphi_0) e^{ig_{K,\varphi_0}(x)} \psi_{\varphi_0} \otimes \Omega\| \\
&\lesssim \|(p^2 + \varepsilon^2 H_f + K) W(\varepsilon^{-1} \varphi_0) e^{ig_{K,\varphi_0}(x)} \psi_{\varphi_0} \otimes \Omega\| \\
&\lesssim \|(p^2 + \varepsilon^2 H_f + K)^{1/2} \psi_{\varphi_0} \otimes \Omega\| \\
&\lesssim K^{\frac{1}{2}}
\end{aligned}$$

$$i\partial_t W(\varepsilon^{-1} \varphi_t)^* = (-\varepsilon^{-1} \phi(i\dot{\varphi}_t) + \varepsilon^{-2} \text{Im}\langle \varphi_t, \dot{\varphi}_t \rangle) W(\varepsilon^{-1} \varphi_t)^*$$

$$\dot{\mu}(t) = \text{Im}\langle \varphi_t, \dot{\varphi}_t \rangle + \|\omega^{1/2} \varphi_t\|_{L^2}^2 + e(\varphi_t)$$

$$\mathcal{L}_{\mathcal{D},K}^\varepsilon(t) i\partial_t \xi_K(t) = \mathcal{L}_{\mathcal{D},K}^\varepsilon(t) \xi_K(t)$$

$$i\dot{\varphi}_t = \omega\varphi_t + \sigma(\psi_{\varphi_t})$$

$$\begin{aligned}
\mathcal{L}_{\mathcal{D},K}^\varepsilon(t) &= e^{-ig_{K,\varphi_t}(x)} W(\varepsilon^{-1} \varphi_t)^* \varepsilon^{-2} H_{\mathcal{D},K}^\varepsilon W(\varepsilon^{-1} \varphi_t) e^{ig_{K,\varphi_t}(x)} \\
&\quad - \varepsilon^{-2} \left(\|\omega^{1/2} \varphi_t\|_{L^2}^2 - e(\varphi_t) \right) - \varepsilon^{-1} \phi \left(\omega\varphi_t + \sigma(\psi_{\varphi_t}) \right) + 2\text{Re}\langle \mathbf{B}_K, \omega\varphi_t + \sigma(\psi_{\varphi_t}) \rangle \\
&= \varepsilon^{-2} \left(h_{\varphi_t} - e(\varphi_t) \right) + \varepsilon^{-1} \left(A_K - \phi \left(\sigma(\psi_{\varphi_t}) \right) \right) \\
&\quad + (H_f + D_K + 2\text{Re}\langle \mathbf{B}_K, \sigma(\psi_{\varphi_t}) \rangle) - \varepsilon \phi(\omega \mathbf{B}_K) + \varepsilon^2 \|\omega^{1/2} B_K\|_{L^2}^2
\end{aligned}$$

$$A_K = \phi(\mathbf{G}_K) + 2a^*(k\mathbf{B}_K) \cdot p + 2p \cdot a(k\mathbf{B}_K)$$

$$D_K = 2a^*(k\mathbf{B}_K)a(k\mathbf{B}_K) + a^*(k\mathbf{B}_K)^2 + a(k\mathbf{B}_K)^2 + 4\pi \ln K$$

$$\delta(t) = \xi_K(t) - \zeta(t)$$

$$\zeta(t) = \psi_{\varphi_t} \otimes \mathbb{U}(t)\Omega$$

$$\partial_t \xi_K(t) = -i\mathcal{L}_{\mathcal{D},K}^\varepsilon(t) \xi_K(t), \partial_t \zeta(t) = (-i\mathbb{H}_{\mathcal{D},K,\infty}(t) + R_{\varphi_t} V_{i\omega\varphi_t}) \zeta(t)$$

$$\|\xi_K(t)\| = \|\zeta(t)\| = 1$$

$$\begin{aligned}
\frac{1}{2} \frac{d}{dt} \|\delta(t)\|^2 &= -\frac{d}{dt} \text{Re}\langle \xi_K(s), \zeta(s) \rangle \\
&= \text{Im}\langle \xi_K(s), (\mathcal{L}_{\mathcal{D},K}^\varepsilon(s) - \mathbb{H}_{\mathcal{D},K,\infty}(s) - iR_{\varphi_s} V_{i\omega\varphi_s}) \zeta(s) \rangle
\end{aligned}$$

$$\begin{aligned}
\|\delta(t)\|^2 &= 2\text{Im} \int_0^t ds \langle \xi_K(s), (\mathcal{L}_{\mathcal{D},K}^\varepsilon(s) - \mathbb{H}_{\mathcal{D},K,\infty}(s) - iR_{\varphi_s} V_{i\omega\varphi_s}) \zeta(s) \rangle \\
&= 2\text{Im}(\mathcal{M}^{(1)} + \mathcal{M}^{(2)} + \mathcal{R}^{(3)} + \mathcal{R}^{(4)} + \mathcal{R}^{(5)})
\end{aligned}$$

$$\mathcal{M}^{(1)} = \int_0^t ds \left\langle \xi_K(s), \varepsilon^{-1} \left(A_K - \phi \left(\sigma(\psi_{\varphi_s}) \right) \right) \zeta(s) \right\rangle$$

$$\mathcal{M}^{(2)} = \int_0^t ds \langle \xi_K(s), P_{\varphi_s} A_K R_{\varphi_s} A_K \zeta(s) \rangle$$

$$\mathcal{R}^{(3)} = \int_0^t ds \langle \xi_K(s), Q_{\varphi_s} (D_K + 2\text{Re}\langle \mathbf{B}_K, \sigma(\psi_{\varphi_s}) \rangle) \zeta(s) \rangle$$

$$\mathcal{R}^{(4)} = \int_0^t ds \langle \xi_K(s), (-iR_{\varphi_s} V_{i\omega\varphi_s}) \zeta(s) \rangle$$

$$\mathcal{R}^{(5)} = \int_0^t ds \left\langle \xi_K(s), \left(-\varepsilon \phi(\omega \mathbf{B}_K) + \varepsilon^2 \|\omega^{1/2} B_K\|_{L^2}^2 \right) \zeta(s) \right\rangle$$



$$P_{\varphi_s} = |\psi_{\varphi_s}\rangle\langle\psi_{\varphi_s}| \text{ and } Q_{\varphi_s} = \mathbf{1} - P_{\varphi_s}$$

$$\mathbb{H}_{\mathcal{D},K,\infty}(s)\zeta(s) = P_{\varphi_s}(H_f + D_K + 2\text{Re}\langle\mathbf{B}_K, \sigma(\psi_{\varphi_s})\rangle - A_K R_{\varphi_s} A_K)\zeta(s)$$

$$\mathcal{R}^{(3)} = \mathcal{R}^{(3.1)} + \mathcal{R}^{(3.2)}$$

$$|\mathcal{R}^\varphi| \lesssim \int_0^t \mathrm{d}s |\langle \xi_K(s), Q_{\varphi_s} \text{Re}\langle \mathbf{B}_K, \sigma(\psi_{\varphi_s}) \rangle \zeta(s) \rangle| \lesssim \|B_K\|_{L^2} \int_0^t \mathrm{d}s \|\sigma(\psi_{\varphi_s})\|_{L^2} \lesssim K^{-1}$$

$$\|B_K\|_{L^2} \lesssim K^{-1} \text{ and } \|\sigma(\psi_{\varphi_s})\|_{L^2} \lesssim 1$$

$$Q_{\varphi_s}D_K\zeta(s) = Q_{\varphi_s}(D_K - 4\pi\ln K)\zeta(s)$$

$$Q_{\varphi_s}\zeta(s) = 0$$

$$\begin{aligned} |\mathcal{R}^{\mathfrak{q}}| &\leq \int_0^t \mathrm{d}s |\langle \xi_K(s), Q_{\varphi_s}(D_K - 4\pi\ln K)\zeta(s) \rangle| \\ &\lesssim \int_0^t \mathrm{d}s \|\langle p \rangle \xi_K(s)\| \left\| \langle p \rangle^{-1} (D_K - 4\pi\ln K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-2} \right\| \left\| \langle p \rangle \left\langle N^{\frac{1}{2}} \right\rangle^2 \zeta(s) \right\| \\ &\lesssim K^{-1/4} \end{aligned}$$

$$\left\| \langle p \rangle \left\langle N^{\frac{1}{2}} \right\rangle^2 \zeta(s) \right\| \lesssim \|\psi_{\varphi_s}\|_{H^1} \left\| \left\langle N^{\frac{1}{2}} \right\rangle^2 \mathbb{U}(s) \Omega \right\| \lesssim 1$$

$$|\mathcal{R}^{(3)}| \lesssim K^{-1/4}$$

$$\begin{aligned} |\mathcal{R}^{\varsigma}| &\lesssim \varepsilon \int_0^t \mathrm{d}s \|\langle p \rangle \xi_K(s)\| \|\langle p \rangle^{-1} \phi(\omega \mathbf{B}_K) \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \langle p \rangle^{-1}\| \|\langle p \rangle \left\langle N^{\frac{1}{2}} \right\rangle \zeta(s)\| \\ &\lesssim \varepsilon K^{-3/4} \end{aligned}$$

$$\left\|\omega^{1/2}B_K\right\|_{L^2}^2\leq CK^{-1}$$

$$|\mathcal{R}^{(5.2)}| \lesssim \varepsilon^2 K^{-1}$$

$$\begin{aligned} Q_{\varphi_s}\xi_K(s) &= R_{\varphi_s}\left(h_{\varphi_s}-e(\varphi_s)\right)\xi_K(s) \\ &= R_{\varphi_s}\left(\varepsilon^2\left(i\partial_s-\mathcal{L}_{\mathcal{D},K}^\varepsilon(s)\right)+h_{\varphi_s}-e(\varphi_s)\right)\xi_K(s) \\ &= R_{\varphi_s}\left(-\varepsilon\left(A_K-\phi\left(\sigma_{\psi_{\varphi_s}}\right)\right)+\varepsilon^2\left(i\partial_s-H_f-D_K-2\text{Re}\langle\mathbf{B}_K,\sigma(\psi_{\varphi_s})\rangle\right)\right. \\ &\quad \left.+\varepsilon^3\phi(\omega\mathbf{B}_K)-\varepsilon^4\left\|\omega^{1/2}B_K\right\|_{L^2}^2\right)\xi_K(s) \end{aligned}$$

$$(i\partial_s-\mathcal{L}_{\mathcal{D},K}^\varepsilon(s))\xi_K(s)=0$$

$$Q_{\varphi_s}\xi_K(s)\text{Ran}(Q_{\varphi_s})\subset L^2\otimes\mathcal{F}$$

$$\varepsilon^2(i\partial_s-\mathcal{L}_{\mathcal{D},K}^\varepsilon(s))+\left(h_{\varphi_s}-e(\varphi_s)\right)$$

$$\mathcal{M}^{(1)} = \int_0^t \mathrm{d}s \left\langle \xi_K(s), \varepsilon^{-1} \left(A_K - \phi \left(\sigma_{\psi_{\varphi_s}} \right) \right) \zeta(s) \right\rangle = \int_0^t \mathrm{d}s \left\langle \xi_K(s), \varepsilon^{-1} Q_{\varphi_s} A_K \zeta(s) \right\rangle$$

$$P_{\varphi_s}+Q_{\varphi_s},Q_{\varphi_s}\phi\left(\sigma(\psi_{\varphi_s})\right)\zeta(s)=\phi\left(\sigma(\psi_{\varphi_s})\right)Q_{\varphi_s}\zeta(s)$$

$$P_{\varphi_s}\Big(A_K-\phi\left(\sigma(\psi_{\varphi_s})\right)\Big)P_{\varphi_s}=0$$

$$\begin{aligned} P_{\varphi_s}(a^*(G_K)+2a^*(k\mathbf{B}_K)\cdot p)P_{\varphi_s}&=P_{\varphi_s}\otimes\int\mathrm{d}k\langle\psi_{\varphi_s},(\mathbf{G}_K(\cdot,k)+2k\mathbf{B}_K(\cdot,k)\cdot p)\psi_{\varphi_s}\rangle a_k^*\\ &=P_{\varphi_s}\otimes a^*\left(\sigma(\psi_{\varphi_s})\right) \end{aligned}$$

