CQP Computational Quantum Physics

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professor : Mark H Fischer

author : walkerchi

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
- $\lambda = \pm 1$: 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 1-body problem

given V ,we want to know ψ according to Schrödinger equation $-\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V(x)\psi(x) = E\psi(x)$

Time-Independent 1 D 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

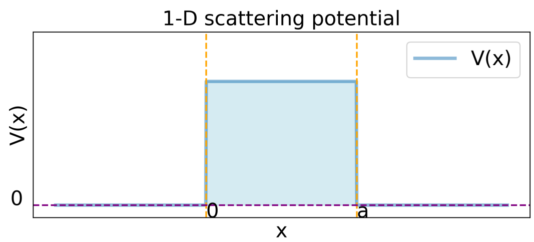
Numerov algorithm

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

- **initial problem for symmetry** $V(x) = V(-x)$
  - $\psi(x) = -\psi(x)$: half integer mesh with $\psi(-\frac{1}{2}\Delta x) = \psi(\frac{1}{2}\Delta x) = 1$
  - $\psi(-x) = -\psi(x)$: integer mesh with $\psi(0) = 0 \quad \psi(\Delta x) = 1$
- **general** $V(x) = 0$ **for** $|x| \geq a$
  - $\psi(-a - \Delta x) = \exp(-\Delta x\sqrt{-2mE}/\hbar) \quad \psi(-a) = 1$

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



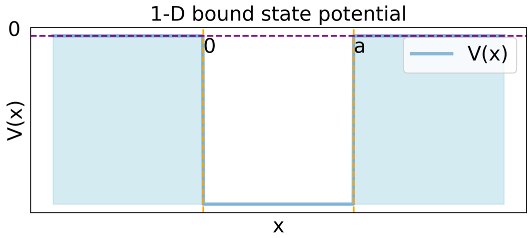
- wave function assumptions :
  - left ($x < 0$) wave function : $\psi_L(x) = \underbrace{Ae^{iqx}}_{\text{origin wave}} + \underbrace{Be^{-iqx}}_{\text{reflection}}$
  - right ($x > a$) wave function : $\psi_R(x) = \underbrace{Ce^{iqx}}_{\text{transmission}}$
  - where q is the wave number $q^2 = \frac{2m[E - V(x)]}{\hbar^2}$
- 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 $V(x) \begin{cases} < 0 & x \in [0, a] \\ = 0 & \text{others} \end{cases}$



- **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 eigenvalue else try another E

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

> Algorithm
>
> 1. try a position $b \in (0, a)$, that $E = V(b),\ \frac{\partial^2 \psi_E}{\partial x^2} = 0$
> 2. use numerov from a to b as ψ_L and from 0 to b as ψ_R
> 3. satisfy $\frac{\psi_L'(b)}{\psi_L(b)} = \frac{\psi_R'(b)}{\psi_R(b)}$ (ψ_L, ψ_R are not normalized), then E is a eigenvalue 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** : $|\phi\rangle = \sum_i^N a_i |u_i\rangle$

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

  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 $U^\top S U = I$
  > - $\vec{b}$: 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

> Notation
>
> - $|\phi_n\rangle$: eigenvector of $H|\phi\rangle = E|\phi\rangle$, $|\psi_0\rangle = \sum c_n |\phi_n\rangle$
> - ε_n : eigenvalue of $H|\phi\rangle = E|\phi\rangle$

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

- **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** : $(\mathbb{1} + \frac{i\Delta t}{2\hbar} H)\psi(\vec{r}, t+\Delta t) = (\mathbb{1} - \frac{i\Delta t}{2\hbar} H)\psi(\vec{r}, t)$
  - H is sparse matrix, using iterative solver (e.g. biconjugate gradient)

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

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

> 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

- $\mathcal{F} = \underbrace{\mathcal{F}_0}_{0 \text{ particles}} \oplus \underbrace{\mathcal{F}_1}_{1 \text{ particles}} \oplus \cdots$

> 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 $\mathcal{S}_- = \mathcal{N}_A \sum_p \mathrm{sgn(p)}$

> Example

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

anti-symmetrized and normalized N single particle wave function product

> Notation
> - $\phi_i(r_j)$: wave function of fermion i at position r_j

Creation and annihilation operators

- $\hat{a}$ **annihilation operator** : remove particle $\hat{a}_i |\phi_j\rangle = \delta_{ij} |0\rangle$
- $\hat{a}^\dagger$ **creation operator** : add particle $|\phi_i\rangle = \hat{a}_i^\dagger |0\rangle$

