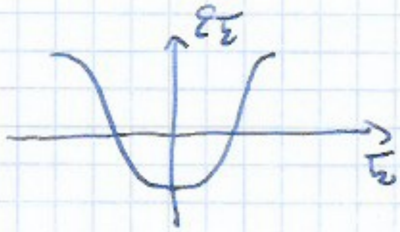
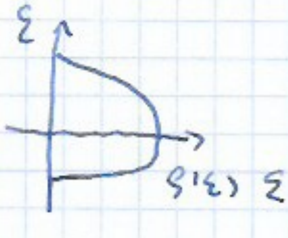
§7. t – J model

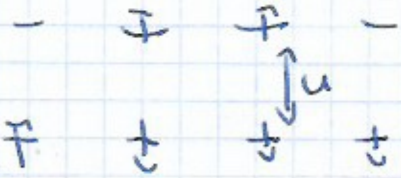
$$H = \sum_{ij\sigma} t_{ij}\, a_{i\sigma}^{\dagger} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \varepsilon \sum_{i\sigma} n_{i\sigma}$$

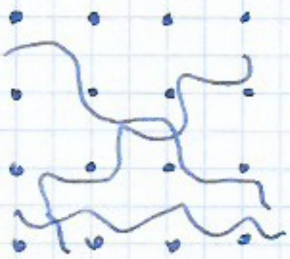
$U = 0$ $\qquad\qquad\qquad\qquad$ $t = 0$

$$H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} \qquad\qquad H = \sum_{i\sigma} \varepsilon n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

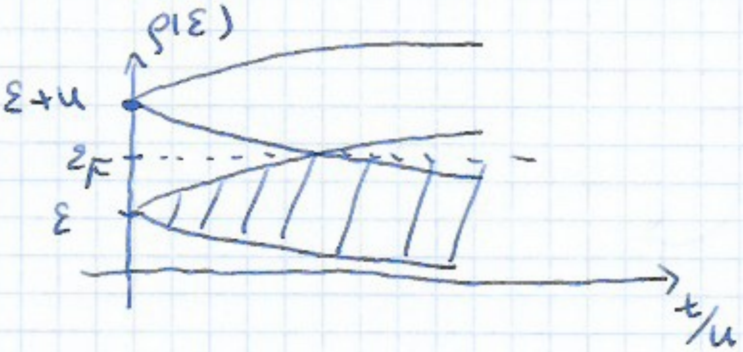








$|\psi\rangle = \prod_{k\sigma} a_{k\sigma}^{\dagger} |0\rangle \qquad\qquad |\psi\rangle = \prod_{i\sigma} \hat{a}_{i\sigma}^{\dagger} |0\rangle$



metal insulator transition

MIT

For two site H we've seen that the ground state is a singlet → antiferromagnetism for large $U \gg t$?

$\frac{N_e}{2N_L} = n \leq 1$ → no double occupied sites

Let's separate low and high energy processes

$$1 = 1 - \hat{n}_{i\bar{\sigma}} + \hat{n}_{i\bar{\sigma}}$$

$$\hat{a}^{\dagger}_{i\sigma}\,\hat{a}_{j\sigma} = \hat{a}^{\dagger}_{i\sigma}\left(1-\hat{n}_{i\bar{\sigma}}+\hat{n}_{i\bar{\sigma}}\right)\hat{a}_{j\sigma}\left(1-n_{j\bar{\sigma}}+n_{j\bar{\sigma}}\right) =$$

$$\text{low} \quad = \hat{a}^{\dagger}_{i\sigma}\left(1-\hat{n}_{i\bar{\sigma}}\right)\hat{a}_{j\sigma}\left(1-n_{j\bar{\sigma}}\right) +$$

$$+ \; \hat{a}^{\dagger}_{i\sigma}\left(1-\hat{n}_{i\bar{\sigma}}\right)\hat{a}_{j\sigma}\,\hat{n}_{j\bar{\sigma}} +$$

$$+ \; \hat{a}^{\dagger}_{i\sigma}\,\hat{n}_{i\bar{\sigma}}\,\hat{a}_{j\sigma}\left(1-\hat{n}_{j\bar{\sigma}}\right) +$$

$$+ \; \hat{a}^{\dagger}_{i\sigma}\,\hat{n}_{i\bar{\sigma}}\,\hat{a}_{j\sigma}\,\hat{n}_{j\bar{\sigma}} \quad \text{high}$$

