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

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

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

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

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

   注意对角矩阵 D 的对角线上能量本征值是升序排列的, 这是为了方便观察基态的能量出现在基矢的什么位置. 如果追加半满条件, 即两个格点共有**两个**电子, 后续通过产生算符作用于真空态得到基态波函数时就会使用**两个**产生算符, 具体是什么产生算符需要看能量最低的两个本征值的位置.

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

根据对角分解有 $H = c^\dagger V D V^{-1} c$, 合并 $V^{-1}c$ 为 γ, 即得到矩阵的新基矢为 $\gamma \equiv V^{-1}c$. 同样的, $c = V\gamma$, 或者写作求和约定 $c_\alpha = \sum_i V_{\alpha i}\gamma_i$. 基态被定义为占据最低能量的态, 而根据对角矩阵可以发现最低能量是二重简并的, 是新基矢 γ 的第 $1,2$ 分量 (γ_1, γ_2) 给出的, 因此基态使用产生算符 $\times|0\rangle$ 写出的话将会是 $\prod_{\min \varepsilon_i}^{2} \gamma_i^\dagger |0\rangle = \gamma_1^\dagger \gamma_2^\dagger |0\rangle$. 那么各粒子数平均值为

$$
\begin{aligned}
\langle n_{1\uparrow}\rangle = \langle c_{1\uparrow}^\dagger c_{1\uparrow}\rangle &= \sum_{\min \varepsilon_i, \min \varepsilon_j} (V_{1\uparrow,i})^\dagger V_{1\uparrow,j} \langle \gamma_i^\dagger \gamma_j\rangle \\
&= \sum_{\min \varepsilon_i, \min \varepsilon_j} (V_{1\uparrow,i})^\dagger V_{1\uparrow,j} \delta_{ij} = \sum_{\min \varepsilon_i}^{2} (V_{1\uparrow,i})^\dagger V_{1\uparrow,i} = (V_{1\uparrow,1})^\dagger V_{1\uparrow,1} + (V_{1\uparrow,2})^\dagger V_{1\uparrow,2} \\
&= 0 \cdot 0 + \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} = \boxed{\frac{1}{2}}
\end{aligned}
$$

同理计算得到 $\langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \frac{1}{2}$. 输入值等于输出值, 迭代成功. 这是顺磁态, 能量为

$$
\begin{aligned}
E_{\text{HF}} &= \sum_{\min \varepsilon_\alpha}^{2} \varepsilon_\alpha - U \cdot \frac{1}{2}\frac{1}{2} \times 2 - V \cdot \left(\frac{1}{2} + \frac{1}{2}\right) \times \left(\frac{1}{2} + \frac{1}{2}\right) = \left(-t + \frac{U}{2} + V\right) \times 2 - \frac{U}{2} - V \\
&= -2t + \frac{U}{2} + V
\end{aligned}
$$

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

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

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

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

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

要找到最低能量的两个态填入电子, 可确认的是 $-t+V < t+V$ 与 $-t+U+V < t+U+V$, 然而 $t+V \sim -t+U+V$ 的相对关系是尚不确定的, 因此需要分类讨论.

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

$$
\begin{aligned}
\langle n_{1\uparrow}\rangle &= \sum_{ij} V_{1i}^* V_{1j} \langle \gamma_i^\dagger \gamma_j\rangle = V_{11}^* V_{11} + V_{13}^* V_{13} = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} + 0 \cdot 0 = \frac{1}{2} \\
\langle n_{1\uparrow}\rangle &= \langle n_{2\uparrow}\rangle = \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = \frac{1}{2}
\end{aligned}
$$

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

(b) When $U > 2t$,

$$
\begin{aligned}
\langle n_{1\uparrow}\rangle &= \sum_{ij} V_{1i}^* V_{1j} \langle \gamma_i^\dagger \gamma_j\rangle = V_{11}^* V_{11} + V_{12}^* V_{12} = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}} + \left(-\frac{1}{\sqrt{2}}\right)\left(-\frac{1}{\sqrt{2}}\right) = 1 \\
\langle n_{1\uparrow}\rangle &= \langle n_{2\uparrow}\rangle = 1, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = 0
\end{aligned}
$$

输出值等于输入值, 迭代成功. 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

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

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

   The effect of $\bar{V} = \alpha U + V$ is still just shifting the energy. 这就和 $\langle n_{1\uparrow}\rangle = \langle n_{2\downarrow}\rangle = 1$ 且 $\langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = 0$ 的情况相似,只是需要替换 $\bar{U} = (1-2\alpha)U$ 和 $\bar{V} = \alpha U + V$, we get

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

   输入值 α 等于输出值 $\langle n_{2\uparrow}\rangle$ 即达成收敛, 这个条件被称为自持方程(self-consistent equation). 能量最低态由 γ 的第 $1, 2$ 分量 (γ_1, γ_2) 给出. 那么

$$\begin{aligned}\langle n_{2\uparrow}\rangle = \langle c_{2\uparrow}^\dagger c_{2\uparrow}\rangle &= \sum_{\min\varepsilon_i, \min\varepsilon_j} (V_{2\uparrow,i})^\dagger V_{2\uparrow,j}\langle\gamma_i^\dagger\gamma_j\rangle = (V_{2\uparrow,1})^\dagger V_{2\uparrow,1} + (V_{2\uparrow,2})^\dagger V_{2\uparrow,2}\\ &= 0\cdot 0 + \left(\frac{2t}{\sqrt{4t^2+(\sqrt{4t^2+\bar{U}^2}+\bar{U})^2}}\right)^2\\ \Rightarrow \alpha &= \frac{4t^2}{4t^2+[\sqrt{4t^2+(1-2\alpha)U^2}+(1-2\alpha)U]^2}\end{aligned}$$

   (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

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

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

   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.