Class 2

Many-fermion systems

- fermionic modes : wavefunction $\phi_i(\underline{r}, \sigma)$ (position, spin)
  - creation operator c_i^+ : "creates" an electron in mode ϕ_i
  - annihilation operator $c_i = (c_i^+)^+$

- many-fermion product states

$$c^+_{i_1} c^+_{i_2} \cdots c^+_{i_n} |0\rangle \Longleftrightarrow \underbrace{\mathcal{A}\left(\phi_{i_1}(\underline{r}_1, \sigma_1)\, \phi_{i_2}(\underline{r}_2, \sigma_2) \cdots \phi_{i_n}(\underline{r}_n, \sigma_n)\right)}_{\text{Slater determinant}}$$

antisymmetrization

$i_1 \neq i_2 \neq \cdots \neq i_n$

- Anticommutation relations $\{A, B\} \equiv AB + BA$

$$\boxed{\{c_i, c_j\} = \{c_i^+, c_j^+\} = \emptyset} \qquad \boxed{\{c_i, c_j^+\} = \delta_{ij}}$$

- Occupation number representation
  - $\rightarrow$ sorting $i_1 < i_2 < \cdots < i_n$
  - $\rightarrow$ $|0\rangle \Longleftrightarrow |0, 0, 0, \ldots, 0\rangle$ ($i = 1\ 2\ 3 \ldots L$)

$$\boxed{|0, 0, \overset{i_1}{1}, 0, 0, \overset{i_2}{1}, 0, \overset{i_3}{1} \ldots\ldots \rangle = c^+_{i_1} c^+_{i_2} c^+_{i_3} \cdots |0\rangle}$$

ordering is important! (sign)

  - $\rightarrow$ action of fermion ops

$$c_j^+ |n_1 n_2 \ldots n_L\rangle = \delta_{n_j, 0} \prod_{i=1}^{j-1} (-1)^{n_i} \cdot |n_1 n_2 \ldots (n_j + 1) \ldots\rangle$$

$$c_j |n_1 n_2 \ldots n_L\rangle = \delta_{n_j, 1} \prod_{i=1}^{j-1} (-1)^{n_i} |n_1 n_2 \ldots (n_j - 1) \ldots\rangle$$

Observation : • the basis is isomorphic to a spin-½ chain

$$|n_1 n_2 \dots n_L\rangle \Longleftrightarrow |\sigma_1 \sigma_2 \dots \sigma_L\rangle$$

$$n_i \in \{0,1\} \Longleftrightarrow \sigma_i \in \{\uparrow \downarrow\}$$

• the anticommutation rules make the Fermi operators non local

The Jordan-Wigner transformation

• Single-mode (~ 1 site) operators:

$$c^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\sigma^x - i\sigma^y) = \sigma^-$$

$$c = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma^x + i\sigma^y) = \sigma^+$$

• Operators in the many-mode Fock space

$$c_j^+ = \underset{\dots}{\phi} \otimes \phi \otimes \dots \otimes \underset{j-1}{\phi} \otimes \underset{j}{c^+} \otimes \underset{j+1}{\mathbb{1}} \otimes \underset{\dots}{\mathbb{1}} \otimes \dots$$

$$c_j = \underbrace{\phi \otimes \phi \otimes \dots \otimes \phi}_{\prod_{i<j}(-1)^{n_i}} \otimes c \otimes \mathbb{1} \otimes \mathbb{1} \otimes \dots$$

$$\boxed{\phi = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^z}$$

$$\boxed{\phi = 1 - 2n}$$

• Consequences: equivalences

Spinless fermion - 1D

$$H = -t\sum_i \left(c_i^+ c_{i+1} + c_{i+1}^+ c_i\right) + V\sum_i n_i n_{i+1}$$

$$c_i^+ c_{i+1} \Longrightarrow \mathbb{1} \otimes \mathbb{1} \otimes \dots \otimes \overbrace{\sigma^- \sigma^z}^{\sigma^-} \otimes \sigma^+ \otimes \mathbb{1} \dots = \sigma_i^- \sigma_{i+1}^+$$

$$c_{i+1}^+ c_i \Longrightarrow \mathbb{1} \otimes \mathbb{1} \otimes \dots \otimes \underbrace{\sigma^z \sigma^+}_{\sigma^+} \otimes \sigma^- \otimes \mathbb{1} \dots = \sigma_i^+ \sigma_{i+1}^-$$

$$n_i n_{i+1} \Longrightarrow \sigma_i^z \sigma_{i+1}^z$$

$$H = -t\sum_i \underbrace{\left(\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+\right)}_{\frac{1}{2}\left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y\right)} + V\sum_i \sigma_i^z \sigma_{i+1}^z \quad \Bigg\} \text{ This is the XXZ model!}$$