We introduce a projection operator onto a single occupied Hilbert space

$$\hat{\Pi}_1 = \prod_{i=1}^{N_L}\left(1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\right) \qquad \text{no double occupancy}$$

$$\hat{\Pi}_2 = \hat{\mathbb{1}} - \hat{\Pi}_1$$

since $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \begin{cases} 0 \\ 1 \end{cases}$

$$\hat{\Pi}_1^2 = \hat{\Pi}_1 \,, \qquad \hat{\Pi}_2^2 = \hat{\Pi}_2$$

$$\hat{\Pi}_1 \cdot \hat{\Pi}_2 = 0$$

Then

$$\hat H = (\hat\Pi_1 + \hat\Pi_2)\,\hat H\,(\hat\Pi_1 + \hat\Pi_2) =$$

$$= \hat\Pi_1 \hat H \hat\Pi_1 + \hat\Pi_2 \hat H \hat\Pi_2 +$$

$$\hat\Pi_1 \hat H \hat\Pi_2 + \hat\Pi_2 \hat H \hat\Pi_1 = \begin{array}{c} \text{low} \\ \left(\begin{array}{c|c} \Pi_1 H \Pi_1 & \Pi_2 H \Pi_1 \\ \hline \Pi_1 H \Pi_2 & \Pi_2 H \Pi_2 \end{array}\right) \\ \text{high} \end{array}$$

and

$$\hat\Pi_1 \hat H \hat\Pi_1 = \sum_{ij\sigma} t_{ij}\, a_{i\sigma}^\dagger (1-\hat n_{i\bar\sigma})\, \hat a_{j\sigma} (1-\hat n_{j\bar\sigma})$$

$$\hat\Pi_2 \hat H \hat\Pi_2 = \sum_{ij\sigma} t_{ij}\, \hat a_{i\sigma}^\dagger\, \hat n_{i\bar\sigma}\, \hat a_{j\sigma}\, \hat n_{j\bar\sigma} + U \sum_i \hat n_{i\uparrow} \hat n_{i\downarrow}$$

$$\hat\Pi_1 \hat H \hat\Pi_2 = \sum_{ij\sigma} t_{ij}\, \hat a_{i\sigma}^\dagger (1-n_{i\bar\sigma})\, \hat a_{j\sigma}\, \hat n_{j\bar\sigma}$$

$$\hat\Pi_2 \hat H \hat\Pi_1 = \sum_{ij\sigma} t_{ij}\, \hat a_{i\sigma}\, \hat n_{j\bar\sigma}\, \hat a_{j\sigma} (1-n_{j\bar\sigma})$$

We want to remove perturbatively the high energy term in the Hamiltonian.

Let's write $\hat H(\lambda) = \hat H_0 + \lambda \hat H_1$

$$\hat H_0 = \hat\Pi_1 \hat H \hat\Pi_1 + \hat\Pi_2 \hat H \hat\Pi_2$$

$$\hat H_1 = \hat\Pi_1 \hat H \hat\Pi_2 + \hat\Pi_2 \hat H \hat\Pi_1$$

$\lambda = 1$ at the end (bookkeeping perturbation terms) canonical (Schrieffer-Wolff, Foldy-Wouthuysen)

$$\hat{\tilde{H}}(\lambda) = e^{-i\lambda\hat{S}} \, \hat{H} \, e^{i\lambda\hat{S}}$$