$$\langle \psi_{\varphi_s}, \mathbf{G}_K \psi_{\varphi_s} \rangle = \sigma(\psi_{\varphi_s}) \mathbf{1}_{|k| \leqslant K}$$

$$2\langle \psi_{\varphi_s}, (k\mathbf{B}_K\cdot p)\psi_{\varphi_s}\rangle = \langle \psi_{\varphi_s}, G\psi_{\varphi_s}\rangle \mathbf{1}_{|k|\geqslant K} = \sigma(\psi_{\varphi_s}) \mathbf{1}_{|k|\geqslant K}(p\cdot \overline{k\mathbf{B}_K}) = \mathbf{G}\mathbf{1}_{|k|\geqslant K}$$

$$\mathcal{M}^{(\Theta)}\!=\!\mathcal{M}^{(\zeta)}+\mathcal{R}^{(\varepsilon)}+\mathcal{R}^{(\epsilon)}+\mathcal{R}^{(\gamma)}$$

$$\mathcal{M}^{(\xi)}=-\int_0^t\mathrm{d}s\left\langle \xi_K(s),\left(A_K-\phi\left(\sigma(\psi_{\varphi_s})\right)\right)R_{\varphi_s}A_K\zeta(s)\right\rangle$$

$$\mathcal{R}^{(\mathfrak{T})}=\varepsilon\int_0^t\mathrm{d}s\langle (i\partial_s-H_f)\xi_K(s),R_{\varphi_s}A_K\zeta(s)\rangle$$

$$\mathcal{R}^{(\mathfrak{J})}=-\varepsilon\int_0^t\mathrm{d}s\langle \xi_K(s),D_KR_{\varphi_s}A_K\zeta(s)\rangle$$

$$\mathcal{R}^{(\aleph\aleph\aleph\gamma)}=\int_0^t\mathrm{d}s\left\langle \xi_K(s),\left(-2\varepsilon\mathrm{Re}\langle \mathbf{B}_K,\sigma(\psi_{\varphi_s})\rangle+\varepsilon^2\phi(\omega\mathbf{B}_K)-\varepsilon^3\left\|\omega^{\frac{1}{2}}B_K\right\|_{L^2}^2\right)R_{\varphi_s}A_K\zeta(s)\right\rangle$$

$$\mathbf{1}=P_{\varphi_s}+Q_{\varphi_s}$$

$$P_{\varphi_s}\phi\left(\sigma(\psi_{\varphi_s})\right)R_{\varphi_s}=0$$

$$\mathcal{M}^{(\kappa)}=-\mathcal{M}^{(\ell)}+\mathcal{R}^{(\mathfrak{H})}$$

$$\mathcal{R}^{(\wp)}=-\int_0^t\mathrm{d}s\left\langle \xi_K(s),Q_{\varphi_s}\left(A_K-\phi\left(\sigma(\psi_{\varphi_s})\right)\right)R_{\varphi_s}A_K\zeta(s)\right\rangle$$

$$\mathbf{1}=\langle p\rangle\langle p\rangle^{-1}\text{ and }\mathbf{1}=\left\langle N^{\frac{1}{2}}\right\rangle^{-1}\left\langle N^{\frac{1}{2}}\right\rangle^1$$

$$\begin{aligned} |\mathcal{R}^{(\wp)}| \leqslant & \varepsilon \int_0^t \mathrm{d} s \Bigg(\left\| \langle p \rangle \xi_K(s) \right\| \left| \langle p \rangle^{-1} D_K \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-2} \right| \left\| \langle p \rangle R_{\varphi_s} \langle p \rangle \right\| \\ & \times \left\| \left\langle N^{\frac{1}{2}} \right\rangle^2 \langle p \rangle^{-1} A_K \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-3} \right\| \left\| \left\langle N^{\frac{1}{2}} \right\rangle^3 \langle p \rangle \zeta(s) \right\| \Bigg) \end{aligned}$$

$$\|\langle p\rangle \xi_K(s)\|\lesssim K^{\frac{1}{2}}$$

$$\left\|\left\langle N^{\frac{1}{2}}\right\rangle^3\langle p\rangle\zeta(s)\right\|\lesssim 1$$

$$\left\|\langle p\rangle R_{\varphi_s}\langle p\rangle\right\|\lesssim 1$$

$$|\mathcal{R}^{(\hbar)}|\lesssim \varepsilon K^{\frac{1}{2}}(\ln\,K)^{\frac{3}{2}}$$

$$\begin{aligned}
& \|\langle p \rangle R_{\varphi_s} \langle p \rangle\| \lesssim 1 \\
& |\mathcal{R}^{(\Re)}| \lesssim (\ln K)^{\frac{1}{2}} \left(\varepsilon K^{-1} + \varepsilon^2 K^{-\frac{1}{2}} \right) \\
& \mathcal{R}^{(\mathcal{M})} = \langle i \xi_K(s), \varepsilon R_{\varphi_s} A_K \zeta(s) \rangle \Big|_{s=0}^{s=t} \\
& \mathcal{R}^{(\otimes)} = -\varepsilon \int_0^t ds \langle \xi_K(s), R_{\varphi_s} [H_f, A_K] \zeta(s) \rangle \\
& \mathcal{R}^{(\Delta)} = \varepsilon \int_0^t ds \langle \xi_K(s), R_{\varphi_s} A_K P_{\varphi_s} (A_K R_{\varphi_s} A_K - D_K - 2\operatorname{Re} \langle \mathbf{B}_K, \sigma(\psi_{\varphi_s}) \rangle) \zeta(s) \rangle \\
& \mathcal{R}^{(*)} = i\varepsilon \int_0^t ds \langle \xi_K(s), (\dot{R}_{\varphi_s} A_K - i R_{\varphi_s} A_K R_{\varphi_s} V_{i\omega\varphi_s}) \zeta(s) \rangle \\
& \|\langle p \rangle^{-1} V_{i\omega\varphi_s} \langle p \rangle^{-1}\| \lesssim \|\varphi_s\|_{\mathfrak{h}_{1/2}} \|\psi_{\varphi_s}\|_{H^1}^2 \lesssim 1 \\
& |\mathcal{R}^{(\boxtimes)}| + |\mathcal{R}^{(\dagger)}| + |\mathcal{R}^{(\ddagger)}| \lesssim \varepsilon (\ln K)^{\frac{3}{2}} \\
& |\mathcal{R}^{(\odot)}| \leq \varepsilon \int_0^t ds \|R_{\varphi_s} \langle p^2 \rangle\| \left\| \langle p \rangle^{-2} [H_f, A_K] \langle p \rangle^{-2} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \left\| \langle p^2 \rangle \left\langle N^{\frac{1}{2}} \right\rangle^2 \zeta(s) \right\| \\
& \lesssim \varepsilon K \\
& \|R_{\varphi_s} \langle p^2 \rangle\| + \|\psi_{\varphi_s}\|_{H^2} \lesssim 1 \\
& |\mathcal{R}^{(1,2)}| \lesssim \varepsilon K \\
& \varphi_s = \varphi_{s,L} + \varphi_{s,>L} \\
& \varphi_{s,L} := \mathbf{1}_{|k| \leq L} \varphi_s \\
& V_{i\omega\varphi_s} = V_{i\omega\varphi_{s,L}} + V_{i\omega\varphi_{s,>L}} \\
& \left| \int_0^t ds \langle \xi_K(s), (-i R_{\varphi_s} V_{i\omega\varphi_{s,>L}}) \zeta(s) \rangle \right| \\
& \leq \int_0^t ds \|R_{\varphi_s}\| \|V_{i\omega\varphi_{s,>L}} \langle p \rangle^{-2}\| \|\langle p \rangle^2 \zeta(s)\| \lesssim L^{-1/4} \\
& \|V_{i\omega\varphi_{s,>L}} \langle p \rangle^{-2}\| \lesssim \|\omega\varphi_{s,>L}\|_{\mathfrak{h}_{-3/4}} \lesssim L^{-1/4} \|\varphi_s\|_{\mathfrak{h}_{1/2}} \lesssim L^{-1/4} \\
& \mathcal{R}^{(\wedge)} = -i\varepsilon \int_0^t ds \left\langle \xi_K(s), \left(-A_K + \phi \left(\sigma(\psi_{\varphi_s}) \right) \right) R_{\varphi_s}^2 V_{i\omega\varphi_{s,L}} \zeta(s) \right\rangle \\
& \mathcal{R}^{(\vee)} = -i\varepsilon^2 \int_0^t ds \langle (i\partial_s - H_f) \xi_K(s), R_{\varphi_s}^2 V_{i\omega\varphi_{s,L}} \zeta(s) \rangle \\
& \mathcal{R}^{(\Delta)} = i\varepsilon^2 \int_0^t ds \langle \xi_K(s), (D_K + 2\operatorname{Re} \langle \mathbf{B}_K, \sigma(\psi_{\varphi_s}) \rangle) R_{\varphi_s}^2 V_{i\omega\varphi_{s,L}} \zeta(s) \rangle \\
& \mathcal{R}^{(\nabla)} = i \int_0^t ds \left\langle \xi_K(s), \left(-\varepsilon^3 \phi(\omega \mathbf{B}_K) + \varepsilon^4 \left\| \omega^{\frac{1}{2}} B_K \right\|_2^2 \right) R_{\varphi_s}^2 V_{i\omega\varphi_{s,L}} \zeta(s) \right\rangle. \\
& |\mathcal{R}^{(\blacksquare)}| + |\mathcal{R}^{(\blacktriangleright)}| + |\mathcal{R}^{(\blacktriangleleft)}| \lesssim \varepsilon \ln K.
\end{aligned}$$

$$\|\langle p \rangle^{-1} V_{i\omega\varphi_{s,L}} \langle p \rangle^{-1}\| \lesssim \|\varphi_s\|_{\mathfrak{h}_{1/2}} \lesssim 1$$

$$\mathcal{R}^{(\perp)} = \varepsilon^2 \left\langle \xi_K(s), R_{\varphi_s}^2 V_{i\omega\varphi_{s,K}} \zeta(s) \right\rangle \Big|_{s=0}^{s=t}$$

$$\mathcal{R}^{(i)} = -i\varepsilon^2 \int_0^t \mathrm{d}s \left\langle \xi_K(s), R_{\varphi_s}^2 V_{i\omega\varphi_{s,L}} P_{\varphi_s} (A_K R_{\varphi_s} A_K - D_K - 2\mathrm{Re}\langle \mathbf{B}_K, \sigma(\psi_{\varphi_s}) \rangle) \zeta(s) \right\rangle$$

$$\mathcal{R}^{(\#)} = i\varepsilon^2 \int_0^t \mathrm{d}s \left\langle \xi_K(s), (2R_{\varphi_s} \dot{R}_{\varphi_s} V_{i\omega\varphi_{s,L}} + R_{\varphi_s}^2 \dot{V}_{i\omega\varphi_{s,L}}) \zeta(s) \right\rangle$$

$$\mathcal{R}^{(\parallel)} = i\varepsilon^2 \int_0^t \mathrm{d}s \left\langle \xi_K(s), (R_{\varphi_s}^2 V_{i\omega\varphi_{s,L}} R_{\varphi_s} V_{i\omega\varphi_s}) \zeta(s) \right\rangle$$

$$\dot{V}_{i\omega\varphi_{s,L}} = V_{i\omega\dot{\varphi}_{s,L}} = V_{\omega^2\varphi_{s,L}} + V_{\omega\sigma_L}$$

$$\sigma_L := \mathbf{1}_{|k| \leq L} \sigma(\psi_{\varphi_s})$$

$$\omega\sigma(\psi_{\varphi_s}) = \omega^{1/2} |\widehat{\psi_{\varphi_s}}|^2$$

$$\|\langle p \rangle^{-1} V_{\omega\sigma_L} \langle p \rangle^{-1}\| \lesssim \|\omega\sigma(\psi_{\varphi_s})\|_{\mathfrak{h}_{-1/2}} = \|\psi_{\varphi_s}\|_{L^4}^2 \lesssim 1.$$