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

- Bosons : commute
  - $\hat{a}_i |n_i\rangle = \sqrt{n_i} |n_i - 1\rangle \quad \hat{a}_i^\dagger |n_i\rangle = \sqrt{n_i + 1} |n_i + 1\rangle$
  - $\hat{a}_i^\dagger \hat{a}_i = n_i$
  - $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \quad [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$
  - $0 \underset{\hat{a}}{\leftarrow} |0\rangle \underset{\hat{a}}{\overset{\hat{a}^\dagger}{\rightleftharpoons}} |1\rangle \underset{\hat{a}}{\overset{\hat{a}^\dagger}{\rightleftharpoons}} |2\rangle \cdots$

- Fermions : anti-commute
  - $\hat{c}_{u_i} |u_i, u_j, \cdots\rangle = |u_j, \cdots\rangle \quad \hat{c}_{u_i} |u_j, \cdots\rangle = |u_i, u_j, \cdots\rangle$
  - $\hat{c}_i^\dagger \hat{c}_i = \hat{n}_i$
    - $n_i = 0 : \hat{c}_i^\dagger \hat{c}_i |u_j, \cdots\rangle = 0$
    - $n_i = 1 : \hat{c}_{u_i}^\dagger \hat{c}_{u_i} |u_i, u_j, \cdots\rangle = |u_i, u_j, \cdots\rangle$
  - $\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij} \quad \{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$
  - $0 \underset{\hat{c}_{u_i}^\dagger}{\leftarrow} |0\rangle \underset{\hat{c}_{u_i}}{\overset{\hat{c}_{u_i}^\dagger}{\rightleftharpoons}} |u_i\rangle \overset{\hat{c}_{u_i}^\dagger}{\rightarrow} 0$

Quantum Spin Model

(TFIM)Transverse field Ising model

$$\hat{H}=\sum_{<ij>}J_{ij}\hat{S}^z_i\hat{S}^z_j-\sum_i\frac{h_i}{2}\hat{S}^x_i$$

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

- 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

$$\begin{aligned}\hat{H}&=\sum_{<ij>}J_{ij}\hat{\vec{S}}_i\cdot\hat{\vec{S}}_j=\sum_{<ij>}J_{ij}\left(\hat{S}^x_i\hat{S}^x_j+\hat{S}^y_i\hat{S}^y_j+\hat{S}^z_i\hat{S}^j_z\right)\\&=\sum_{<ij>}J_{ij}\left[\frac{1}{2}\left(\hat{S}^+_i\hat{S}^-_j+\hat{S}^-_i\hat{S}^+_j\right)+\hat{S}^z_i\hat{S}^z_j\right]\end{aligned}$$

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

- 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

$$\hat{H}=\sum_{<ij>}J_{ij}\left(\hat{S}^x_i\hat{S}^x_j+\hat{S}^y_i\hat{S}^y_j+\Delta\hat{S}^z_i\hat{S}^z_j\right)$$

- 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

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

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

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*
>
> $$\vec{r}_0 = \frac{\vec{v}}{||\vec{v}||} \quad \beta_m \vec{r}_m = H\vec{r}_{m-1} - \alpha_{m-1}\vec{r}_{m-1} - \beta_{m-1}\vec{r}_{m-2} \quad \alpha_n = \vec{r}_n^\dagger H \vec{r}_n \quad \beta_n = |\vec{r}_n^\dagger H \vec{r}_{n-1}|$$
>
> 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 ^ (3<<i)`

> 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.

> Notation
>
> - $\hat{S}^\pm : \hat{S}^\pm = \hbar\sigma^\pm = \hbar(\sigma_x \pm i\sigma_y)$

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

- 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* $\rho_A = \sum_\alpha \lambda_\alpha^2 |\phi_\alpha\rangle_A \langle\phi_\alpha|_A \rightarrow S - \sum_\alpha \lambda_\alpha^2 \mathrm{log}\lambda_\alpha^2$

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

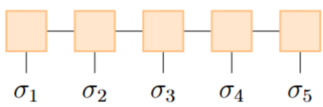
Area law of entanglement : entanglement entropy scales as $S \propto L^{D-1}$