unitary $\rightarrow$ $\hat{S}^{\dagger} = \hat{S}$ - Hermitian

$$e^{\pm i\lambda\hat{S}} = 1 \pm i\lambda\hat{S} - \frac{1}{2}\lambda^2\hat{S}^2 + \dots$$

$$\hat{\tilde{H}}(\lambda) = \hat{H}_0 + \lambda\left(\hat{H}_1 + i[\hat{H}_0, \hat{S}]\right) +$$

$$+ \frac{1}{2}\lambda^2\left(2i[\hat{H}_1, \hat{S}] - [[\hat{H}_0, \hat{S}], \hat{S}]\right) + \dots$$

Transformation $\hat{S}$ is defined by vanishing of $O(\lambda)$ term

$$\boxed{\hat{H}_1 + i[\hat{H}_0, \hat{S}] = 0}$$

And then

$$\hat{\tilde{H}}(\lambda) = \hat{H}_0 + \frac{1}{2} i\lambda^2 [\hat{H}_1, \hat{S}] + \dots$$

proof

$$2i[\hat{H}_1, \hat{S}] - [[\hat{H}_0, \hat{S}], \hat{S}] =$$

$$= 2i[\hat{H}_1, \hat{S}] - i[\hat{H}_1, \hat{S}] = i[\hat{H}_1, S] \quad \square$$

Let's find $\hat{S}$:

$$\hat{P}_\mu \,/\, \hat{H}_1 + i\,\hat{H}_0 \underbrace{\ }_{\hat{P}_1+\hat{P}_2} \hat{S} - i\,\hat{S} \underbrace{\ }_{\hat{P}_1+\hat{P}_2} \hat{H}_0 = 0 \,/\, \hat{P}_\nu$$

$$\hat{P}_\mu \hat{H}_1 \hat{P}_\nu + i\,\hat{P}_\mu \hat{H}_0 (\hat{P}_1+\hat{P}_2)\hat{S}\hat{P}_\nu - i\,\hat{P}_\mu \hat{S}(\hat{P}_1+\hat{P}_2)\hat{H}_0 \hat{P}_\nu = 0$$

$$\Rightarrow (\hat{\Pi}_\mu \hat{H} \hat{\Pi}_\mu)(\hat{\Pi}_\mu \hat{S} \hat{\Pi}_\nu) - (\hat{\Pi}_\mu \hat{S} \hat{\Pi}_\nu)(\hat{\Pi}_\nu \hat{H} \hat{\Pi}_\nu) =$$

$$= i\,(\hat{\Pi}_\mu \hat{H} \hat{\Pi}_\nu)(1-\delta_{\mu\nu})$$

For $\mu = \nu$

$$(\hat{\Pi}_\mu \hat{H} \hat{\Pi}_\mu)(\hat{\Pi}_\mu \hat{S} \hat{\Pi}_\mu) - (\hat{\Pi}_\mu \hat{S} \hat{\Pi}_\mu)(\hat{\Pi}_\mu \hat{H} \hat{\Pi}_\mu) = 0$$

Since $\hat{\Pi}_\mu \hat{S} \hat{\Pi}_\mu$ commutes with $\hat{\Pi}_\mu \hat{H} \hat{\Pi}_\mu = \hat{H}_0$
we can choose solution such that

$$\hat{\Pi}_\mu \hat{S} \hat{\Pi}_\mu = 0$$

For $\mu \neq \nu$

$$\hat{\Pi}_1 \hat{S} \hat{\Pi}_2 = \left[-i\,\hat{\Pi}_1 \hat{H} \hat{\Pi}_2 + (\hat{\Pi}_1 \hat{H} \hat{\Pi}_1)(\hat{\Pi}_1 \hat{S} \hat{\Pi}_2)\right](\hat{\Pi}_2 \hat{H} \hat{\Pi}_2)^{-1}$$

