CQP Computational Quantum Physics

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Quantum Basics

Hilbert space : $\mathcal{H}=\mathbb{C}^{2^n}$

wave function : $|\phi\rangle\in\mathcal{H}$

- a spin-$\frac{1}{2}$ system, $\mathcal{H}=\mathbb{C}^2$, $\phi=\alpha|\uparrow\rangle+\beta|\downarrow\rangle\quad |\alpha|^2+|\beta|^2=1$
- basic state : $|\uparrow\rangle=\begin{bmatrix}1\\0\end{bmatrix}\quad|\downarrow\rangle=\begin{bmatrix}0\\1\end{bmatrix}\quad|\rightarrow\rangle=\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$

pauli matrices : $\sigma_x=\begin{bmatrix}0&1\\1&0\end{bmatrix}\sigma_y=\begin{bmatrix}0&-i\\i&0\end{bmatrix}\sigma_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix}$

- $\sigma_i=\sigma_i^\dagger$: Hermitian
- $\sigma_i=\sigma_i^{-1}$: involutory
- $\sigma_i^2=I$
- $|\sigma_i|=-1$: determinant
- $\mathrm{Tr}(\sigma_i)=0$: trace
- $\lambda=\pm1$: eigen values, eigen vectors are positive negative axes in Bloch sphere
- $[\sigma_i,\sigma_j]=2i\epsilon_{ijk}\sigma_k$: commutation, ϵ_{ijk} : Levi-Civita symbol
- $\{\sigma_i,\sigma_j\}=2\delta_{ij}I$: anti-commutation, δ_{ij} : kronecker delta

Operators :

- **spin operator** : $\hat{S}_x=\frac{\hbar}{2}\sigma_x\quad\hat{S}_y=\frac{\hbar}{2}\sigma_y\quad\hat{S}_z=\frac{\hbar}{2}\sigma_z$
  - spin pointing along direction $\vec{e}=[e_x,e_y,e_z]$ $\vec{e}\cdot\hat{\vec{S}}=\frac{\hbar}{2}\begin{bmatrix}e_z&e_x-ie_y\\e_x+ie_y&-e_z\end{bmatrix}$
- **position operator** : $\hat{q}\,|\psi(q)\rangle=q\psi(q)$
- **momentum operator** : $\hat{p}=-i\hbar\frac{\mathrm{d}}{\mathrm{d}q}$
- **hamiltonian operator** : $\hat{H}=-\frac{\hbar^2}{2m}\nabla^2+V$
- **kinetic operator** : $\hat{T}=\frac{(\hat{p})^2}{2m}=\frac{-i\hbar^2}{2m}\nabla^2$
- **potential operator** : $\hat{V}=V$

Schrödinger equation : $i\hbar\partial_t|\psi(t)\rangle=\hat{H}|\psi(t)\rangle$

- for stationary problem : $\hat{H}|\psi\rangle=E|\psi\rangle\quad\psi(t)=e^{-iEt/\hbar}|\psi(0)\rangle$
- external potential : $i\hbar\partial_t\psi(\hat{r})=-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})+V(\vec{r})\psi(\vec{r})$

> Notation
>
> - $\hat{H}$ Hamilton operator
> - E energy of the system
> - V potential

> Example
>
> - harmonic oscillator : $\frac{1}{2}(\hat{p}^2+\hat{q}^2)|\psi\rangle=E|\psi\rangle$
>   - $V(\hat{q})=\frac{1}{2}\hat{q}^2$
>   - $\psi(q)=\frac{1}{\sqrt{2^n n!\sqrt{\hbar\pi}}}e^{-q^2/2}H_n\left(\frac{1}{\sqrt{\hbar}}q\right)$
>   - $E=\hbar(n+\frac{1}{2})$

Density matrix : $\hat{\rho}=\sum_{i,j}p_{i,j}|\psi_i\rangle\langle\psi_j|$

- purity of the system $\mathrm{Tr}(\hat{\rho}^2)$
- for a pure state without noise : $\hat{\rho}_{\text{pure}}=|\psi\rangle\langle\psi|$

> Example
>
> $\hat{\rho}_\rightarrow=|\rightarrow\rangle\langle\rightarrow|=\begin{bmatrix}\frac{1}{2}&\frac{1}{2}\\\frac{1}{2}&\frac{1}{2}\end{bmatrix}$
>
> $\mathrm{Tr}(\hat{\rho}_\rightarrow)=1$
>
> $\hat{\rho}_{\uparrow\downarrow}=|\uparrow\rangle\langle\downarrow|=\begin{bmatrix}\frac{1}{2}&0\\0&\frac{1}{2}\end{bmatrix}$

> $\mathrm{Tr}(\hat{\rho}_{\uparrow\downarrow}) = \frac{1}{2}$

- unitary time evolution : $i\hbar\partial_t\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)]$
- thermal density matrix : $\hat{\rho}_\beta = \frac{1}{\sum_i e^{-\beta E_i}} \sum_i e^{-\beta E_i} |i\rangle \langle i| = \frac{1}{\mathrm{Tr}(e^{-\beta\hat{H}})} e^{-\beta\hat{H}}$

measurement : $\langle\psi|\hat{A}|\psi\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$

- measure non commute operator : $[\hat{A}, \hat{B}] = i\hbar \Leftrightarrow \Delta A \cdot \Delta B \geq \frac{\hbar}{2}$

Quantum one body problem

Time-Independent 1D Schrödinger equation

stationary assumption : $\psi(t) = e^{-iEt/\hbar}|\psi(0)\rangle$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + V(x)\psi(x) = E\psi(x) \to H\psi(x) = E\psi(x)$$

for special form

$$\psi''(x) + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

given V, m, E we want to know ψ

Numerov algorithm

$$\left(1 + \frac{(\Delta x)^2}{12}k_{n+1}\right)\psi_{n+1} = 2\left(1 - \frac{5(\Delta x)^2}{12}k_n\right)\psi_n - \left(1 + \frac{(\Delta x)^2}{12}k_{n-1}\right)\psi_{n-1} + O[(\Delta x)^6]$$
$$k = \frac{2m}{\hbar^2}(E - V(x))$$

- **initial problem for symmetry** $V(x) = V(-x)$
  - even solution : half integer mesh with $\psi_{-\frac{1}{2}} = \psi_{\frac{1}{2}} = 1$
  - odd solution : integer mesh with $\psi_0 = 0, \psi(x_1) = 1$
- **potential** V **vanish at large distance**
  - start from the vanishing exact solution

1D scattering problem

a particle approaching the potential barrier $V(x)\begin{cases}\neq 0 & x \in [0, a] \\ = 0 & \text{others}\end{cases}$ from the left

- wave function assumptions :
  - left ($x < 0$) wave function : $\psi_L(x) = Ae^{iqx} + Be^{-iqx}$
  - right ($x > a$) wave function : $\psi_R(x) = Ce^{iqx}$
  - where q is the wave number $q^2 = \frac{2m[E - V(x)]}{\hbar^2}$
- solution :

> Algorithm
>
> 1. set $C = 1$, use Numerov algorithm starting at $a + \Delta x$ from right to left
> 2. match the numerical solution on the left $x < 0$ to determine A and B

- probability :
  - reflection probaility : $R = \frac{|B|^2}{|A|^2}$
  - transition probability : $T = \frac{|C|^2}{|A|^2}$

Bound state

particles are confined due to potential $V(x) = \begin{cases}0 & x \in (0, a) \\ \infty & \text{otherwise}\end{cases}$

- **shooting method for eigen solver**

> Algorithm
>
> 1. try a energy E
> 2. use numerov algorithm from $x = 0$ to $x_f \gg a$
> 3. satisfy $\psi_E(x_f) \approx 0$ then E is a eigen value else try another E

- **Improved Method - Integration from Both Sides**

> Algorithm
>
> 1. try a position $b \in (0, a)$, that $E = V(b)$, $\psi_E''(b) = 0$

2. use numerov from a to b as ψ_L and from 0 to b as ψ_R
3. satisfy $\frac{\psi'_L(b)}{\psi_L(b)} = \frac{\psi'_R(b)}{\psi_R(b)}$, then E is a eigen value else try another b

Time-independent nD Schrödinger equation

Factorization techniques :

