- Spinless fermions: Taking into account Fermi algebra

Interlude: Jordan Wigner transformation in 1D

- Map spin-$\frac{1}{2}$ operators $\vec{S}^{(j)} = \frac{\vec{\sigma}^{(j)}}{2}$ to spinless fermions $\{\psi_i, \psi_j^\dagger\} = \delta_{ij}$
- Rule of thumb (up to fermionic signs): $S_-^{(j)} \sim \psi_j$; $S_+^{(j)} \sim \psi_j^\dagger$

  (Full story for hardcore bosons)
- Fermionic algebra requires non-local mappings with Jordan-Wigner strings:

$$S_+^{(j)} = F_1 \cdots F_{j-1} \psi_j^\dagger, \text{ with } F_j = e^{i\pi S_+^{(j)} S_-^{(j)}} = e^{i\pi \overbrace{\psi_j^\dagger \psi_j}^{n_j}} =$$

$$= (-1)^{n_j}, \text{ where } S_z^{(j)} \simeq \psi_j^\dagger \psi_j - \frac{1}{2} = n_j - \frac{1}{2}, \text{ since } S_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix},$$

$$\text{and } S_+ S_- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

- Binary representation of occupation number states:
  Simply identify occupation numbers $n_j \in \{0, 1\}$ with the bits of the integer $I_{\{n_j\}} = \sum_{j=1}^{N} n_j 2^{N-j}$

- Examples for the action of operators:

  ↳ Nearest neighbor hopping:

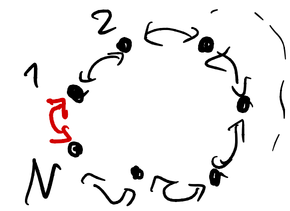
identical unless $(1-n_i)=0$

$$\psi_i^\dagger \psi_{i+1} |\ldots, n_i, n_{i+1}, \ldots\rangle = n_{i+1} (-1)^{\sum_{j<i+1} n_j} (1-n_i) (-1)^{\sum_{j<i} n_j} \ldots$$

$$\ldots |\ldots, 1-n_i, 1-n_{i+1}, \ldots\rangle$$

$$= n_{i+1}(1-n_i) |\ldots, 1-n_i, 1-n_{i+1}, \ldots\rangle$$

⇝ Fermionic signs cancel out for nearest neighbor hopping, except for PBC when hopping between sites 1 and N:



$$\psi_1^+ \psi_L |n_1, \dots, n_L\rangle = n_L \underbrace{(-1)^{\sum_{j<L} n_j}}_{(-1)^{\#\text{particles}-1}} (1-n_1)\,|1-n_1, \dots, 1-n_L\rangle$$

unless $n_L = 0$.

⇝ extra sign for <u>even</u> total number of particles.

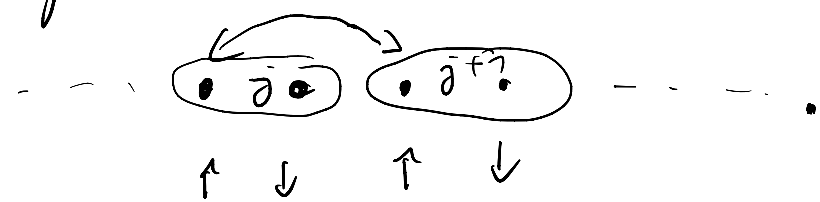
↳ Next-nearest neighbor hopping:

$$\psi_i^+ \psi_{i+2} |\dots, n_i, n_{i+1}, n_{i+2}, \dots\rangle = n_{i+2}(1-n_i)(-1)^{\sum_{j<i+2} n_j}(-1)^{\sum_{j<i} n_j} \cdot |\dots 1-n_i, n_{i+1}, 1-n_{i+2}, \dots\rangle$$

$$= n_{i+2}(1-n_i)(-1)^{n_{i+1}}|\dots 1-n_i, n_{i+1}, 1-n_{i+2}, \dots\rangle$$

⇝ Extra sign if $n_{i+1} = 1$ from hopping over fermion on intermediate site $i+1$.

- Models of spinful fermions (or fermions with further internal degrees of freedom) can be mapped to the spinless case (e.g. even sites for spin ↓ and odd sites for spin ↑) at the expense of somewhat non-local terms in simple operators



B.2: Krylov Space Construction and Basic Lanczos Algorithm

$|E_0\rangle$

- Primary goal: Find the ground state of a given QMB model more efficiently than by full diagonalization.

- Physically intuitive method: Imaginary time propagation

$$|E_0\rangle = \lim_{\beta \to \infty} \frac{e^{-\beta H}|\psi_i\rangle}{|\quad '' \quad|}$$

with a random initial state $|\psi_i\rangle$.