we solve it iteratively with

$$\hat{\Pi}_1 \hat{S}^{(0)} \hat{\Pi}_2 = 0$$

$$\hat{\Pi}_1 \hat{S}^{(1)} \hat{\Pi}_2 = (-i\,\hat{\Pi}_1 \hat{H} \hat{\Pi}_2)\cdot(\hat{\Pi}_2 \hat{H} \hat{\Pi}_2)^{-1}$$

$$\hat{\Pi}_1 \hat{S}^{(2)} \hat{\Pi}_2 = \left[-i\,\hat{\Pi}_1 \hat{H} \hat{\Pi}_2 + (\hat{\Pi}_1 \hat{H} \hat{\Pi}_1)(-i\,\hat{\Pi}_1 \hat{H} \hat{\Pi}_2)\cdot(\hat{\Pi}_2 \hat{H} \hat{\Pi}_2)^{-1}\right]\cdot (\hat{\Pi}_2 \hat{H} \hat{\Pi}_2)^{-1}$$

$$\hat{\Pi}_1 \hat{S}^{(2)} \hat{\Pi}_2 = \left[1 + \frac{\hat{\Pi}_1 \hat{h} \hat{\Pi}_1}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2} \right] \cdot \frac{(-i \hat{\Pi}_1 \hat{h} \hat{\Pi}_2)}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2}$$

$$\hat{\Pi}_1 \hat{S}^{(3)} \hat{\Pi}_2 = \left[-i \hat{\Pi}_1 \hat{h} \hat{\Pi}_2 + \hat{\Pi}_1 \hat{h} \hat{\Pi}_1 \cdot \left[1 + \frac{\hat{\Pi}_1 \hat{h} \hat{\Pi}_1}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2} \right] \frac{(-i \hat{\Pi}_1 \hat{h} \hat{\Pi}_2)}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2} \right] \cdot \frac{1}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2} =$$

$$= \left[1 + \frac{\hat{\Pi}_1 \hat{h} \hat{\Pi}_1}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2} + \frac{(\hat{\Pi}_1 \hat{h} \hat{\Pi}_1)^2}{(\hat{\Pi}_2 \hat{h} \hat{\Pi}_2)^2} \right] \frac{(-i \hat{\Pi}_1 \hat{h} \hat{\Pi}_2)}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2}$$

Continuing, up to first order in $\frac{t_{ij}}{U} \sim \hat{\Pi}_1 \hat{h} \hat{\Pi}_2$ we find

$$\boxed{\hat{\Pi}_1 \hat{S} \hat{\Pi}_2 =} \frac{-i \hat{\Pi}_1 \hat{h} \hat{\Pi}_2}{1 - \frac{\hat{\Pi}_1 \hat{h} \hat{\Pi}_1}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2}} \frac{1}{\hat{\Pi}_2 \hat{h} \hat{\Pi}_2} \simeq$$

$$\simeq \frac{-i \hat{\Pi}_1 \hat{h} \hat{\Pi}_2}{\langle \hat{\Pi}_2 \hat{h} \hat{\Pi}_2 \rangle - \langle \hat{\Pi}_1 \hat{h} \hat{\Pi}_1 \rangle} = \boxed{\frac{-i \hat{\Pi}_1 \hat{h} \hat{\Pi}_2}{U}}$$

Similarly

$$\boxed{\hat{\Pi}_2 \hat{S} \hat{\Pi}_1 = \frac{-i \hat{\Pi}_2 \hat{h} \hat{\Pi}_1}{U}}$$