- **along coordinate axes** : $\psi(\vec{r}) = \psi_x(x)\psi_y(y)\psi_z(z)$
- **spherical symmetry** : $\psi(\vec{r}) = \frac{u(r)}{r}Y_{lm}(\theta,\phi) \quad l \in \mathbb{N}_0, m \in \mathbb{Z}, |m| \leq l$
  apply to the Schrodinger equation : $\left(-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right)u(r) = Eu(r)$

> Notation
>
> - l : azimuthal quantum number, magnitude of the orbital angular momentum
> - m : magnetic quantum number, projection of the angular momentum vector along a chosen axis
> - μ : mass

Solving methods :

- **finite difference**

> Example : three dimensional Schrodinger
>
> $$\nabla^2\psi(\vec{r}) + 2m[E - V(\vec{r})]\psi(\vec{r}) = 0$$
> $$\Downarrow$$
> $$\begin{aligned} 0 = \frac{1}{(\Delta x)^2}[&\psi(x_{n+1},y_n,z_n) + \psi(x_{n-1},y_n,z_n) \\ &+ \psi(x_n,y_{n+1},z_n) + \psi(x_n,y_{n-1},z_n) \\ &+ \psi(x_n,y_n,z_{n+1}) + \psi(x_n,y_n,z_{n-1})] \\ &+ \left\{2m[E - V(\vec{r})] - \frac{6}{(\Delta x)^2}\right\}\psi(x_n,y_n,z_n) \end{aligned}$$

- **variational approaches** : $|\phi\rangle = \sum_i^N a_i |u_i\rangle$

$$\langle\phi|\phi\rangle E^* = \langle\phi|\hat{H}|\phi\rangle \rightarrow \underbrace{\langle u_i|u_j\rangle}_{S_{ij}}E^* = \underbrace{\langle u_i|\hat{H}|u_j\rangle}_{H_{ij}} \rightarrow U^\top HU\hat{b} = E^*\vec{b}$$

more basis more accurate

> Notation
>
> - $|u_i\rangle$ basis
> - a_i : basis coefficient, $\vec{a} = [a_1, \cdots, a_n]^\top$
> - U : nomalization matrix for S that $U^\top SU = I$
> - $\vec{b}$: eigen vector, $\vec{b} = U^{-1}\vec{a}$

- **finite element method**
  - irregular geometries
  - higher accuracy

Time dependent Schrödinger Equation

$$i\partial_t|\psi\rangle = \hat{H}|\psi\rangle$$

Spectral method : $|\psi_t\rangle = \sum_n c_n e^{-i\varepsilon_n(t-t_0)/\hbar}|\phi_n\rangle$

> Algorithm
>
> 1. eigen value ε_n and eigen vector $|\phi_n\rangle$ for stationary problem $\hat{H}|\phi\rangle = E|\phi\rangle$
> 2. represent initial wave function in eigen vectors $|\psi_0\rangle = \sum_n c_n|\phi_n\rangle$
> 3. the evolution state $|\psi_t\rangle = \sum_n c_n e^{-i\varepsilon_n(t-t_0)/\hbar}|\phi_n\rangle$

limitations :

- the diagonalization of H is complex, so this method is only useful for small problems

Direct numerical integration : $\left(\mathbb{1} + \frac{i\Delta t}{2\hbar}H\right)\psi(\vec{r}, t+\Delta t) = \left(\mathbb{1} - \frac{i\Delta t}{2\hbar}H\right)\psi(\vec{r},t)$

- **forward euler** : $|\psi(t_{n+1})\rangle = |\psi(t_n)\rangle - \frac{i\Delta t}{\hbar}\hat{H}|\psi(t_n)\rangle$
  - numerically unstable
  - violet conservation of $\langle\phi|\phi\rangle$
- **implicit method** : $\left(\mathbb{1} + \frac{i\Delta t}{2\hbar}H\right)\psi(\vec{r}, t+\Delta t) = \left(\mathbb{1} - \frac{i\Delta t}{2\hbar}H\right)\psi(\vec{r},t)$
  - H is sparse matrix, using iterative solver (e.g. biconjugate gradient)

Split-operator method : $\psi(\vec{q}) \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftharpoons}} \psi(\vec{p}) \Rightarrow \hat{H} = \hat{T}(\vec{p}) + \hat{V}(\vec{q})$

$$e^{-it\hat{H}/\hbar} = e^{-i\Delta t\hat{V}/2\hbar}\left[e^{-i\Delta t\hat{T}/\hbar}e^{-i\Delta t\hat{V}/\hbar}\right]^{N-1}e^{-i\Delta t\hat{T}/\hbar}e^{-i\Delta t\hat{V}/2\hbar}$$

> Algorithm
>
> 1. $\psi(\vec{q}) \leftarrow e^{-i\Delta t V(\vec{q})/2\hbar}\psi_0(\vec{q})$
> 2. loop N-1 timesteps
>   1. $\psi(\vec{p}) \overset{\mathcal{F}}{\leftarrow} \psi(\vec{q})$
>   2. $\psi(\vec{p}) \leftarrow e^{-i\Delta t\hbar\|\vec{p}\|^2/2m}\psi(\vec{p})$
>   3. $\psi(\vec{q}) \overset{\mathcal{F}^{-1}}{\leftarrow} \psi(\vec{p})$
>   4. $\psi(\vec{q}) \leftarrow e^{-i\Delta t V(\vec{q})/\hbar}\psi(\vec{q})$
> 3. $\psi(\vec{p}) \overset{\mathcal{F}}{\leftarrow} \psi(\vec{q})$
> 4. $\psi(\vec{p}) \leftarrow e^{-i\Delta t\hbar\|\vec{p}\|^2/2m}\psi(\vec{p})$
> 5. $\psi(\vec{q}) \overset{\mathcal{F}^{-1}}{\leftarrow} \psi(\vec{p})$
> 6. $\psi(\vec{q}) \leftarrow e^{-i\Delta t V(\vec{q})/2\hbar}$

> Notation
>
> - $\vec{p}$: momentum in hamilton expression
> - $\vec{q}$: position in hamilton expression
> - $\hat{T}$: kinetic operator , $\hat{T} = \frac{\hat{(\vec{p})}^2}{2m} = \frac{-i\hbar^2}{2m}\nabla^2$
> - $\hat{V}$: potential operator , $\hat{V} = V$
> - $\mathcal{F}$: fourier operator , $\mathcal{F}\psi(\vec{q}) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{-\infty}^{+\infty}\psi(\vec{q})e^{-i\vec{p}\cdot\vec{q}}\mathrm{d}\vec{q}$
> - $\mathcal{F}^{-1}$: inverse fourier operator , $\mathcal{F}^{-1}\psi(\vec{p}) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{-\infty}^{+\infty}\psi(\vec{p})e^{-i\vec{p}\cdot\vec{q}}\mathrm{d}\vec{p}$

Quantum n-body problem

Hilbert space for n particles: $\mathcal{H}^N = \mathcal{H}^{\otimes N}$

Indistinguishable Particles

Bosons and Fermions :

- **fermions** : $\psi(\vec{r}_1, \vec{r}_2) = -\psi(\vec{r}_2, \vec{r}_1)$

$$\Psi^A = \mathcal{N}_A \sum_p \mathrm{sign}(p)\psi(\vec{r}_{p(1)}, \cdots, \vec{r}_{p(N)})$$

  > Notation
  >
  > - Ψ^A : n particle fermions wave function
  > - $\mathcal{N}_A$: normalization factor
  > - p : permutation

  - *Pauli exclusion principle* : $\Psi^A(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_1, \vec{r}_2) - \psi(\vec{r}_2, \vec{r}_1) \neq 0$
  - spinful, generalized coordinate $r = (\vec{r}, \sigma)$

- **bosons** : $\psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2, \vec{r}_1)$

$$\Psi^S = \mathcal{N}_S \sum_p \psi(\vec{r}_{p(1)}, \cdots, \vec{r}_{p(N)})$$

  > Notation
  >
  > - Ψ^S : n particle bosons wave function
  > - $\mathcal{N}_S$: normalization factor

Fock space: $\mathcal{F} = \bigoplus_{N=0}^{\infty}\mathcal{S}_{\pm}\mathcal{H}^N$

possible particle configurations for a given type of particle

> Notation
>
> - $\oplus$: direct sum, e.g. $\mathbf{A} \oplus \mathbf{B} = \begin{bmatrix}\mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{B}\end{bmatrix}$
> - $S_{\pm}$: symmetrization for bosons $\mathcal{S}_+\mathcal{N}_S\sum_p$ / antisymmetrization operator for fermions $\mathcal{S}_- = \mathcal{N}_A\sum_p \mathrm{sgn(p)}$