$$\begin{aligned} \left| \varepsilon^2 \int_0^t \mathrm{d}s \left\langle \xi_K(s), R_{\varphi_s}^2 \dot{V}_{i\omega\varphi_{s,L}} \zeta(s) \right\rangle \right| &\lesssim \varepsilon^2 \sup_{|s| \leq T} \left(\|V_{\omega^2\varphi_{s,L}} \langle p \rangle^{-2}\| + \|\langle p \rangle^{-1} V_{\omega\sigma_L} \langle p \rangle^{-1}\| \right) \\ &\lesssim \varepsilon^2 \sup_{|s| \leq T} \left(\|\omega^2\varphi_{s,L}\|_{\mathfrak{h}_{-3/4}} + 1 \right) \lesssim \varepsilon^2 L^{3/2} \end{aligned}$$

$$|\mathcal{R}^{(4)}| \lesssim \varepsilon \ln K + \varepsilon^{2/7}.$$

$$A_K = \phi(\mathbf{G}_K) + (A_K - \phi(\mathbf{G}_K))$$

$$\mathcal{R}^{(\Lambda)} = - \int_0^t \mathrm{d}s \left\langle \xi_K(s), Q_{\varphi_s} \phi \left(\mathbf{G}_K - \sigma(\psi_{\varphi_s}) \right) R_{\varphi_s} \phi(\mathbf{G}_K) \zeta(s) \right\rangle$$

$$\mathcal{R}^{(\Xi)} = \int_0^t \mathrm{d}s \left\langle \xi_K(s), Q_{\varphi_s} \phi \left(\mathbf{G}_K - \sigma(\psi_{\varphi_s}) \right) R_{\varphi_s} (A_K - \phi(\mathbf{G}_K)) \zeta(s) \right\rangle$$

$$\mathcal{R}^{(\Pi)} = - \int_0^t \mathrm{d}s \left\langle \xi_K(s), Q_{\varphi_s} (A_K - \phi(\mathbf{G}_K)) R_{\varphi_s} A_K \zeta(s) \right\rangle$$

$$\begin{aligned} |\mathcal{R}^{(\kappa)}| &\lesssim (\ln K)^{\frac{1}{2}} \int_0^t \mathrm{d}s \|\langle p \rangle \xi_K(s)\| \left\| \langle p \rangle^{-1} \phi \left(\mathbf{G}_K - \sigma(\psi_{\varphi_s}) \right) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \|\langle p \rangle R_{\varphi_s} \langle p \rangle\| \\ &\times \left\| \left\langle N^{\frac{1}{2}} \right\rangle \langle p \rangle^{-1} (A_K - \phi(\mathbf{G}_K)) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-2} \right\| \left\| \left\langle N^{\frac{1}{2}} \right\rangle^2 \langle p \rangle \zeta(s) \right\| \\ &\lesssim (\ln K)^{\frac{1}{2}} K^{-\frac{1}{4}} \end{aligned}$$

$$|\mathcal{R}^{(\omega)}| \lesssim (\ln K)^{\frac{1}{2}} K^{-\frac{1}{4}}$$

$$\phi\left(\omega\sigma(\psi_{\varphi_s})\right)\left[H_f,\phi\left(\sigma(\psi_{\varphi_s})\right)\right]$$

$$\|\sigma(\psi)\mathbf{1}_{|k|\geq L}\|_{L^2}\lesssim L^{-1}\|\psi\|_{H^2}$$

$$\|\omega\sigma(\psi)\mathbf{1}_{|k|\leq L}\|_{L^2}\lesssim (\ln L)^{\frac{1}{2}}\|\psi\|_{H^2}$$

$$e^{-ikx} = |k|^{-4} \left[(k \cdot p), [(k \cdot p), e^{-ikx}] \right]$$

$$\|\sigma(\psi)\mathbf{1}_{|k|\geq L}\|_{L^2}^2 = \int_{|k|\geq L} dk \omega^{-1}(k) |\langle \psi, e^{-ik(\cdot)} \psi \rangle|^2 \lesssim \|\psi\|_{H^2} \int_{|k|\geq L} \frac{dk}{|k|^5}$$

$$\|\omega\sigma(\psi)\mathbf{1}_{|k|\leq L}\|_{L^2} \lesssim 1 + \|\omega\sigma(\psi)\mathbf{1}_{2\leq |k|\leq K}\|_{L^2}$$

$$\|\omega\sigma(\psi)\mathbf{1}_{2\leq |k|\leq L}\|_{L^2}^2 = \int_{2\leq |k|\leq K} dk \omega(k) |\langle \psi, e^{-ik(\cdot)} \psi \rangle|^2 \lesssim \|\psi\|_{H^2} \int_{2\leq |k|\leq L} \frac{dk}{|k|^3}$$

$$\sigma_K\colon=\sigma(\psi_{\varphi_s})\mathbf{1}_{|k|\leq K}$$

$$\sigma_K\colon=\sigma(\psi_{\varphi_s})\mathbf{1}_{|k|>K}$$

$$\mathcal{R}^{(\rho)} = - \int_0^t \mathrm{d} s \langle \xi_K(s), Q_{\varphi_s} \phi(\mathbf{G}_K - \sigma_K) R_{\varphi_s} \phi(\mathbf{G}_K) \zeta(s) \rangle$$

$$\mathcal{R}^{(\lambda)} = \int_0^t \mathrm{d} s \langle \xi_K(s), Q_{\varphi_s} \phi(\sigma_{>K}) R_{\varphi_s} \phi(\mathbf{G}_K) \zeta(s) \rangle$$

$$\begin{aligned} |\mathcal{R}^{(\Theta)}| &\lesssim \int_0^t \mathrm{d} s (\|\sigma_{>K}\|_{L^2} \|R_{\varphi_s} \langle p \rangle\| \\ &\quad \times \left\| \langle p \rangle^{-1} \phi(\mathbf{G}_K) \langle p \rangle^{-1} \left\langle N^{\frac{1}{2}} \right\rangle^{-1} \right\| \left\| \langle p \rangle \left\langle N^{\frac{1}{2}} \right\rangle \zeta(s) \right\| \\ &\lesssim K^{-1} (\ln K)^{1/2} \end{aligned}$$

$$L_K\coloneqq \phi(\mathbf{G}_K-\sigma_K)R_{\varphi_s}\phi(\mathbf{G}_K)$$

$$\mathcal{R}^{(\sigma)} = \int_0^t \mathrm{d} s \left\langle \xi_K(s), \varepsilon \left(A_K - \phi(\sigma_{\psi_s}) \right) R_{\varphi_s} L_K \zeta(s) \right\rangle$$

$$\mathcal{R}^{(\sigma)} = -\varepsilon^2 \int_0^t \mathrm{d} s \langle (i\partial_s - H_f) \xi_K(s), R_{\varphi_s} L_K \zeta(s) \rangle$$

$$\mathcal{R}^{(\aleph)} = \int_0^t \mathrm{d} s \langle \xi_K(s), \varepsilon^2 (D_K + 2\varepsilon^2 \mathrm{Re} \langle \mathbf{B}_K, \sigma(\psi_{\varphi_s}) \rangle) R_{\varphi_s} L_K \zeta(s) \rangle$$

$$\mathcal{R}^{(2)} = \int_0^t \mathrm{d} s \left\langle \xi_K(s), \left(-\varepsilon^3 \phi(\omega \mathbf{B}_K) + \varepsilon^4 \|\omega^{1/2} B_K\|_{L^2}^2 \right) R_{\varphi_s} L_K \zeta(s) \right\rangle$$

$$|\mathcal{R}^{(i)}| + |\mathcal{R}^{(l)}| + |\mathcal{R}^{(v)}| \lesssim \varepsilon (\ln K)^{\frac{3}{2}} + \varepsilon^2 (\ln K)^2$$

$$\mathcal{R}^{(\Gamma)} = -i\varepsilon^2 \langle \xi_K(s), R_{\varphi_s} L_K \zeta(s) \rangle \Big|_0^t$$

$$\mathcal{R}^{(\mathbb{L})} = -\varepsilon^2 \int_0^t \mathrm{d} s \langle \xi_K(s), R_{\varphi_s} [H_f, L_K] \zeta(s) \rangle$$

$$\mathcal{R}^{(*)} = \varepsilon^2 \int_0^t \mathrm{d} s \langle \xi_K(s), R_{\varphi_s} L_K P_{\varphi_s} (A_K R_{\varphi_s} A_K - D_K - 2\mathrm{Re} \langle \mathbf{B}_K, \sigma(\psi_{\varphi_s}) \rangle) \zeta(s) \rangle$$

$$\mathcal{R}^{(\mathfrak{h})} = -i\varepsilon^2 \int_0^t \mathrm{d} s \langle \xi_K(s), (\dot{R}_{\varphi_s} L_K + R_{\varphi_s} \dot{L}_K) \zeta(s) \rangle$$

$$[H_f, L_K] = \phi^-(\omega \mathbf{G}_K - \omega \sigma_K) R_{\varphi_s} \phi(\mathbf{G}_K) + \phi(\mathbf{G}_K - \sigma_K) R_{\varphi_s} \phi^-(\omega \mathbf{G}_K)$$



$$\phi^{-}(\mathbf{F})=a^{*}(\mathbf{F})-a(\mathbf{F})$$

$$\left\|\langle p\rangle^{-1}\left\langle N^{\frac{1}{2}}\right\rangle^m\phi^{-}(\mathbf{G}_K-\sigma_K)\left\langle N^{\frac{1}{2}}\right\rangle^{-m-1}\langle p\rangle^{-1}\right\|\lesssim(\ln K)^{\frac{1}{2}}+1,$$

$$\left\|\langle p\rangle^{-1}\left\langle N^{\frac{1}{2}}\right\rangle^m\phi^{-}(\omega\mathbf{G}_K-\omega\sigma_K)\left\langle N^{\frac{1}{2}}\right\rangle^{-m-1}\langle p\rangle^{-1}\right\|\lesssim K+\ln K.$$

$$|\mathcal{R}^{(6)}|\leqslant \varepsilon^2 K \ln\,K$$

$$|\mathcal{R}^{(\mathfrak{U})}|\lesssim \varepsilon^2 K \ln\,K + (\ln\,K)^{\frac{1}{2}} K^{-1/4}$$

$$\|\delta(t)\|^2\lesssim (\ln K)^{1/2}K^{-1/4}+\varepsilon K+\varepsilon^2K\ln K+\varepsilon^{2/7}$$

$$\Psi_t^\varepsilon=e^{-it\varepsilon^{-2}H^\varepsilon+i\varepsilon^{-2}\mu(t))}\Psi_0$$

$$\Psi_0=\psi_{\varphi_0}\otimes W(\varepsilon^{-1}\varphi_0)\Omega$$

$$\Phi_t=\psi_{\varphi_t}\otimes W(\varepsilon^{-1}\varphi_t)\mathbb{U}(t)\Omega$$

$$\gamma_{\rm particle}^\varepsilon\left(t\right)=\mathrm{Tr}_{\mathcal{F}}|\Psi_t^\varepsilon\rangle\langle\Psi_t^\varepsilon|\text{ and }|\psi_{\varphi_t}\rangle\langle\psi_{\varphi_t}|=\mathrm{Tr}_{\mathcal{F}}|\Phi_t\rangle\langle\Phi_t|$$

$$\begin{aligned}\gamma_{\rm particle}^\varepsilon\left(t\right)-|\psi_{\varphi_t}\rangle\langle\psi_{\varphi_t}|=&\mathrm{Tr}_{\mathcal{F}}|\Psi_t^\varepsilon\rangle\langle\Psi_t^\varepsilon|-\mathrm{Tr}_{\mathcal{F}}|\Phi_t\rangle\langle\Phi_t|\\&=\mathrm{Tr}_{\mathcal{F}}|\Psi_t^\varepsilon\rangle\langle\Psi_t^\varepsilon-\Phi_t|+\mathrm{Tr}_{\mathcal{F}}|\Psi_t^\varepsilon-\Phi_t\rangle\langle\Phi_t|\end{aligned}$$

$$\left|\mathrm{Tr}_{L^2}|\gamma_{\mathrm{el}}^\varepsilon(t)-|\psi_t\rangle\langle\psi_t|\right|\leqslant 2\|\Psi_t^\varepsilon-\Phi_t\|\leqslant C\varepsilon^{1/10}\ln\frac{1}{\varepsilon}$$

