PHYSICS 231

Homework 4

Due in class, Monday November 7

1. **Periodic Potentials in One Dimension**
   Ashcroft and Mermin, Ch. 8, Problem 1. (The question is too long to type out.)

2. **Level splitting in a two-dimensional model**
   As discussed in class, a periodic potential only mixes plane-wave states whose wave vectors differ by a reciprocal lattice vector $\mathbf{G}$. Writing the wave function as

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{G}} c_{\mathbf{k}+\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}, \tag{1}$$

   the equation for the energy eigenvalue, $\lambda_{\mathbf{k}}$, is (see AM Eq. (8.41))

$$\left(\epsilon^0_{\mathbf{k}} - \lambda_{\mathbf{k}}\right) c_{\mathbf{k}} + \sum_{\mathbf{G}} U_{\mathbf{G}} c_{\mathbf{k}-\mathbf{G}} = 0, \tag{2}$$

   where $\epsilon^0_{\mathbf{k}} = \hbar^2 k^2/2m$, is the unperturbed energy.

   Consider a square lattice with lattice spacing a and crystal potential

$$U(x, y) = -4U \cos(2\pi x/a) \cos(2\pi y/a). \tag{3}$$

   (a) What are the non-zero Fourier components of the crystal potential.

   (b) Find, approximately, the energy gap at the corner point, $(\pi/a, \pi/a)$, of the Brillouin zone. *n.b.* It is sufficient to solve a 2×2 determinental equation.

3. **Density of States for an Anisotropic Band**
   Consider a band with an anisotropic dispersion relation,

$$\epsilon(\mathbf{k}) = \left(\frac{\hbar^2}{2}\right)\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right). \tag{4}$$

   This could occur, for example in an crystal with orthorhombic symmetry. A similar situation occurs in metals and semiconductors when the minimum of the band is not at $\mathbf{k} = 0$, but at some non-zero wave vector $\mathbf{k}_0$ (in which case $\mathbf{k}$ above should be replaced by $\mathbf{k} - \mathbf{k}_0$).

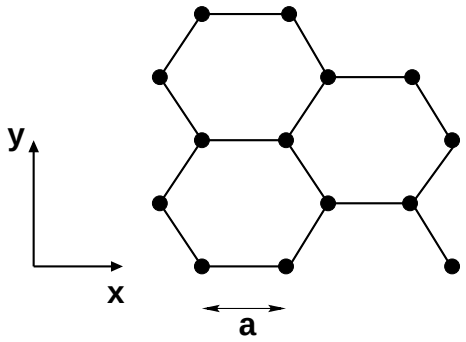
   (a) Using the fact that the ellipsoid $(x/a)^2 + (y/b)^2 + (z/c)^2 = 1$ has volume $(4\pi/3)abc$, calculate the density of states $g(\epsilon)$.
   Hint: The density of levels, $g(\epsilon)$, is given by $dh(\epsilon)/d\epsilon$, where $h(\epsilon)$ is the number of levels per unit volume with energy *less than* ϵ.

   (b) Using the standard between the coefficient of T in the specific heat, i.e. the value of γ where $C_V = \gamma T$, and the density of states at the Fermi energy, show, for a fixed density of electrons that, γ is proportional to an effective mass

$$m^* = (m_x m_y m_z)^{1/3}. \tag{5}$$

4. **A model for the band structure of graphene**

It has recently been possible to produce samples of graphene a single atomic layer thick. The physics of graphene is very rich, so this material is intensively studied at present. Here we will derive the unusual dispersion relation of graphene in the vicinity of the Fermi energy, which leads to many of its striking properties.



Graphene is a honeycomb array of carbon atoms, see figure. It has 4 electrons in the 2s and 2p shells (the "core" electrons in the 1s shell do not participate for the purposes of this question). Three of the electrons form sp^2 orbitals which point to the neighbors of the hexagonal array and provide the chemical bonding. The remaining electron, in a $2p^z$ orbital, can give rise to conduction, i.e. there is one electron per atom in a potentially unfilled band. In this question we only consider these electrons. As we discussed in class, there are two atoms per unit cell, so there are two electrons per unit cell.

(a) How many bands will these electrons fill?

(b) What is the Bravais lattice? Specify two basis vectors of the Bravais lattice.

(c) Determine two basis vectors of the reciprocal lattice. What lattice does this correspond to? Draw the first Brillouin zone, indicating the value of $\mathbf{k}$ at the edge of the zone in the x- and the y-directions.

(d) Determine the band structure in the tight binding approximation.

(e) Explain where the Fermi energy lies, and describe the dispersion relation of the electrons in the vicinity of the Fermi energy.

(f) What is the density of states at the Fermi energy (explain your result). Hence explain whether graphene is a metal, insulator, semiconductor (an insulator with a small bandgap), or a semi-metal (a metal with a small density of states at the Fermi energy)?

5. Consider a two-dimensional square lattice with lattice constant a.

(a) Write down, in units of π/a, the radius of the circle that can accommodate m free electrons per primitive cell.

(b) Construct a table listing which of the first four zones of the square lattice are completely full, which are completely empty, and which are partially full, for $m = 1, 2, \cdots, 6$.

(c) Draw pictures, in suitable primitive cells, of all branches of the Fermi surface for $m = 1, 2, 3$.

Hint: See the discussion on higher Brillouin zones in Ashcroft and Mermin p. 162-165, and Fig. 9.15.