10.12.18

<u>identical</u> <u>particles</u>

The hamiltonian $\hat{H}$ is symmetric in the variable $1 \dots N$

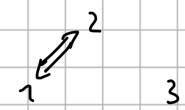
The permutation group of the permutations of N objects is called S_N. The order of S_N is $|S_N| = N!$

The symmetric group S_N is generated by two elements:

A transposition and a cyclic permutation

Exampl: S_3 generators $(2,1)$, $(2,3,1)$

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} \to (2,1)$$



$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \to (2,3,1)$$

representation theory: group $\to$ set of matrices with the same multiplication laws

$$(2,1) \to \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (2,3,1) \to \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The wave-function of N particles depends on the coordinates and spin of the particles

$$\psi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2, \dots, \vec{r}_N \vec{\sigma}_N)$$

The transposition can (only) change the sign of wave function. (i.e. ± 1)

$P_{ij}\, \psi(\vec{r}_1 \vec{\sigma}_1, \dots, \vec{r}_N \vec{\sigma}_N)$ $\qquad (P_{ij})^2 \psi = \psi$ $\qquad P_{ij} \in S_N$

$\hat{H}$ is symmetric in $1, \dots, N$ $\longrightarrow$ $[H, P] = 0$ $\qquad$ Bosons

For <u>two</u> particls: $\qquad$ Fermions

$$\psi_S(1,2) = \psi(1,2) + \psi(2,1) \qquad +1$$

$$\psi_A(1,2) = \psi(1,2) - \psi(2,1) \qquad -1$$

For $N > 2$ the experimental finding is that only the totally symmetric and totally symmetric are allowed!

The spin-statistics (Pauli) says that the totally antisymmetric wave functions are realized by half integer spin and symmetric with integer spin.

For two fermions $\psi(\vec{r}_1\sigma_1, \vec{r}_1\sigma_1) = -\psi(\vec{r}_1\sigma_1, \vec{r}_1\sigma_1) = 0$

$\rightarrow$ Pauli-exclusion prinzip

<u>Non-interchanging particles Hamiltonian</u>

$$\hat{H} = \hat{H}_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_3 \cdots \otimes \mathbb{1}_N + \cdots \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes \cdots \otimes \hat{H}_N$$

<u>Fermions</u> (totally antisymmetric wave functions)

$$\psi_{\underbrace{k_1\vec{\sigma}_1}_{\alpha_1}}(\vec{r}_1)\, \psi_{k_2\vec{\sigma}_2}(\vec{r}_2) \cdots \psi_{k_N\vec{\sigma}_N}(\vec{r}_N)$$

$$\psi(\vec{r}_1\vec{\sigma}_1, \ldots, \vec{r}_N\vec{\sigma}_N) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} (-1)^{\pi}\, \psi_{\alpha\pi(1)}(\vec{r}_1) \cdots \psi_{\alpha\pi(N)}(\vec{r}_N)$$

slater-determinant

$$\psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{\alpha_1}(\vec{r}_1) & \cdots & \psi_{\alpha_1}(\vec{r}_N) \\ \vdots & \ddots & \vdots \\ \psi_{\alpha_N}(\vec{r}_1) & \cdots & \psi_{\alpha_N}(\vec{r}_N) \end{vmatrix}$$

For $N=2$: $\psi = \frac{1}{\sqrt{2}}\left(\psi_{\alpha_1}(\vec{r}_1)\psi_{\alpha_2}(\vec{r}_2) - \psi_{\alpha_1}(\vec{r}_2)\psi_{\alpha_2}(\vec{r}_1)\right)$

