Physics 4250: Assignment #12

DUE: Thursday December 8, 2016

Problems:

1. **Read chapter 20**

2. **Read the hand-out and summarize the important physics discussed on these pages.**

3. **Tight-Binding Model**

   (a) **3D lattice:** Suppose you have a cubic lattice with the primitive lattice vectors: $\vec{a}_1 = \hat{x}a$, $\vec{a}_2 = \hat{y}a$, and $\vec{a}_3 = \hat{z}a$.

   i. What are the reciprocal lattice vectors?

   ii. Suppose you have Born - von Karman boundary conditions and a finite lattice such that the translational symmetry of the entire crystal is: $\vec{R} = \hat{x}n_1 2a + \hat{y}n_2 4a + \hat{z}n_3 6a$. What are the allowed wavevectors within the first Brillouin zone?

   (b) **2D lattice:** Suppose you have a square lattice with the primitive lattice vectors: $\vec{a}_1 = \hat{x}a$ and $\vec{a}_2 = \hat{y}a$.

   i. What are the reciprocal lattice vectors?

   ii. Suppose you have Born - von Karman boundary conditions and a finite lattice such that the translational symmetry of the entire crystal is: $\vec{R} = 4n_1(\vec{a}_1 + \vec{a}_2) + 2n_2(\vec{a}_1 - \vec{a}_2)$. What are the allowed wavevectors within the first Brillouin zone?

   (c) **1D lattice:** Suppose you have a one-dimensional lattice with the primitive lattice vector: $\vec{a}_1 = \hat{x}a$.

   i. What is the reciprocal lattice vector?

   ii. Suppose you have Born - von Karman boundary conditions and a finite lattice such that the translational symmetry of the entire crystal is: $\vec{R} = 4n_1\vec{a}_1$. What are the allowed wavevectors within the first Brillouin zone?

   iii. Suppose you have a spin up electron and a spin down electron on this lattice. What are the second quantization wavefunctions for this system, where $|0\rangle$ is the vacuum state?

   iv. Suppose the Hamiltonian is the single-band Hubbard model;

$$\hat{H} = \epsilon \sum_{i=1}^{4} \sum_{\sigma} \hat{n}_{i,\sigma} + t \sum_{i=1}^{4} \sum_{\sigma} c_{i,\sigma}^{\dagger} \left[c_{i+1,\sigma} + c_{i-1,\sigma} \right] + U \sum_{i=1}^{4} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \tag{1}$$

   where $\epsilon > U > t > 0$. Write the Hamiltonian in matrix form using the wavefunctions given in part (iii).

   v. Apply Bloch's theorem to the parts (iii) and (iv). What are the new wavefunctions and Hamiltonian?

   vi. Apply perturbation theory to the Hamiltonian in part (v). What are the energies (eigenvalues)?