Proof: With $|\psi_i\rangle = \sum_\lambda c_\lambda |E_\lambda\rangle$, $e^{-\beta H}|\psi_i\rangle = \sum_\lambda e^{-\beta E_\lambda} c_\lambda |E_\lambda\rangle$

$$\overset{E_0 \text{ non-deg.}}{=} e^{-\beta E_0}\left(c_0|E_0\rangle + \sum_{\lambda\neq 0} e^{-\beta\underbrace{(E_\lambda - E_0)}_{>0}} c_\lambda |E_\lambda\rangle\right)$$

$$\leadsto \lim_{\beta\to\infty} \frac{e^{-\beta H}|\psi_i\rangle}{\|\ \text{"}\ \|} = \lim_{\beta\to\infty} \frac{\cancel{e^{-\beta E_0}}\left(c_0|E_0\rangle + \sum_{\lambda\neq 0} e^{-\beta(E_\lambda - E_0)} c_\lambda |E_\lambda\rangle\right)}{\cancel{e^{-\beta E_0}}\sqrt{|c_0|^2 + \sum_{\lambda\neq 0}|c_\lambda|^2 e^{-2\beta(E_\lambda - E_0)}}}$$

$$= \underbrace{\frac{c_0}{|c_0|}}_{\text{global phase factor}} |E_0\rangle \,. \quad \square$$

- Simple imaginary time propagation algorithm:
  - Use $e^{-\beta H} = \lim_{n\to\infty}\left(1 - \frac{\beta}{n} H\right)^n$

$$\boxed{\dim \mathcal{H} =: D}$$

$\rightsquigarrow$ For small $\frac{\beta}{n} =: \delta\tau$ we have $e^{-\delta\tau H} = (1 - \delta\tau H) + \mathcal{O}(\delta\tau^2)$

$\rightsquigarrow$ Simplest algorithm: Iterate $|\psi\rangle \rightarrow \dfrac{(1-\delta\tau H)|\psi\rangle}{|\quad '' \quad|}$

until converged.

$\rightsquigarrow$ Basic refinement: Reduce $\delta\tau$ while converging.

– Next level of sophistication: Use $e^{-\delta\tau H} \underset{+\mathcal{O}(\delta\tau^3)}{\approx} 1 - \delta\tau H + \frac{1}{2}\delta\tau^2 H^2$

$= (1 - d_1 H)(1 - d_2 H)$ with $d_1 + d_2 = \delta\tau$, $d_1 \cdot d_2 = \frac{\delta\tau^2}{2}$,

i.e. $\boxed{\begin{aligned} d_1 &= \delta\tau\,\frac{(1+i)}{2} \\ d_2 &= \delta\tau\,\frac{(1-i)}{2} \end{aligned}}$ $\rightsquigarrow$ Error in every (double) step reduced from $\mathcal{O}(\delta\tau^2)$ to $\mathcal{O}(\delta\tau^3)$

$$\left[\,(1 - d_1 H)(1 - d_2 H) \stackrel{\downarrow}{=} 1 - \underbrace{(d_1 + d_2)}_{=\delta\tau} H + \underbrace{d_1 d_2}_{=\frac{1}{2}\delta\tau^2} H^2 \quad \checkmark\,\right]$$

- Cost of imaginary time propagation: $\mathcal{O}\big((\dim \mathcal{H})\, \underset{\uparrow}{F} \cdot \beta\big)$

terms in H

↳ Pros and Cons:

+ very easy to implement
+ Numerically very stable
+ Simultaneous convergence of eigenstates and eigenvalues.

- Many iterations are needed (typically $\mathcal{O}(10^4 - 10^5)$).
- Only ground state directly accessible.

- If we truncate the series $e^{-\beta H}|\psi_i\rangle = \lim_{n\to\infty} \sum_{\ell=0}^{n} \frac{(-\beta H)^\ell}{\ell!}|\psi_i\rangle$ at finite n, we obtain a polynomial of degree n in H, acting on $|\psi_i\rangle$.

$\rightsquigarrow \sum_{\ell=0}^{n} \frac{(-\beta H)^\ell}{\ell!} |\varphi_i\rangle$ lies in the subspace of $\mathcal{H}$ spanned by $\langle\langle |\varphi_i\rangle, H|\varphi_i\rangle, H^2|\varphi_i\rangle, \ldots, H^n|\varphi_i\rangle \rangle\rangle$, known as the $(n+1)$-th Krylov space $K_{n+1}(H, |\varphi_i\rangle)$.