Operators in the occupation # representation

$$\hat{F} = \sum_{i=1}^{N} \hat{F}_i = \sum_{i=1}^{N} \underbrace{F_{\alpha\beta}\, |\alpha\rangle_i \langle\beta|_i}$$

this operator is acting on the i-th Hilbert space

$$\hat{F}_1 \otimes \mathbb{1}_2 \cdots \otimes \mathbb{1}_N + \cdots + \mathbb{1}_1 \otimes \cdots \otimes \hat{F}_N \quad , \quad \hat{F}_1 = \hat{F}_2 = \cdots = \hat{F}_N = \hat{F}_S$$

$$\xrightarrow{1} \frac{1}{\sqrt{N!\, n_1! \cdots n_N!}} \sum_{\alpha\,\beta} F_{\alpha\beta} |\alpha\rangle\langle\beta| \sum_{\pi \in S_N} |\varphi_{\alpha_1}(\vec{r}_{\pi(1)})\rangle \cdots |\varphi_{\alpha_N}(\vec{r}_{\pi(N)})\rangle$$

$$\hat{F}\,|n_1, \dots, n_N\rangle = C \sum_{\alpha\beta} F_{\alpha\beta}\, |n_1, \dots, n_\alpha + 1, \dots, n_\beta - 1, \dots\rangle$$

Calculate the normalization:

$$\hat{F}\,|n_1, n_2, \dots\rangle = \sum_{\alpha\beta} F_{\alpha\beta} \sqrt{n_\alpha + 1}\,\sqrt{n_\beta}\; |\dots\, \underbrace{n_\alpha + 1 \dots n_\beta - 1}_{\text{are the only quantum number that change}} \dots\rangle$$

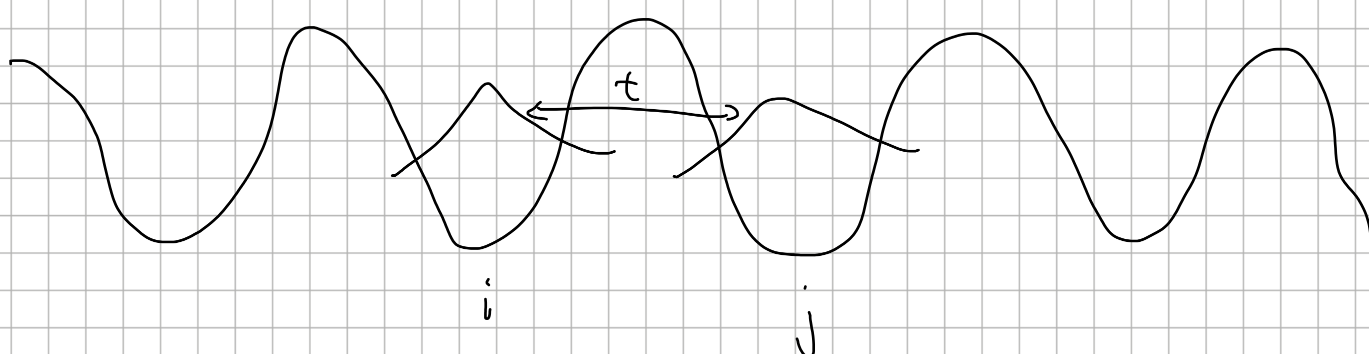
Bosonic case: $\hat{b}_\beta\,|n_1, \dots, n_\beta \dots\rangle = \sqrt{n_\beta}\;|\dots\, n_\beta - 1 \dots\rangle$

$$\hat{b}_\alpha^{+}\,|n_1, \dots, n_\alpha, \dots\rangle = \sqrt{n_\alpha + 1}\;|\dots\, n_\alpha + 1, \dots\rangle$$

$$\Rightarrow \hat{F} = \sum_{\alpha\beta} F_{\alpha\beta}\, b_\alpha^{+} b_\beta$$

kinetic energy: $\hat{H} = \sum_k \frac{\hbar^2 k^2}{2m}\, b_k^{+} b_k$

Bosons on a lattice



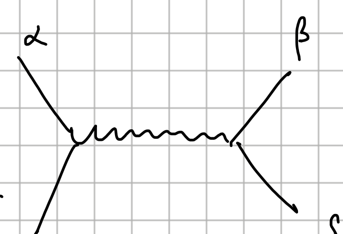
$$\hat{H} = -t \sum_{\langle i,j\rangle} b_i^{+} b_j$$