	Bosons	**Spinless Fermions**	**Spinful Fermions**	**Spin-$\frac{1}{2}$**
Fock space dimension	∞(bosons can take same position)	2^N	4^N	2^N

Slater determinant : $\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & \cdots & \phi_N(r_1) \\ \vdots & \ddots & \vdots \\ \phi_r(r_N) & \cdots & \phi_N(r_N) \end{vmatrix}$

anti-symmetrized and normalized N single particle wave function product

Creation and annihilation operators

- $\hat{a}$ **annihilation operator** : remove particle $\hat{a}_i \left|\phi_j\right\rangle = \delta_{ij} \left|\text{null}\right\rangle$
- $\hat{a}^\dagger$ **creation operator** : add particle $\left|\phi_i\right\rangle = \hat{a}_i^\dagger \left|\text{null}\right\rangle$

> Notation
>
> - $\left|\text{null}\right\rangle$: vacuum state with no particles, $\left|\text{null}\right\rangle = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
> - $[\cdot, \cdot]$: commute, $[A, B] = AB - BA$
> - $\{\cdot, \cdot\}$: anti-commute, $\{A, B\} = AB + BA$

- Bosons : commute
  - $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$
  - $[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$
- Fermions : anti-commute
  - $\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}$
  - $\{\hat{a}_i, \hat{a}_j\} = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0$

Quantum Spin Model

(TFIM)Transverse field Ising model

$$\hat{H} = \sum_{<ij>} J_{ij} \hat{S}_i^z \hat{S}_j^z - \sum_i \frac{h_i}{2} \hat{S}_i^x$$

$$\hat{S}_i^z \hat{S}_j^z = I \otimes \cdots \otimes \underbrace{\hat{S}^z}_{n=i} \otimes \cdots \otimes \underbrace{\hat{S}^z}_{n=j} \otimes \cdots \otimes \mathbb{1} I$$

- quantum phase transition between a spontaneously symmetry-broken and a disordered phase
- extension of the classical Ising model by adding a magnetic field in the x direction

> Notation
>
> - $< ij >$: connection between particle i and particle j
> - J_{ij} : interacting constant between particle i and particle j
> - h_i : external magenatic field on particle i
> - $\hat{S}^x$: spin operator in x direction, $\hat{S}^x = \frac{1}{2}\hbar\sigma_x = \frac{1}{2}\hbar \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
> - $\hat{S}^z$: spin operator in z direction, $\hat{S}^z = \frac{1}{2}\hbar\sigma_z = \frac{1}{2}\hbar \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

Heisenberg model

$$\begin{aligned} \hat{H} &= \sum_{<ij>} J_{ij} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j = \sum_{<ij>} J_{ij} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_z^j \right) \\ &= \sum_{<ij>} J_{ij} \left[\frac{1}{2} \left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+ \right) + \hat{S}_i^z \hat{S}_j^z \right] \end{aligned}$$

> Notation
>
> - $\hat{S}^\pm$: raising/lowering operator , $\hat{S}^\pm = \hbar\sigma^\pm = \hbar(\sigma_x \pm i\sigma_y)$
>   - $\hat{S}^+\hat{S}^+ \left|\downarrow\right\rangle = \hat{S}^+ \left|\uparrow\right\rangle = \left|\text{null}\right\rangle \quad \left|\uparrow\right\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \left|\downarrow\right\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \left|\text{null}\right\rangle = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
>   - $(\sigma^\pm)^2 = 0$: a spin can be flipped only only once
> - $\hat{M}^z$: total magnetization , $\hat{M}^z = \sum_i \hat{S}_i^z$

- conserve total magentization
- Hamitonian has $SU(2)$ symmetry

> Example : two particles ($\{\left|\uparrow\uparrow\right\rangle, \left|\uparrow\downarrow\right\rangle, \left|\downarrow\uparrow\right\rangle, \left|\downarrow\downarrow\right\rangle\}$)
>
> $$\hat{H} = \begin{bmatrix} \frac{1}{4}J_{ij} & 0 & 0 & 0 \\ 0 & -\frac{1}{4}J_{ij} & \frac{1}{2}J_{ij} & 0 \\ 0 & \frac{1}{2}J_{ij} & -\frac{1}{4}J_{ij} & 0 \\ 0 & 0 & 0 & \frac{1}{4}J_{ij} \end{bmatrix}$$

XXZ model

$$\hat{H} = \sum_{<ij>} J_{ij} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right)$$

- conserve total magentization $\hat{M}^z$

> Notation
>
> - Δ : hyperparameter
>
> | $\Delta = 0$ | $\Delta = 1$ | $\Delta \to \infty$ |
> | --- | --- | --- |
> | XY model | Heisenberg model | Ising model |

Jordan-Wigner Transformation

mapping spin models to spinless fermions, derive from XXZ model

$$\hat{H} = \frac{1}{2}\sum_{<ij>} J_{ij}\left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i + 2\Delta \hat{n}_i \hat{n}_j\right)$$

> Notation
>
> - $\hat{c}_i / \hat{c}_i^\dagger$: Jordan-Wigner transformation operator, $\hat{c}_i = \prod_{j<i}\left(\sigma_j^z\right)\sigma_i^+ \qquad \hat{c}_i^\dagger = \prod_{j<i}\left(\sigma_j^z\right)\sigma_i^-$
>   - $\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}$
>   - $\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$
> - $\hat{n}_i$: number operator, $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$

Brute-force method

[ED]Exact Diagonalization

diagonalizing the Hamiltonian matrix

- full spectrum $N \approx 20$
- Lanczos algorithm $N \approx 40$

Lanczos algorithm

- storage complexity $\mathcal{O}(2^N)$ compared to dense matrix eigen solvers of $\mathcal{O}(2^N)^2$
- ghost state : low-lying eigen values result from round of error that $\vec{r}_n$ is not fully orthogonal

> Algorithm
>
> 1. find the orthogonalized basis $\vec{r}_i$ using *Gram-Schmidt orthogonalization*
>
> $\vec{r}_0 = \dfrac{\vec{v}}{\|\vec{v}\|} \quad \beta_m \vec{r}_m = H\vec{r}_{m-1} - \alpha_{m-1}\vec{r}_{m-1} - \beta_{m-1}\vec{r}_{m-2} \quad \alpha_n = \vec{r}_n^\dagger H \vec{r}_n \quad \beta_n = |\vec{r}_n^\dagger H \vec{r}_{n-1}|$
>
> 2. express Hamiltonian H in tridiagonal matrix
>
> $$H^M = \begin{bmatrix} \alpha_0 & \beta_1 & \cdots & 0 & 0 \\ \beta_1 & \alpha_1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \alpha_{M-1} & \beta_M \\ 0 & 0 & \cdots & \beta_M & \alpha_M \end{bmatrix}$$
>
> 3. eigendecomposite the H^M
> 4. transform the eigenvectors to the original basis
>   - for memory constraint, only store the last three $\vec{r}_n$ and recompute $\vec{r}_n$ iteratively to perform basis transformation

Spin-$\frac{1}{2}$ hamitonians

two possible state $|\uparrow\rangle$ and $|\downarrow\rangle$ bitwise operation (xor) rather than vector

- $\hat{S}_i^z \hat{S}_{i+1}^z$: `s = s ^ (s>>1)`
- $\hat{S}_i^+ \hat{S}_{i+1}^-$: `s = s ^ (r<<3)`

> Example
>
> assume state $s = 011_2$
>
> then for heisenberg model $\tilde{s} = 011_2 \oplus 010_2 = 010_2$ where $\oplus$ is bitwise xor here.

symmetries

block diagonalize the Hamitonian and solve within the symmetries' eigenspaces.

