Class 1: Exact diagonalization

Tutorial example: XXZ-model in 1D

$$H = \sum_{i=1}^{L-1} J \cdot \left(S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta \cdot S^z_i S^z_{i+1} \right) + J\left(S^x_L S^x_1 + S^y_L S^y_1 + \Delta S^z_L S^z_1 \right)$$

for periodic B.C.

anisotropy

spin-1/2 operators:

$$S^{x,y,z} = \frac{1}{2}\sigma^{x,y,z}$$

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Pauli matrices

L=2 minimal toy-model

$$H = J\left(S^x_1 S^x_2 + S^y_1 S^y_2 + \Delta S^z_1 S^z_2 \right)$$

$$S^a_1 = S^a \otimes 1\!\!1_{2\times2} \qquad a \in \{x, y, z\}$$

$$S^a_2 = 1\!\!1_{2\times2} \otimes S^a$$

$$\Downarrow$$

$$S^a_1 S^a_2 = \left(S^a \otimes 1\!\!1_{2\times2}\right)\left(1\!\!1_{2\times2} \otimes S^a\right) = S^a \otimes S^a$$

Kronecker (tensor) product

$$\underline{\underline{A}} = \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & & \\ A_{n1} & \cdots & A_{nn} \end{pmatrix} \qquad \underline{\underline{B}} = \begin{pmatrix} B_{11} & \cdots & B_{1m} \\ \vdots & & \\ B_{m1} & \cdots & B_{mm} \end{pmatrix}$$

$$\underline{\underline{A}} \otimes \underline{\underline{B}} = \begin{pmatrix} A_{11}\underline{\underline{B}} & \cdots & A_{1n}\underline{\underline{B}} \\ \vdots & & \\ A_{n1}\underline{\underline{B}} & \cdots & A_{nn}\underline{\underline{B}} \end{pmatrix}$$

acts on basis $|e_i\rangle \otimes |f_j\rangle$ ordered lexicographically.

Product basis:

$|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle \sim \{|e_1\rangle \otimes |e_2\rangle\}$

Lexicographic (~binary) ordering

00, 01, 10, 11

$$H = J\left(\underbrace{S^x \otimes S^x}_{} + \underbrace{S^y \otimes S^y}_{} + \Delta \cdot \underbrace{S^z \otimes S^z}_{} \right)$$

$$\frac{1}{4}\begin{pmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{pmatrix} \quad \frac{1}{4}\begin{pmatrix} & & & -1 \\ & & +1 & \\ & +1 & & \\ -1 & & & \end{pmatrix} \quad \frac{1}{4}\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}$$

$$\Rightarrow \quad \boxed{H_{L=2} = \frac{J}{4}\begin{pmatrix} \Delta & & & \\ & -\Delta & 2 & \\ & 2 & -\Delta & \\ & & & \Delta \end{pmatrix}}$$

Note: $S^z_{tot} = S^z_1 + S^z_2 = \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{pmatrix}$

$[S^z_{tot}, H] = \emptyset$ U(1) symmetry

$\rightarrow$ good quantum number

L>2 case

$$H = \sum_{i=1}^{L} J \left(S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta S^z_i S^z_{i+1} \right)$$

Periodic BC

$$S^a_{L+1} \equiv S^a_1$$

$$S^a_i = \mathbb{1}_{2\times 2} \otimes \mathbb{1}_{2\times 2} \otimes \dots \otimes \mathbb{1}_{2\times 2} \otimes \underset{\substack{\uparrow \\ \text{position } i}}{S^a} \otimes \mathbb{1}_{2\times 2} \otimes \dots \otimes \mathbb{1}_{2\times 2}$$

Product basis:

$|\uparrow\uparrow\uparrow \dots \uparrow\uparrow\rangle$, $|\uparrow\uparrow\uparrow \dots \uparrow\downarrow\rangle$ ....

$$\boxed{\dim \mathcal{H} = 2^L}$$

IMPORTANT QUESTIONS

- GAPPED OR GAPLESS ?
- Ground state structure (long range order ? Correlators ?)
- Excitation spectrum ?
- Quasiparticles ?

Full diagonalization (MATLAB DEMO)

- All eigenstates and energies
- up to $\dim \mathcal{H} \sim 10^3 - 10^4$ $L = 10 - 13$

"Curse of dimensionality"

→ Maybe too much ? ⟹ Usually we only need ground state and low energy excitations

ITERATIVE EIGENSOLVERS

Power method : random initial state $|\psi_0\rangle$

$$|\psi_{GS}\rangle \sim \left(H - \underset{\substack{\uparrow \\ \text{some shift maybe necessary, if}}}{b \cdot \mathbb{1}} \right)^n |\psi_0\rangle$$

$|E_{min}| < |E_{max}|$

What is needed ?

- store 1 vector
- iterate $|\psi_n\rangle = \underset{\substack{\uparrow \\ \text{action with the Hamiltonian}}}{(H - b\mathbb{1})} |\psi_{n-1}\rangle$
  - Sparse matrix ? (many zeros)
    ↳ (i, j, H_{ij}) storage is more efficient
  - "function" $fun_H(\psi) = H \cdot |\psi\rangle$

PROBLEM: poor scaling $|\psi_n\rangle = c_n|\psi_{GS}\rangle + |\tilde{\psi}_n\rangle$ $\qquad \frac{\|\tilde{\psi}_n\|}{|c_n|} \sim \left(\frac{E^b_{GS} + GAP}{E^b_{GS}}\right)^n$

Better approach: The Lánczos Algorithm

- init state (random, or good guess for GS) $|\psi_0\rangle$ $\quad (\langle\psi_0|\psi_0\rangle = 1)$
- Basic Idea: search the eigenstates in the Krylov subspace: $\mathcal{K}^n_{\psi_0} = \text{span}\left(|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle \dots H^n|\psi_0\rangle\right)$

