0.1 Homework 4

0.1.1 Mean-field Solutions for Extended Hubbard Model

The Hamiltonian of the extended Hubbard model can be written as:

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \textbf{h.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j\rangle} n_i n_j$$

where:

- $c_{i\sigma}^{\dagger}$ **and** $c_{i\sigma}$ **are the fermionic creation and annihilation operators for an eletron with spin** σ **at site** i**.**
- $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ **is the number operator for electrons with spin** σ **at site** i**.**
- $n_i = \sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}$ **is the number operator for total electrons at site** i**.**
- $U > 0$ **is the strength of the on-site interaction between electrons.**
- $V > 0$ **is the strength of the interaction between electrons at neighboring sites.**
- $t > 0$ **is the hopping strength of the electrons.**

We consider the case of half-filling for two lattice sites ($\langle N\rangle = \langle n_{1\uparrow} + n_{1\downarrow} + n_{2\uparrow} + n_{2\downarrow}\rangle$**). In the mean-field approximation, calculate the ground state energy** E_{MF}**. Please consider initial mean-field values with following four cases.**

In the mean-field approximation, the Hamiltonian can be written as

$$\begin{aligned}
\hat{H} &= -t \sum_{\langle i,j\rangle,\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j\rangle} n_i n_j \\
&= -t \sum_{\langle i,j\rangle,\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + U \sum_{i} \left(n_{i\uparrow} \langle n_{i\downarrow}\rangle + n_{i\downarrow} \langle n_{i\uparrow}\rangle - \langle n_{i\uparrow}\rangle \langle n_{i\downarrow}\rangle \right) \\
&+ V \sum_{\langle i,j\rangle} \left(n_i \langle n_j\rangle + n_j \langle n_i\rangle - \langle n_i\rangle \langle n_j\rangle \right) \\
&= c^{\dagger} \begin{bmatrix}
U\langle n_{1\downarrow}\rangle + V\langle n_2\rangle & & -t & \\
& U\langle n_{1\uparrow}\rangle + V\langle n_2\rangle & & -t \\
-t & & U\langle n_{2\downarrow}\rangle + V\langle n_1\rangle & \\
& -t & & U\langle n_{2\uparrow}\rangle + V\langle n_1\rangle
\end{bmatrix} c
\end{aligned}$$

1. **Case 1: Paramagnetic(PM). Initial mean-field value** $\langle n_{i\sigma}\rangle = \dfrac{1}{2}$**.**

   For this case, the interactions are weak, so we expect that the hopping term is dominant. Thus we have

   $$\langle n_{i\uparrow}\rangle = \langle n_{i\downarrow}\rangle = \frac{1}{2}, \quad \text{for all } i.$$

   $$\begin{bmatrix}
   U\frac{1}{2} + V & & -t & \\
   & U\frac{1}{2} + V & & -t \\
   -t & & U\frac{1}{2} + V & \\
   & -t & & U\frac{1}{2} + V
   \end{bmatrix} = UDU^{-1}$$

   Except for the different diagnoal elements, this matrix is very similar to the case in the lecture. We can get

   $$U = \frac{1}{\sqrt{2}} \begin{bmatrix}
   1 & & -1 & \\
   1 & & -1 & \\
   & 1 & & 1 \\
   & 1 & & 1
   \end{bmatrix}, \quad D = \begin{bmatrix}
   -t + \frac{U}{2} + V & & & \\
   & -t + \frac{U}{2} + V & & \\
   & & t + \frac{U}{2} + V & \\
   & & & t + \frac{U}{2} + V
   \end{bmatrix}$$

   $$E_{\text{MF}} = -2t + \frac{U}{2} + V$$

2. **Case 2: Ferromagnetic(FM). Initial mean-field value $\langle n_{i\uparrow}\rangle = 1$ and $\langle n_{i\downarrow}\rangle = 0$.**

When U is large, we expect no double occupancy. For this case, the mean-field values are chosen as

$$\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = 1, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = 0.$$

$$\begin{bmatrix} V & & -t & \\ & U+V & & -t \\ -t & & V & \\ & -t & & U+V \end{bmatrix} = \begin{bmatrix} & & -t & \\ & U & & -t \\ -t & & & \\ & -t & & U \end{bmatrix} + V\mathbb{I} = UDU^{-1}$$

The effect of V is still just shifting the energy, and we get

$$U = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 & & \\ & & 1 & -1 \\ 1 & 1 & & \\ & & 1 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} -t+V & & & \\ & t+V & & \\ & & -t+U+V & \\ & & & t+U+V \end{bmatrix}$$

(a) When $-t+U+V < t+V \iff U < 2t$,

$$\langle n_{1\uparrow}\rangle = \sum_{ij} V_{1i}^* V_{1j} \langle \gamma_i^\dagger \gamma_j\rangle = V_{11}^* V_{11} + V_{13}^* V_{13} = \frac{1}{2}$$

$$\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = \frac{1}{2}$$

which implies the system is still in PM phase and $E_{\text{MF}} = -2t + \dfrac{U}{2} + V$.