> Example : Transverse Field Ising Model
>
> 1. parity operator : $\hat{P} = \bigotimes_i \sigma_i^x$, the eigen values are ± 1
> 2. $|\psi\rangle = \hat{P}^M |\psi\rangle$: for random state ψ, apply operator for M times we find the initial state again
> 3. eigen state becomes : $\sum_{i=0}^{M} \hat{P}^i |\psi\rangle$
> 4. construct hamiltonian H from eigen state and eigen vector

Time evolution

Trotter-Suzuki decomposition : $e^{-i\hat{H}\Delta t/\hbar} = \prod_{k=1}^{K} e^{-i\hat{h}_k\Delta t/\hbar} + \mathcal{O}(\Delta t^2)$

- time-indepedent assumption : $|\psi(t+\Delta t)\rangle = e^{-i\hat{H}\Delta t/\hbar}|\psi(t)\rangle$
- non-commuting decomposition : $\hat{H} = \sum_{k=1}^{K}\hat{h}_k \quad [\hat{h}_i, \hat{h}_j] \neq 0 \quad i \neq j$
- second order version : $e^{-i\hat{H}\Delta t/\hbar} = \left(\prod_{k=1}^{K} e^{-i\hat{h}_k\Delta t/2\hbar}\right)\left(\prod_{k=K}^{1} e^{-i\hat{h}_k\Delta t/2\hbar}\right) + \mathcal{O}(\Delta t^3)$

> Example : $K = 2$
>
> $|\psi(t+\Delta t)\rangle = e^{-i\hat{h}_1\Delta t/2\hbar}e^{-i\hat{h}_2\Delta t/\hbar}e^{-i\hat{h}_1\Delta t/2\hbar}|\psi\rangle$

> Example : Transverse Field Ising Model
>
> $\hat{H} = \underbrace{\sum_{<ij>} J_{ij}\sigma_i^z\sigma_j^z}_{\hat{h}_1} - \underbrace{\sum_i h_i\sigma_i^x}_{\hat{h}_2}$
>
> $e^{-i\hat{h}_1\Delta t/\hbar} = \bigotimes_{<ij>} e^{-i\Delta t J_{ij}s_i^z s_j 6z/\hbar}$
>
> $e^{-i\hat{h}_2\Delta t/\hbar} = \begin{bmatrix}\cos(\Delta t h_i/\hbar) & i\sin(\Delta t h_i/\hbar)\\ i\sin(\Delta t h_i/\hbar) & \cos(\Delta t h_i/\hbar)\end{bmatrix}$
>
> (since $e^A = 1 + A + \frac{A^2}{2!} + \cdots$)

> Notation
>
> - $[\cdot,\cdot]$: commute operator, $[A,B] = AB - BA = 0 \rightarrow A, B$ commute
> - $< i, j >$: means i, j are neighbors
> - J_{ij} : connection between site i and j
> - h_i : magenatic field at site i
> - $\hat{h}_k$: non-commuting term
> - s_i : eigen value for σ_i^z

Imaginary-time evlotion: $it \rightarrow \tau$

- time-indepedent assumption : $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle \rightarrow |\psi(t)\rangle = e^{-\tau\hat{H}}|\psi(0)\rangle$
- converges to the ground state by suppressing the amplitudes of excited states exponentially fast in the product $\Delta E_k \tau$.

Magnus expansian : $\hat{U}(\Delta t) = e^{-i\bar{H}_t\Delta t/\hbar} + \mathcal{O}(\Delta t^2) \quad H_t = \bar{H}_t^1 + \bar{H}_t^2 + \cdots$

- time-depdent assumption : $|\psi(t')\rangle = U(t',t)|\psi(t)\rangle$
- $\bar{H}_t^1 = \frac{1}{\Delta t}\int_t^{t+\Delta t}\hat{H}(s)ds$ and $H_t^2 = -\frac{i}{\Delta t}\int_t^{t+\Delta t}ds\int_t^s dl\left[\hat{H}(s), \hat{H}(l)\right]$

> Notation
>
> - U : evolution operator, $\hat{U}(t',t) = e^{-i\int_t^{t'}\hat{H}(s)\mathrm{d}s/\hbar} \quad t' > t$

Matrix Product States

Bipartite entanglement

Reduced density matrix : $\rho_A = \mathrm{Tr}_B(|\psi\rangle\langle\psi|) \quad |\psi\rangle \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$

> Notation
>
> - $\otimes$: kronecker product, e.g. $\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} \otimes \begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix} = \begin{bmatrix}1 & 1 & 0 & 0\\ 1 & 1 & 0 & 0\\ 0 & 0 & 1 & 1\\ 0 & 0 & 1 & 1\end{bmatrix}$
> - Tr_B : partial trace over subsystem B, e.g. $\mathrm{Tr}_B\begin{bmatrix}A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12}\\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22}\\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12}\\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22}\end{bmatrix} = \begin{bmatrix}\sum_{ii}B_{ii}A_{11} & \sum_{ii}B_{ii}A_{12}\\ \sum_{ii}B_{ii}A_{21} & \sum_{ii}B_{ii}A_{22}\end{bmatrix}$

Entanglement : $S = -\mathrm{Tr}(\rho_A\log\rho_A) = -\mathrm{Tr}(\rho_B\log\rho_B)$

using *Schmidt decomposition* $\rho_A = \sum_\alpha \lambda_\alpha^2 |\phi_\alpha\rangle_A\langle\phi_\alpha|_A \rightarrow S - \sum_\alpha \lambda_\alpha^2 \log\lambda_\alpha^2$

- product state (zero entanglement) : $S = 0 \Leftrightarrow \lambda_1 = 1, \lambda_{\alpha>1} = 0$
- maximally entangled state : $S = \frac{N}{2}\log d \Leftrightarrow \lambda_i = 1/\sqrt{d^{N/2}}$
- random state : $S \approx \frac{N}{2}\log d - \frac{1}{2}$

Area law of entanglement : entanglement entropy scales as $S \propto L^{D-1}$

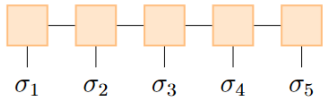
> Example : 1-D entanglement
>
> $S \sim \mathrm{const}$

> Notation

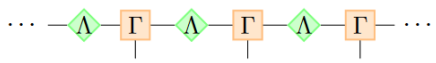
- S : entanglement entropy
- d : Hilbert space dimension
- λ : eigen value
- N : number of sites
- D : dimension of the entanglement system
- L : linear dimension of system

Matrix Product state

[MPS]Matrix Product State : $|\psi\rangle = \sum_s \mathrm{Tr}(A_1^{s_1}\cdots A_N^{s_N})\,|s_1\cdots s_N\rangle$



- canonical form (normalization) : $A = \Lambda\Gamma$

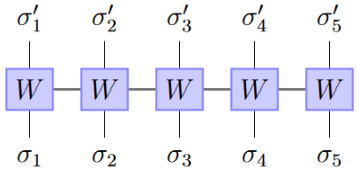


> Example : GHZ or 'cat' state
>
> $$|GHZ\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle^{\otimes N} + |\uparrow\rangle^{\otimes N}) = \frac{1}{Z}\left(\mathrm{Tr}\left((A^{\uparrow})^N\right)|\uparrow\rangle^{\otimes N} + \mathrm{Tr}\left((A^{\downarrow})^N\right)|\downarrow\rangle^{\otimes N}\right)$$
>
> where Z is a norm and $A^{\downarrow} = \begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}$ $A^{\uparrow} = \begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}$

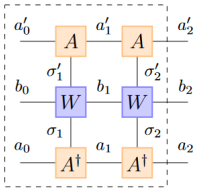
> Example : AKLT state
>
> ground state of spin-1 Hamiltonian : $\hat{H} = \sum_j \hat{\vec{S}}_j \cdot \hat{\vec{S}}_{j+1} + \frac{1}{3}\left(\hat{\vec{S}}_j \cdot \hat{\vec{S}}_{j+1}\right)^2$
>
> with matrices : $A^{+} = \sqrt{\frac{2}{3}}\sigma^{+} = \begin{bmatrix}0 & \sqrt{\frac{2}{3}}\\ 0 & 0\end{bmatrix}$ $A^{0} = \frac{-1}{\sqrt{3}}\sigma^{z} = \begin{bmatrix}-\frac{1}{\sqrt{3}} & 0\\ 0 & \frac{1}{\sqrt{3}}\end{bmatrix}$ $A^{-} = -\sqrt{\frac{2}{3}}\sigma^{-} \begin{bmatrix}0 & 0\\ -\sqrt{\frac{2}{3}} & 0\end{bmatrix}$
>
> the corresponding $|+\rangle$, $|-\rangle$, $|0\rangle$ are three states for spin-1 particle not for spin-$\frac{1}{2}$ particle

