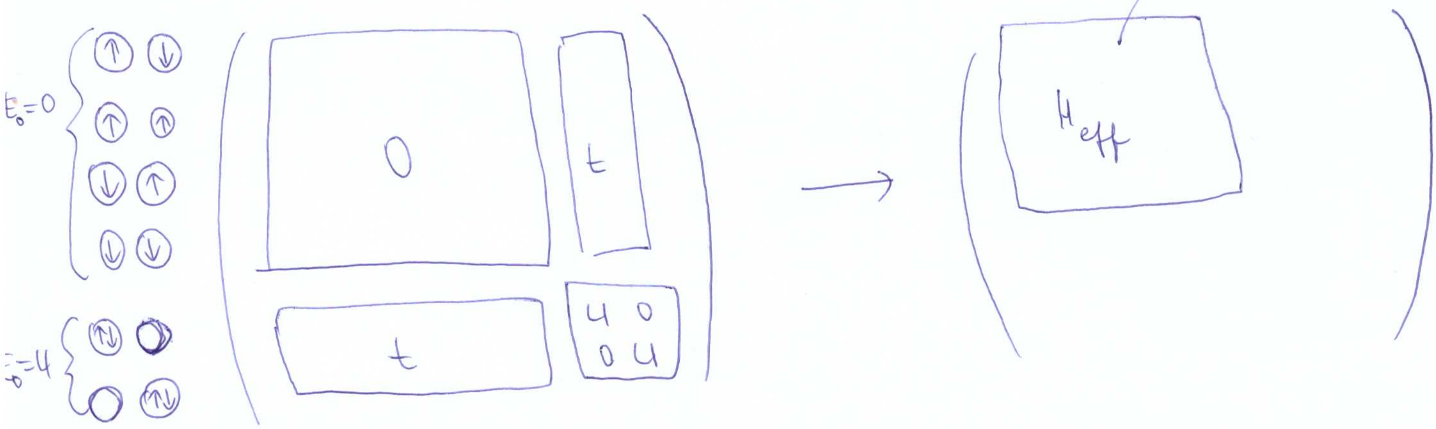
3. Heisenbergův hamiltonián jako efektivní hamiltonián Hubbardova modelu

Pomocí poruchové teorie druhého řádu ukažte, že efektivním hamiltoniánem Hubbardova modelu pro molekulu H_2

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

v limitě $t/U \ll 1$ (poruchou jsou členy s t) je antiferomagnetický Heisenbergův hamiltonián $H_{eff} = J \hat{S}_1 \cdot \hat{S}_2$ s výměnnou konstantou $J = 4t^2/U$.



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

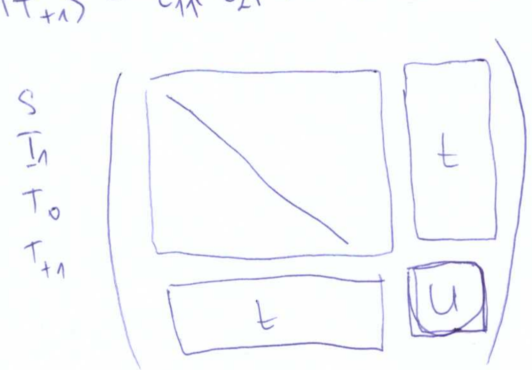
$$|S_1\rangle = c_{1\uparrow}^{+} c_{1\downarrow}^{+} |vac\rangle$$

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

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

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

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



Efektivní hamiltonián v podprostoru vymezeném stavy $|S\rangle$, $|T_{-1}\rangle$, $|T_0\rangle$, $|T_{+1}\rangle$. Kvůli spinovej symetrii musí být efektivní hamiltonián z těchto stavů vyjádřený v bázi sestavené diagonální. Stačí tedy určit jeho diagonální maticové elementy pomocou poruchovej teorie druhého řádu

<

$$\langle \psi | H_{eff} | \psi \rangle = - \sum_n \frac{\langle \psi | H_t | n \rangle \langle n | H_t | \psi \rangle}{E_{exc,n}}$$

kde $|\psi\rangle$ jsou jednotlivé nízkoenergiové stavy $|S\rangle, |T_{-1}\rangle, |T_0\rangle, |T_{+1}\rangle$

$|n\rangle$ jsou stavy s dvojnásobným obsazením $|S_1\rangle$ a $|S_2\rangle$ s exc. ener U

$|\psi\rangle = |T_{-1}\rangle$

$$H_t |T_{-1}\rangle = t\left[c_{1\uparrow}^+ c_{2\uparrow} + c_{2\uparrow}^+ c_{1\uparrow} + c_{1\downarrow}^+ c_{2\downarrow} + c_{2\downarrow}^+ c_{1\downarrow}\right] c_{1\downarrow}^+ c_{2\downarrow}^+ |vac\rangle$$

$$= 0$$

$|\psi\rangle = |T_{+1}\rangle$

$$H_t |T_{+1}\rangle = t\left[c_{1\uparrow}^+ c_{2\uparrow} + c_{2\uparrow}^+ c_{1\uparrow} + c_{1\downarrow}^+ c_{2\downarrow} + c_{2\downarrow}^+ c_{1\downarrow}\right] c_{1\uparrow}^+ c_{2\uparrow}^+ |vac\rangle$$

$$= 0$$

$|\psi\rangle = |T_0\rangle$

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

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

$$= \frac{t}{\sqrt{2}}\left[- c_{1\uparrow}^+ c_{1\downarrow}^+ + c_{1\uparrow}^+ c_{1\downarrow}^+ + c_{2\uparrow}^+ c_{2\downarrow}^+ - c_{2\uparrow}^+ c_{2\downarrow}^+\right] |vac\rangle = 0$$

$|\psi\rangle = |S\rangle$

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

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

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

$$= \frac{2t}{\sqrt{2}}\left[\underbrace{c_{1\uparrow}^+ c_{1\downarrow}^+ |vac\rangle}_{|S_1\rangle} + \underbrace{c_{2\uparrow}^+ c_{2\downarrow}^+ |vac\rangle}_{|S_2\rangle}\right]$$

$$\langle S | H_{eff} | S \rangle = - \frac{\langle S | H_t | S_1 \rangle \langle S_1 | H_t | S \rangle}{U} - \frac{\langle S | H_t | S_2 \rangle \langle S_2 | H_t | S \rangle}{U} =$$

$$= -2 \cdot \left[\frac{\frac{4t^2}{2}}{U} \right] = - \frac{4t^2}{U}$$