- Let's add interactions to the tight-binding model

$$H = H_0 + H_I \text{ with } H_0 = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \psi^{\dagger}_{i,\sigma} \psi_{j,\sigma} - \mu \sum_{j,\sigma} \psi^{\dagger}_{j,\sigma} \psi_{j,\sigma} =$$

NN

Fermi-Hubbard model

$$= \sum_{k,\sigma} c^{\dagger}_k \left(\sum_{\nu=1}^{d} -2t \cos k_{\nu} \right) - \mu) c_k .$$

$$\text{and } H_I = U \sum_j (\hat{n}_{j,\uparrow} - \rho)(\hat{n}_{j\downarrow} - \rho) \quad \text{with } \hat{n}_{j,\sigma} = \psi^{\dagger}_{j,\sigma} \psi_{j,\sigma}$$

Filling factor ρ constant

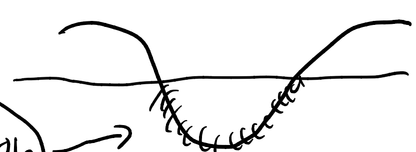
⇝ Describes tightly bound electrons (single-band approximation) with short-ranged interaction (screening length $\leq a$).

Bose-Hubbard model: $\quad H = -J \sum_{\langle i,j \rangle} b^{\dagger}_i b_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$

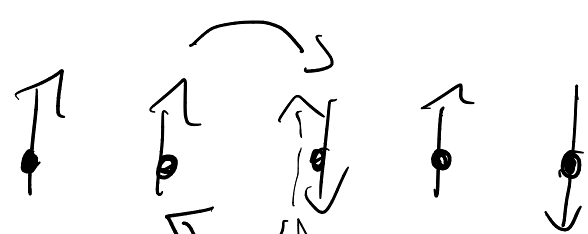
- Heisenberg spin model from Fermi-Hubbard model:
  - Consider $\rho = \frac{1}{2}$ (half-filling) and $\frac{U}{t} \gg 1$ (strong correlation).
  - Basic idea: Treat H_0 as a perturbation to the ground state of H_I.

    ⇝ Start from the 2^L-fold degenerate ground state of H_I, in which a single particle is frozen to each lattice site (all 2^L spin configurations having 0 energy).

    ⇝ Perform 2nd order degenerate perturbation theory calculation in H_0



<0 energy from delocalization



virtual double occupation

$\rightsquigarrow$ Effective Hamiltonian within the previously degenerate sub-space of frozen spins:

$$H_J = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad \text{with} \quad J = \frac{4t^2}{U} > 0$$

(Antiferromagnetic coupling)

and $S_j^\alpha = \psi^+_{j,\sigma} \frac{\tau^\alpha_{\sigma,\sigma'}}{2} \psi_{j,\sigma'}$, τ^α standard Pauli matrix i.e. $\tau^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\tau^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\tau^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

A.3: Practical calculation of observables in free systems

• One-body observable (in system of N identical particles):

$$\mathcal{O} = \sum_{i=1}^{N} \mathbb{1} \otimes \cdots \underset{\substack{\uparrow \\ \text{pos. } i}}{\mathcal{O}} \otimes \cdots \mathbb{1} \equiv \sum_{i=1}^{N} \mathcal{O}^{(i)} \underset{\substack{\uparrow \\ \text{2nd Q.}}}{=} \sum_{\alpha, \beta} \mathcal{O}_{\alpha\beta}\, a_\alpha^\dagger a_\beta \quad \text{with}$$

$$\mathcal{O}_{\alpha\beta} = \langle \alpha | \mathcal{O} | \beta \rangle$$

single particle states

– Fermions: System in state $|\psi\rangle = S_- |\alpha_1, \ldots, \alpha_N\rangle$

$$\rightsquigarrow \boxed{\langle \psi | \mathcal{O} | \psi \rangle = \sum_{i=1}^{N} \langle \alpha_i | \mathcal{O} | \alpha_i \rangle}$$

since in

$$\langle \psi | \mathcal{O} | \psi \rangle = \frac{1}{N!} \sum_{P, P'} (-1)^{|P| + |P'|} \underbrace{\langle \alpha_1, \ldots, \alpha_N | P^\dagger \mathcal{O} P' | \alpha_1, \ldots, \alpha_N \rangle}_{= 0 \text{ unless } P = P'.}$$

- Bosons: System in state $|\Psi\rangle = \frac{S_+}{\sqrt{n_1! \cdots}} |\alpha_1, \dots, \alpha_N\rangle$

$\rightsquigarrow \langle\Psi|O|\Psi\rangle = \sum_{i=1}^{N} \langle\alpha_i|O|\alpha_i\rangle$ for similar reasons as in fermionic case as long as $\langle\alpha_i|\alpha_j\rangle \in \{0,1\}$.