> Notation
>
> - A_i : a rank-3 tensor, $A_i \in \mathbb{C}^{D\times 2\times 2}$, D is the number of basis state for single site.
>
> $A_i^{s_i}$ means when the site i is in state s_i, there is a 2×2 matrix for product
>
>   For translationally symmetric $A_i = A$
> - σ^{+} : creation / raising operator , $\sigma^{+} = \begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}$
>   - $\sigma^{+}|\downarrow\rangle = |\mathrm{null}\rangle$
>   - $\sigma^{+}|\uparrow\rangle = |\downarrow\rangle$
> - σ^{-} : annihilation / lowering operator, $\sigma^{-} = \begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}$
>   - $\sigma^{-}|\downarrow\rangle = |\uparrow\rangle$
>   - $\sigma^{-}|\uparrow\rangle = |\mathrm{null}\rangle$
> - $|\mathrm{null}\rangle$: vaccum state, no particle
> - $|+\rangle$: for spin-1 , $|+\rangle = |\uparrow\uparrow\rangle$
> - $|-\rangle$: for spin-1 , $|-\rangle = |\downarrow\downarrow\rangle$
> - $|0\rangle$: for spin-1 , $|0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

[MPO]Matrix Product Operator : $\hat{O} = \sum_{\sigma_i,\sigma_i'}\left[W_1^{\sigma_1\sigma_1'}\cdots W_N^{\sigma_N\sigma_N'}\right]|\sigma_1\ldots\sigma_N\rangle\langle\sigma_1'\cdots\sigma_N'|$



- computing $\langle\psi|\hat{O}|\psi\rangle$:



> Example : single site operator
>
> $\hat{O}_j = I \otimes \cdots \otimes \underbrace{\hat{O}}_{\text{site } j} \otimes \cdots \otimes I$
>
> $W_i^{\sigma_i,\sigma'_i} = \langle \sigma_i | \hat{O} | \sigma'_i \rangle$

> Example : paramagnetic system $\hat{H} = -\sum_i h\hat{S}_i^z$
>
> $\hat{H} = (-h\hat{S}^z \otimes I \otimes \cdots \otimes I) + \cdots + (I \otimes \cdots \otimes I \otimes -h\hat{S}^z)$
>
> $W_1 = \begin{bmatrix} -hS^z & I \end{bmatrix} \quad W_i = \begin{bmatrix} I & 0 \\ -hS^z & I \end{bmatrix} \quad W_N = \begin{bmatrix} I \\ -hS^z \end{bmatrix}$

> Example : Transverse field Ising model $\hat{H} = -\sum_i \hat{S}_i^z \hat{S}_{i+1}^z + h\sum_i \hat{S}_i^x$
>
> $W_1 = \begin{bmatrix} hS^x & -S^z & I \end{bmatrix} \quad W_i = \begin{bmatrix} I & 0 & 0 \\ S^z & 0 & 0 \\ hS^x & -S^z & I \end{bmatrix} \quad W_N = \begin{bmatrix} I \\ S^z \\ hS^x \end{bmatrix}$

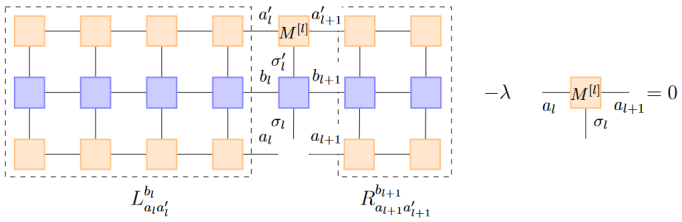
> Notation
>
> - W_i a rank-4 tensor, $W_i \in \mathbb{C}^{D\times D\times 2\times 2}$
>
> $W_i^{\sigma_i\sigma_j}$ means for site i when the left state is σ_i and right state σ_j there is a 2×2 matrix for product

[DMRG]Density matrix renormalization group

find the ground state that $\underset{|\psi\rangle}{\operatorname{argmin}} \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$

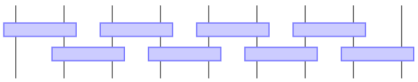
- left normalization : $A^\dagger A = I \quad A' = U\Sigma V^\dagger \to A = U$
- right normalization : $BB^\dagger = I \quad B' = U\Sigma V^\dagger \to B = V^\dagger$
- substitution algorithm : imaginary time evolution, but converge slower

> Algorithm
>
> 1. random initialize $|\psi\rangle$ as right-normalized
> 2. build R_1
> 3. repeat until energy converge $\mathrm{Var}(H) < \epsilon$
> 1. right sweep for $l = 1, \ldots, L-1$
> 1. solve eigen value for M_l

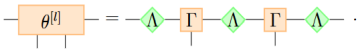


> 2. left normalize M_l
> 3. build L_l
> 2. Left sweep for $l = L, \ldots, 2$
> 1. solve eigen value for M_l
> 2. right normalize M_l
> 3. build R_l

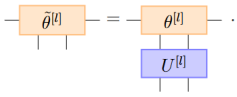
[TEBD]Time evolving block decimation

$U(\Delta t) =$  .

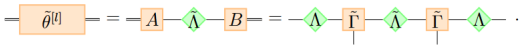
> Algorithm
>
> 1. two site tensor contraction



2. apply evolution gate



3. split into single site tensor



4. truncation : keep $\chi_{\max}$ eigen value and renormalize $\sum_i \Lambda_i i^2 = 1$

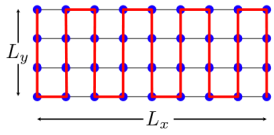
Computation errors :

- truncation error : main error, grows exponentially
- Trotter error : can be avoid reducing Δt and higher expension
- small eigen value : at step 3 $\Lambda^{-1}A$ and $B\Lambda^{-1}$
- imaginary time evolution : canonical form only retrained when $\Delta\tau \to 0$

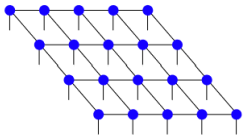
Further topics

Two-dimensional system

- converting two dimension system as chain



- [PEPS]projected entangled pair state

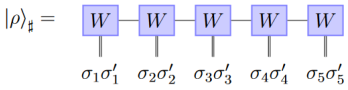


  - chanllenging computationally
  - lack a canonical form

Mixed state and open quantum system dynamics

- mixed state unitary time evolution is governed by $\hat{H}$: $\partial_t\hat{\rho}(t) = -i[\hat{H}, \hat{\rho}(t)]$
- *open quantum system* : coupled to an environment or bath

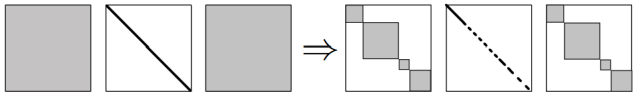
  which can be described by *Lindblad equation* : $\partial_t\hat{\rho} = \hat{\mathcal{L}}\hat{\rho} = -i[\hat{H}, \hat{\rho}] + \sum_i \gamma_i \left(\hat{L}_i\hat{\rho}\hat{L}_i^\dagger - \frac{1}{2}\{\hat{L}_i^\dagger\hat{L}_i, \hat{\rho}\}\right)$



> Notation
>
> - $\hat{L}_i$: jump operator, the system operators directly coupled to the bath, e.g. creation, annilation
> - $\hat{\mathcal{L}}$: Lindbladian, could be considered as a linear operator $|\rho(t)\rangle = e^{-i\hat{\mathcal{L}}t}|\rho_0\rangle$

Symmetries

schmidt eigenstates belong to a fixed magnetization sector



[TDVP]Time-dependent variational principle

- action function : $S = \int_{t_1}^{t_2} \langle\psi(t)|i\partial_t - \hat{H}|\psi(t)\rangle \mathrm{d}t \to \partial_t A_i = -iH_iA_i$
- analogue to DMRG algorithm, but better at simulate long-ranged

Quantum Monte Carlo

Monte Carlo Basics

Monte Carlo

- error $\frac{1}{\sqrt{N}}$

Markov Chain : $P_{XY} = T(X \to Y)A(X \to Y) \quad A(X \to Y) = \min\left(1, \frac{W(Y)}{W(X)}\right)$