Hence, for $\Delta = 1$

$$\hat{\tilde{H}} = \hat{\Pi}_1 \hat{H} \hat{\Pi}_1 + \hat{\Pi}_2 \hat{H} \hat{\Pi}_2 -$$

$$- \frac{1}{U} \left[(\hat{\Pi}_1 \hat{H} \hat{\Pi}_2)(\hat{\Pi}_2 \hat{H} \hat{\Pi}_1) - (\hat{\Pi}_2 \hat{H} \hat{\Pi}_1)(\hat{\Pi}_1 \hat{H} \hat{\Pi}_2) \right] =$$

$$= \hat{\Pi}_1 \hat{\tilde{H}} \hat{\Pi}_1 + \hat{\Pi}_2 \hat{\tilde{H}} \hat{\Pi}_2$$

For $n \leq 1$ the relevant part is

$$\hat{\Pi}_1 \hat{H} \hat{\Pi}_1 - \frac{1}{U} \hat{\Pi}_1 \hat{H} \hat{\Pi}_2 \hat{H} \hat{\Pi}_1$$

Explicitly

$$\hat{\Pi}_1 \hat{H} \hat{\Pi}_1 = \sum_{ij\sigma} t_{ij} \hat{a}^+_{i\sigma} (1 - \hat{n}_{i\bar{\sigma}}) \hat{a}_{j\sigma} (1 - \hat{n}_{j\bar{\sigma}})$$

$$\hat{\Pi}_1 \hat{H} \hat{\Pi}_2 \hat{H} \hat{\Pi}_1 = \sum_{ij\sigma} t_{ij} \hat{a}_{i\sigma} (1 - \hat{n}_{i\bar{\sigma}}) \hat{a}_{j\sigma} n_{j\bar{\sigma}} \cdot$$

$$\cdot \sum_{kl\sigma'} t_{lk} \hat{a}^+_{l\sigma'} n_{l\bar{\sigma}'} \hat{a}_{k\sigma'} (1 - n_{k\bar{\sigma}'})$$

Since no double occupancy in initial and final state term $\underline{l = j}$!

Separating $\sigma' = \sigma$ and $\sigma' = \bar{\sigma}$

$$\hat{\Pi}_1 \hat{H} \hat{\Pi}_2 \hat{H} \hat{\Pi}_1 = \sum_{ijk\sigma}{}' t_{ij} t_{jk} \Big[\hat{a}^+_{i\sigma} (1-\hat{n}_{i\bar\sigma}) \hat{a}_{j\sigma} n_{j\bar\sigma} \hat{a}^+_{j\sigma} n_{j\bar\sigma} \hat{a}_{k\sigma} (1-n_{k\bar\sigma})$$

$$+ \hat{a}^+_{i\sigma} (1-n_{i\bar\sigma}) \hat{a}_{j\sigma} n_{j\bar\sigma} \hat{a}^+_{j\bar\sigma} (1-n_{j\sigma}) \hat{a}_{k\bar\sigma} (1-n_{k\sigma}) \Big]$$

line up: $a^+_{j\sigma} \leftrightarrow n_{j\bar\sigma}$, $n^2_{j\bar\sigma} = n_{j\bar\sigma}$, $a_{j\sigma} a^+_{j\sigma} = 1 - n_{j\sigma}$

line down: $n_{j\bar\sigma} a^+_{j\bar\sigma} = a^+_{j\bar\sigma}$, $\hat{a}_{j\bar\sigma} \hat{a}^+_{j\sigma} = -S_j^{\sigma}$,

$$\hat{\Pi}_1 \hat{H} \hat{\Pi}_2 \hat{H} \hat{\Pi}_1 = \sum_{ijk\sigma}{}' t_{ij} t_{jk} \Big[\hat{a}^+_{i\sigma} (1-n_{i\bar\sigma}) n_{j\bar\sigma} (1-n_{j\sigma}) \hat{a}_{k\sigma} (1-n_{k\bar\sigma}) +$$

$$+ \hat{a}^+_{i\bar\sigma} (1-n_{i\sigma}) (-S_j^{\bar\sigma}) a_{k\bar\sigma} (1-n_{k\sigma}) \Big]$$

