3. Heisenbergův hamiltonián jako efektivní hamiltonián Hubbardova modelu

- pomocí poruch. teorie II. řádu ze hamiltonián

$$H = t\cdot\sum_{\sigma=\uparrow\downarrow}\left(c^+_{1\sigma}c_{2\sigma}+c^+_{2\sigma}c_{1\sigma}\right) + U\left(n_{1\uparrow}n_{1\downarrow}+n_{2\uparrow}n_{2\downarrow}\right)$$

v limitě $t/U \ll 1$ (poruchou jsou členy s t) je antiferomagnetický Heisenbergův hamiltonián

výměnná konstanta

$$H_{eff} = J\cdot\hat{S}_1\cdot\hat{S}_2 \quad ; \text{ kde } J = 4t^2/U$$

jednotlivé možné stavy:

singlet:

$$|S\rangle = \frac{1}{\sqrt{2}}\left(c^+_{1\uparrow}c^+_{2\downarrow} - c^+_{1\downarrow}c^+_{2\uparrow}\right)|vac\rangle$$

triplety:

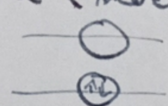
$$|T_{-1}\rangle = c^+_{1\downarrow}c^+_{2\downarrow}|vac\rangle$$

$$|T_0\rangle = \frac{1}{\sqrt{2}}\left(c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{1\downarrow}c^+_{2\uparrow}\right)|vac\rangle$$

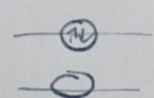
$$|T_{+1}\rangle = c^+_{1\uparrow}c^+_{2\uparrow}|vac\rangle$$

stavy s dvojnásobným obsazením (mezistavy)

$$|S_1\rangle = c^+_{1\uparrow}c^+_{1\downarrow}|vac\rangle$$



$$|S_2\rangle = c^+_{2\uparrow}c^+_{2\downarrow}|vac\rangle$$



- kvůli spin. symetrii musí být ef. ham. v bázi z těchto stavů diagonální ⇒ určujeme pouze diagonální maticové elementy pomocí poruch. teorie II. řádu:

$$\langle\Psi|H_{eff}|\Psi\rangle = -\sum_m \frac{\langle\Psi|H|m\rangle\langle m|H|\Psi\rangle}{E_{ex,m}} ,$$

kde $|\Psi\rangle$ jsou $|S\rangle, |T_{-1}\rangle, |T_0\rangle, |T_{+1}\rangle$

a $|m\rangle$ je $|S_1\rangle, |S_2\rangle$

$|4\rangle$:

$$H|S\rangle = \left[t\cdot\left(c^+_{1\uparrow}c_{2\uparrow} + c^+_{2\uparrow}c_{1\uparrow}\right) + t\cdot\left(c^+_{1\downarrow}c_{2\downarrow} + c^+_{2\downarrow}c_{1\downarrow}\right)\right]\cdot\frac{1}{\sqrt{2}}\cdot\left(c^+_{1\uparrow}c^+_{2\downarrow} - c^+_{1\downarrow}c^+_{2\uparrow}\right)|vac\rangle$$

$$= \frac{t}{\sqrt{2}}\Big[\Big(\underbrace{c^+_{1\uparrow}c_{2\uparrow}c^+_{1\uparrow}c^+_{2\downarrow}}_{=0} + c^+_{2\uparrow}c_{1\uparrow}c^+_{1\uparrow}c^+_{2\downarrow} - c^+_{1\uparrow}c_{2\uparrow}c^+_{1\downarrow}c^+_{2\uparrow} \underbrace{- c^+_{2\uparrow}c_{1\uparrow}c^+_{1\downarrow}c^+_{2\uparrow}}_{=0}$$
$$+ c^+_{1\downarrow}c_{2\downarrow}c^+_{1\uparrow}c^+_{2\downarrow} + \underbrace{c^+_{2\downarrow}c_{1\downarrow}c^+_{1\uparrow}c^+_{2\downarrow}}_{=0} - \underbrace{c^+_{1\downarrow}c_{2\downarrow}c^+_{1\downarrow}c^+_{2\uparrow}}_{=0} - c^+_{2\downarrow}c_{1\downarrow}c^+_{1\downarrow}c^+_{2\uparrow}\Big)\Big]|vac\rangle$$

využijeme komutační relace:

$$\{c_i; c_j^+\} = \delta_{ij} \quad ; \quad \{c_i^+, c_j^+\} = 0$$

tedy

$i \neq j$: $c_i c_j^+ + c_j^+ c_i = 0$, $\quad c_i c_j^+ = -c_j^+ c_i$

$i = j$: $c_i c_i^+ = 1 - c_i^+ c_i$

$c_i^+ c_j^+ = -c_j^+ c_i^+$

$c_{i\alpha}|vac\rangle = 0$; $c^+_{j\alpha}c^+_{j\alpha}|vac\rangle = 0$ (2 e^- nemohou být ve stejném stavu)

$$= \frac{t}{\sqrt{2}}\left[c^+_{2\uparrow}c_{1\uparrow}c^+_{1\uparrow}c^+_{2\downarrow} - c^+_{1\uparrow}c_{2\uparrow}c^+_{1\downarrow}c^+_{2\uparrow} + c^+_{1\downarrow}c_{2\downarrow}c^+_{1\uparrow}c^+_{2\downarrow} - c^+_{2\downarrow}c_{1\downarrow}c^+_{1\downarrow}c^+_{2\uparrow}\right]|vac\rangle$$

$$c^+_{2\uparrow}c_{1\uparrow}c^+_{1\uparrow}c^+_{2\downarrow}|vac\rangle = c^+_{2\uparrow}\left(1 - c^+_{1\uparrow}c_{1\uparrow}\right)c^+_{2\downarrow}|vac\rangle = c^+_{2\uparrow}c^+_{2\downarrow} - c^+_{2\uparrow}c^+_{1\uparrow}c_{1\uparrow}c^+_{2\downarrow}|vac\rangle$$

$$= c^+_{2\uparrow}c^+_{2\downarrow}|vac\rangle + c^+_{2\uparrow}c^+_{1\uparrow}c^+_{2\downarrow}\underbrace{\left(c_{1\uparrow}|vac\rangle\right)}_{=0} = c^+_{2\uparrow}c^+_{2\downarrow}|vac\rangle$$

$$-c^+_{1\uparrow}c_{2\uparrow}c^+_{1\downarrow}c^+_{2\uparrow}|vac\rangle = c^+_{1\uparrow}c^+_{1\downarrow}c_{2\uparrow}c^+_{2\uparrow}|vac\rangle = c^+_{1\uparrow}c^+_{1\downarrow}|vac\rangle - c^+_{1\uparrow}c^+_{1\downarrow}c^+_{2\uparrow}\overbrace{\left(c_{2\uparrow}|vac\rangle\right)}^{0}$$

$$= c^+_{1\uparrow}c^+_{1\downarrow}|vac\rangle$$

$$c^+_{1\downarrow}c_{2\downarrow}c^+_{1\uparrow}c^+_{2\downarrow}|vac\rangle = -c^+_{1\downarrow}c^+_{1\uparrow}c_{2\downarrow}c^+_{2\downarrow}|vac\rangle = -c^+_{1\downarrow}c^+_{1\uparrow}|vac\rangle + 0$$

$$-c^+_{2\downarrow}c_{1\downarrow}c^+_{1\downarrow}c^+_{2\uparrow}|vac\rangle = -c^+_{2\downarrow}\left(1 - c^+_{1\downarrow}c_{1\downarrow}\right)c^+_{2\uparrow}|vac\rangle = -c^+_{2\downarrow}c^+_{2\uparrow}|vac\rangle + 0$$

$$H|S\rangle = \frac{t}{\sqrt{2}}\left(c^+_{2\uparrow}c^+_{2\downarrow} + c^+_{1\uparrow}c^+_{1\downarrow} - c^+_{1\downarrow}c^+_{1\uparrow} - c^+_{2\downarrow}c^+_{2\uparrow}\right)|vac\rangle$$

$$= \frac{t}{\sqrt{2}}\left(2c^+_{2\uparrow}c^+_{2\downarrow} + 2c^+_{1\uparrow}c^+_{1\downarrow}\right)|vac\rangle = \frac{2t}{\sqrt{2}}\left(c^+_{2\uparrow}c^+_{2\downarrow} + c^+_{1\uparrow}c^+_{1\downarrow}\right)|vac\rangle$$

$$= \frac{2t}{\sqrt{2}}\left(|S_2\rangle + |S_1\rangle\right)$$

$|T_{-1}\rangle$:

$$H|T_{-1}\rangle = t\cdot\left(c^+_{1\uparrow}c_{2\uparrow} + c^+_{2\uparrow}c_{1\uparrow} + c^+_{1\downarrow}c_{2\downarrow} + c^+_{2\downarrow}c_{1\downarrow}\right)\cdot c^+_{1\downarrow}c^+_{2\downarrow}|vac\rangle$$