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

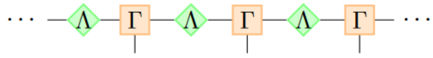
> Notation
>
> - S : entanglement entropy
> - d : Hilbert space dimension
> - λ : eigen value
> - N : number of sites
> - D : dimension of the entanglement system
> - L : linear dimension of system

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) : $A = \Lambda\Gamma$

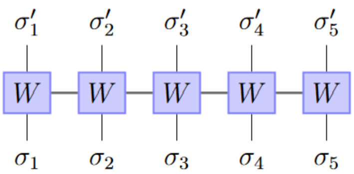


> Example : GHZ or 'cat' state
>
> $$|GHZ\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle^{\otimes N} + |\uparrow\rangle^{\otimes N}) = \frac{1}{Z}\left(\mathrm{Tr}\left((A^{\uparrow})^N\right)|\uparrow\rangle^{\otimes N} + \mathrm{Tr}\left((A^{\downarrow})^N\right)|\downarrow\rangle^{\otimes N}\right)$$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

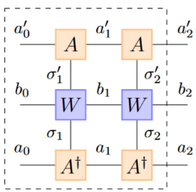
> Example : AKLT state
>
> ground state of spin-1 Hamiltonian : $\hat{H} = \sum_j \hat{\vec{S}}_j \cdot \hat{\vec{S}}_{j+1} + \frac{1}{3}\left(\hat{\vec{S}}_j \cdot \hat{\vec{S}}_{j+1}\right)^2$
>
> with matrices :
>
> $A_i^+ = A^+ = \sqrt{\frac{2}{3}}\sigma^+ = \begin{bmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix}$ $\quad A_i^0 = A^0 = \frac{-1}{\sqrt{3}}\sigma^z = \begin{bmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{bmatrix}$ $\quad A_i^- = A^- = -\sqrt{\frac{2}{3}}\sigma^- \begin{bmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{bmatrix}$
>
> 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 , $\sigma^+ = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$
>   - $\sigma^+ |\downarrow\rangle = 0$
>   - $\sigma^+ |\uparrow\rangle = |\downarrow\rangle$
> - σ^- : annihilation / lowering operator, $\sigma^- = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$
>   - $\sigma^- |\downarrow\rangle = |\uparrow\rangle$
>   - $\sigma^- |\uparrow\rangle = 0$
> - $|+\rangle$: 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 $\hat{H} = -\sum_i h\hat{S}_i^z$
>
> $\hat{H} = (-h\hat{S}^z \otimes I \otimes \cdots \otimes I) + \cdots + (I \otimes \cdots \otimes I \otimes -h\hat{S}^z)$
>
> $W_1 = \begin{bmatrix} -hS^z & I \end{bmatrix}$ $\quad W_i = \begin{bmatrix} I & 0 \\ -hS^z & I \end{bmatrix}$ $\quad W_N = \begin{bmatrix} I \\ -hS^z \end{bmatrix}$

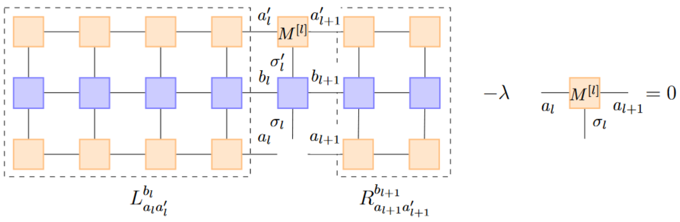
> Example : Transverse field Ising model $\hat{H} = -\sum_i \hat{S}_i^z\hat{S}_{i+1}^z + h\sum_i \hat{S}_i^x$
>
> $W_1 = \begin{bmatrix} hS^x & -S^z & I \end{bmatrix}$ $\quad W_i = \begin{bmatrix} I & 0 & 0 \\ S^z & 0 & 0 \\ hS^x & -S^z & I \end{bmatrix}$ $\quad W_N = \begin{bmatrix} I \\ S^z \\ hS^x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

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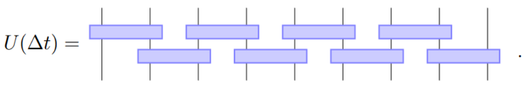
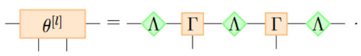
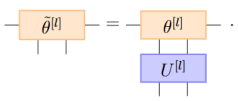
>
>   2. left normalize M_l
>   3. build L_l
>   2. Left sweep for $l = L, \dots, 2$
>   1. solve eigen value for M_l
>   2. right normalize M_l
>   3. build R_l