- Erogodicity : $T(X \to Y) > 0 \quad \forall X, Y$
- Normalization : $\sum_Y T(X \to Y) = 1$
- Reversibility : $T(X \to Y) = T(Y \to X)$, if T not satisfy this, then $A(X \to Y) = \min\left(\frac{W(Y)T(Y \to X)}{W(X)T(X \to Y)}\right)$

> Notation
>
> - T : transition probability
> - W : static distribution
> - A : accept probability

Classical Ising model

symmetry-braking phase transition at a finite temperature

$$H = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j - \sum_i h\sigma_i \quad \sigma_i = \pm 1$$

> Notation
>
> - J_{ij} : coupling constant
>   - $J_{ij} \geq 0$: symmetry-broken state
> - h_i : external field
> - $< i, j >$: means i, j are connected
> - c : cluster, $|c|$ means the number of spins inside a cluster

> Algorithm : **Swendsen-Wang**
>
> 1. two neighboring parallel spins connected with probability $p = 1 - e^{-2\beta J}$
> 2. cluster labeling. e.g., Hoshen-Kopelman algorithm
> 3. measurement : $\langle m^2 \rangle_{C'} = \frac{1}{N^2}\sum_c |c|$
> 4. cluster flipped with probability $\frac{1}{2}$

> Algorithm : **Wolff**
>
> 1. random site
> 2. recursive find parallel neighbor add it to the cluster with $p = 1 - e^{-2\beta J}$
> 3. measurement : $\langle m^2 \rangle_{C'} = \frac{1}{N}|c_0|$, since only one cluster
> 4. flip all spins in the clster

- *Swendsen-Wang* will result in many small clusters in high dimension, but Wolff will result in one large cluster

Quantum spin system thermodynamics

$$\langle \hat{m} \rangle = \frac{1}{Z}\mathrm{Tr}\left(\hat{m}e^{-\beta\hat{H}}\right) = \frac{1}{Z}\sum_C m(C)W(C) \quad Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \sum_C W(C)$$

> Notation
>
> - $\hat{m}$: magnetization
> - β : reverse of temperature $\beta = \frac{1}{\kappa_B T}$
> - Z : partition sum
> - $m(C)$: magnetization of a configuration C
> - $W(C)$: weight of a configuration C

spin-$\frac{1}{2}$ in a magnetic field : $\hat{H} = -h\hat{S}^z - \Gamma\hat{S}^x = \begin{bmatrix} -\frac{h}{2} & -\frac{\Gamma}{2} \\ -\frac{\Gamma}{2} & \frac{h}{2} \end{bmatrix}$

> Notation
>
> - h : longitudinal field
> - Γ : transverse field

Discrete-time path integral : $\beta = \Delta\tau M$

expand to first order $e^{-\Delta\tau\hat{H}} = \hat{U} + \mathcal{O}(\Delta\tau^2) \to Z \approx \mathrm{Tr}\left(\hat{U}^M\right)$

> Notation

- $\hat{U}$: transfer matrix : $\hat{U} = I - \Delta\tau\hat{H} = \begin{bmatrix} 1+\frac{\Delta\tau h}{2} & \frac{\Delta\tau\Gamma}{2} \\ \frac{\Delta\tau\Gamma}{2} & 1-\frac{\Delta\tau h}{2} \end{bmatrix}$
- $\Delta\tau$: discrete time step
- M : resolution
- E_0 : ground energy

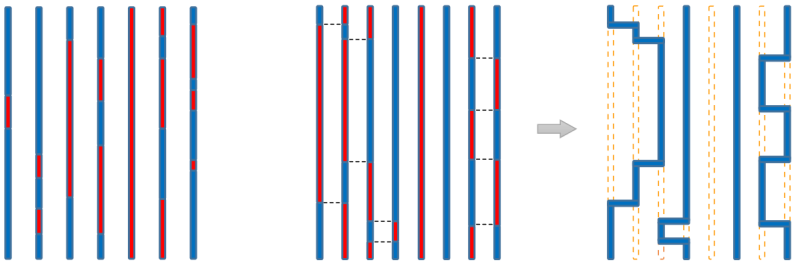
> Example : 1D classical Ising model (0D transverse field Ising model)
>
> $H = -J\sum_i^M \sigma_i\sigma_{i+1} - h\sum_i \sigma_i$ with periodic boundary condition $\sigma_{M+1} = \sigma_1$
>
> - $\beta J = -\frac{1}{2}\log(\Delta\tau\Gamma/2)$: off diagonal
> - $\beta h = \log(1+\Delta\tau h/2)$: diagonal
> - $\beta E_0 = M\beta J$

Continous-time path integral : $\Delta\tau \to 0$???

d -dimensional quantum spin model $\Leftrightarrow$ $d+1$- dimensional classical Ising model

quantum XY model

spin flip-flops proportional to β



no spin conservation (1D TFIM) | with spin conservation (XY model)

negative sign problem : positive off diagonal

Variational Monte Carlo

variational principle : $|\psi(\theta)\rangle = \sum_n \psi_n(\theta)\,|n\rangle$

energy expectation(MCMC) : $E_\theta = \frac{\sum_n |\psi_n(\theta)|^2 E_1(n)}{\sum_n |\psi_n(\theta)|^2}$

> Notation
>
> - $E_1(n)$: local energy $E_1(n) = \sum_m \langle n|\hat{H}\,|m\rangle\psi_m(\theta)\psi_n(\theta)$
> - G_{kl} : metric tensor

[SGD]Stochastic Graident Descent : $\theta \leftarrow \theta - \lambda\nabla_\theta E_\theta$

Stochastic Reconfiguration : $\theta \leftarrow \theta - \Delta\tau G^{-1}\nabla_\theta E_\theta$

- to avoid small value inverse : $G' = \sqrt{\beta^2 I + G^\dagger G} \quad \beta \in \mathbb{R}$

Jastrow States : $\psi_n(\theta) = \exp\left(\sum_i a_i\sigma_i + \sum_{<ij>} J_{ij}\sigma_i\sigma_j\right) \quad \theta = \{a, J\}$

[NQS]Neural Quantum States : $\psi_n(\theta) = \mathrm{MLP}(\{\sigma_1, \cdots, \sigma_N\})$

[MFPWF]Mean-field projected wave function : $|\psi(\theta)\rangle = \mathcal{P}_G\left[\sum_{i,j}\sum_{s,s'} F_{ij}^{ss'}\hat{c}_{i,s}^\dagger\hat{c}_{j,s'}^\dagger\right]^{N/2}|0\rangle \quad \theta = F_{ij}^{ss'} \in \mathbb{R}^{2N\times 2N}$

represent spin as pesudo-fermions : $\hat{S}_i^{\{x,y,z\}} = \frac{1}{2}\sum_{ss'}\hat{c}_{i,s}\sigma_{ss'}^\alpha\hat{c}_{i,s'}$

> Notation
>
> - $\mathcal{P}_G$: Gutzwillller projection operator
> - $\hat{c}_{i,s}, \hat{c}_{i,s}^\dagger$: fermionic operator
> - s, s' : spin of the site, $\uparrow$ or $\downarrow$
> - i, j : index of the site

Path integrals in quantum statistical mechanics

$\rho_{\text{free}}(\vec{R}, \vec{R}', \Delta\tau) = \left\langle \vec{R}\middle| e^{-\Delta\tau\hat{T}} \middle|\vec{R}'\right\rangle = \left(\frac{2\pi\hbar^2\Delta\tau}{m}\right)^{-Nd/2}\exp\left(-\frac{|\vec{R}-\vec{R}'|^2}{2\hbar^2\Delta\tau/m}\right)$

$Z = \int \mathrm{d}\vec{R}\rho(\vec{R}, \vec{R}) = \int\left(\prod_{j=1}^M \mathrm{d}\vec{R}_j\right)\prod_{j=1}^M\left[\left(\frac{2\pi\hbar^2\Delta\tau}{m}\right)^{-Nd/2}\exp\left(-\frac{\vec{R}_j-\vec{R}_{j+1}}{2\hbar^2\Delta\tau/m} - \Delta\tau V(\vec{R}_j)\right)\right]$

> Notation
>
> - ρ_{free} : density matrix of free particles
> - Z : partition function