To preserve the statistics of the wave

$$[\hat{b}_\alpha^{+}, \hat{b}_\beta] = \delta_{\alpha\beta}\,, \qquad [\hat{b}_\alpha, \hat{b}_\beta] = [\hat{b}_\alpha^{+}, \hat{b}_\beta^{+}] = 0$$

Two particle operator:

$$\hat{G} = \frac{1}{2}\sum_{i\neq j} G_{ij} = \sum_{i\neq j}\sum_{\alpha\beta\gamma\delta} G_{\alpha\beta\gamma\delta}\, \underbrace{|\alpha\rangle|\beta\rangle\langle\gamma|\langle\delta|}_{b_\alpha^{+} b_\beta^{+} b_\gamma b_\delta}$$



12.12.2018

Bosons single- and two-particle operators

$b_\alpha \quad b_\alpha^+ \qquad [b_\alpha, b_\beta^+] = \delta_{\alpha\beta} \qquad [b_\alpha, b_\beta] = 0 \qquad [b^+_\alpha, b^+_\beta] = 0$

typical Hamiltonian: $\hat{H} = \sum_{\alpha\beta} T_{\alpha\beta} b_\alpha^+ b_\beta + \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} b_\alpha^+ b_\beta^+ b_\gamma b_\delta + \cdots$

singel-particle term   two-...   three-...

Fermions: $|n_1, n_2, \ldots\rangle \qquad n_i = 0$ or 1

$$\hat{F}|n_1, n_2, \ldots\rangle = \sum_{\alpha\beta} F_{\alpha\beta} |n_1, \ldots, n_\alpha + 1, \ldots, n_\beta - 1, \ldots\rangle \sqrt{(n_\alpha+1) \bmod 2} \cdot \sqrt{n_\beta}\,(-1)^{k_{\alpha\beta}}$$

$k_{\alpha\beta}$ = distance between α and β

fermions state in occupation number $\to$ binary system

Example: $|\phi\rangle = |1, 1, 0, 0, 1, 0, \ldots\rangle$

$\hat{F}_{32}|\phi\rangle = |1, 0, 1, 0, 1, 0, \ldots\rangle$

$\hat{F}_{41}|\phi\rangle = -|0, 1, 0, 1, 1, 0, \ldots\rangle$

c_α, e.g. $\alpha = (\vec{k}, \sigma) \qquad c_\alpha c_\beta^+ + c_\beta^+ c_\alpha = \delta_{\alpha\beta} \qquad \Rightarrow \qquad \{c_\alpha, c_\beta^+\} = \delta_{\alpha\beta}$

$c_\alpha^+ \qquad c_{k\sigma} c^+_{k'\sigma'} + c^+_{k'\sigma'} c_{k\sigma} = \delta_{\sigma\sigma'} \delta(\vec{k} - \vec{k}')$

$\{c_\alpha, c_\beta\} = 0 \Rightarrow c_\alpha c_\beta = -c_\beta c_\alpha$

$\{c_\alpha^+, c_\beta^+\} = 0 \Rightarrow c_\alpha^+ c_\beta^+ = -c_\beta^+ c_\alpha^+$

Field operators:

Bosons: $\hat{\psi}(\vec{r}) = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \hat{b}_{\vec{k}}$ Fermions: $\hat{\psi}_\sigma(\vec{r}) = \sum e^{i\vec{k}\cdot\vec{r}} \hat{c}_{k\sigma}$

$\hat{\psi}^+(\vec{r}) = \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \hat{b}^+_{\vec{k}}$ $\hat{\psi}^+_\sigma(\vec{r}) = \sum e^{-i\vec{k}\cdot\vec{r}} \hat{c}^+_{k\sigma}$

$$\{\hat{\psi}_\sigma(\vec{r}), \hat{\psi}^+_{\sigma'}(\vec{r}')\} = \sum_{kk'} e^{i\vec{k}\cdot\vec{r} - i\vec{k}'\cdot\vec{r}'} \{c_{k\sigma}, c^+_{k'\sigma'}\} = \delta_{\sigma\sigma'} \delta(\vec{r} - \vec{r}')$$

$$\{\hat{\psi}_\sigma(\vec{r}), \hat{\psi}_{\sigma'}(\vec{r}')\} = 0$$

$$\hat{H} = \sum_\sigma \int d^3r\, \hat{\psi}^+_\sigma(\vec{r}) \left(-\frac{\hbar^2}{2m}\Delta\right) \hat{\psi}_\sigma(\vec{r}) = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} c^+_{k\sigma} c_{k\sigma}$$