- Examples (Matlab): • spinless fermion

Symmetries & Quantum numbers

Spinless fermion

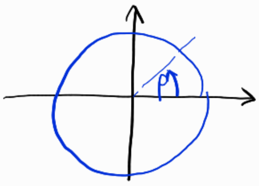
$$\hat{H} = -t\sum_i \left(c_i^+ c_{i+1} + c_{i+1}^+ c_i\right) + V\sum_i n_i n_{i+1}$$

$$\hat{N}_{tot} = \sum_i n_i = \sum_i c_i^+ c_i \qquad [H, N_{tot}] = \emptyset$$

from $[n_i, n_j] = \emptyset$

$[n_i, c_j] = -\delta_{ij} c_j$

This is a $U(1)$ symmetry



$$\hat{U}_\rho = e^{i\hat{N}_{tot}\rho}$$

N_{tot} sectors $\Longleftrightarrow$ Irreducible representations of $U(1)$ group

$U(1)$ is Abelian: irreps are 1D

$$\Gamma_\rho^N = e^{iN\rho}$$

XXZ-model

$$H = J\sum_i \left(S_i^x S_{i+1}^x + S_i^y S_i^{y+1} + \Delta S_i^z S_{i+1}^z\right)$$

$$S_{tot}^z = \sum_i S_i^z \qquad [H, S_{tot}^z] = \emptyset$$

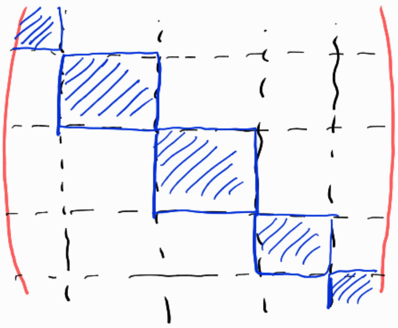
this is again a $U(1)$ symmetry

$$\hat{U}_\rho = e^{i\rho\hat{S}_{tot}^z}$$

How to exploit U(1) in our numerics?

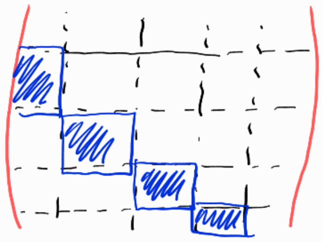
- Use symmetric basis locally:
  - fermion model $|0\rangle, |1\rangle$: $n = 0, 1$
  - spin model $|\uparrow\rangle, |\downarrow\rangle$: $S^z = +\frac{1}{2}, -\frac{1}{2}$
- The product basis states are immediately eigenstates of N_{tot} / S_{tot}^z

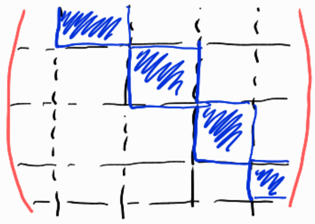
- Collect states to Quantum number sectors.
  - After sorting states:

$H =$ 

$N_{bt} = 0$
1
2
⋮

  - Fermi operators change charge by ± 1 :

$c_i^+ =$ 

$c_i =$ 

  - Spin models:

$S_i^+ \quad S_i^- \Rightarrow$ these change spin by ± 1

$S_i^x \quad S_i^y \Rightarrow$ no definit spin change
↳ more blocks

How to store?

(A) : pointer matrix (cell array) for blocks

- Simple : 1 pointer / cell for every possible block
- Matrix product: easy to implement
- Pointer is stored for $\emptyset$-blocks too !

↳ This can be expensive for
  - More symmetries
  - Higher rank tensors

(B) : block-sparse storage

example c^+:

sec_f	sec_i	pointer/cell
2	1	{ }
3	2	{ }

- Memory efficient
- Matrix product : more complicated (lookups, task lists)

Non-Abelian symmetries

Heisenberg-model (XXZ with $\Delta = 1$)

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right)$$

edges of a lattice

$\Rightarrow$ SU(2) symmetry

$$[H, S^x_{tot}] = [H, S^y_{tot}] = [H, S^z_{tot}] = \emptyset$$

- Symmetry op is

$$\hat{U}(\vec{n}, \varphi) = e^{i \varphi \vec{n} \cdot \vec{S}_{tot}}$$

irreducible representations are characterized by eigenvalue of $S^2_{tot} = \vec{S}_{tot} \cdot \vec{S}_{tot}$

- Energy eigenstates

$$\hat{H} \, | \alpha; S_\alpha, s^z \rangle = E_\alpha | \alpha; S_\alpha, s^z \rangle$$

$$S^2_{tot} | \alpha; S_\alpha, s^z \rangle = S_\alpha (S_\alpha + 1) | \alpha; S_\alpha, s^z \rangle$$

$$S^z_{tot} | \alpha; S_\alpha, s^z \rangle = s^z | \alpha; S_\alpha, s^z \rangle$$

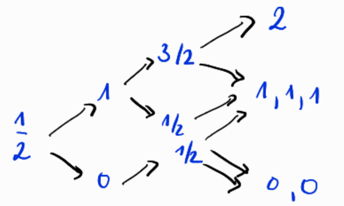
How to exploit?

