EXACT DIAGONALIZATION

PART II. MANY-PARTICLE SYSTEMS

N constituents (spins, electrons, ...)

$$H^{(N)} = \underbrace{\mathcal{H} \otimes \mathcal{H} \otimes \cdots}_{N \text{ times } \mathcal{H}}$$

$\dim(\mathcal{H}) = d$ $\boxed{\dim(\mathcal{H}^N) = d^N}$! Terrible :(
It can be very large number

for Spin 1/2

$d = 2 \longrightarrow |\uparrow\rangle, |\downarrow\rangle$

$\dim(\mathcal{H}^N) = 2^N$

for $N = 30$, $2^{30} \approx 10^9 \Rightarrow$ approximately 16 GB of memor to store $|\psi\rangle_N$

Sparse Hamiltonians

$\hat{A} \in M \times M$ M^2 entries

$\hat{H} \in M \times M \longrightarrow M = 2^N$ $N^\alpha \times M$ entries

Hamiltonian

where $\alpha = 1, 2, 3, 4$

Basis

$$|S_1, S_2, \dots, S_N\rangle = |S_1\rangle \otimes |S_2\rangle \otimes \dots |S_N\rangle$$

$$\sigma_i^z |S_1, \dots, S_N\rangle = \underbrace{s_i}_{\text{eigenvalue of } S_i} |S_1 \dots S_N\rangle$$

$$s_i = \pm 1$$

Transverse Field Ising Model

$$\hat{H} = \sum_{\underbrace{\langle i,j \rangle}_{\text{nearest neighbours}}} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_{i=1}^{N} \hat{\sigma}_i^x$$

The meaning of $\hat{\sigma}_i^\alpha$

$$\hat{\sigma}_i^\alpha = \underbrace{\hat{I} \otimes \hat{I} \dots \otimes I}_{i-1} \otimes \hat{\sigma}^\alpha \otimes \underbrace{I \otimes \dots \otimes I}_{N-i}$$

$$= \hat{I}(2^{i-1}) \otimes \hat{\sigma}^\alpha \otimes \hat{I}(2^{N-i})$$

Matrix Elements

$$\langle s_1 \dots\dots s_N | \hat{H} | s_1' \dots s_N' \rangle = H(\vec{s}, \vec{s}\,')$$

$$\langle S_1 \dots S_N | \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z | s_1' \dots s_N' \rangle = \delta_{S,S'} \sum_{\langle i,j \rangle} J_{ij} \overbrace{S_i S_j}^{\text{eigenvalues}}$$

when $S = S'$

(diagonal matrix elements)

$$\langle s_1 \dots s_N | \sigma_i^x | s_1' \dots s_N' \rangle = \delta_{s_1, s_1'} \delta_{s_2, s_2'} \dots \delta_{s_i, -s_i'} \dots \delta_{s_N, s_N'}$$

$$\# \text{Non-zero} = 2^N + N.2^N = (N+1)\,2^N \Rightarrow \alpha = 1$$

Sparse Matrix

$$\hat{H}|v\rangle = |v'\rangle$$

cost $\rightarrow$ $O(N^\alpha \times 2^N)$

order

dense matrix cost $\sim \Theta(2^N \times 2^N)$

Find the Ground State

ITERATIVE METHODS

→ Power Method

$k = 1, \ldots\ldots p$ steps

can not be normalized

$$|v_{k+1}\rangle = \underbrace{(\Lambda\hat{I} - \hat{H})}_{\text{non unitary}} |v_k\rangle$$

$|v_0\rangle$ = Initial Condition

$$|v_p\rangle \xrightarrow{p\infty} |E_0\rangle$$

→ ground state

Proof

$$|v_0\rangle = \sum_{\ell=1}^{2^N} c_\ell |E_\ell\rangle$$

$$E_0 \leq E_1 \leq \ldots\ldots \leq E_N$$

$$\boxed{|v_p\rangle = (\Lambda I - \hat{H})^p |v_0\rangle}$$

$$= \sum_{l=0}^{2^N-1} c_\ell (\Lambda - E_\ell)^p |E_\ell\rangle$$

$$\langle E_0|v_p\rangle = c_0 (\Lambda - E_0)^p$$

$$\boxed{\Lambda > E_{N-1}}$$

$$\frac{|\langle E_0 | u_p \rangle|^2}{\langle u_p | u_p \rangle} = \frac{|c_0|^2 (\Lambda - E_0)^{2p}}{|c_0|^2 (\Lambda - E_0)^{2p} + |c_1|^2 (\Lambda - E_1)^{2p} + \dots}$$