$$= t\cdot\left(c^+_{1\uparrow}c_{2\uparrow}c^+_{1\downarrow}c^+_{2\downarrow} + c^+_{2\uparrow}c_{1\uparrow}c^+_{1\downarrow}c^+_{2\downarrow} + c^+_{1\downarrow}c_{2\downarrow}c^+_{1\downarrow}c^+_{2\downarrow} + c^+_{2\downarrow}c_{1\downarrow}c^+_{1\downarrow}c^+_{2\downarrow}\right)|vac\rangle$$

$$= 0$$

$$H|T_{+1}\rangle = t\cdot\left(c^+_{1\uparrow}c_{2\uparrow} + c^+_{2\uparrow}c_{1\uparrow} + c^+_{1\downarrow}c_{2\downarrow} + c^+_{2\downarrow}c_{1\downarrow}\right)\cdot c^+_{1\downarrow}c^+_{2\downarrow}|vac\rangle = 0$$

- výsledný stav musí být vždy singlet

$$H|T_0\rangle = t\cdot\left[c^+_{1\uparrow}c_{2\uparrow} + c^+_{2\uparrow}c_{1\uparrow} + c^+_{1\downarrow}c_{2\downarrow} + c^+_{2\downarrow}c_{1\downarrow}\right]\cdot\frac{1}{\sqrt{2}}\left(c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{1\downarrow}c^+_{2\uparrow}\right)|vac\rangle$$

$$= \frac{t}{\sqrt{2}}\Big[c^+_{1\uparrow}c_{2\uparrow}c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{1\uparrow}c_{2\uparrow}c^+_{1\downarrow}c^+_{2\uparrow} + c^+_{2\uparrow}c_{1\uparrow}c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{2\uparrow}c_{1\uparrow}c^+_{1\downarrow}c^+_{2\uparrow}$$
$$+ c^+_{1\downarrow}c_{2\downarrow}c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{1\downarrow}c_{2\downarrow}c^+_{1\downarrow}c^+_{2\uparrow} + c^+_{2\downarrow}c_{1\downarrow}c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{2\downarrow}c_{1\downarrow}c^+_{1\downarrow}c^+_{2\uparrow}\Big]|vac\rangle$$

$$(1 - c^+_{1\uparrow}c_{1\uparrow})$$

$$= \frac{t}{\sqrt{2}}\Big[c^+_{1\uparrow}c_{2\uparrow}c^+_{1\downarrow}c^+_{2\uparrow} + c^+_{2\uparrow}c_{1\uparrow}c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{1\downarrow}c_{2\downarrow}c^+_{1\uparrow}c^+_{2\downarrow} + c^+_{2\downarrow}c_{1\downarrow}c^+_{1\downarrow}c^+_{2\uparrow}\Big]|vac\rangle$$

$$= \frac{t}{\sqrt{2}}\Big[-c^+_{1\uparrow}c^+_{1\downarrow} + c^+_{2\uparrow}c^+_{2\downarrow} - c^+_{1\downarrow}c^+_{1\uparrow} + c^+_{2\downarrow}c^+_{2\uparrow}\Big]|vac\rangle$$

$$= \frac{t}{\sqrt{2}}\Big[-c^+_{1\uparrow}c^+_{1\downarrow} + c^+_{1\uparrow}c^+_{1\downarrow} + c^+_{2\downarrow}c^+_{2\uparrow} - c^+_{2\downarrow}c^+_{2\uparrow}\Big]|vac\rangle = 0$$

$$\langle S|H_{eff}|S\rangle = -\frac{\langle S|H|S_1\rangle\langle S_1|H|S\rangle}{u} - \frac{\langle S|H|S_2\rangle\langle S_2|H|S\rangle}{u}$$

$$= -\frac{\left(\langle S_1| + \langle S_2|\right)\frac{2t}{\sqrt{2}}|S_1\rangle\langle S_1|\frac{2t}{\sqrt{2}}\left(|S_1\rangle + |S_2\rangle\right)}{u}$$

$$-\frac{\left(\langle S_1| + \langle S_2|\right)\frac{2t}{\sqrt{2}}|S_2\rangle\langle S_2|\frac{2t}{\sqrt{2}}\left(|S_1\rangle + |S_2\rangle\right)}{u}$$

$$= -\frac{4t^2}{2u} - \frac{4t^2}{2u} = -\frac{4t^2}{u} = J$$