- PROBLEM: our product basis states are eigenstates of S^z_{tot} but not eigenstates of S^2_{tot}.

$\Downarrow$

Basis rotation is necessary

S_{tot} :

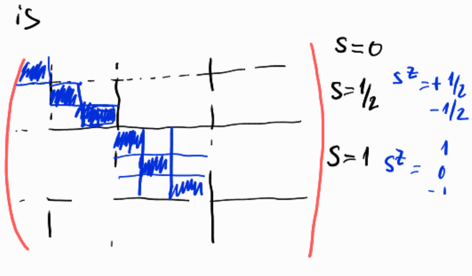


$\rightarrow$ Complicated combination of spins

$\rightarrow$ Clebsh-Gordan coefficients are needed

Once the rotation is done, the Hamiltonian is

$H =$



Translationally invariant models (PBC)

$c^+_{L+1} \equiv c^+_1$

$$H = -t\sum_{i=1}^{L}\left(c^+_i c_{i+1} + c^+_{i+1} c_i\right) + V\sum_{i=1}^{L} n_i n_{i+1}$$

Transform to momentum space

$$\tilde{c}^+_k = \sum_x \frac{e^{ikx}}{\sqrt{L}} c^+_x \qquad c^+_x = \sum_k \frac{e^{-ikx}}{\sqrt{L}} \tilde{c}^+_k \qquad k = \frac{2\pi}{L}\cdot m$$

$$\sum_{x=1}^{L}\left(c^+_{x+1} c_x + c^+_x c_{x+1}\right) = \sum_k 2\cos(k)\, \tilde{c}^+_k \tilde{c}_k$$

$$n_x = c^+_x c_x = \sum_{k,k'} \frac{e^{i(k'-k)x}}{L} \tilde{c}^+_k \tilde{c}_{k'}$$

$$H = \sum_k -2t\cos(k)\, \tilde{c}^+_k \tilde{c}_k + \sum_{\substack{k_1 k_1' \\ k_2 k_2'}} \frac{e^{i(k_2'-k_2)}}{L} \delta^{\mathrm{mod}\,2\pi}_{k_1+k_2,\, k_1'+k_2'} \tilde{c}^+_{k_1} \tilde{c}_{k_1'} \tilde{c}^+_{k_2} \tilde{c}_{k_2'}$$

In momentum space we get a new Q-number: k

↳ similar to $U(1)$, but $k_{tot} = \sum_k k\, \tilde{c}^+_k \tilde{c}_k$ mod 2π

Spin models

$$H = \sum_i \left(J_1 \vec{S}_i \vec{S}_{i+1} + J_2 \vec{S}_i \vec{S}_{i+2}\right)$$

↳ Jordan-Wigner: $c^+ c^+ c^+ c c c$ 3-body ☹

Idea: <u>translation operator</u>

$$T\,|\sigma_1 \sigma_2 \dots \sigma_L\rangle = |\sigma_2 \sigma_3 \dots \sigma_L \sigma_1\rangle$$

$$T^+ = T^{-1} \quad \text{(unitary)}$$

$$T \vec{S}_i T^{-1} = \vec{S}_{i+1} \implies [H, T] = \emptyset$$

T generates the C_L group. Eigenvalues: e^{ik} $\quad k = \frac{2\pi}{L}\cdot m$

How to exploit?

- Basis formation: → cycles $\underbrace{|\sigma_1 \sigma_2 \dots \sigma_L\rangle}_{|A_1\rangle}, \underbrace{|\sigma_2 \sigma_3 \dots \sigma_L \sigma_1\rangle}_{|A_2\rangle} \dots \underbrace{|\sigma_L \sigma_1 \sigma_2 \dots \sigma_{L-1}\rangle}_{|A_L\rangle}$

  ↳ k-states from cycle

$$|\tilde{A}_k\rangle = \frac{1}{\sqrt{L}}\left(|A_1\rangle + e^{-ik}|A_2\rangle + e^{-2ik}|A_3\rangle + \dots\right)$$

- H is block diagonal for k-sectors