[TEBD] Time evolving block decimation



> Algorithm
>
> 1. two site tensor contraction
>
> 
>
>
> 2. apply evolution gate
>
> 
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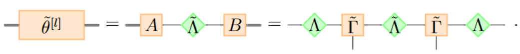
>
> 3. split into single site tensor
>
> 
>
>
> 4. truncation : keep $\chi_{\max}$ eigen value and renormalize $\sum_i \Lambda_i i^2 = 1$

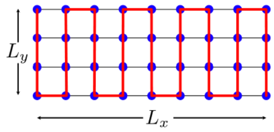
Computation errors :

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

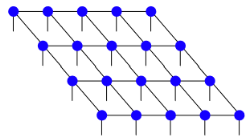
Further topics

Two-dimensional system

- converting two dimension system as chain



- [PEPS] projected entangled pair state

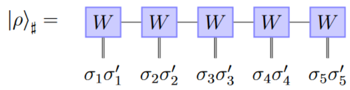


  - challenging computationally
  - lack a canonical form

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

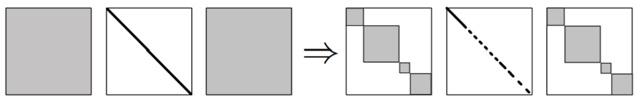
  which can be described by *Lindblad equation* : $\partial_t \hat{\rho} = \hat{\mathcal{L}}\hat{\rho} = -i[\hat{H}, \hat{\rho}] + \sum_i \gamma_i \left(\hat{L}_i \hat{\rho} \hat{L}_i^\dagger - \frac{1}{2}\{\hat{L}_i^\dagger \hat{L}_i, \hat{\rho}\} \right)$



> 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 : $S = \int_{t_1}^{t_2} \langle \psi(t)| i\partial_t - \hat{H} |\psi(t)\rangle \mathrm{d}t \rightarrow \partial_t A_i = -iH_i A_i$
- 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 : $P_{XY} = T(X \rightarrow Y)A(X \rightarrow Y) \quad A(X \rightarrow Y) = \min\left\{1, \frac{W(Y)}{W(X)}\right\}$

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

> 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
> - β : inverse temperature, $\beta=\frac{1}{\kappa_B T}$
> - m : magnetization

> 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 : $\langle m^2\rangle_{C'}=\frac{1}{N^2}\sum_c|c|^2$
> 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
> - $\beta E_0=M\beta J$

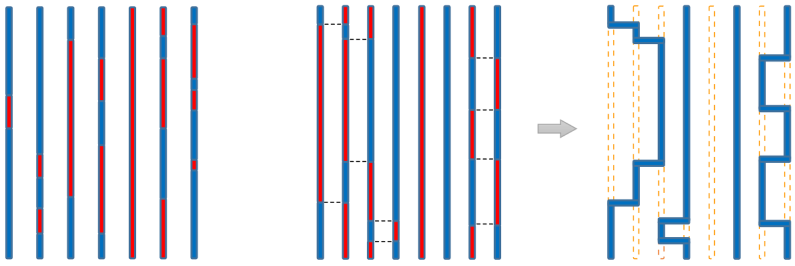
Continous-time path integral : $\Delta\tau\to 0$???

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

> Example : 1D classical Ising model (0D transverse field Ising model)

quantum XY model : $\hat{H} = -\sum_{<i,j>} \frac{J_{xy}}{2}(\hat{S}_i^+\hat{S}_j^- + \hat{S}_i^-\hat{S}_j^+)$

spin flip-flops (blue line) proportional to β which is a constant not grow bigger as $\Delta\tau \to 0$



negative sign problem : positive off diagonal lead to negative probabilities

- solution : $\langle\hat{A}\rangle_W = \frac{\sum_C A(C)W(C)}{\sum_C W(C)} = \frac{\sum_C A(C)\mathrm{sign}(W)|W(C)|/\sum_C|W(C)|}{\sum_C \mathrm{sign}(W)|W(C)|/\sum_C|W(C)|}$
- error : $\beta\uparrow, L\uparrow \to \epsilon\uparrow$ error ϵ increase with inverse temperature β and system size L

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 $G_{kl} = \langle\hat{O}_k^*\hat{O}_l\rangle_\theta - \langle\hat{O}_k^*\rangle_\theta\langle\hat{O}_l\rangle_\theta$
> - O : logarithm wave-function derivative $O = \nabla_\theta\psi_n(\theta)/\psi_n(\theta)$
>   - $\hat{O} = \sum_n O(n)\,|n\rangle\,\langle n|$

