P502 **Problem set # 4** **Due: Nov. 22, 14:30**

---

1. (15 points) *"Krönig-Penney model"*

Consider an electron in one dimension in the presence of a potential defined by

$$V(x) = V_0 \sum_{n=-\infty}^{\infty} \theta(x - na)\theta(na + b - x)$$

where $\theta(x)$ is the step function and $0 < b < a$.

a) Sketch the potential. Focusing on a single unit cell write down the boundary conditions for the electron wavefunction that lead to Bloch state in this unit cell.

b) Solve the Schrödinger equation in this cell by taking linear superpositions of plane waves and imposing the boundary conditions. Find the condition for the Bloch index k.

c) Transform the barriers into delta functions by taking the limit

$$b \to 0, \quad V_0 \to \infty, \quad V_0 b = W_0 a(\hbar^2/ma^2)$$

with W_0 characterizing the strength of the delta functions. Find the condition on k in this limit. It is useful to introduce a momentum scale $K = \sqrt{2mE/\hbar^2}$.

d) Produce plots of two lowest energy bands for $W_0 = 0.5$. Display the bands in the reduced and extended zone schemes.

2. (15 points) *"Density of States in the Tight Binding Model"*

Consider electrons in a tight binding approximation with nearest neighbor hopping t and on-site energy $E_0 = 0$ on a cubic lattice in dimensions $d = 1, 2, 3$. Analyze and sketch the density of states (DOS) resulting from this band structure for $d = 1, 2, 3$.

Note: As you will quickly discover the momentum integrals involved in this calculation cannot be evaluated in the closed form. One has to determine DOS approximately. The approach is to (i) Taylor-expand the energy dispersion near the bottom and the top of the band and calculate DOS near these two points; (ii) locate the van Hove singularities inside the band and determine their degree of divergence. Finally, (iii) assuming that DOS is smooth away from the singularities, sketch the overall DOS.

3. (15 points) *"The Hubbard Model"* The simplest lattice model that includes electron-electron interactions is the Hubbard model, defined by the Hamiltonian

$$H = E_0 \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

The first two terms describe the familiar tight binding model with nearest neighbor hopping. The last term represents the effects of Coulomb interaction which is assumed to be screened so that electrons interact only when they occupy the same lattice site ($n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the operator for number of electrons with spin $\sigma = \uparrow, \downarrow$ on the site i). Despite its apparent

simplicity the Hubbard model can be solved exactly only in one dimension and even this solution is technically very difficult. Here we shall consider a mean-field solution which is a reasonable approximation in the case of weak coupling ($U \ll t$).

a) Perform the Hartree-Fock decoupling of the interaction term and write the full mean-field Hamiltonian.

b) From now on focus on the Hartree terms and discard the more complicated Fock terms. In this approximation write the Hamiltonian in terms of two mean fields defined as

$$N_i = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle, \quad M_i = \langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle, \tag{2}$$

and discuss their physical significance.

c) Now specialize to the 2-dimensional square lattice. It is known that near the half filling (i.e. with ≈ 1 electron per site) the metallic state of the $U \to 0$ Hubbard model is unstable toward formation of the antiferromagnetic spin density wave (AF-SDW), a state characterized by uniform charge density ($N_i = N$ =const) but staggered magnetic moments on the neighboring sites, $M_i = (-1)^{i_x + i_y} M$. Find the energy spectrum of this AF-SDW state. For exact half filling is this a metal or an insulator?

Hint: Notice that constant N can be absorbed into E_0 and therefore may be ignored when solving for the spectrum. Also notice that in the above approximation there is no interaction between spin up and spin down electrons and therefore the problem can be solved for each spin orientation separately.