For $\underline{k=i}$

$$\sum_{ij\sigma}{}' t_{ij}^2 \Big[\hat{n}_{i\sigma} (1-\hat{n}_{i\bar\sigma}) \hat{n}_{j\sigma} (1-\hat{n}_{j\bar\sigma}) - S_i^{\sigma} S_j^{\bar\sigma} \Big]$$

Let $\hat{n}_{i\sigma} = \dfrac{\hat{n}_i}{2} + \sigma \hat{S}_i^z$,

$$\hat{n}_{i\sigma} (1-n_{i\bar\sigma}) = \frac{\hat{\nu}_i}{2} + \sigma \hat{S}_i^z$$

with $\hat{\nu}_i = \sum_\sigma \hat{n}_{i\sigma} (1-\hat{n}_{i\bar\sigma})$

Then

$$\hat{\Pi}_1 \hat{H} \hat{\Pi}_2 \hat{H} \hat{\Pi}_1 = \sum_{ij}{}' 2 t_{ij}^2 \Big\{ \frac{1}{4} \hat{\nu}_i \hat{\nu}_j - \hat{S}_i^z \hat{S}_j^z - \frac{1}{2} \sum_\sigma S_i^{\sigma} S_j^{\bar\sigma} \Big\} =$$

$$= \sum_{ij}{}' 2t_{ij}^2 \Big[\frac{1}{4} \hat{\nu}_i \hat{\nu}_j - \vec{S}_i \cdot \vec{S}_j \Big]$$

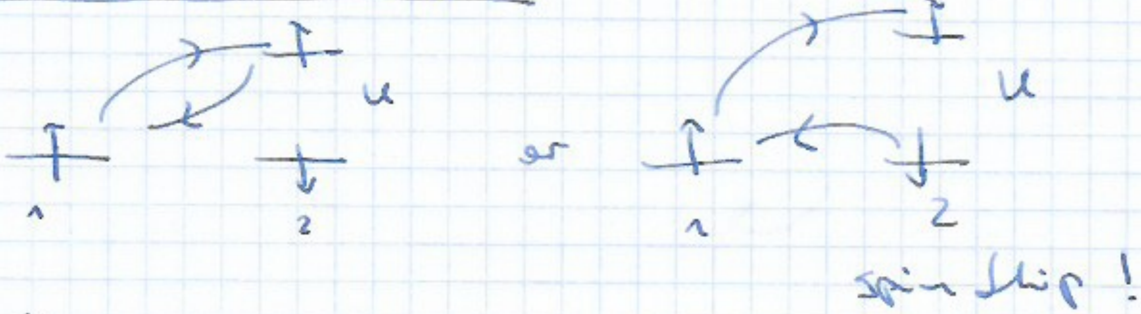
At half-filling $\hat{\nu}_i = \hat{\nu}_j = 1$ so $\hat{\nu}_i \hat{\nu}_j = \text{const.}$

Similarly $k \neq j$

Finally, <u>t-J model</u> $\quad \underline{t_{ij}/U \ll 1}$

$$\boxed{\begin{aligned}\tilde{H}_{tJ} = {} & \sum_{ij\sigma}{}' t_{ij}\, \hat{a}^+_{i\sigma}(1-\hat{n}_{i\bar\sigma})\,\hat{a}_{j\sigma}(1-\hat{n}_{j\bar\sigma}) + \\ & + \sum_{ij}{}' \frac{2t_{ij}^2}{U}\left(\vec{S}_i\cdot\vec{S}_j - \tfrac{1}{4}\hat{\nu}_i\hat{\nu}_j\right) - \\ & - \sum_{ijk\sigma}{}'' \frac{t_{ij}t_{jk}}{U}\Big[\hat{a}^+_{i\sigma}(1-\hat{n}_{i\bar\sigma})\,\hat{n}_{j\bar\sigma}(1-\hat{n}_{j\sigma})\,\hat{a}_{k\sigma}(1-\hat{n}_{k\bar\sigma}) + \\ & \qquad + \hat{a}^+_{i\sigma}(1-\hat{n}_{i\bar\sigma})\,\hat{S}_j^{\bar\sigma}\,\hat{a}_{k\bar\sigma}(1-n_{k\sigma})\Big]\end{aligned}}$$