- $\vec{R}_j : (\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N)$, N particles position at time j
- $\hat{T}, \hat{V}$: kinetic, potential terms of Hamiltonian $\hat{H}$

path sampling method : $A(X \to X') = \min\left\{1, \frac{\exp(-m[(\vec{r}^i_{j-1}-\vec{r}^{i'}_j)^2+(\vec{r}^{i'}_j-\vec{r}^i_{j+1})^2]/2\hbar^2\Delta\tau)}{\exp(-m[(\vec{r}^i_{j-1}-\vec{r}^i_j)^2+(\vec{r}^i_j-\vec{r}^i_{j+1})^2]/2\hbar^2\Delta\tau)} \cdot \exp(-\Delta\tau[V(\vec{R}'_j)-V(\vec{R}_j)])\right\}$

The accept probability of *Metropolis algorithm* is defined above

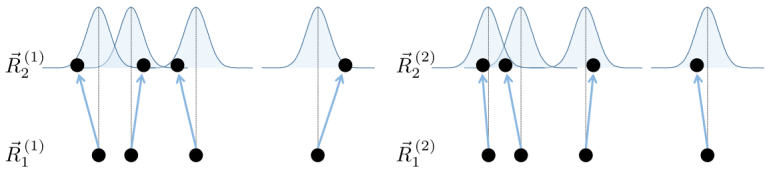
Notation

- $\vec{r}^i_j$: position of particle i at time j
- $\vec{r}^{i'}_j$: displaced position of particle i at time j
- $\vec{R}_j : (\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N)$, N particles position at time j
- V : potential energy, in most cases it's sum of single-particle and two-particle terms : $\hat{V} = \sum_i^N v_{\text{ext}}(\hat{\vec{r}}^i) + \sum_{i<j} v(\hat{\vec{r}}^i - \hat{\vec{r}}^j)$

Boson symmetry :

$\rho_{\text{Bose}} = \frac{1}{N!}\sum_P \rho(\vec{R}_1, P\vec{R}_2, \beta)$

[DMC]Diffusion Monte Carlo



Algorithm

1. $w_0^\alpha \leftarrow 1, \vec{R}_0^\alpha \leftarrow \vec{R}_0$
2. update loop
    1. $\vec{R}_k^\alpha \sim \mathcal{N}(\vec{R}_{k-1}^\alpha, \frac{\Delta\tau}{m})$: diffusion update
    2. $w_k^\alpha \leftarrow w_{k-1}^\alpha e^{-\frac{\Delta\tau}{2}[V(\vec{R}_k^\alpha)+V(\vec{R}_{k-1}^\alpha))]}$
    3. clone $\lfloor \frac{w_k^\alpha}{\mathbb{E}_\alpha[w_k^\alpha]} + r \rfloor$ times for walker α

- maximum clones $\Leftrightarrow \Delta\tau$ too large
- scale $w^\alpha \to \exp(E_t\Delta\tau)w^\alpha$ where E_t is trial energy $V(\vec{R}) - V(\vec{R}) - E_t$, when $E_t = E_0$ stability will achieve.

Importance sampling : $\vec{R}_{k-1} \leftarrow \vec{R}_{k-1} + \frac{\hbar^2\Delta\tau}{2m}\frac{\nabla\phi_t(\vec{R}_{k-1})}{\phi(\vec{R}_{k-1})}$

before update, add a dift : $\vec{R}_{k-1} \leftarrow \vec{R}_{k-1} + \frac{\hbar^2\Delta\tau}{2m}\frac{\nabla\phi_t(\vec{R}_{k-1})}{\phi(\vec{R}_{k-1})}$

Notation

- ϕ_t : trial wavefunction $\phi_t(\vec{R}) = \prod_{i<j} f_z(|\vec{r}_i - \vec{r}_j|)$
- f_z : Jastrow factor, two particle coorelations

Fermionic systems : $\phi_{t'}(\vec{R}) = \phi_t(\vec{R})\det_{l,n}[e^{i\vec{k}_l\cdot\vec{r}_n}]$

ϕ_0 could be negative, when $\phi \to -\phi$ should be applied

Notation

- n : particle index
- $\vec{k}_l$: wave vectors compatible with periodic boundary conditions

Electronic-structure problem

Full Hamiltonian of matter

$$\hat{H} = \underbrace{-\sum_j^{N_e}\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_j}}_{\hat{T}_e} \underbrace{-\sum_l^{N_n}\frac{\hbar^2}{2M_l}\nabla^2_{\vec{R}_l}}_{\hat{T}_n} + \underbrace{\frac{1}{2}\sum_{i\neq j}^{N_e}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}}_{V_{ee}} + \underbrace{\frac{1}{2}\sum_{l\neq m}^{N_n}\frac{Z_lZ_me^2}{|\vec{R}_l-\vec{R}_m|}}_{V_{nn}} \underbrace{-\sum_{j=1}^{N_e}\sum_{l=1}^{N_n}\frac{Z_le^2}{|\vec{r}_j-\vec{R}_l|}}_{V_{en}} + V_{SO}$$

Adiabatic (Born-Oppenheimer) approximation : $M_l \gg m \quad |\vec{R}_l - \vec{R}_m| \ll |\vec{r}_i - \vec{r}_j|$

$$\hat{H} = \underbrace{\sum_{j=1}^{N_e}\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_j}}_{\hat{T}_e} \underbrace{-\sum_{j=1}^{N_e}\sum_{j=1}^{N_n}\frac{Z_le^2}{|\vec{r}_j-\vec{R}_l|}}_{V_{en}} + \underbrace{\frac{1}{2}\sum_{i\neq j}^{N_e}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}}_{V_{ee}}$$

Non-interacing (mean-field) approximation : $\hat{H}_{\text{sp}} = -\frac{\hbar^2}{2m}\nabla^2_{\vec{r}} + V_{\text{eff}}(\vec{r})$

non-interacting electrons assumption, $V_{en} + V_M + V_{ee} \to V_{\text{eff}}$

Hatree-Fock approximation :

use a Slater determinant for non-interacting system

$$\langle\Phi|\hat{H}|\Phi\rangle = \underbrace{\sum_{i,\sigma}\int \mathrm{d}^3\vec{r}\;\phi_i^{\sigma *}(\vec{r})[-\frac{\hbar^2}{2m}\nabla^2 + V_{en}(\vec{r})]\sigma_i^{\sigma}(\vec{r}) + V_M}_{\hat{T}_e}$$

$$\left.\begin{aligned} &+\sum_{i,j,\sigma,\sigma'} e^2\int \mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{r}'\;\phi_i^{\sigma *}(\vec{r})\;\phi_j^{\sigma' *}(\vec{r}')\frac{1}{|\vec{r}-\vec{r}'|}\phi_i^{\sigma}(\vec{r})\phi_j^{\sigma'}(\vec{r}') \quad \text{Hatree interaction} \\ &-\sum_{i,j,\sigma} e^2\int \mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{r}'\;\phi_i^{\sigma *}(\vec{r})\;\phi_j^{\sigma *}(\vec{r})\frac{1}{|\vec{r}-\vec{r}'|}\phi_j^{\sigma}(\vec{r})\phi_i^{\sigma}(\vec{r}') \quad \text{exchange interaction} \end{aligned}\right\} V_{ee}$$

$The integration shows that the wave function \$\psi$

> Notation
>
> - i, j : index of the single particle state
> - σ, σ' : spin of the electron, $\uparrow$ or $\downarrow$
> - $\phi_i^{\sigma}(\vec{r})$: dnotes for particle i of state σ , the wave function value at position $\vec{r}$

Configuration-Interaction : $|\Phi_0\rangle = \left(1 + \sum_{i,\mu}\alpha_\mu^i\hat{c}_i^\dagger\hat{c}_\mu + \sum_{i<j,\mu<\nu}\alpha_{\mu,\nu}^{ij}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_\mu\hat{c}_\nu\right)|\Phi_{\mathrm{HF}}\rangle$

add interations between electrons correctly and allow calculation of excited state

> Notation
>
> - $|\Phi_{\mathrm{HF}}\rangle$: Hartree-Fock ground state, which is from the Hartree-Fock approximation, $|\Phi_{\mathrm{HF}}\rangle = \prod_{\mu=1}^{N}\hat{c}_\mu^\dagger|\mathrm{nulll}\rangle$
> - $\hat{c}^\dagger, \hat{c}$: creation / annihilation operator

