Lecture 2: Exact Diagonalization: Symmetries & Observables.

Hilbert-spaces with non-trivial symmetry

symmetry group G of operations

elements $g \in G$

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can induce non-trivial transformations on basic configurations / many-body states $|\mu\rangle$

$$\langle g(\mu) | H | g(\mu) \rangle = \langle \mu | H | \mu \rangle$$

$$\langle g(\mu) | \mu \rangle \neq 1.$$

* spins on lattice
  - translations C° 1° 8_6
  - mirror-reflections 3° 4° 5°
  - discrete rotations 0° 1° 2°

  $\Rightarrow$ permutations of site-numbers R_4, M_{11}, M_1, T

* particles in orbitals $\Rightarrow$ unitary transformations

$$\tilde{\phi}_i = U_{ij} \phi_j$$

Symmetry group can connect multiple configurations
$\Rightarrow$ select one representative $|r\rangle$ only among these; typically smallest / largest numerical representation.
$\Rightarrow$ create symmetrized state

$$|\tilde{r}\rangle = \frac{1}{\mathcal{N}\sqrt{|G|}} \sum_{g \in G} \chi(g) \; | g(r) \rangle$$

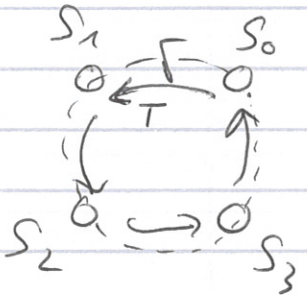
χ_{rg} = matrix rep. of transformation. (symmetry)

where we defined the norm $\mathcal{N} = \sqrt{\sum_{g \in G, g(r)=r} \chi(r)}$

group-elements under which r is invariant.

This is a bit abstract, so let's do an example

4 spins on chain with PBC.



T = translation $\begin{pmatrix} S_0 \to S_1 \\ S_1 \to S_2 \\ S_2 \to S_3 \\ S_3 \to S_0 \end{pmatrix}$

$$G = \{ T^0, T^1, T^2, T^3 \} \qquad |G| = 4$$

$$g = T^n \qquad \chi(g) = e^{iK\frac{n}{4}}$$

valid momenta (rep's) of translation group $K = 0, \pm\frac{\pi}{2}, \pi$

1/ sector, e.g. $K=0 \Rightarrow \chi(r) = e^{i\cdot 0} = 1$ $\quad k=\pi \Rightarrow \chi(r) = (-1)^n$

$K = \pm\frac{\pi}{2} \Rightarrow \chi(r) = e^{\pm i\frac{\pi}{2}n} = (\pm i)^n$

$S_z = +2 \to |1\,1\,1\,1\rangle = |r\rangle$

$$T^0|r\rangle = T^1|r\rangle = T^2|r\rangle = T^3|r\rangle$$

$$\Rightarrow \mathcal{N}_{|1111\rangle}(k=0) = \sqrt{4} = 2$$

$$\mathcal{N}_{|1111\rangle}\left(k=\tfrac{\pi}{2}\right) = \sqrt{i + i^2 + i^3 + i^4} = 0$$

$$\mathcal{N}_{|1111\rangle}(k=\pi) = \sqrt{(-1) + (-1)^2 + (-1)^3 + (-1)^4} = 0$$

only $k=0$ state exists

$$|\tilde{r}\rangle = \frac{1}{2\sqrt{4}} \cdot 4|1111\rangle = |1111\rangle.$$

$S_z = 1$ $\quad r = |0\,111\rangle$ $\quad T^0|r\rangle = |r\rangle$ only

$$\mathcal{N} = \sqrt{\chi(0)} = 1$$

$$|\tilde{r}\rangle = \frac{1}{\sqrt{4}}\left(|0111\rangle + \chi_k(1)|1011\rangle + \chi_k(2)|1101\rangle + \chi_k(3)|1110\rangle \right)$$

$S_z = 0$ $\quad r = |01\,01\rangle$

$$T^0 |r\rangle = |r\rangle$$
$$T^1 |r\rangle \neq |r\rangle$$
$$T^2 |r\rangle = |r\rangle$$
$$\Big\} \; N = \sqrt{\chi(0) + \chi(2)}$$

$$N_{|01\,01\rangle}(k=0) = \sqrt{2}$$

$$N_{|01\,01\rangle}\left(k = \pm\tfrac{\pi}{2}\right) = \sqrt{\pm(i + i^3)} = 0$$

$$N_{|01\,01\rangle}(k=\pi) = \sqrt{1 + (-1)^2} = \sqrt{2}$$

$$|r_{k=0}\rangle = \frac{1}{\sqrt{2}\sqrt{4}} \left(2\,|01\,01\rangle + 2\,|10\,10\rangle \right)$$

$$|r_{k=\pi}\rangle = \frac{1}{\sqrt{2}} \left(|01\,01\rangle - |10\,10\rangle \right)$$

Δ $\quad r' = |00\,11\rangle \Rightarrow k=0$ or $k = \pm\frac{\pi}{2}$ with $N=1$.