$$N_{\leqslant L}=\int_{|k|\leqslant L}a_k^*a_k\,\mathrm{d}k,0\leqslant L\leqslant K$$

$$\left\|H_f^{1/2}\xi_K(t)\right\|^2\leqslant C\varepsilon^{-2}\ln K$$

$$\left\|\varepsilon H_f^{1/2}\xi_K(t)\right\|\leqslant \left\|(\varepsilon^2H_f+1)^{1/2}e^{-it\varepsilon^{-2}H_{\mathcal{D},K}^\varepsilon W(\varepsilon^{-1}\varphi_0)}e^{ig_{K,\varphi_0}(x)}\psi_{\varphi_0}\otimes\Omega\right\|.$$

$$H_{\mathcal{D},K}^\varepsilon=U_K^\varepsilon(U_L^\varepsilon)^*H_{\mathcal{D},L}^\varepsilon U_L^\varepsilon(U_K^\varepsilon)^*$$

$$U_L^\varepsilon(U_K^\varepsilon)^*\varepsilon^2H_fU_K^\varepsilon(U_L^\varepsilon)^*\lesssim \varepsilon^2H_f+\varepsilon^4(K^{-1/2}+L^{-1/2})\lesssim \varepsilon^2H_f+1,$$

$$\left\|\omega^{-1/2}B_K\right\|_{L^2}\lesssim K^{-1/2}$$

$$\left\|\varepsilon H_f^{1/2}\xi_K(t)\right\|\lesssim \left\|(\varepsilon^2H_f+1)^{1/2}e^{-it\varepsilon^{-2}H_{\mathcal{D},L}^\varepsilon U_L^\varepsilon(U_K^\varepsilon)^*W(\varepsilon^{-1}\varphi_0)}e^{ig_{K,\varphi_0}(x)}\psi_{\varphi_0}\otimes\Omega\right\|$$

$$\varepsilon^2H_f\lesssim H_{\mathcal{D},L}^\varepsilon+L$$

$$\left\|\varepsilon H_f^{1/2}\xi_K(t)\right\|\lesssim \left\|(H_{\mathcal{D},L}^\varepsilon+L)^{1/2}U_L^\varepsilon(U_K^\varepsilon)^*W(\varepsilon^{-1}\varphi_0)e^{ig_{K,\varphi_0}(x)}\psi_{\varphi_0}\otimes\Omega\right\|$$

$$H_{\mathcal{D},K}^\varepsilon\lesssim p^2+\varepsilon^2H_f+\ln K(N+1)$$

$$\left\|\varepsilon H_f^{1/2}\xi_K(t)\right\|\lesssim \left\|(p^2+\varepsilon^{-2}H_f+\varepsilon^2\ln K(N+1)+L)^{1/2}W(\varepsilon^{-1}\varphi_0)e^{ig_{K,\varphi_0}(x)}\psi_{\varphi_0}\otimes\Omega\right\|$$

$$\left\| \varepsilon H_f^{1/2} \xi_K(t) \right\| \lesssim L^{1/2} + (\ln K)^{1/2}$$

$$\left\| N_{\leq L} \xi_K(t) \right\| \leq C \varepsilon^{-2} L^2$$

$$f(t) := \varepsilon^4 \left\| N_{\leq L} \xi_K(t) \right\|^2 + \varepsilon^2 L^2 \left\| N_{\leq L}^{1/2} \xi_K(t) \right\|^2$$

$$\xi_K(0) = \psi_{\varphi_0} \otimes \Omega$$

$$i\partial_t \xi_K(t) = \mathcal{L}_{\mathcal{D},K}^\varepsilon(t) \xi_K(t)$$

$$\mathcal{L}_{\mathcal{D},K}^\varepsilon(t) = i\varepsilon^4 \int_0^t ds \langle \xi_K(s), [\mathcal{L}_{\mathcal{D},K}^\varepsilon(s), N_{\leq L}^2] \xi_K(s) \rangle$$

$$\varepsilon^{-1} \phi(\mathbf{G}_K) = i\varepsilon^2 L^2 \int_0^t ds \langle \xi_K(s), [\mathcal{L}_{\mathcal{D},K}^\varepsilon(s), N_{\leq L}] \xi_K(s) \rangle$$

$$\{|k| \geq K\} \subset \{|k| \geq L\}$$

$$[\mathcal{L}_{\mathcal{D},K}^\varepsilon(t), N_{\leq L}] = \varepsilon^{-1} \phi^-(\mathbf{G}_L)$$

$$[\mathcal{L}_{\mathcal{D},K}^\varepsilon(t), N_{\leq L}^2] = \varepsilon^{-1} (N_{\leq L} \phi^-(\mathbf{G}_L) + \phi^-(\mathbf{G}_L) N_{\leq L})$$

$$\phi^-(\mathbf{G}_L) = a^*(\mathbf{G}_L) - a(\mathbf{G}_L)$$

$$\|\phi(\mathbf{G}_L) \xi_K(s)\| \lesssim L \left\| (N_{\leq L} + 1)^{1/2} \xi_K(s) \right\|$$

$$|(I)| \lesssim \varepsilon^3 L \int_0^t ds \left\| N_{\leq L} \xi_K(s) \right\| \left\| (N_{\leq L} + 1)^{1/2} \xi_K(s) \right\| \lesssim \int_0^t f(s) ds + \varepsilon^2$$

$$\|a(\mathbf{G}_L) \xi_K(s)\| \lesssim L \left\| N_{\leq L}^{1/2} \xi_K(s) \right\|$$

$$|(II)| \lesssim \varepsilon L^3 \int_0^t ds \left\| N_{\leq L}^{1/2} \xi_K(s) \right\| \leq \int_0^t f(s) ds + L^4$$

$$f(t) \lesssim \int_0^t f(s) ds + L^4$$

$$g(t) := \left\| N^{1/2} W(\varepsilon^{-1} \varphi_t)^* e^{-i\varepsilon^{-2} t H^\varepsilon} \Psi_K^\varepsilon(\varphi_0) \right\|^2$$

$$\Psi_K^\varepsilon(\varphi_0) = W(\varepsilon^{-1} \varphi_0) (U_K^\varepsilon)^* \psi_{\varphi_0} \otimes \Omega$$

$$U_K^\varepsilon N (U_K^\varepsilon)^* \lesssim N + \varepsilon^2 \|B_K\|_{L^2}^2$$

$$g(t) \lesssim \left\| N^{1/2} U_K^\varepsilon W(\varepsilon^{-1} \varphi_t)^* e^{-i\varepsilon^{-2} t H^\varepsilon} \Psi_K^\varepsilon(\varphi_0) \right\|^2 + \varepsilon^2 K^{-1}$$

$$U_K^\varepsilon W(\varepsilon^{-1} \varphi_t)^* e^{-it\varepsilon^{-2} H^\varepsilon} \Psi_K^\varepsilon(\varphi_0) = e^{-i\varepsilon^{-2} \mu(t)} \xi_K(t)$$

$$N = N_{\leq L} + N_L \text{ with } N_L = \int_{|k|>L} a_k^* a_k \, dk$$

$$\langle \xi_K(t), N_L \xi_K(t) \rangle \leq L^{-1} \langle \xi_K(t), H_f \xi_K(t) \rangle \leq \varepsilon^{-2} (\ln K) L^{-1}$$

$$g(t) \lesssim \langle \xi_K(t), N_{\leq L} \xi_K(t) \rangle + \varepsilon^{-2} (\ln K) L^{-1} + \varepsilon^2 K^{-1}$$



$$\zeta(t) = \psi_{\varphi_t} \otimes \mathbb{U}(t)\Omega, \text{ with } \|N\zeta(t)\| \lesssim 1$$

$$\begin{aligned} \langle \xi_K(t), N_{\leq L} \xi_K(t) \rangle &= \langle \xi_K(t) - \zeta(t), N_{\leq L} \xi_K(t) \rangle + \langle \zeta(t), N_{\leq L} \xi_K(t) \rangle \\ &\leq \| \xi_K(t) - \zeta(t) \| \| N_{\leq L} \xi_K(t) \| + \| N_{\leq L} \zeta(t) \| \\ &\lesssim \varepsilon^{-2} L^2 \| \xi_K(t) - \zeta(t) \| + 1 \end{aligned}$$

$$\|\delta(t)\| = \|\xi_K(t) - \zeta(t)\| \leq \varepsilon^{1/10} \ln \frac{1}{\varepsilon}$$

$$\langle \xi_K(t), N_{\leq L} \xi_K(t) \rangle \lesssim \varepsilon^{-19/10} \left(\ln \frac{1}{\varepsilon} \right) L^2 + 1$$

$$\langle \xi_K(t), N \xi_K(t) \rangle \lesssim \varepsilon^{-19/10} \left(\ln \frac{1}{\varepsilon} \right) L^2 + 1 + \varepsilon^{-2} \left(\ln \frac{1}{\varepsilon} \right) L^{-1} + \varepsilon^{1/5}$$

$$U_{K,\Lambda}^\varepsilon := \exp \left(\varepsilon a^*(\mathbf{B}_{K,\Lambda}) - \varepsilon a(\mathbf{B}_{K,\Lambda}) \right), \mathbf{B}_{K,\Lambda}(x,k) := \mathbf{B}_K(x,k) \mathbf{1}_{\{|k| \leq \Lambda\}}.$$

$$\begin{aligned} U_{K,\Lambda}^\varepsilon p^2 (U_{K,\Lambda}^\varepsilon)^* &= p^2 + \varepsilon \left(2a^*(k\mathbf{B}_{K,\Lambda}) \cdot p + 2p \cdot a(k\mathbf{B}_{K,\Lambda}) - \phi(k^2\mathbf{B}_{K,\Lambda}) \right) \\ &\quad + \varepsilon^2 \left(2a^*(k\mathbf{B}_{K,\Lambda})a(k\mathbf{B}_{K,\Lambda}) + a(k\mathbf{B}_{K,\Lambda})^2 + a^*(k\mathbf{B}_{K,\Lambda})^2 + \|k\mathbf{B}_{K,\Lambda}\|_{L^2}^2 \right), \\ U_{K,\Lambda}^\varepsilon (\varepsilon^2 H_f) (U_{K,\Lambda}^\varepsilon)^* &= \varepsilon^2 H_f - \varepsilon^3 \phi(\omega\mathbf{B}_{K,\Lambda}) + \varepsilon^4 \|\omega^{1/2} \mathbf{B}_{K,\Lambda}\|_{L^2}^2, \end{aligned}$$

$$U_{K,\Lambda}^\varepsilon (\varepsilon \phi(\mathbf{G}_\Lambda)) (U_{K,\Lambda}^\varepsilon)^* = \varepsilon \phi(\mathbf{G}_\Lambda) - 2\varepsilon^2 \text{Re} \langle \mathbf{G}_\Lambda, \mathbf{B}_{K,\Lambda} \rangle.$$

$$\varepsilon^2 \|k\mathbf{B}_{K,\Lambda}\|_{L^2}^2 - 2\varepsilon^2 \text{Re} \langle \mathbf{G}_\Lambda, \mathbf{B}_{K,\Lambda} \rangle = 4\pi\varepsilon^2 (\ln K - \ln \Lambda),$$

$$\phi(\mathbf{G}_\Lambda) - \phi(k^2\mathbf{B}_{K,\Lambda}) = \phi(\mathbf{G}_K).$$

$$\begin{aligned} H_{\mathcal{D},K,\Lambda}^\varepsilon &:= U_{K,\Lambda}^\varepsilon (H_\Lambda^\varepsilon + 4\pi\varepsilon^2 \ln \Lambda) (U_{K,\Lambda}^\varepsilon)^* \\ &= p^2 + \varepsilon \left(\phi(\mathbf{G}_K) + 2a^*(k\mathbf{B}_{K,\Lambda}) \cdot p + 2p \cdot a(k\mathbf{B}_{K,\Lambda}) \right) \\ &\quad + \varepsilon^2 \left(H_f + 2a^*(k\mathbf{B}_{K,\Lambda})a(k\mathbf{B}_{K,\Lambda}) + a(k\mathbf{B}_{K,\Lambda})^2 + a^*(k\mathbf{B}_{K,\Lambda})^2 + 4\pi \ln K \right) \\ &\quad - \varepsilon^3 \phi(\omega\mathbf{B}_{K,\Lambda}) + \varepsilon^4 \|\omega^{1/2} \mathbf{B}_{K,\Lambda}\|_{L^2}^2. \end{aligned}$$