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

- $\nabla_\theta\langle E\rangle_\theta = 2\mathrm{Re}\left\{\sum_n W(n)[E_1(n) - E_\theta]O(n)\right\}$

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

wave function form for spin system

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

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

- $\psi_n(\theta) = (N/2)!\mathrm{Pf}(X)$

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

Path integrals in quantum statistical mechanics

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

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

> 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 $\hat{H}, \hat{T} = -\frac{\hbar^2}{2m}\partial_x^2$

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

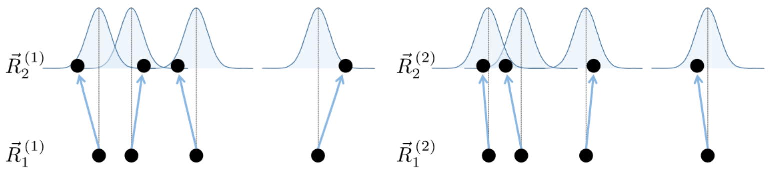
$H = \sum_j \sum_i \frac{m}{2(\hbar\Delta\tau)^2}(\vec{r}^i_j - \vec{r}^i_{j+1})^2 + \sum_j V(\vec{R}_j)$

> 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. $\vec{R}_k^\alpha \sim \mathcal{N}(\vec{R}^\alpha_{k-1}, \frac{\Delta\tau}{m})$: diffusion update
>   2. $w_k^\alpha \leftarrow w^\alpha_{k-1} e^{-\frac{\Delta\tau}{2}[V(\vec{R}^\alpha_k)+V(\vec{R}^\alpha_{k-1})]}$
>   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 $V(\vec{R}) \leftarrow V(\vec{R}) - E_t$, when $E_t = E_0$ stability will achieve.

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

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

> 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

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

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

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

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

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

$$\left.\begin{array}{ll} + \sum_{i,j,\sigma,\sigma'} e^2 \int \mathrm{d}^3\vec{r}\,\mathrm{d}^3\vec{r}'\,\phi_i^{\sigma *}(\vec{r})\,\phi_j^{\sigma' *}(\vec{r}')\frac{1}{|\vec{r}-\vec{r}'|}\phi_i^{\sigma}(\vec{r})\phi_j^{\sigma'}(\vec{r}') & \text{Hatree interaction} \\ - \sum_{i,j,\sigma} e^2 \int \mathrm{d}^3\vec{r}\,\mathrm{d}^3\vec{r}'\,\phi_i^{\sigma *}(\vec{r})\,\phi_j^{\sigma *}(\vec{r})\frac{1}{|\vec{r}-\vec{r}'|}\phi_j^{\sigma}(\vec{r})\phi_i^{\sigma}(\vec{r}') & \text{exchange interaction} \end{array}\right\} V_{ee} \quad The integration shows that the wave function \$\psi$$

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

> Notation
>
> - $v_{\mathrm{ext}}(\vec{r})$: 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 :

find a 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 : $V_{\mathrm{eff}}(\vec{r}) = \int \mathrm{d}^3 r' \frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|} + \mu^{\mathrm{XC}}(\vec{r}) + \nu_{\mathrm{ext}}(\vec{r})$
> 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, $\mu^{\mathrm{XC}} = \frac{\mathrm{dE}^{\mathrm{XC}}}{\mathrm{dn}}$
> - 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

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

- plane waves basis : $\psi_{\vec{k}}(\vec{r}) = \exp(-i\vec{k} \cdot \vec{r})$
- low temperature : Wigner crystal
    - better basis will be 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 $C(U) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & & \\ 0 & 0 & \multicolumn{2}{c}{U} \end{bmatrix}$

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

- 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** : $|\Psi\rangle = |n_{N-1}, \cdots, n_0\rangle \leftrightarrow |z_{N-1}, \cdots, z_0\rangle \quad z_i = \left[\sum_{j=0}^{i} n_i\right] \mathrm{mod}\ 2$
  $\hat{c}_i \leftrightarrow X_{N-1} \cdots X_{i+1}(X_i Z_{i-1} + iY_i) \quad \hat{c}_i^\dagger \leftrightarrow X_{N-1} \cdots X_{i+1}(X_i Z_{i-1} - iY_i)$
    - 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