$S_z = -1$ $\quad r = |0001\rangle$ $\quad N = 1$

$$|\tilde{r}_k\rangle = \frac{1}{2}\left(|0001\rangle + \chi_k(1)\,|0010\rangle + \chi_k(2)\,|0100\rangle + \chi_k(3)\,|1000\rangle \right)$$

$S_z = -2$ $\quad N = 2$, as $S_z = +2$.

$\Rightarrow$ 16 states total

can fix k if $[H, T] = 0$

so the biggest space we need to diagonalize has dimension 2!

Other benefits:

- Get access to lowest eigenstates in all symmetry sectors: much easier to calculate than many eigenvalues from the same matrix!

Hamiltonian matrix:

decompose H into elementary terms $H = \sum_\alpha h^\alpha$

e.g. (a) spin-model $H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$ on nearest-neighbors $\langle i,j \rangle$

in spin-$\frac{1}{2}$ basis $|\uparrow\rangle, |\downarrow\rangle$ $\quad S_z |\sigma_i\rangle = \sigma |\sigma_i\rangle$

$$\vec{S}_i \cdot \vec{S}_j = \frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z$$

$\Rightarrow$ $\underbrace{h_{(i,j,+1,-1,z)}}_{\alpha}$ act with $S_i^+ S_j^-$ or $S_i^- S_j^+$ or $\underbrace{S_i^z S_j^z}_{\text{diagonal.}}$

typical sparsity off-diagonal: $2 \times \frac{c}{2} \cdot N_s = c \cdot N_s$

c: connectivity $\quad$ $(c=4)$

N_s: # of sites.

(b) two-body interaction in FQHE or other

$$H = \int d\underline{r}\, d\underline{r}' \; \hat{\rho}(r) \; V(r-r') \; \hat{\rho}(r')$$

expand $\hat{\rho}(r) = \hat{c}^\dagger(r)\, \hat{c}(r)$

$\hat{c}(r) = \sum_i \phi_i(r)\, \hat{a}_i$ for orbitals i

$$\Rightarrow H = \sum_{ijkl} V_{ijkl}\, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l$$

typical sparsity if interactions are long-range (Coulomb)

# of entries per line $\propto (N_{orb}-N)(N_{orb}-N-1)(N-1)N \propto N_{orb}^4$

$\Rightarrow$ more difficult numerically than spin-systems.

Each term acting on a basis-state yields a unique target

$$h^\alpha |\mu\rangle = h^\alpha(\mu) |\nu\rangle$$

Basic algorithm: (review) - ask if we can skip this.

create empty target-vector $|\varphi'\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$

take previous factors vector $|\varphi_i\rangle = \sum_\mu \varphi_i^\mu |\mu\rangle = \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_d \end{pmatrix}$

- loop over initial index n
  - loop over α
    - look up $\mu(n) = |\mu\rangle$
    - calculate $|\nu\rangle$, $h^\alpha(\mu)$
    - find index m of $|\nu\rangle$
    - add to target vector at position m

$$\varphi'[m] \mathrel{+}= \varphi_i[n] * h^\alpha(\mu)$$

  - Done
- Done

With symmetries, the technique becomes more challenging:

have to deal with representatives

$|\mu\rangle \to |r\rangle$ $\qquad$ $|\nu\rangle \to |s\rangle$

in general: $h^\alpha |r\rangle = h^\alpha(r) |\nu\rangle$

$\neq |s\rangle$, but $|s\rangle = |g^*(\nu)\rangle$

i.e. $\exists$ element $g^* \in G \mid g^*(\nu) = s$.

we can thus evaluate matrix elements between the Bloch-states directly as follows:

$$\langle \tilde{s} | h^\alpha | \tilde{r} \rangle = \frac{N_s}{N_r} \chi(g^*) h^\alpha(r)$$

let us show this (if there is time)

$$\langle \tilde{s} | h^\alpha | \tilde{r} \rangle = \frac{1}{|G| N_r N_s} \sum_{g,h \in G} \langle g(s) | \bar{\chi}(g)\, h^\alpha\, \chi(h) | h(r) \rangle$$

$$= \frac{1}{|G| N_r N_s} \sum_{g,h \in G} \bar{\chi}(g)\chi(h) \langle \overbrace{h^{-1}(g(s))}^{g'} | h^\alpha | \cancel{h} \rangle$$