17.12.2018

Bosonic coherent state:

$$\hat{b}_k |k\rangle = \phi_k |k\rangle$$ particle number is not fixed!

$$|\phi\rangle = \sum_{n_{\alpha_1} \cdots n_{\alpha_N}} \phi_{n_{\alpha_1} \cdots n_{\alpha_N}} |n_{\alpha_1}, \ldots, n_{\alpha_N}\rangle$$

$$\hat{b}_{\alpha_i} |\phi\rangle = \sum_{n_{\alpha_1} \cdots n_{\alpha_N}} \phi_{n_{\alpha_1} \cdots n_{\alpha_N}} \hat{b}_{\alpha_i} |n_{\alpha_1} \cdots n_{\alpha_N}\rangle$$

$$= \sum_{n_{\alpha_1} \cdots n_{\alpha_N}} \phi_{n_{\alpha_1} \cdots n_{\alpha_N}} \sqrt{n_{\alpha_i}} |n_{\alpha_1}, \ldots, (n_{\alpha_i}-1), \ldots n_{\alpha_N}\rangle$$

$$\hat{b}_{\alpha_i} |\phi\rangle = \phi_{\alpha_i} |\phi\rangle = \sum_{n_1 \cdots n_{\alpha_N}} \phi_{n_{\alpha_i}} \phi_{n_{\alpha_1} \cdots (n_{\alpha_i}-1) \cdots n_{\alpha_N}} |n_{\alpha_1} \cdots (n_{\alpha_i}-1) \cdots n_{\alpha_N}\rangle$$

Mistake!

$$\phi_{\alpha_i} \phi_{n_{\alpha_1} \cdots n_{\alpha_N}} = \sqrt{n_{\alpha_i}} \phi_{n_{\alpha_1} \cdots (n_{\alpha_i}-1) \cdots n_{\alpha_N}}$$

$$\Rightarrow \phi_{n_{\alpha_1} \cdots n_{\alpha_N}} = \frac{\phi_{\alpha_1}^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \frac{\phi_{\alpha_2}^{n_{\alpha_2}}}{\sqrt{n_{\alpha_2}!}} \cdots \frac{\phi_{\alpha_N}^{n_{\alpha_N}}}{\sqrt{n_{\alpha_N}!}}$$

$$\rightarrow |n_{\alpha_1} \cdots n_{\alpha_N}\rangle = \frac{(\hat{b}^{\dagger}_{\alpha_1})^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \cdots \frac{(\hat{b}^{\dagger}_{\alpha_N})^{n_{\alpha_N}}}{\sqrt{n_{\alpha_N}!}} |0\rangle$$

$$|\phi\rangle = \sum_{n_{\alpha_1} \cdots n_{\alpha_N}} \frac{(\phi_{\alpha_1} \hat{b}^{\dagger}_{\alpha_1})^{n_{\alpha_1}}}{n_{\alpha_1}!} \cdots \frac{(\phi_{\alpha_N} \hat{b}^{\dagger}_{\alpha_N})^{n_{\alpha_N}}}{n_{\alpha_N}!} |0\rangle$$

$$\boxed{|\phi\rangle = \exp\left(\sum_{\alpha} \phi_{\alpha} \hat{b}^{\dagger}_{\alpha}\right) |0\rangle}$$ coherent state $\phi_\alpha \in \mathbb{C}$

expectation value:

$$\langle\phi| = \langle 0| \exp\left(\sum_{\alpha} \phi^*_{\alpha} \hat{b}_{\alpha}\right)$$