[DFT] Density functional theory

Hohenberg-Kohn Theorem : for electron system $\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\sum_j\nabla_j^2}_{\hat{T}_e} + \underbrace{\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}}_{\hat{V}_{ee}} + \underbrace{\int v_{\mathrm{ext}}(\vec{r})n(\vec{r})\mathrm{d}\vec{r}}_{\hat{V}_{\mathrm{ext}}}$

- **Uniqueness** : $n_0(\vec{r}) \Leftrightarrow \nu_{\mathrm{ext}}(\vec{r})$
- **Variational** : $n_0 = \underset{n}{\operatorname{argmin}}\;E = \underset{n}{\operatorname{argmin}}\;\langle\Psi|\hat{H}|\Psi\rangle$

> Notation
>
> - $\nu_{\mathrm{ext}}(\vec{r})$: external potential density
> - $n_0(\vec{r})$: ground state electron density
> - $n(\vec{r})$: electron density $\sum_j|\phi_j(\vec{r})|^2$

Kohn-Sham solution :

non-interacting system that has the same particle density as the interacting one

> Algorithm
>
> 1. initial guess V_{eff}^0
> 2. solve ϕ_j (eigen vector) from KS1 : $\left[-\frac{\hbar^2}{2m_e}\nabla^2 + V_{\mathrm{eff}}(\vec{r})\right]\phi_j(\vec{r}) = \varepsilon_j\phi_j(\vec{r})$
> 3. $n(\vec{r}) \leftarrow \sum_i|\phi_j(\vec{r})|^2$
> 4. revise V_{eff} from KS 2 : $V_{\mathrm{eff}}(\vec{r}) = \int \mathrm{d}^3r'\frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|} + \mu^{\mathrm{XC}}(\vec{r}) + \nu_{\mathrm{ext}}(\vec{r})$
> 5. goto 2 if $|V_{\mathrm{eff}}^{\mathrm{new}} - V_{\mathrm{eff}}^{\mathrm{odd}}| \geq \mathrm{threshold}$

> Notation
>
> - μ^{XC} : functional derivative of the exchange-correlation energy, $\mu^{\mathrm{XC}} = \frac{\mathrm{dE}^{\mathrm{XC}}}{\mathrm{d}n}$
> - E^{XC} : exchange-correlation energy, $E^{\mathrm{XC}} = \langle\Phi|\hat{T}|\Phi\rangle - E_k + \langle\Phi|\hat{V}_{ee}|\Phi\rangle - E_c$ with approximation (local density approximation) $E^{\mathrm{XC}} \approx \int n(\vec{r})\varepsilon^{\mathrm{XC}}(n(\vec{r}))\mathrm{d}\vec{r} = \int n(\vec{r})[\varepsilon^X(n(\vec{r})) + \varepsilon^C(n(\vec{r}))]\mathrm{d}\vec{r}$
>   - uniform electron gas : $\varepsilon(n(\vec{r})) = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}n(\vec{r})^{1/3}$
>   - Monte carlo -> interpolation
> - E_C : Hartree energy $E_C = \frac{1}{2}\int e^2\frac{n(\vec{r})n(\vec{r}')}{|\vec{r}-\vec{r}'|}\mathrm{d}\vec{r}\mathrm{d}\vec{r}'$
> - E_K : kinetic energy $E_K = -\frac{\hbar^2}{2m}\sum_j\langle\phi_j|\nabla^2|\phi_j\rangle$

Basis functions

Atoms and molecules

- [STO] Slater Type Orbitals : $\psi_{nlm}^i(r,\theta,\phi) \propto r^{n-1}e^{-\xi_i r}Y_{lm}(\theta,\phi)$
  - two nuclei no closed form
- [GTO] Gauss Type Orbitals : $\psi_{nlm}^i(\vec{r}) \propto x^l y^m z^n e^{-\xi_i r^2}$
  - gaussian product still gaussian easy to integral

Free electron gas

$$\hat{H} = \underbrace{-\sum_{i=1}^{N_e} \frac{\hbar^2}{2m} \nabla_{\vec{r}_i}^2}_{\hat{T}} + \underbrace{e^2 \sum_{i<j} \frac{1}{|\vec{r} - \vec{r}'|}}_{\hat{V}_{ee}}$$

- plane waves basis : $\psi_{\vec{k}}(\vec{r}) = \exp(-i\vec{k} \cdot \vec{r})$
- low temperature : Wigner crystal
  - eigenfunctions of harmonic oscillatiors centered around

Pseudo-potentials

- only model outer shell with basis, use pseudo potential to model inner shell since they are not involved in chemical bond

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Quantum Computing

Quantum Computer

quantum gates

- one-qubit gate

X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
name	matrix	name	matrix	name	matrix
$H = \frac{X+Z}{\sqrt{2}}$	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$	$S = T^2$	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$

- two-quitbit gate $C(U) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & & \\ 0 & 0 & & U \end{bmatrix}$

measurement : $|\langle z_1 z_2 \dots | \psi \rangle|^2$

- repeated $\mathcal{O}(1000)$ times

errors

- coupling to environment $\Rightarrow$ mixed density matrix
- gate error
- read out measurement error

Representing the Hilbert space

Spin-$\frac{1}{2}$ system : directly mapped to a qubit

Fermionic system

- **Jordan-Wigner Transformation** : $|\Psi\rangle = |n_{N-1}, \cdots, n_0\rangle \leftrightarrow |z_{N-1}, \cdots, z_0\rangle \quad n_i = z_i$
  $\hat{c}_i \leftrightarrow A_i Z_{i-1} \cdots Z_0 \quad \hat{c}_i^\dagger \leftrightarrow A_i^\dagger Z_{i-1} \cdots Z_0 \quad A_i = \frac{(X_i + iY_i)}{2}$
  - measuring parity requires $\mathcal{O}(N)$ operators
  - updating an occupation number requires $\mathcal{O}(1)$ operators
- **Parity Encoding** : $|\Psi\rangle = |n_{N-1}, \cdots, n_0\rangle \leftrightarrow |z_{N-1}, \cdots, z_0\rangle \quad z_i = \left[\sum_{j=0}^{i} n_i\right] \bmod 2$
  $\hat{c}_i \leftrightarrow X_{N-1} \cdots X_{i+1} (X_i Z_{i-1} + iY_i) \quad \hat{c}_i^\dagger \leftrightarrow X_{N-1} \cdots X_{i+1} (X_i Z_{i-1} - iY_i)$
  - measuring parity requires $\mathcal{O}(1)$ operators
  - updating an occupation requires $\mathcal{O}(N)$ operators
- **Bravyi-Kitaev** : a hypbrid of **Parity** and **Jordan-Wigner**

> Notation
>
> - n_i : fermionic orbitals/site occupation number $n_i \in \{0, 1\}$
> - $\hat{c}_i, \hat{c}_i^\dagger$: creation operator, annihilation operator

Variational quantum solver

extract the spectrum of an operator

[QFT] Quantum fourier transform

- exact solution
- vast number of gate operations

[VQE] Variational Quantum Eigensolver : $\min_\theta \frac{\langle \Psi(\theta) | \hat{H} | \Psi(\theta) \rangle}{\langle \Psi(\theta) | \Psi(\theta) \rangle}$

- quantum computer : expectation evaluation

- classical computer : optimization COBYLA (no SGD since no gradient)

[UCC] Unitary Coupled Cluster : $|\Psi(\theta)\rangle = e^{\hat{T}(\theta)-\hat{T}^{\dagger}(\theta)}\,|\Psi_0\rangle$

- a good choice for variational state
- huge circuit depth
- much depend on the choice of state $|\Phi_0\rangle$

[UCCSD] Unitary Coupled Cluster with Single and Double excitation

- $\hat{T}(\theta) \approx \hat{T}_1(\theta_1) + \hat{T}_2(\theta_2)$
  - $\hat{T}_1(\theta_1) = \sum_{i,j} \theta_{1,i,j} \hat{c}_i^{\dagger} \hat{c}_j$
  - $\hat{T}_2(\theta_2) = \sum_{i,j} \theta_{2,i,j,k,l} \hat{c}_i^{\dagger} \hat{c}_k^{\dagger} \hat{c}_j \hat{c}_l$

> Notation
>
> - $\hat{T}(\theta)$: excitation operator
> - $|\Psi_0\rangle$: Hartree-Fock/single Slater detereminant state