$$= \frac{1}{1 + \left|\frac{c_1}{c_0}\right|^2 \left(\frac{\Lambda - E_1}{\Lambda - E_0}\right)^{2p} + \dots + \left|\frac{c_m}{c_0}\right|^2 \left(\frac{\Lambda - E_{N-1}}{\Lambda - E_0}\right)^{2p}}$$

small

$$= 1 - \left|\frac{c_1}{c_0}\right|^2 \left(\frac{\Lambda - E_1}{\Lambda - E_0}\right)^{2p} + \dots$$

when $p \to \infty$ it goes 1.

→ Lanchoz Method

Krylov Subspace

$$\{ |U_1\rangle , \dots , |U_p\rangle \}$$

$$|U_i\rangle = \hat{H}^i |U_0\rangle$$

$$\langle U_i | U_j \rangle \neq \delta_{i,j}$$

$$|v_1\rangle, |v_2\rangle, \quad \ldots\ldots \quad |v_p\rangle$$

$$\beta_{m+1} |v_{m+1}\rangle = \hat{H} |v_n\rangle - \alpha_n |v_n\rangle - \beta_n |v_{n-1}\rangle$$

$$\langle v_i | v_j \rangle = \delta_{ij}$$

$$\alpha_n = \langle v_n | \hat{H} | v_n \rangle$$

$$\beta_n = | \langle v_n | \hat{H} | v_{n-1} \rangle |$$

$$\hat{T}^{(p)} = \begin{pmatrix} \alpha_1 & \beta_2 & & 0 \\ \beta_2 & \alpha_2 & & \\ & & \ddots & \beta_p \\ 0 & & \beta_p & \alpha_p \end{pmatrix}$$

$$\text{Eigenvalues of } \hat{T}^{(p)} \overset{p \to \infty}{\simeq} \text{Eigenvalues of } \hat{H}$$

Quantum Dynamics

$$|\psi(t)\rangle = e^{-i\hat{H}t} |\psi(0)\rangle \quad , \quad t_n = t_0 + n\Delta_t$$

Taylor Expansion:

$$|\psi(t+\Delta t)\rangle = \left[I - i\hat{H}\Delta_t - \frac{1}{2}\hat{H}\Delta t^2 + \dots \quad \Delta t^s \right] |\psi(t)\rangle + O(\Delta_t^{s+1})$$

$$\left.\begin{aligned} |r_k\rangle &= -i\frac{\Delta t}{k}\hat{H}|r_{k=0}\rangle \\ |\Delta_k\rangle &= |\Delta_{k-1}\rangle + |r_k\rangle \end{aligned}\right\} \quad \begin{aligned} &k = 1, 2, \dots, s \\ &|r_0\rangle = |\Delta_0\rangle = |\psi(t)\rangle \end{aligned}$$

$$|\Delta_s\rangle = |\psi(t+\Delta t)\rangle$$

Unitary Scheme

$$\hat{H} = \hat{\sum_k} \hat{h}_k \qquad [\hat{h}_k, \hat{h}_{k'}] = (1 - \delta_{kk'})$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(x)$$

Ex. TFI

$$\hat{h}_x = \sum_i \hat{\sigma}_i^x$$

$$\hat{h}_{zz} = \sum_{\langle i,j\rangle} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z \quad , \quad n = 2$$

Trotter-Suzuki Formula

$$\exp[-i\Delta_t \hat{H}] \simeq e^{-i\Delta_t \hat{h}_1} e^{-i\Delta_t \hat{h}_2} \cdots e^{-i\Delta_t \hat{h}_n} + O(\Delta_t^2)$$

$\Rightarrow$ 1^{st} order Trotter Formula

$$\exp[-i\Delta t\, \hat{H}] \simeq e^{-i\frac{\Delta t}{2}\hat{h}_1} e^{-i\frac{\Delta t}{2}\hat{h}_2} \cdots e^{-i\frac{\Delta t}{2}\hat{h}_n} e^{-i\frac{\Delta t}{2}h_{n-1}} \cdots e^{-i\frac{\Delta t}{2}\hat{h}_1} + O(\Delta t^3)$$