$$\pm (H_{\mathcal{D},K,\Lambda}^\varepsilon - p^2 - \varepsilon^2 H_f) \leq \delta (p^2 + \varepsilon^2 H_f) + C_\delta K$$

$$Q(p^2 + H_f)\Lambda_2 \geq \Lambda_1 \geq \Lambda_0 \text{ and } K \geq K_0$$

$$\pm (H_{\mathcal{D},K,\Lambda_2}^\varepsilon - H_{\mathcal{D},K,\Lambda_1}^\varepsilon) \leq C\Lambda_1^{-1/4} (p^2 + \varepsilon^2 H_f).$$

$$H_{\mathcal{D},K}^\varepsilon = H_{\mathcal{D},K,\infty}^\varepsilon Q(p^2 + H_f)$$

$$s - \lim_{\Lambda \rightarrow \infty} e^{-itH_{\mathcal{D},K,\Lambda}^\varepsilon} = e^{-itH_{\mathcal{D},K}^\varepsilon} \ (\forall t \in \mathbb{R})$$

$$U_{K,\Lambda}^\varepsilon \xrightarrow{\Lambda \rightarrow \infty} U_{K,\infty}^\varepsilon$$

$$H^\varepsilon := (U_{K,\infty}^\varepsilon)^* H_{\mathcal{D},K}^\varepsilon U_{K,\infty}^\varepsilon$$

$$s - \lim_{\Lambda \rightarrow \infty} e^{-itH_\Lambda^\varepsilon} e^{-it4\pi\varepsilon^2 \ln \Lambda} = e^{-itH^\varepsilon} \ (t \in \mathbb{R})$$



$$\mathcal{E}_{\text{field}}(u) := e(u) + \|u\|_{\mathfrak{h}_{1/2}}^2,$$

$$E_* = \mathcal{E}_{\text{field}}(\varphi_*)$$

$$\varphi_* = -\omega^{-1}\sigma(\psi_*)$$

$$\mathcal{E}_{\text{P}}(\psi) = \langle \psi, p^2 \psi \rangle - \left\| \omega^{-1/2} \sigma(\psi) \right\|_{L^2}^2.$$

$$\mathcal{M} \colon = \{T_y \varphi_* \colon y \in \mathbb{R}^3\}, (T_y u)(k) \colon = e^{-ik \cdot y} u(k).$$

$$\mathcal{E}_{\text{field}}(u) - E_* \geqslant c \text{dist}_{\mathfrak{h}_{1/2}}(u, \mathcal{M})^2 \ \forall u \in \mathfrak{h}_{1/2}.$$

$$\mathcal{E}_{\text{field}}(u) \leqslant \mathcal{E}_{\text{P}}(\psi) + \left\| \omega^{1/2} u + \omega^{-1/2} \sigma(\psi) \right\|_{L^2}^2.$$

$$\psi = T_y \psi_*$$

$$\varphi_* = -\omega^{-1}\sigma(\psi_*)$$

$$\mathcal{E}_{\text{field}}(u) - E_* \leqslant \left\| u - T_y \varphi_* \right\|_{\mathfrak{h}_{1/2}}^2,$$

$$\mathcal{E}_{\text{field}}(u) - E_* \leqslant \text{dist}_{\mathfrak{h}_{1/2}}(u, \mathcal{M})^2.$$

$$\mathcal{E}_{\text{field}}(\varphi_t) = \mathcal{E}_{\text{field}}(\varphi_0) \text{ for all } t \in (-T_-, T_+)$$

$$\begin{aligned} \text{dist}_{\mathfrak{h}_{1/2}}(\varphi_t, \mathcal{M})^2 &\leqslant c^{-1}(\mathcal{E}_{\text{field}}(\varphi_t) - E_*) \\ &= c^{-1}(\mathcal{E}_{\text{field}}(\varphi_0) - E_*) \\ &\leqslant c^{-1} \text{dist}_{\mathfrak{h}_{1/2}}(\varphi_0, \mathcal{M})^2 \end{aligned}$$

$$\text{dist}_{\mathfrak{h}_{1/2}}(\varphi_0, \mathcal{M}) \leqslant \eta$$

$$\|\varphi_t - \varphi_*\|_{\mathfrak{h}_{1/2}} \leqslant c^{-1} \eta$$

$$\Delta(\varphi_t) \geqslant \frac{1}{2} \Delta(\varphi_*) > 0 \ \forall t \in (-T_-, T_+)$$

$$\liminf_{t \rightarrow T_+} \Delta(\varphi_t) > 0$$

$$(\psi_0, \varphi_0) \in H^s \times \mathfrak{h}_{s-1/2}$$

$$\|\psi_t\|_{L^2} = \|\psi_0\|_{L^2}$$

$$\mathcal{E}(\psi_t, \varphi_t) = \mathcal{E}(\psi_0, \varphi_0)$$

$$(\psi_0, \varphi_0) \in H^1 \times \mathfrak{h}_{1/2}$$

$$\sup_{t \in \mathbb{R}} \left(\|\psi_t\|_{H^1} + \|\varphi_t\|_{\mathfrak{h}_{1/2}} \right) < \infty$$

$$H^1 \times \mathfrak{h}_{1/2} = \mathcal{O}(\varepsilon^{-2})$$

$$\varphi_0 \in \mathfrak{h}_0 \cap \mathfrak{h}_{1/2}$$

$$e(\varphi_0) < 0$$



$$\psi_{\varphi_t} \geq 0$$

$$(\psi_t^\varepsilon, \varphi_t^\varepsilon)(\psi_{\varphi_0}, \varphi_0)$$

$$\left\| \exp \left(i\varepsilon^{-2} \int_0^t e(\varphi_{\varepsilon^{-2}s}) ds \right) \psi_{\varepsilon^{-2}t} - \psi_{\varphi_t} \right\|_{L^2} + \|\varphi_{\varepsilon^{-2}t} - \varphi_t\|_{L^2} \leq C\varepsilon^{2/7}$$

$$e(\varphi_s^\varepsilon)=\inf\sigma(h_{\varphi_s}^\varepsilon)$$

$$u_t^\varepsilon:=\psi_{\varepsilon^{-2}t}^\varepsilon \text{ and } w_t^\varepsilon:=\varphi_{\varepsilon^{-2}t}^\varepsilon$$

$$i\partial_t u_t^\varepsilon = \varepsilon^{-2} h_{w_t^\varepsilon} u_t^\varepsilon, i\partial_t w_t^\varepsilon = \omega w_t^\varepsilon + \sigma(u_t^\varepsilon)$$

$$\|w_t^\varepsilon-\varphi_0\|_{\mathfrak{h}_{1/2}}\leqslant\|(e^{-i\omega t}-1)\varphi_0\|_{\mathfrak{h}_{1/2}}+\int_0^{|t|}\|\sigma(u_s^\varepsilon)\|_{\mathfrak{h}_{1/2}}\,\mathrm{d}s$$

$$\sup_{\varepsilon>0}\sup_{t\in\mathbb{R}}\|u_t^\varepsilon\|_{H^1}\leq C\,)$$

$$\inf_{\varepsilon>0}\inf_{|t|\leqslant T}\Delta\left(w_t^\varepsilon\right)>|t|\leqslant T$$

$$e(w_t^\varepsilon)<h_{w_t^\varepsilon}\psi_{w_t^\varepsilon}$$

$$\left\| e^{i\varepsilon^{-2}\int_0^te(w_s^\varepsilon)ds}u_t^\varepsilon-\psi_{w_t^\varepsilon}\right\|_{L^2}\leq C\varepsilon^{2/7},|t|\leq T$$

$$\|w_t^\varepsilon-\varphi_t\|_{\mathfrak{h}_{1/2}}\leq CT$$

$$\|\psi_{w_t}^\varepsilon-\psi_{\varphi_t}\|_{H^1}\leq C\|w_t^\varepsilon-\varphi_t\|_{\mathfrak{h}_{1/2}}$$

$$\left\| e^{i\varepsilon^{-2}\int_0^te(w_s^\varepsilon)ds}u_t^\varepsilon-\psi_{\varphi_t}\right\|_{L^2}\leq C\varepsilon+C\|w_t^\varepsilon-\varphi_t\|_{L^2}$$

$$\|w_t^\varepsilon-\varphi_t\|_{L^2}\leq \int_0^{|t|}\|\sigma(u_s^\varepsilon)-\sigma(\psi_{\varphi_s})\|_{L^2}\,\mathrm{d}s$$

$$\leq C\int_0^{|t|}\left\| e^{i\varepsilon^{-2}\int_0^se(w_r^\varepsilon)dr}u_s-\psi_{\varphi_s}\right\|_{L^2}\,\mathrm{d}s$$

$$\leq C\varepsilon^{2/7}+C\int_0^{|t|}\|w_s^\varepsilon-\varphi_s\|_{L^2}\,\mathrm{d}s$$

$$\|w_t^\varepsilon-\varphi_t\|_{L^2}\leq C\varepsilon^{2/7}$$

$$\Delta\left(w_t^\varepsilon\right)>0$$

$$\begin{aligned} &\|R_{w_t^\varepsilon}\|+\left\|\langle p\rangle R_{w_t^\varepsilon}^{1/2}\right\|+\left\|\langle p^2\rangle R_{w_t^\varepsilon}\right\|+\left\|\psi_{w_t^\varepsilon}\right\|_{H^2}\leq C,\\ &\left\|\dot{\psi}_{w_t^\varepsilon}\right\|_{L^2}+\left\|\dot{\sigma}(\psi_{w_t^\varepsilon})\right\|_{L^2}+\left\|\dot{R}_{w_t^\varepsilon}\right\|+\left\|\langle p\rangle \dot{R}_{w_t^\varepsilon}\langle p\rangle\right\|\leq C, \end{aligned}$$

$$R_{w_t^\varepsilon}=Q_{w_t^\varepsilon}\left(h_{w_t^\varepsilon}-e(w_t^\varepsilon)\right)^{-1}Q_{w_t^\varepsilon}$$

$$Q_{w_t^\varepsilon}=\mathbf{1}-|\psi_{w_t^\varepsilon}\rangle\langle\psi_{w_t^\varepsilon}|$$