↑ redundant coverage of h. in sum over $h^{-1}g$.

$$= \frac{1}{N_r N_s} \sum_{g' \in G} \bar{\chi}(g')\chi(\mathbb{1}) \langle g'(s) | h^\alpha(r) | \underbrace{r}_{= |g^*(s)\rangle} \rangle$$

$$= \frac{1}{N_r N_s} \sum_{g'} \bar{\chi}(g')\, h^\alpha(r)\, \cancel{\chi(g^*)} \langle g'(s) | s \rangle$$

(remember $\sum_g \chi(g) = N^2$)

$$= \frac{N_s}{N_r} h^\alpha(r) \chi(g^*).$$

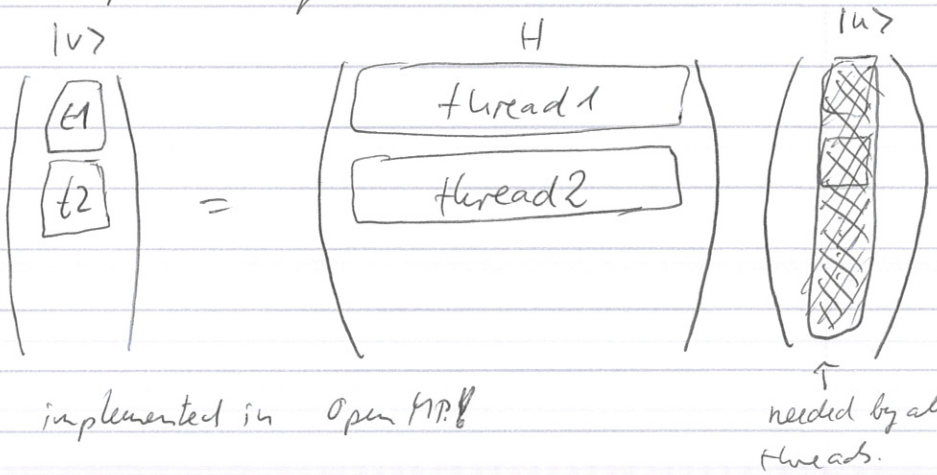
Algorithm for calculating H with symmetries:

- apply loop over operators h^α
- → evaluate $h^\alpha(r)$, $|v\rangle$
- search representative $|\tilde{s}\rangle$ for $|v\rangle$ as well as the group element g^* linking the two
- then look up index for $|s\rangle$.

- crucial for efficiency
  - full look-up of g^*, $|s\rangle$ for all $|v\rangle$ (memory intensive)
  - factorise symmetry group to speed up search of g^*
  - brute force (cycle through all g in worst case, or when there are few g ($|G|$ small)

Note on parallelization:

better to loop over final vector index:



⇒ easily implemented in OpenMP!

Other observables:

works like the Hamiltonian:

$$\langle \psi | \mathcal{O} | \psi \rangle = \underbrace{\langle \psi | \underbrace{\left(\mathcal{O} | \psi \rangle \right)}_{\text{matrix-vector multiplication}}}_{\text{scalar product}}$$

possible for any operator that can be written as an expectation value in a known eigenstate.

However, it is possible also to go beyond this!

A useful trick is the continued fraction method, which gives access to the diagonal elements of Green's functions.

Continued fraction method:

e.g. $G_{xx}(\omega) = \langle x \left| \frac{1}{\omega + i\varepsilon - H} \right| x \rangle$

Spectral function

$$S_{particle} = -\frac{1}{\pi} \mathrm{Im} \langle \phi_0 | \underbrace{c_q}_{hole} \frac{1}{\omega + i\varepsilon - H} \underbrace{c_q^+}_{c_q^+} | \phi_0 \rangle$$

dynamical spin structure factor

$$S_{spin} = \frac{1}{\pi} \mathrm{Im} \langle \phi_0 | \underbrace{S_q^-}_{S_q^+} \frac{1}{\omega + i\varepsilon - H} S_q^+ | \phi_0 \rangle$$

Recipe: tri-diagonalize H from $v_1 = \frac{|x\rangle}{\sqrt{\langle x|x\rangle}}$

$$\Rightarrow G_{xx} = \cfrac{\langle x|x\rangle}{\omega + i\varepsilon - \alpha_1 - \cfrac{\beta_2^2}{\omega + i\varepsilon - \alpha_2 - \cfrac{\beta_3^2}{\omega + i\varepsilon - \alpha_3 + \ddots}}}$$