  ↳ • orthogonalization (Lánczos)

- $|\tilde{\phi}_0\rangle := H|\psi_0\rangle$
- $\alpha_0 := \langle\tilde{\phi}_0|\psi_0\rangle$
- $|\phi_0\rangle = |\tilde{\phi}_0\rangle - \alpha_0|\psi_0\rangle$ $\qquad$ note: $\langle\phi_0|\psi_0\rangle = 0$

for $i = 1:n$

- $\beta_i := \||\phi_{i-1}\rangle\| = \sqrt{\langle\phi_{i-1}|\phi_{i-1}\rangle}$
- if $\beta_i \neq \emptyset$

  $|\psi_i\rangle = \dfrac{|\phi_{i-1}\rangle}{\beta_i}$

  else

  $|\psi_i\rangle$ = random unit vector orthogonalized on $\{|\psi_0\rangle, |\psi_1\rangle \dots |\psi_{i-1}\rangle\}$

  end
- $|\tilde{\phi}_i\rangle := H|\psi_i\rangle - \beta_i|\psi_{i-1}\rangle$
- $\alpha_i := \langle\tilde{\phi}_i|\psi_i\rangle$
- $|\phi_i\rangle = |\tilde{\phi}_i\rangle - \alpha_i|\psi_i\rangle$

end (for)

Statement: $\langle \psi_i | \psi_j \rangle = \delta_{ij}$

Proof:

i) $\langle \psi_1 | \psi_0 \rangle = \emptyset$ (by construction)

ii) $i > 0$

$$|\psi_{i+1}\rangle = \frac{|\phi_i\rangle}{\beta_{i+1}} = \frac{H|\psi_i\rangle - \beta_i|\psi_{i-1}\rangle - \alpha_i|\psi_i\rangle}{\beta_{i+1}}$$

$\alpha_i \to \langle \psi_i | H | \psi_i \rangle$

normalization

$$\Longrightarrow \boxed{H|\psi_i\rangle = \beta_{i+1}|\psi_{i+1}\rangle + \alpha_i|\psi_i\rangle + \beta_i|\psi_{i-1}\rangle}$$

iii) $\langle \psi_j | \psi_{i+1} \rangle = ?$ $\quad j \leq i$ is enough

Inductive proof: Suppose $\langle \psi_j | \psi_i \rangle = \delta_{ij}$

$\to$ Show $\langle \psi_j | \psi_{i+1} \rangle = \emptyset$

- $j = i$

$$\langle \psi_i | \psi_{i+1} \rangle = \frac{\langle \psi_i | H | \psi_i \rangle - \beta_i \underbrace{\langle \psi_i | \psi_{i-1} \rangle}_{\emptyset} - \langle \psi_i | H | \psi_i \rangle}{\beta_{i+1}} = \underline{\underline{\emptyset}}$$

- $j < i$

$$\langle \psi_j | \psi_{i+1} \rangle = \underbrace{\langle \psi_j | H | \psi_i \rangle} - \beta_i \underbrace{\langle \psi_j | \psi_{i-1} \rangle}_{\delta_{i-1,j}} - \alpha_i \underbrace{\langle \psi_j | \psi_i \rangle}_{\emptyset}$$

$$\downarrow$$

$$\beta_{j+1}\langle \psi_{j+1}| + \alpha_j \langle \psi_j | + \beta_j \langle \psi_{j-1} |$$

$$\langle \psi_j | H | \psi_i \rangle = \beta_{j+1} \langle \psi_{j+1} | \psi_i \rangle + \alpha_j \underbrace{\langle \psi_j | \psi_i \rangle}_{\emptyset} + \beta_j \underbrace{\langle \psi_{j-1} | \psi_i \rangle}_{\emptyset}$$

$$\Longrightarrow \langle \psi_j | \psi_{i+1} \rangle = \beta_{j+1} \underbrace{\langle \psi_{j+1} | \psi_i \rangle}_{\delta_{j+1,i}} - \beta_i \underbrace{\langle \psi_j | \psi_{i-1} \rangle}_{\delta_{j,i-1}} = \underline{\underline{\emptyset}} \ !$$

→ We proved, that $\{|\psi_i\rangle\}$ is orthonormal set.

→ $$\langle\psi_j|H|\psi_i\rangle = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & \\ & \beta_2 & \alpha_2 & \beta_3 & \\ & & \beta_3 & \ddots & \\ & & & & \ddots \end{pmatrix}$$ tridiagonal matrix!

Numerical issues (see slides and MatLab demo)

⇒ orthogonality lost numerically $\langle\psi_j|\psi_i\rangle_{num} \neq \delta_{ij}$

↳ 'Ghost' states (fake degeneracies)

⇒ Still good for ground state.

↳ diagonalize $\langle\psi_i|H|\psi_j\rangle$ up to $i<M, j<M$

↳ $|\psi_{GS}\rangle \sim v_0|\psi_0\rangle + v_1|\psi_1\rangle + \ldots = \sum_{\alpha=0}^{M-1} v_\alpha|\psi_\alpha\rangle$

eigenvector $\begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ \vdots \\ v_{M-1} \end{pmatrix}$

⇒ Re-orthogonalization may helps.

$\boxed{\text{Matlab eigs() ⇒ uses Lánczos}}$

Computational resources

→ original Lánczos:
- 3 vector in memory
- $2 \times N_{iter}$ $H|\psi\rangle$ calls

→ keeping all vectors in memory:
- N_{iter} vectors
- N_{iter} $H|\psi\rangle$ calls

re-orthogonalization is possible

↳ cost: $\frac{N_{iter}\cdot(N_{iter}-1)}{2}\cdot \dim \mathcal{H} \times 2$