$$\begin{aligned}
\partial_t \psi_{w_t^\varepsilon} &= R_{w_t^\varepsilon} V_{i\omega w_t^\varepsilon} \psi_{w_t^\varepsilon} \\
\tilde{u}_t^\varepsilon &:= e^{i \int_0^t e(w_s^\varepsilon) ds} u_t^\varepsilon \\
\|\tilde{u}_t^\varepsilon - \psi_{w_t^\varepsilon}\|_{L^2}^2 &= 2\text{Im} \int_0^t \left\langle \tilde{u}_s^\varepsilon, \left(\varepsilon^{-2} (h_{w_s^\varepsilon} - e(w_s^\varepsilon)) - i R_{w_s^\varepsilon} V_{i\omega w_s^\varepsilon} \right) \psi_{w_s^\varepsilon} \right\rangle ds \\
&= -2\text{Im} \int_0^t \langle \tilde{u}_s^\varepsilon, R_{w_s^\varepsilon} V_{i\omega w_s^\varepsilon} \psi_{w_s^\varepsilon} \rangle ds \\
h_{w_s^\varepsilon} \psi_{w_s^\varepsilon} &= e(w_s^\varepsilon) \psi_{w_s^\varepsilon} \\
w_s^\varepsilon &= w_{s,L}^\varepsilon + w_{s,>L}^\varepsilon \\
w_{s,L}^\varepsilon &:= w_s^\varepsilon \mathbf{1}_{|k| \leq L} \\
\left| \int_0^t \left\langle \tilde{u}_s^\varepsilon, R_{w_s^\varepsilon} V_{i\omega w_{s,>L}^\varepsilon} \psi_{w_s^\varepsilon} \right\rangle ds \right| &\lesssim L^{-1/4} \\
Q_{w_s^\varepsilon} \tilde{u}_s^\varepsilon &= R_{w_s^\varepsilon} (h_{w_s^\varepsilon} - e(w_s^\varepsilon)) \tilde{u}_s^\varepsilon = i\varepsilon^2 R_{w_s^\varepsilon} \partial_s \tilde{u}_s^\varepsilon \\
i\partial_t \tilde{u}_t^\varepsilon &= (h_{w_t^\varepsilon} - e(w_t^\varepsilon)) \tilde{u}_t^\varepsilon \\
\|\tilde{u}_t^\varepsilon - \psi_{w_t^\varepsilon}\|_{L^2}^2 &= -2\text{Im} \int_0^t \left\langle i\partial_s \tilde{u}_s^\varepsilon, R_{w_s^\varepsilon}^2 V_{i\omega w_{s,L}^\varepsilon} \psi_{w_s^\varepsilon} \right\rangle ds \\
&= 2\varepsilon^2 \text{Im} \left\langle \tilde{u}_s^\varepsilon, R_{w_s^\varepsilon}^2 V_{i\omega w_{s,L}^\varepsilon} \psi_{w_s^\varepsilon} \right\rangle \Big|_0^t \\
&\quad + 2\varepsilon^2 \text{Im} \int_0^t \left\langle \tilde{u}_s^\varepsilon, \left(2\dot{R}_{w_s^\varepsilon} R_{w_s^\varepsilon} + \dot{V}_{i\omega w_{s,L}^\varepsilon} + R_{w_s^\varepsilon}^2 V_{i\omega w_{s,L}^\varepsilon} R_{w_s^\varepsilon} V_{i\omega w_{s,L}^\varepsilon} \right) \psi_{w_s^\varepsilon} \right\rangle ds \\
\|\tilde{u}_t^\varepsilon - \psi_{w_t^\varepsilon}\|_{L^2}^2 &\lesssim L^{-1/4} + \varepsilon^2 L^{3/2} \lesssim \varepsilon^{2/7}
\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.

REFERENCIAS BIBLIOGRÁFICAS.

Théotime Girardot, Derivation of the Hartree dynamics for a N-particles fermionic

2D system interacting via long-range electric and magnetic two-body singular potentials in a dilute regime, arXiv:2507.16300v1 [math-ph] 22 Jul 2025.

Rabah Abdelmouheymen KHAMADJA, FROM VQE TO SQD : MODERN QUANTUM ALGORITHMS FOR ELECTRONIC STRUCTURE PROBLEMS, arXiv:2509.21555v1 [quant-ph] 25 Sep 2025.



- Simon H. Hille y Attila Szabó, TeMFpy: a Python library for converting fermionic mean-field states into tensor networks, arXiv:2510.05227v1 [cond-mat.str-el] 6 Oct 2025.
- Paul A. Johnson, Charles-Émile Fecteau, Samuel Nadeau, Mauricio Rodríguez-Mayorga y Pierre-François Loos, Connections between Richardson-Gaudin States, Perfect-Pairing, and Pair Coupled-Cluster Theory, arXiv:2510.06144v1 [physics.chem-ph] 7 Oct 2025.
- Alfred Li, Ankit Mahajan y Sandeep Sharma, Fokker-Planck equation governing the distribution of walkers in AFQMC, arXiv:2510.19914v1 [physics.chem-ph] 22 Oct 2025.
- Gerald V. Dunne, Slater Decomposition of Laughlin States, arXiv:cond-mat/9306022v1 8 Jun 1993.
- Håkon Emil Kristiansen, Håkon Kvernmoen, Simen Kvaal y Thomas Bondo Pedersen, Configuration weights in coupled-cluster theory, arXiv:2411.00690v2 [physics.chem-ph] 27 Feb 2025.
- Yuri Alexandre Aoto y Márcio Fabiano da Silva, Calculating the distance from an electronic wave function to the manifold of Slater determinants through the geometry of Grassmannians, arXiv:2012.05283v1 [quant-ph] 9 Dec 2020.
- Bin Yan, Rachel E. Wooten, Kevin M. Daily y Chris H. Greene, Hyperspherical Slater determinant approach to few-body fractional quantum Hall states, arXiv:1611.05305v1 [cond-mat.str-el] 16 Nov 2016.
- Clemens Giuliani, Jannes Nys, Rocco Martinazzo, Giuseppe Carleo y Riccardo Rossi, Precise Quantum Chemistry calculations with few Slater Determinants, arXiv:2503.14502v2 [physics.chem-ph] 2 May 2025.
- Chong Hian Chee, Daniel Leykam, Adrian M. Mak y Dimitris G. Angelakis, Shallow quantum circuits for efficient preparation of Slater determinants and correlated states on a quantum computer, arXiv:2301.07477v5 [quant-ph] 26 Jul 2023.]
- PIETRO SILVI, DAVIDE ROSSINI, ROSARIO FAZIO, GIUSEPPE E. SANTORO y VITTORIO GIOVANNETTI, Matrix Product State representation for Slater Determinants and Configuration Interaction States, arXiv:1205.4154v2 [quant-ph] 5 Nov 2012.
- CHIARA BOCCATO, FRANCESCA PIERONI y DARIO TREVISAN, ON DISTANCES AMONG SLATER DETERMINANT STATES AND DETERMINANTAL POINT PROCESSES, arXiv:2504.08971v1 [math-ph] 11 Apr 2025.



- John Kearney, Hojin Yoo y Kathryn M. Zurek, Is a Higgs Vacuum Instability Fatal for High-Scale Inflation, arXiv:1503.05193v1 [hep-th] 17 Mar 2015.
- G. F. Bertsch y L. M. Robledo, Symmetry Restoration in Hartree-Fock-Bogoliubov Based Theories, Phys. Rev. Lett. **108**, 042505 — Published 26 January 2012.
- S.V. Molodtsov y G.M. Zinovjev, Bogolyubov-Hartree-Fock approach to studying the QCD ground state, arXiv:0811.4405v3 [hep-ph] 11 Aug 2009.
- Marcel Griesemer y Fabian Hantsch, Unique Solutions to Hartree-Fock Equations for Closed Shell Atoms, arXiv:1012.5179v1 [math-ph] 23 Dec 2010.
- Niels Benedikter, Effective Dynamics of Interacting Fermions from Semiclassical Theory to the Random Phase Approximation, arXiv:2203.11255v3 [math-ph] 5 Jul 2022.
- P. A. M. Guichon, J. R. Stone y A. W. Thomas, Hartree-Fock Formulation of the QMC Model at Finite Temperature, arXiv:2310.19262v1 [nucl-th] 30 Oct 2023.
- Ettore Vitali, Peter Rosenberg y Shiwei Zhang, Monte Carlo Methods in the Manifold of Hartree-Fock-Bogoliubov Wave Functions, arXiv:2409.11571v1 [cond-mat.str-el] 17 Sep 2024.
- Stefan Vuckovic, John Kozłowski y Kieron Burke, Density functional analysis: The theory of density-corrected DFT, arXiv:1908.05721v1 [physics.chem-ph] 15 Aug 2019.
- I. C. Danchev, A. N. Antonov, D. N. Kadrev, M. K. Gaidarov, P. Sarriguren y E. Moya de Guerra, Symmetry energy properties of neutron-rich nuclei from the coherent density fluctuation model applied to nuclear matter calculations with Bonn potentials, arXiv:2006.01471v1 [nucl-th] 2 Jun 2020.
- CYRIL MALÉZÉ, SCATTERING FOR THE ONE DIMENSIONAL HARTREE FOCK EQUATION, arXiv:2406.17715v3 [math.AP] 10 Mar 2025.
- Google AI Quantum and Collaborators, Hartree-Fock on a superconducting qubit quantum computer, arXiv:2004.04174v2 [quant-ph] 20 Apr 2020.
- SOHEI ASHIDA, CONVERGENCE OF SCF SEQUENCES FOR THE HARTREE-FOCK EQUATION, arXiv:2205.10300v4 [math.AP] 25 Jan 2023.



- Nikolai Kaschewski y Axel Pelster, The Weighted Hartree-Fock-Bogoliubov method for interacting fermions: An application to ultracold Fermi superfluids, arXiv:2508.18801v1 [cond-mat.quant-gas] 26 Aug 2025.
- Andreas Erbs Hillers-Bendtsen y Todd J. Martinez, Accelerating Hartree-Fock and Density Functional Theory Calculations using Tensor Hypercontraction. (arXiv)
- Federico Rossi y Henrik Koch, Convex Hartree-Fock theory: A simple framework for ground state conical intersections, arXiv:2508.21453v1 [physics.chem-ph] 29 Aug 2025.
- Yaolong Zhang, Bin Jiang y Hua Guo, SchrödingerNet: A Universal Neural Network Solver for The Schrödinger Equation. (arXiv)
- Jong-Kwon Ha y Ryan J. MacDonell, Supplemental Material for Analog Quantum Simulation of Coupled Electron-Nuclear Dynamics in Molecules. (arXiv)
- Xuezhi Bian, Yanze Wu, Tian Qiu, Tao Zhen y Joseph E. Subotnik, A semiclassical non-adiabatic phase-space approach to molecular translations and rotations: A new picture of surface hopping and electronic inertial effects, arXiv:2410.01156v1 [physics.chem-ph] 2 Oct 2024.
- Jan Biedermann y Lukas Janssen, Dirac quantum criticality in twisted double bilayer transition metal dichalcogenides, arXiv:2509.04561v1 [cond-mat.mes-hall] 4 Sep 2025.
- Pujita Das, Parth Bahuguna, Tulika Maitra y Narayan Mohanta, Superconducting pairing symmetries in charge-ordered kagomé metals, arXiv:2509.04571v1 [cond-mat.supr-con] 4 Sep 2025.
- Rahul Ghosh, Quantum Phases in a Two-Dimensional Generalized interacting SSH Model, arXiv:2509.05655v1 [cond-mat.str-el] 6 Sep 2025.
- E. Rule, I. A. Chernyshev, I. Stetcu, J. Carlson y R. Weiss, Recursive algorithm for constructing antisymmetric fermionic states in first quantization mapping, arXiv:2509.07279v1 [quant-ph] 8 Sep 2025.
- Giorgio Visentin y François Mauger, Configuration-interaction calculations with density-functional theory molecular orbitals for modeling valence- and core-excited states in molecules, arXiv:2509.08245v1 [physics.chem-ph] 10 Sep 2025.
- M. Rothman, B. Johnson-Toth, G. Hagen, M. Heinz y T. Papenbrock, NuLattice: Ab initio computations of atomic nuclei on lattices, arXiv:2509.08771v1 [nucl-th] 10 Sep 2025.

- Bilal Hawashin, Julian Kleeschulte, David Kurz y Michael M. Scherer, Relativistic Mott transition, high-order van Hove singularity, and mean-field phase diagram of twisted double bilayer WSe₂, arXiv:2509.09398v1 [cond-mat.mes-hall] 11 Sep 2025.
- Usuf Rahaman, Investigation of ground state properties and shape evolution in Hf isotopes using the CDFT approach, arXiv:2509.12565v1 [nucl-th] 16 Sep 2025.
- Ibrahim E. Awad, Abd Al-Aziz A, Abu-Saleh, Gurleen Cheema, Joshua W. Hollett y Raymond A. Poirier, Atomic Radial Correlation Energy Density Components, arXiv:2509.12580v1 [physics.chem-ph] 16 Sep 2025.
- Shi-jing, Suo Qiu, H. Sagawa y Xian-Rong Zhou, Charge symmetry breaking effect in mirror Λ hypernuclei with Skyrme-Hartree-Fock model, arXiv: 2509.13655v2 [nucl-th] 23 Oct 2025.
- Félix Desrochers, Joe Huxford, Mark R. Hirsbrunner y Yong Baek Kim, Electronic Crystal Phases in the Presence of Non-Uniform Berry Curvature and Tunable Berry Flux : The λN -Jellium model, isoarXiv: 2509.15300v1 [cond-mat.str-el] 18 Sep 2025.
- Xuan Zeng, Ru-You Zheng, Zhi-Wei Liu, Li-Sheng Geng y Xian-Rong Zhou, Hypernuclear structure with the new leading order covariant chiral hyperon-nucleon force, arXiv:2509.16878v1 [nucl-th] 21 Sep 2025.
- Xin Lu, Yuanfan Yang, Zhongqing Guo y Jianpeng Liu, General Many-Body Perturbation Framework for Moiré Systems, arXiv:2509.19764v3 [cond-mat.str-el] 22 Oct 2025.
- Jian Kang, Minxuan Wang y Oskar Vafek, Orbital magnetization and magnetic susceptibility of interacting electrons, therearXiv: 2509.20626v1 [cond-mat.str-el] 25 Sep 2025.
- Alan A. Dzhiyev y N. V. Antonenko, Isoenergetic description of induced fission pathways within energy-density functional theory, arXiv:2509.22006v1 [nucl-th] 26 Sep 2025.
- Hopersky A.N, Nadolinsky A.M, Novikov S.A y Koneev R.V, Two-photon ionization of the *K-shell* of a heavy beryllium-like atomic ion. (arXiv)
- Peyman Najafi, Aaron Villanueva y Hilbert Kappen, Path Integral Quantum Control for Quantum Chemistry Applications, arXiv:2509.24104v1 [quant-ph] 28 Sep 2025.

