Hubbard Model for Hydrogen Atom Lattice

Consider a *simple cubic lattice* with a hydrogen atom at each lattice site. Assuming that the only relevant electronic state at the hydrogen site is the $1s$ state, one can describe the system by a model Hamiltonian

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where i represents the lattice site at $\mathbf{R}_i$, $\langle ij \rangle$ the pair of nearest-neighbor sites $\mathbf{R}_j = \mathbf{R}_i + \boldsymbol{\delta}$, ($\boldsymbol{\delta}$ being $\pm a\mathbf{e}_\alpha$ with $\alpha = x, y, z$) and σ corresponds to the spin index. In this model, while the on-site Coulomb interaction U is independent of the lattice constant, the hopping integral t can be *assumed* to depend on the lattice constant a:

$$t(a) = \frac{A}{a^\gamma}$$

with $\gamma > 0$. Thus, as a varies from 0 to ∞, one can take the limit of either $U \to 0$ or $t \to 0$.

a) **Density-of-States:**
First, considering the free electron limit, i.e., $U \to 0$, show that the kinetic part of the Hamiltonian $\mathcal{H}$ in Eq. (1) can be represented by

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} \varepsilon_{0\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{2}$$

where the summation over $\mathbf{k}$ is limited to the first Brillouin zone. Also, obtain that the density-of-state (DOS) at energy ε can be written by

$$D_0(\varepsilon) = \frac{B(\varepsilon/2t)}{t}$$

where $B(x)$ is defined by

$$B(x) = \int_{|\eta|<\pi} \frac{\mathrm{d}^3\vec{\eta}}{(2\pi)^3}\ \delta\left(x + \sum_{\alpha=x,y,z} \cos\eta_\alpha\right) .$$

Here it is noted that the DOS at E_F becomes

$$D_0(\varepsilon_\mathrm{F} = 0) = \frac{B(0)}{t} .$$

Hint: To find the expression in th plane-wave-state representation, one may use the following transformation:

$$c_{i\sigma} = \sum_{\mathbf{k}\in\mathbf{B.Z.}} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{R}_i} c_{\mathbf{k}\sigma}$$

and the identity

$$\sum_i \mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} = \delta_{\mathbf{k},\mathbf{k}'}$$

where $\mathbf{k}$ and $\mathbf{k}'$ belong to the first Brillouin zone.

b) **Stoner Theory:**
When U is small, one can take the Fermi sphere as a *starting* point in considering the effect of Coulomb interaction. Thus, one can rewrite the Eq. (1) by

$$\mathcal{H} = \sum_{\mathrm{k}\sigma} \varepsilon_{0\mathrm{k}} c^{\dagger}_{\mathrm{k}\sigma} c_{\mathrm{k}\sigma} + U \sum_{\mathrm{q}} n_{-\mathrm{q}\uparrow}\ n_{\mathrm{q}\downarrow} \tag{3}$$

where $n_{\mathrm{q}\sigma} = \sum_{\mathrm{k}\in\mathrm{B.Z.}} c^{\dagger}_{\mathrm{k}\sigma} c_{\mathrm{k}-\mathrm{q},\sigma}$.
Assuming a *mean field* solution for the ferromagnetic (FM) ground state,

$$\langle n_{\mathrm{q}\sigma} \rangle = \delta_{\mathrm{q},0} \bar{n}_{\sigma}\ , \tag{4}$$

show that the *mean field* Hamiltonian can be written by

$$\bar{\mathcal{H}} = \sum_{\mathrm{k}\sigma} \bar{\varepsilon}_{\mathrm{k}\sigma} c^{\dagger}_{\mathrm{k}\sigma} c_{\mathrm{k}\sigma}$$

with the *spin-dependent* energy term

$$\bar{\varepsilon}_{\mathrm{k}\sigma} = \varepsilon_{0\mathrm{k}} + U \bar{n}_{-\sigma}\ .$$

Based on the Stoner theory of ferromagnetism, one expects that the ground state of this system changes from paramagnetic to ferromagnetic at a critical value of $a = a_{\mathrm{c}}$. Find a_{c} in terms of A, $B(0)$, γ, and U, and discuss the energetics of the ground states as a function of a.

c) **Superexchange Interaction:**
Now let us consider the ground state of Eq. (1) in the limit of $t \to 0$, i.e., $a \to \infty$. An appropriate starting Hamiltonian becomes

$$\mathcal{H}_U = \sum_i n_{i\uparrow}\ n_{i\downarrow}$$

This limit represents a collection of atoms far apart from each other. Thus the ground state should be a mere superposition of electron in the ground state of each hydrogen atom. Following the perturbation-theory arguments for the superexchange mechanism discussed during the class, show that the ground state can be determined by the spin-Hamiltonian

$$\mathcal{H}_{\mathrm{spin}} = J_{\mathrm{AF}} \sum_{\langle ij \rangle} \mathrm{S}_i \cdot \mathrm{S}_j$$

with the antiferromagnetic (AF) exchange interaction, i.e., $J_{\mathrm{AF}} > 0$. Obtain the expression of J_{AF} in terms of t and U.

d) **Conflicting Results:**
In Question (b), we showed that the ground state becomes FM for $a > a_{\mathrm{c}}$, i.e., for small t, but this result conflicts with the AF ground state as described by the AF spin Hamiltonian in Question (c) even for the same range of a, i.e., t. Discuss the possible causes of such conflicts, for example, in terms of energetics (total energy) and magnetic instability. (**Hint:** One may repeat the calculations Question (b) for the AF instability.)