<u>Kinetic AF/exchange</u>



three site processes

$\Rightarrow$ AF in $n=0$ (half) state $\quad \uparrow \; \downarrow \; \uparrow \; \downarrow$

Projected operators

$$\hat{b}_{i\sigma} = \hat{a}_{i\sigma}(1-\hat{n}_{i\bar{\sigma}})$$

$$\hat{b}^{+}_{i\sigma} = \hat{a}^{+}_{i\sigma}(1-\hat{n}_{i\bar{\sigma}})$$

$$\hat{\nu}_{i\sigma} = \hat{b}^{+}_{i\sigma}\hat{b}_{i\sigma} = \hat{n}_{i\sigma}(1-n_{i\bar{\sigma}})$$

$$\hat{\nu}_{i} = \sum_{\sigma}\hat{b}^{+}_{i\sigma}\hat{b}_{i\sigma}$$

$$\hat{S}_i^{\sigma} = \hat{a}^{+}_{i\sigma}(1-n_{i\bar{\sigma}})a_{i\bar{\sigma}}(1-n_{i\sigma}) = \hat{b}^{+}_{i\sigma}\hat{b}_{i\bar{\sigma}}$$

$$\bar{S}_i^{z} = \frac{1}{2}\sum_{\sigma}\hat{n}_{i\sigma} = \frac{1}{2}\sum_{\sigma}\sigma\hat{b}^{+}_{i\sigma}\hat{b}_{i\sigma}$$

$$\{\hat{b}_{i\sigma}, \hat{b}^{+}_{j\sigma'}\} = \delta_{ij}\left[(1-n_{i\bar{\sigma}})\delta_{\sigma\sigma'} + (1-\delta_{\sigma\sigma'})S_i^{\bar{\sigma}}\right]$$

$$\boxed{\begin{aligned} H_{tJ} &= \sum_{ij\sigma}{}' t_{ij}\hat{b}^{+}_{i\sigma}\hat{b}_{j\sigma} + \\ &+ \sum_{ij}{}' \frac{2t_{ij}^2}{U}\left(\bar{S}_i\cdot\bar{S}_j - \frac{1}{4}\nu_i\nu_j\right) - \\ &- \sum_{ijk\sigma}{}'' \frac{t_{ij}t_{jk}}{U}\left(\hat{b}^{+}_{i\sigma}\hat{\nu}_{j\bar{\sigma}}\hat{b}_{k\sigma} + \hat{b}_{i\sigma}\hat{S}_i^{\bar{\sigma}}\hat{b}_{k\bar{\sigma}}\right) \end{aligned}}$$

Real space pairing $n < 1$ dopped Mott insulator

$$\hat{B}^{+}_{ij} = \frac{1}{\sqrt{2}}\left(\hat{b}^{+}_{i\uparrow}\hat{b}^{+}_{j\downarrow} - \hat{b}^{+}_{i\downarrow}b^{+}_{j\uparrow}\right)$$

$$\hat{B}_{ij} = \frac{1}{\sqrt{2}}\left(\hat{b}_{i\downarrow}\hat{b}_{j\uparrow} - \hat{b}_{i\uparrow}\hat{b}_{j\downarrow}\right)$$

real space Cooper singlet pair of electrons

$$\boxed{H_{tJ} = \sum_{ij}{}' t_{ij}\hat{b}^{+}_{i\sigma}\hat{b}_{j\sigma} - \sum_{ijk}\frac{t_{ij}t_{jk}}{U}\hat{B}^{+}_{ij}\hat{B}_{kj}}$$

→ Superconductivity in $U>0$ case!