- R. Folprecht, Knapp, G. De Gregorio, R. Mancino, P. Vesely y N. Lo Iudice, Bulk and spectroscopic nuclear properties within an ab initio renormalized random-phase approximation framework, arXiv:2510.00878v1 [nucl-th] 1 Oct 2025.
- Xiaoyu Liu, Chong Wang, Xiao-Wei Zhang, Ting Cao y Di Xiao, Orbital Magnetization in Correlated States of Twisted Bilayer Transition Metal Dichalcogenides, efarXiv: 2510.01727v1 [cond-mat.mes-hall] 2 Oct 2025.
- Yanek Verghis, Denis Sedov, Jakob Weßling, Prathyush P. Poduval y Mathias S. Scheurer, Vestigial pairing from fluctuating magnetism and triplet superconductivity, arXiv:2510.02474v1 [cond-mat.supr-con] 2 Oct 2025.
- Nicolau Sobrosa, Miguel Goncalvez, Eduardo V. Castro, Pedro Ribeiro y Bruno Amorim, Ground state and excitations of quasiperiodic 1D narrow-band moiré systems – a mean field approach, inarXiv: 2510.04132v1 [cond-mat.str-el] 5 Oct 2025.
- Claudia D. Alvarado, Eduardo Chiumiento, Homogeneous spaces in Hartree-Fock-Bogoliubov theory, arXiv:2402.15606v1 [math.FA] 23 Feb 2024.
- A. I.Komech, On the Hartree-Fock dynamics in wave-matrix picture, arXiv:1407.5208v4 [math-ph] 4 Jun 2015.
- Sahil Gulania, Stephen K. Gray, Yuri Alexeev, Bo Peng y Niranjana Govind, Hybrid algorithm for the time-dependent Hartree-Fock method using the Yang-Baxter equation on quantum computers, arXiv:2309.00737v1 [quant-ph] 1 Sep 2023.
- James Daniel Whitfield y Zoltán Zimborás, On the NP-completeness of the Hartree-Fock method for translationally invariant systems, arXiv:1408.3459v2 [quant-ph] 30 Dec 2014.
- B. R. Quea, J. M. Zhang, H. F. Song y Y. Liu, Hartree-Fock approximation for bosons with symmetry-adapted variational wave functions, arXiv:2502.15863v1 [cond-mat.quant-gas] 21 Feb 2025.
- Jia Liu, Yi Fei Niu y Wen Hui Long, Configuration-interaction relativistic Hartree-Fock model, arXiv:2411.05370v3 [nucl-th] 11 Apr 2025.
- CHARLES COLLOT, ELENA DANESI, ANNE-SOPHIE DE SUZZONI y CYRIL MALEZE, STABILITY OF HOMOGENEOUS EQUILIBRIA OF THE HARTREE-FOCK EQUATION,

FOR ITS EQUIVALENT FORMULATION FOR RANDOM FIELDS, arXiv:2310.03442v2 [math.AP] 15 Oct 2024.

Ichio Kikuchi y Akihito Kikuchi, Symbolic, numeric and quantum computation of Hartree-Fock equation, arXiv:2401.00019v2 [quant-ph] 18 Jun 2024.

Amir Ayati, Hugh G. A. Burton y Stijn De Baerdemacker, Spin-Symmetry Projected constrained Unrestricted Hartree-Fock, arXiv:2412.16458v1 [quant-ph] 21 Dec 2024.

Alexis Ralli, Tim Weaving, Peter V. Coveney y Peter J. Love, Bridging Quantum Chemistry and MaxCut: Classical Performance Guarantees and Quantum Algorithms for the Hartree-Fock Method, arXiv:2506.04223v1 [quant-ph] 4 Jun 2025.

Vlad-Mihai Ene, Ilinca Lianu y Ioan Grosu, Hartree-Fock approximation for non-Coulomb interactions in three and two-dimensional systems, arXiv:2408.14967v1 [cond-mat.quant-gas] 27 Aug 2024.

Matteo Castagnola, Rosario R. Riso, Yassir El Moutaoukal y Enrico Ronca, Strong coupling quantum electrodynamics Hartree-Fock response theory, arXiv:2502.14511v1 [physics.chem-ph] 20 Feb 2025.

Klaas Giesbertz, Hartree-Fock & Density Functional Theory, arXiv:2010.10243v2 [physics.ed-ph] 7 Feb 2023.

Fei Xu, Multilevel correction type of adaptive finite element method for Hartree-Fock equation, arXiv:2510.10879v1 [math.NA] 13 Oct 2025.

Sunilkumar V. Rajat, Sandeep Gautam y Arko Roy, Finite-temperature phase diagram and collective modes of coherently coupled Bose mixtures, arXiv:2510.11671v1 [cond-mat.quant-gas] 13 Oct 2025.

N. Ebrahimian, Absorbed power in ultracold polarized Fermi mixtures at normal-superfluid separation phase: Mass-imbalanced effect. (arXiv).

Yasuhiro Tanaka y Hitoshi Seo, Photoinduced melting dynamics and collective mode in a correlated charge-order system, arXiv:2510.16855v1 [cond-mat.str-el] 19 Oct 2025.

Yulong Pan y Michael Lindsey, Fast adaptive discontinuous basis sets for electronic structure, arXiv:2510.21213v1 [physics.comp-ph] 24 Oct 2025.



- Xuepeng Wang, Johannes S. Hofmann y Debanjan Chowdhury, Intertwined Orders, Quantum Criticality and Skyrmions in Tunable Topological Bands, arXiv:2510.21913v1 [cond-mat.str-el] 24 Oct 2025.
- Fei Xu, Effective approximations for Hartree–Fock exchange potential, arXiv:2509.00733v1 [physics.chem-ph] 31 Aug 2025.
- Paul Haubenwallner y Matthias Heller, Fully numerical Hartree-Fock calculations for atoms and small molecules with quantics tensor trains, arXiv:2503.08430v2 [physics.chem-ph] 11 Jun 2025.
- Ericka Roy Miller y Shane M. Parker, Numerically Stable Resonating Hartree-Fock, arXiv:2411.00712v2 [physics.chem-ph] 13 Mar 2025.
- E. Langmann y J. Lenells, Update of Hartree–Fock theory for Hubbard-like models, arXiv:2506.16525v1 [cond-mat.str-el] 19 Jun 2025.
- Volker Bach, Hartree–Fock Theory, Lieb’s Variational Principle and their Generalizations, arXiv:2209.10189v1 [quant-ph] 21 Sep 2022.
- D. S. Rosa, T. Frederico, R. M. Francisco y G. Krein, Reliability of the Born-Oppenheimer approximation in noninteger dimensions, arXiv:2408.01776v1 [cond-mat.quant-gas] 3 Aug 2024.
- X. L. Huang, S. L. Wu, L. C. Wang y X. X. Yi, Born-Oppenheimer approximation for open quantum systems within the quantum trajectory approach, arXiv:1003.1177v2 [quant-ph] 17 Apr 2010.
- Haci Akbas y O. Teoman Turgut, Born-Oppenheimer Approximation for a Singular System, arXiv:1602.02811v2 [math-ph] 29 Mar 2016.
- John Bonini, Iman Ahmadabadi y Johannes Flick, Cavity-Born Oppenheimer Approximation for Molecules and Materials via Electric Field Response, arXiv: 2407.14613v1 [physics.chem-ph] 19 Jul 2024.
- Marit R. Fiechter y Jeremy O. Richardson, Understanding the Cavity Born–Oppenheimer Approximation, arXiv:2401.03532v1 [physics.chem-ph] 7 Jan 2024.
- Haowu Duan, Alex Kovner y Michael Lublinsky, Born-Oppenheimer Renormalization group for High Energy Scattering: the Setup and the Wave Function, arXiv:2412.05085v1 [hep-ph] 6 Dec 2024.
- Haowu Duan, Alex Kovner y Michael Lublinsky, Born-Oppenheimer Renormalization group for High Energy Scattering: CSS, DGLAP and all that, arXiv:2412.05097v1 [hep-ph] 6 Dec 2024.

- Anjiao Gu y Shi Jin, Quantum simulation of a class of highly-oscillatory transport equations via Schrödingerisation, arXiv:2501.10176v2 [math.NA] 4 Sep 2025.
- D. Germani, B. Grinstein y A.D. Polosa, Tetraquarks in the Born-Oppenheimer approximation, arXiv:2501.13249v2 [hep-ph] 3 Apr 2025.
- Jakob Hoffmann, Lasse Müller y Marc Wagner, arXiv:2501.16188v1 [hep-lat] 27 Jan 2025.
- Galit Cohen, Rachel Steinitz-Eliyahu, E. K. U. Gross, Sivan Refaely-Abramson y Ryan Requist, Non-adiabaticity from first principles: the exact-factorization approach for solids, arXiv:2502.07439v1 [cond-mat.mtrl-sci] 11 Feb 2025.
- Robert Stanton, Mehmet Cagri Kaymak y Anders M. N. Niklasson, Shadow Molecular Dynamics for a Charge-Potential Equilibration Model, arXiv:2502.09602v1 [physics.chem-ph] 13 Feb 2025.
- Max Hays, Junghyun Kim y William D. Oliver, Non-degenerate noise-resilient superconducting qubit, arXiv:2502.15459v1 [quant-ph] 21 Feb 2025.
- Kamran Behnia, Phonon thermal Hall as a lattice Aharonov-Bohm effect, arXiv:2502.18236v5 [cond-mat.mes-hall] 29 Sep 2025.
- Muhammad Naeem Anwar, arXiv:2502.20329v1 [hep-ph] 27 Feb 2025.
- Richard F. Lebed y Steven R. Martinez, Meson-Meson Molecular Binding Potentials in the Diabatic Dynamical Diquark Model, arXiv:2502.20567v2 [hep-ph] 15 Apr 2025.
- Ville J Harkonen, Beyond Born-Oppenheimer Green's function theories: absolute and relational, arXiv:2503.01417v1 [cond-mat.other] 3 Mar 2025.
- Aleksander P. Wozniak, Ludwik Adamowicz, Thomas Bondo Pedersen y Simen Kvaal, Rothe Time Propagation for Coupled Electronic and Rovibrational Quantum Dynamics, arXiv:2503.09813v1 [physics.chem-ph] 12 Mar 2025.
- A. Becker, G. M. Koutentakis y P. Schmelcher, Dynamical probe of the pseudo Jahn-Teller effect in one-dimensional confined fermions, arXiv:2503.09835v2 [cond-mat.quant-gas] 24 Jun 2025.
- Hervé Bergeron, Przemysław Małkiewicz y Patrick Peter, Non-Gaussianities as a Signature of Quantumness of Quantum Cosmology, arXiv:2503.14570v1 [gr-qc] 18 Mar 2025.
- Bowen Kang, Xi Xia y Tao Guo, Hidden heavy flavor tetraquarks in the Born-Oppenheimer approximation, arXiv:2503.10173v2 [hep-ph] 6 Apr 2025.