(b) When $U > 2t$,

$$\langle n_{1\uparrow}\rangle = \sum_{ij} V_{1i}^* V_{1j} \langle \gamma_i^\dagger \gamma_j\rangle = V_{11}^* V_{11} + V_{12}^* V_{12} = 1$$

$$\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = 1, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = 0$$

Now the system is in FM phase and $E_{\text{FM}} = V$.

3. **Case 3: Anti-ferromagnetic(AFM). Initial mean-field value $\langle n_{1\uparrow}\rangle = \langle n_{2\downarrow}\rangle = 1-\alpha$ and $\langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = \alpha$.**

Another choice when U is large is to give

$$\langle n_{1\uparrow}\rangle = \langle n_{2\downarrow}\rangle = 1-\alpha, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = \alpha.$$

$$\begin{bmatrix} \alpha U+V & & -t & \\ & (1-\alpha)U+V & & -t \\ -t & & (1-\alpha)U+V & \\ & -t & & \alpha U+V \end{bmatrix}$$
$$= \begin{bmatrix} & & -t & \\ & (1-2\alpha)U & & -t \\ -t & & (1-2\alpha)U & \\ & -t & & \end{bmatrix} + (\alpha U+V)\mathbb{I} = UDU^{-1}$$

The effect of $\bar{V} = \alpha U + V$ is still just shifting the energy. Similar to the contents in the lecture note, mark $\bar{U} = (1-2\alpha)U$ and shift each eigenenergy with $\bar{V}$, we get

$$\begin{aligned} E_{\text{MF}} &= \bar{U} - \sqrt{4t^2+\bar{U}^2} + 2\alpha U + 2V - 2\alpha(1-\alpha)U - V \\ &= (1-2\alpha+2\alpha^2)U - \sqrt{4t^2+\bar{U}^2} + V \end{aligned}$$

and the self-consistent equation is

$$\alpha = \frac{4t^2}{4t^2 + [\sqrt{4t^2+(1-2\alpha)U^2} + (1-2\alpha)U]^2}$$

(a) When $U \gg t$, we get $\alpha \approx 0$ and $E_{\text{MF}} \approx -\dfrac{4t^2}{U} + V$. This corresponds to an AFM solution, which is lower than FM.

(b) When $U \ll t$, we get $\alpha \approx \frac{1}{2}$ and back to the PM solution.

4. **Case 4: Charge density wave(CDW). Initial mean-field value $\langle n_{1\uparrow}\rangle = \langle n_{1\downarrow}\rangle = 1-\alpha$ and $\langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \alpha$.**

When V is much stronger, we expect a double occupancy will occur. Thus the mean-field values are chosen as

$$\langle n_{1\uparrow}\rangle = \langle n_{1\downarrow}\rangle = 1-\alpha, \quad \langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \alpha.$$

$$\begin{bmatrix} (1-\alpha)U+2\alpha V & & -t & \\ & (1-\alpha)U+2\alpha V & & -t \\ -t & & \alpha U+2(1-\alpha)V & \\ & -t & & \alpha U+2(1-\alpha)V \end{bmatrix} = UDU^{-1}$$

The result is a little complicated and one can solve the matrix by Mathematica easily. Note $\beta = (1-2\alpha)(U-2V)$ and $\gamma = 2t$, we have

$$D = \frac{1}{2}\left((U+2V)\mathbb{I} + \sqrt{\beta^2+\gamma^2}\begin{bmatrix} -1 & & & \\ & -1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}\right)$$

The self-consistent equation is

$$1-\alpha = \frac{2\beta^2+\gamma^2-2\beta\sqrt{\beta^2+\gamma^2}}{2\beta^2+2\gamma^2-2\beta\sqrt{\beta^2+\gamma^2}}$$

(a) When $\beta^2 \gg \gamma^2 \iff V \gg \frac{U}{2}$ and $V \gg t$, we have

$$\begin{aligned} \alpha \approx 0, \quad \langle n_{1\sigma}\rangle = 1, \quad \langle n_{2\sigma}\rangle = 0; \\ H_{\text{MF}} \approx U. \end{aligned}$$

(b) When $\beta^2 \ll \gamma^2 \iff V \ll t$ and $U \ll t$, we have $\langle n_{i\sigma}\rangle = \dfrac{1}{2}$ which corresponds to the PM solution.