Proof: EV's of $\omega + i\varepsilon - H$ given approximately by EV's of tri-diagonal matrix.

$$\underbrace{\begin{pmatrix} \omega + i\varepsilon - \alpha_1 & -\beta_2 & & \\ -\beta_2 & \omega + i\varepsilon - \alpha_2 & -\beta_3 & \\ & -\beta_3 & \omega + i\varepsilon - \alpha_3 & \\ & & & \ddots \end{pmatrix}}_{\equiv D_0}$$

Matrix with first n rows & columns eliminated D_n

$$\langle x | (\omega + i\varepsilon - H)^{-1} | x \rangle = \frac{\det D_1}{\det D_0}$$

$$\alpha_1 = \langle v_1 | H | v_1 \rangle$$

$$\det D_n = (\omega + i\varepsilon + \alpha_{n+1}) \det D_{n+1} - \beta_{n+2}^2 \det D_{n+2}$$

$$\det D_0 = (\omega + i\varepsilon + \alpha_1) \det D_1 - \beta_2^2 \det D_2$$

$$G_{xx}(\omega) = \langle x|x\rangle \det D_1 / \det D_0 = \frac{\langle x|x\rangle}{\frac{\det D_0}{\det D_1}}$$

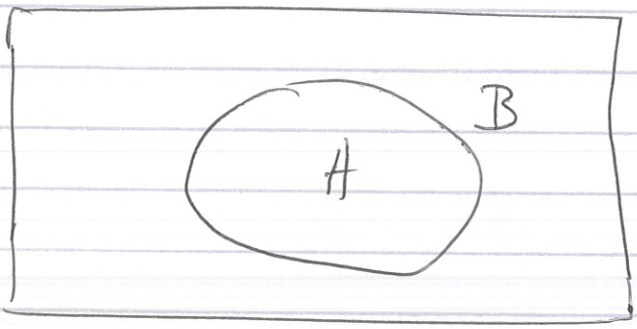
$$= \frac{\langle x|x\rangle}{\omega + i\varepsilon + \alpha_1 - \frac{\beta_2^2}{\det D_1}}$$

↑ expand to get continued fraction.

take $i\varepsilon \to 0$.

Entanglement:

Quantum-state of one part of the system depends on state of the rest
⇒ partition system in two parts:



Knowing the wave function for the entire system A ∪ B, we can extract information on its entanglement properties:

decompose:

simply element of state-vector

$$|\psi\rangle = \sum_{i,j} \kappa_{ij} \; |\chi_i^A\rangle \otimes |\chi_j^B\rangle$$

(basis states in A, basis states in B)

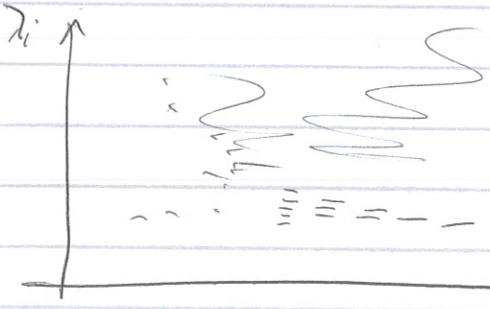
↓ SVD (LAPACK dgesdd)

$$= \sum_i \lambda_i \; |\hat{\chi}_i^A\rangle \otimes |\hat{\chi}_i^B\rangle$$

positive "Schmidt eigenvalues" $\lambda_i = e^{-\xi_i}$

Classify eigenstates $\hat{\chi}_i^A$ using their known quantum numbers, such as $N_\#^A$, S_z^A, $\underline{K}^A$, L_z^A, ...
Plot of $\xi_i = -\ln \lambda_i$ as fct of these gives extra info!

e.g.



e.g. Laughlin state on sphere

also, entanglement entropy $S_{A-B} = -\sum_i \lambda_i \ln \lambda_i$

Background: Singular Value Decomposition:

Any real or complex matrix A possesses a decomposition into singular values

$$A \in \mathbb{K}[l \times m] \qquad l \geq m$$

$\exists$ unitary matrix $Y \in K[l \times l]$
and $X \in K[m \times m]$
such that

$$A = Y \Sigma X^H$$

where Σ has the simple form

$$\Sigma = \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix}, \quad \Sigma_1 = \mathrm{diag}(\lambda_1, \ldots, \lambda_m)$$

(and X, Y unitary)

Singular values are eigenvalues for the right- or left- singular vectors, respectively

$$A x = \lambda y$$

$$A^T y = \lambda x$$

i.e.

$$A^T A x = \lambda^2 x$$

(semi-)

which proves that the eigenvalues are positive definite.