$$\hat{b}^{\dagger}_{\alpha} |\phi\rangle = \partial_{\phi_\alpha} |\phi\rangle$$

overlap of coherent states:

$$|\phi\rangle = \sum_{n_{\alpha_1} \cdots n_{\alpha_N}} \phi_{\alpha_1 \cdots \alpha_N} |n_{\alpha_1} \cdots n_{\alpha_N}\rangle$$

$$|\phi'\rangle = \sum_{n_{\alpha_1} \cdots n_{\alpha_N}} \phi'_{\alpha_1 \cdots \alpha_N} |n_{\alpha_1} \cdots n_{\alpha_N}\rangle$$

$$\langle \phi' | \phi \rangle = \sum_{n_{\alpha_1} \cdots n_{\alpha_N}} \frac{(\phi'^*_{\alpha_1} \phi_{\alpha_1})^{n_{\alpha_1}}}{n_{\alpha_1}!} \cdots \frac{(\phi'^*_{\alpha_N} \phi_{\alpha_1})^{n_{\alpha_N}}}{n_{\alpha_N}!} \in \mathbb{C}$$

$$(\hat{b}_\alpha \hat{b}_\alpha^+)^n = \hat{b}_\alpha^{n-1} \hat{b}_\alpha \hat{b}_\alpha^+ \hat{b}_\alpha^{+n-1} = \hat{b}_\alpha^{n-1} (1 + \hat{n}_\alpha) \hat{b}_\alpha^{+n-1}$$

$$= \exp\Big(\sum_\alpha \phi'^*_\alpha \phi_\alpha \Big)$$

Representation of the operator $\mathbb{1}$ in this space: (normalisation)

$$\boxed{\mathbb{1} = \int d\phi^*_\alpha \, d\phi_\alpha \, e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \underbrace{|\phi\rangle\langle\phi|}_{\text{projector}}}$$

Grassman-variables and Fermion coherent states

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0 \qquad \xi_\alpha^2 = 0$$

$$(\xi_\alpha)^* = \xi^*_\alpha \qquad \text{conjugation}$$

$\{\xi_\alpha\}$ are generators $(\alpha = 1, \ldots, n)$

conjugation of product

$$(\xi_{\alpha_1} \ldots \xi_{\alpha_N})^* = \xi^*_{\alpha_N} \xi^*_{\alpha_{n-1}} \cdots \xi^*_{\alpha_1}$$

algebra generated by $1, \xi, \xi^*, \xi^* \xi$

Any function of ξ, ξ^* has the form:

$$A(\xi^*, \xi) = a_0 + a_1 \xi + \bar{a}_1 \xi^* + b \, \xi^* \xi$$

$$\partial_\xi \xi = 1 \qquad \partial_\xi 1 = 0$$

$$\partial_\xi A(\xi^*, \xi) = a_1 - b \xi^*$$

$$\partial_{\xi^*} A(\xi^*, \xi) = \bar{a}_1 + b \xi$$

$$\partial^2_{\xi\xi^*} A(\xi^*, \xi) = -\partial^2_{\xi^*\xi} A(\xi^*, \xi) = -b$$

$$\int d\xi \, 1 = 0 \qquad \int d\xi \, \xi = 1$$

$$\int d\xi \, A(\xi^*, \xi) = \int d\xi \, (a_0 + a_1 \xi + \bar{a}_1 \xi^* + b \xi^* \xi) = a_1 - b \xi^*$$

$$\int d\xi^* \int d\xi \, A(\xi^*, \xi) = -b$$

Define δ-function:

higher orders disappear

$$\delta(\xi, \xi') = \int d\eta \exp(-\eta(\xi - \xi')) = \int d\eta \, (1 - \eta(\xi - \xi'))$$
$$= -(\xi - \xi')$$

