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.**

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

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

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

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