- Kiyoharu Kawana, Phases and propagation of closed p-brane, arXiv:2503.14902v1 [hep-th] 19 Mar 2025.
- Mirko Daumann y Thomas Dahm, Particle pairing causes subdiffusion of heavy particles in the imbalanced Hubbard model, arXiv:2503.15409v2 [cond-mat.stat-mech] 22 Jul 2025.
- Thomas Schnappinger y Markus Kowalewski, Molecular Polarizability under Vibrational Strong Coupling, arXiv:2503.17102v1 [physics.chem-ph] 21 Mar 2025.
- Nadine C. Bradbury, Titouan Duston, Zhen Tao, Jonathan I. Rawlinson, Robert Littlejohn y Joseph Subotnik, Symmetry Breaking as Predicted by a Phase Space Hamiltonian with a Spin Coriolis Potential, arXiv:2504.03100v2 [physics.chem-ph] 28 May 2025.
- Rhiannon A. Zarotiadis, Joseph E. Lawrence y Jeremy O. Richardson, Nonadiabatic ring-polymer instanton rate theory: a generalized dividing-surface approach, arXiv:2505.04770v1 [physics.chem-ph] 7 May 2025.
- David Linteau, Saverio Moroni, Giuseppe Carleo y Markus Holzmann, Universal neural wave functions for high-pressure hydrogen, arXiv:2504.07062v1 [cond-mat.str-el] 9 Apr 2025.
- Yaser Tavakoli, Ahad Khaleghi Ardabili y Sara Mosaddegh, Fermions in a loop quantum cosmological spacetime, arXiv:2505.06695v2 [gr-qc] 30 Sep 2025.
- S. GHERGHE, I. MOYANO y I.M. SIGAL, ON THE TIME-DEPENDENT BORN-OPPENHEIMER APPROXIMATION, arXiv:2505.18701v1 [quant-ph] 24 May 2025.
- Lei Liu, Yanmei Xiao y Tao Guo, Hydrogen-like structures in the strong interaction, arXiv:2505.22177v1 [hep-ph] 28 May 2025.
- Simon Euchner y Igor Lesanovsky, Rydberg atom arrays as quantum simulators for molecular dynamics, arXiv:2506.09865v1 [quant-ph] 11 Jun 2025.
- Titouan Duston, Nadine Bradbury, Zhen Tao y Joseph E. Subotnik, Conical Intersections and Electronic Momentum As Viewed From Phase Space Electronic Structure Theory, arXiv:2506.11963v1 [physics.chem-ph] 13 Jun 2025.
- Maxime Labat, Guillaume Jeanmairet y Emmanuel Giner, Prediction of the aqueous redox properties of functionalized quinones using a new QM/MM variational formulation, arXiv:2506.12448v1 [physics.chem-ph] 14 Jun 2025.



CLAUDIO CACCIAPUOTI, ANDREA POSILICANO y HAMIDREZA SABERBAGHI, THE BORN-OPPENHEIMER APPROXIMATION FOR A 1D 2+1 PARTICLE SYSTEM WITH ZERO-RANGE INTERACTIONS, arXiv:2506.21457v1 [math-ph] 26 Jun 2025.

Eric W. Fischer, Cavity Born-Oppenheimer Coupled Cluster Theory: Towards Electron Correlation in the Vibrational Strong Light-Matter Coupling Regime, arXiv:2507.10100v2 [physics.chem-ph] 4 Sep 2025.

Olimpia Lombardi, Sebastian Fortin, Juan Camilo Martínez González y Hernán Accorinti, What are we talking about when we discuss the Born-Oppenheimer approximation. (arXiv)

LINO BENEDETTO, QUANTUM ERGODICITY FOR CONTACT METRIC STRUCTURES, arXiv:2507.18216v3 [math.AP] 18 Sep 2025.

O. Jonathan Fajen, Oscar Granas, Todd J. Martinez y Anders M. N. Niklasson, Shadow excited state molecular dynamics with the Δ SCF method, arXiv:2507.21461v1 [physics.chem-ph] 29 Jul 2025.

Kratika Mazde, Lisa Mickel y Patrick Peter, Quantum cosmological background superposition and perturbation predictions, arXiv:2508.06231v1 [gr-qc] 8 Aug 2025.

Dil K. Limbu, Sandip Bhusal, Diana M. Castaneda-Bagatella y Farnaz A. Shakib, Diagonal Born–Oppenheimer Corrections in Condensed-Phase Ring Polymer Surface Hopping, arXiv:2509.10629v1 [physics.chem-ph] 12 Sep 2025.

Morris Brooks y David Mitrouskas, Adiabatic Klein–Gordon Dynamics for the Renormalized Nelson Model, arXiv:2509.14226v1 [math-ph] 17 Sep 2025.

Xiaohan Dan, Zhuoran Long, Tianyin Qiu, Jan Paul Menzel, Qiang Shi y Victor Batista, Nonadiabatic H-Atom Scattering Channels on Ge(111) Elucidated by the Hierarchical Equations of Motion, arXiv:2509.16916v1 [cond-mat.mtrl-sci] 21 Sep 2025.

Julian Stetzler, Sophya Garashchuk y Vitaly Rassolov, Factorized electron-nuclear dynamics with effective complex potential: on-the-fly implementation for H₂ in a laser field, arXiv:2510.07483v1 [physics.chem-ph] 8 Oct 2025.

Nora Brambilla, Gastão Krein, Jaume Tarrus Castella y Antonio Vairo, The Born-Oppenheimer approximation in an effective field theory language, arXiv:1707.09647v2 [hep-ph] 22 Jan 2018.



- Bernardo Barrera, Daniel P. Arovas, Anushya Chandran y Anatoli Polkovnikov, The Moving Born-Oppenheimer Approximation, arXiv:2502.17557v2 [quant-ph] 7 Apr 2025.
- Jakob Gunther, Alberto Baiardi, Markus Reiher y Matthias Christandl, More quantum chemistry with fewer qubits, arXiv:2308.16873v4 [quant-ph] 3 Nov 2024.
- Ludwig Nutzel, Alexander Gresch, Lukas Hehn, Lucas Marti, Robert Freund, Alex Steiner, Christian D. Marciniak, Timo Eckstein, Nina Stockinger, Stefan Wolf, Thomas Monz, Michael Kuhn y Michael J. Hartmann, Solving an Industrially Relevant Quantum Chemistry Problem on Quantum Hardware, arXiv: 2408.10801v1 [quant-ph] 20 Aug 2024.
- Dominic W. Berry, Maria Kieferov, Artur Scherer, Yuval R. Sanders, Guang Hao Low, Nathan Wiebe, Craig Gidney y Ryan Babbush, Improved Techniques for Preparing Eigenstates of Fermionic Hamiltonians, arXiv:1711.10460v2 [quant-ph] 21 Dec 2017.
- Dave Wecker, Bela Bauer, Bryan K. Clark, Matthew B. Hastings y Matthias Troyer, Can quantum chemistry be performed on a small quantum computer?, arXiv:1312.1695v2 [quant-ph] 6 Jan 2014.
- Yangjun Wu, Xiansong Xu, Dario Poletti, Yi Fan, Chu Guo y Honghui Shang, A real neural network state for quantum chemistry, arXiv: 2301.03755v1 [quant-ph] 10 Jan 2023.
- Ka-Wa Yip, Kubra Yeter-Aydeniz y Sijia S. Dong, Variational Quantum Annealing for Quantum Chemistry, arXiv:2503.15473v1 [quant-ph] 19 Mar 2025.
- Jonathan Romero, Ryan Babbush, Jarrod R. McClean, Cornelius Hempel, Peter Love y Alan Aspuru-Guzik, Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz, arXiv:1701.02691v2 [quant-ph] 10 Feb 2018.
- Mario Motta y Julia E. Rice, Emerging quantum computing algorithms for quantum chemistry, arXiv:2109.02873v2 [quant-ph] 13 Nov 2021.
- Matthew Otten, Matthew R. Hermes, Riddhish Pandharkar, Yuri Alexeev, Stephen K. Gray y Laura Gagliardi, Localized Quantum Chemistry on Quantum Computers, arXiv: 2203.02012v1 [quant-ph] 3 Mar 2022.
- Mohammad Haidar, Hugo D. Nogueira y Jean-Philippe Karr, Quantum Computing Approach to Atomic and Molecular Three-Body Systems, arXiv:2510.18005v1 [quant-ph] 20 Oct 2025.



- Zhong-Xia Shang, Han-Sen Zhong, Yu-Kun Zhang, Cheng-Cheng Yu, Xiao Yuan, Chao-Yang Lu, Jian-Wei Pan y Ming-Cheng Chen, Boson sampling enhanced quantum chemistry, arXiv:2403.16698v2 [quant-ph] 18 Apr 2024.
- Juan Miguel Arrazola, Olivia Di Matteo, Nicolas Quesada, Soran Jahangiri, Alain Delgado y Nathan Killoran, Universal quantum circuits for quantum chemistry, arXiv:2106.13839v2 [quant-ph] 10 Jun 2022.
- Tian Xue, Jacob P. Covey y Matthew Otten, Efficient algorithms for quantum chemistry on modular quantum processors, arXiv:2506.13332v1 [quant-ph] 16 Jun 2025.
- Seunghoon Lee, Joonho Lee, Huanchen Zhai, Yu Tong, Alexander M. Dalzell, Ashutosh Kumar, Phillip Helms, Johnnie Gray, Zhi-Hao Cui, Wen-Yuan Liu, Michael Kastoryano, Ryan Babbush, John Preskill, David R. Reichman, Earl T. Campbell, Edward F. Valeev, Lin Lin y Garnet Kin-Lic Chan, Is there evidence for exponential quantum advantage in quantum chemistry?, arXiv:2208.02199v3 [physics.chem-ph] 14 Nov 2022.
- Ingrid von Glehn, James S. Spencer y David Pfau, A Self-Attention Ansatz for Ab-initio Quantum Chemistry, arXiv:2211.13672v2 [physics.chem-ph] 19 Apr 2023.
- Yudong Cao, Jonathan Romero, Jonathan P. Olson, Matthias Degroote, Peter D. Johnson, Maria Kieferova, Ian D. Kivlichan, Tim Menke, Borja Peropadre, Nicolas P. D. Sawaya, Sukin Sim, Libor Veis y Alan Aspuru-Guzik, Quantum Chemistry in the Age of Quantum Computing, arXiv:1812.09976v2 [quant-ph] 28 Dec 2018.
- Smik Patel, Praveen Jayakumar, Tzu-Ching Yen y Artur F. Izmaylov, Quantum Measurement for Quantum Chemistry on a Quantum Computer, arXiv:2501.14968v2 [quant-ph] 29 May 2025.
- Stepan Fomichev, Kasra Hejazi, Modjtaba Shokrian Zini, Matthew Kiser, Joana Fraxanet, Pablo Antonio Moreno Casares, Alain Delgado, Joonsuk Huh, Arne-Christian Voigt, Jonathan E. Mueller y Juan Miguel Arrazola, Initial state preparation for quantum chemistry on quantum computers, arXiv:2310.18410v2 [quant-ph] 9 Feb 2024.
- Samuele Piccinelli, Alberto Baiardi, Max Rossmannek, Almudena Carrera Vazquez, Francesco Tacchino, Stefano Mensa, Edoardo Altamura, Ali Alavi, Mario Motta, Javier Robledo-Moreno, William Kirby, Kunal Sharma, Antonio Mezzacapo y Ivano Tavernelli.



Quantum chemistry with provable convergence via randomized sample-based quantum diagonalization,
arXiv:2508.02578v1 [quant-ph] 4 Aug 2025.

Sam McArdle, Suguru Endo, Alan Aspuru-Guzik, Simon C. Benjamin y Xiao Yuan, Quantum
computational chemistry, arXiv:1808.10402v3 [quant-ph] 27 Jan 2020.

Garnet Kin-Lic Chan, Quantum chemistry, classical heuristics, and quantum advantage,
arXiv:2407.11235v1 [quant-ph] 15 Jul 2024.

Michael A. Jones, Harish J. Vallury, Charles D. Hill y Lloyd C. L. Hollenberg, Chemistry beyond the
Hartree–Fock energy via quantum computed moments, www.nature.com/scientificreports.