The function has the desired properties:

$$f(\xi) = f_0 + f_1 \xi$$
$$\int d\xi' \, \delta(\xi, \xi') f(\xi') = -\int d\xi' (\xi - \xi')(f_0 + f_1 \xi')$$
$$= f_0 + f_1 \xi$$
$$= f(\xi)$$

$$\langle f | g \rangle := \int d\xi^* \int d\xi \, e^{-\xi \xi^*} f^*(\xi) g(\xi^*)$$ scalar product in function space

$$= \int d\xi^* \int d\xi \, (1 - \xi \xi^*)(f_0^* + f_1^* \xi)(g_0 + g_1 \xi^*)$$

$$= f_0^* g_0 + f_1^* g_1$$ ← positive semi-definite

coherent states

- They don't exist!

$$|\psi\rangle = \sum_\alpha \chi_\alpha \, |\phi_\alpha\rangle$$ ← state in Fock-space

↑ Grassman variable

to complete the construction in analogy with bosonic case we need

c, c^+ are fermionic creation and annihilation operators

$$\{\xi, c\} = \{\xi^*, c^+\} = \{\xi^*, c\} = \{\xi, c^+\} = 0$$

The coherent state is given by:

$$|\xi\rangle = \exp(-\sum_\alpha \xi_\alpha c_\alpha^+) |0\rangle$$

$$|\xi\rangle = \prod_\alpha (1 - \xi_\alpha c_\alpha^+) |0\rangle$$

($\xi_\alpha c_\alpha^+$ and $\xi_\beta c_\beta^+$ commute if $\alpha \neq \beta$)

Check if $|\xi\rangle$ is a coherent state

$$c_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle$$ — the CS of fermions are not real, not observable!

$$\left(c_\alpha (1 - \xi_\alpha c_\alpha^+) |0\rangle = \xi_\alpha |0\rangle \right)$$

$$\left(\xi_\alpha (1-\xi_\alpha c_\alpha^\dagger)|0\rangle = \xi_\alpha |0\rangle \right)$$

Overlap between two coherent fermions states:

$$\langle \xi|\xi'\rangle = \langle 0|\prod_\alpha (1+\xi_\alpha^* c_\alpha)(1-\xi'_\alpha c_\alpha^\dagger)|0\rangle = \prod_\alpha (1+\xi_\alpha^*\xi'_\alpha)$$

$$= e^{\sum_\alpha \xi_\alpha^* \xi'_\alpha}$$

$$\prod_\alpha \int d\xi_\alpha^* \int d\xi_\alpha \, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} |\xi\rangle\langle\xi| = \mathbb{1}$$

19.12.2018 (*)

Basic model: Bosonic Hubbard-model

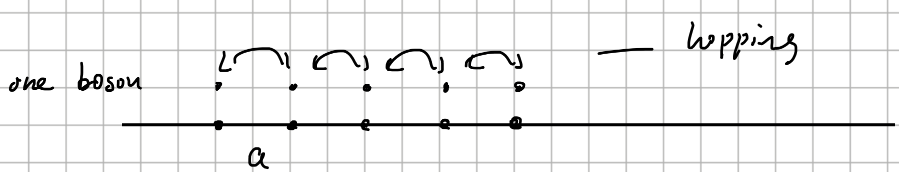
$$\hat{H} = -t \sum_{\langle ij\rangle} b_i^\dagger b_j + \frac{1}{2} U \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$

i and j are neighbors

hopping term (putting particle to the neighboring lattic)

chemical potential

$\rightarrow$ not exact solvable (wenn $n_i > 1$); not all operators are diagonalbar at the same time



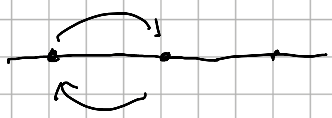
$U/t \rightarrow \infty$, bosons are stuck $\Rightarrow$ Mott insulator

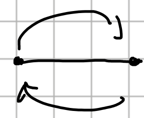
Idee: perturbation in t/U

ground state energy $\langle \phi|\hat{H}|\phi\rangle = E_0$

$$E_0 = U\left(a_2 \left(\frac{t}{U}\right)^2 + a_4 \left(\frac{t}{U}\right)^4 + \dots\right)$$

only t^{2n}, hopping to another site and back topological clusters (connected at the lattice)





→ Calculate the Hamiltonian with each cluster