More complicated situation for Bosons in non-orthogonal states: Example: 2 particles in states $|\alpha\rangle$ and $|\gamma\rangle = \frac{1}{\sqrt{2}}(|\alpha\rangle + |\beta\rangle)$ with $\langle\alpha|\beta\rangle = 0$.

$$|\Psi\rangle = \frac{a_\alpha^+ \left(\frac{1}{\sqrt{2}}(a_\beta^+ + a_\alpha^+)\right)|0\rangle}{\| \quad " \quad \|} =$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{2}\,|n_\alpha = 2\rangle + |n_\alpha = 1, n_\beta = 1\rangle\right) =$$

$$= \frac{1}{\sqrt{3}}\left(\sqrt{2}\,|n_\alpha = 2\rangle + |n_\alpha = 1, n_\beta = 1\rangle\right)$$

$$\rightsquigarrow \langle\psi|O|\psi\rangle = \frac{1}{3}\Big(5\underbrace{\langle\alpha|O|\alpha\rangle}_{O_{\alpha\alpha}} + 2O_{\alpha\beta} + 2O_{\beta\alpha} + O_{\beta\beta}\Big) =$$

$$\neq \langle\alpha|O|\alpha\rangle + \langle\gamma|O|\gamma\rangle$$

- Time evolution operator (as an exponential) requires some extra care, even for free systems:

$$\mathcal{U}(t) = e^{-iHt} = e^{-it\sum_{j=1}^{N} h^{(j)}} = u(t) \otimes u(t) \cdots\cdots \otimes u(t) \quad \text{with}$$

N identical factors $u(t) = e^{-iht}$.

$\rightsquigarrow$ $\mathcal{U}(t)$ <u>not</u> of conventional single particle form $\sum_{i=1}^{N} o^{(i)}$, even if H is.

- Application to time-evolved expectation values of one-body operators:

$$\langle \Psi_0 | \mathcal{U}^\dagger(t)\, O\, \mathcal{U}(t) | \Psi_0 \rangle \overset{\text{Heisenberg pict.}}{=} \langle \Psi_0 | \underbrace{\left(\sum_{i=1}^{N} u^\dagger(t)\, o^{(i)}\, u(t) \right)}_{O(t)} | \Psi_0 \rangle =$$

$$= \sum_{\alpha} \langle \alpha | o(t) | \alpha \rangle = \sum_{\alpha} \langle \alpha(t) | o | \alpha(t) \rangle .$$

single particle states occupied in $|\Psi_0\rangle$

Schrödinger picture

with $|\alpha(t)\rangle = u(t)|\alpha\rangle$

– Application to overlaps between time-evolved and initial states (auto-correlations)

$$\langle\Psi_0|\Psi(t)\rangle = \langle\Psi_0|\mathcal{U}(t)|\Psi_0\rangle = \frac{1}{N!}\sum_{P,P'}(-1)^{|P|+|P'|}\langle\alpha_1,\dots,\alpha_N|\cdots$$

$|\Psi(t)\rangle = \mathcal{U}(t)|\Psi_0\rangle$

Fermions

$$\cdots P^{\dagger}\,\mathcal{U}(t)\,P'|\alpha_1,\dots,\alpha_N\rangle = \frac{1}{N!}\sum_{P,P'}(-1)^{|P|+|P'|}\langle\alpha_1,\dots,\alpha_N|\mathcal{U}(t)P^{\dagger}P'|\cdots$$

$[P,O]=0$

$$\cdots\alpha_1,\dots,\alpha_N\rangle = \sum_{\tilde{P}}(-1)^{\tilde{P}}\langle\alpha_1,\dots,\alpha_N|\,\mathcal{U}(t)\,\tilde{P}\,|\alpha_1,\dots,\alpha_N\rangle =$$

$$= \sum_{\tilde{P}}(-1)^{\tilde{P}}\prod_{i=1}^{N}\langle\alpha_i|u(t)|\alpha_{\tilde{P}(i)}\rangle = \det\left(\left(\langle\alpha|u(t)|\beta\rangle\right)_{\alpha\beta}\right).$$

$\mathcal{U}(t) = u(t)\otimes u(t)\otimes\dots\otimes u(t)$

α,β states initially occupied by particles