Applied Physics 195 / Physics 195 — Assignment #7

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Date: November 6th, 2015

Due: **5pm <u>SHARP</u> (4:50pm + 10 min grace period)**, November 13th, 2015; slide your work under through the door at Maxwell-Dworkin Room 131.

Problem 1 (100 pt): Nearly free electron model — 2D case

Consider a 2D square lattice crystal with a lattice constant a. Let the periodic potential energy for an electron propagating in this crystal be given by:

$$V(x, y) = A \left[\cos\left(\frac{2\pi x}{a} \right) + \cos\left(\frac{2\pi y}{a} \right) \right] \tag{1}$$

with $A > 0$.

(a) Draw the 1st, 2nd, 3rd, and 4th Brillouin zones in the Bloch $\vec{k}$ space.

(b) By using the nearly free electron approximation, calculate all—two—single-electron energy eigenvalues at the mid point of each edge of the 1st Brillouin zone boundary to the first non-vanishing order. What is the band gap at these points?

(c) Again resorting to the nearly free electron approximation, evaluate all single-electron energy eigen values at each corner of the 1st Brillouin zone boundary to the first non-vanishing order. You should get 4 energy eigen values (though some roots may be degenerate) for each corner; can you give a brief physical interpretation as to why 4 roots arise at these corner points of the zone boundary?

(d) Assume that this 2D crystal is made out of divalent atoms (two valence electrons per atom; by the way, assume one atom per unit cell). This 2D crystal can be a metal or an insulator depending on whether bands overlap or not. Show that the condition for this crystal to be a metal is given by

$$A < \frac{\hbar^2 \pi^2}{3ma^2} \tag{2}$$

where m is the intrinsic electron mass. To prove this, you should first evaluate the maximum energy of the 1st band and the minimum energy value of the higher bands. You can obtain this information from parts (b) and (c). Assume that $A < \hbar^2 \pi^2 / (ma^2)$.

Problem 2 (200 pt): Band structure of graphene

Figure 1(a) shows the honeycomb net of carbon atoms in graphene, the one-atom thick monolayer of graphite. Each carbon atom has 4 valence electrons. 3 of them participate in covalent bonding—σ bonding with sp^2 orbitals—to form the 2D crystal. The remaining one valence electron per atom—π electron—gives the electronic property to graphene. This problem is concerned with the π electronic band structure.

(a) As discussed in Lecture #7, the honeycomb net is not a Bravais lattice, and hence graphene should be described with the lattice-with-a-basis formalism. The conventionally used Bravais lattice in this case is the lattice spanned by the primitive lattice vectors $\vec{a}_1$ and $\vec{a}_2$ shown in Fig. 1(a); the corresponding primitive unit cell then contains two carbon atoms as a basis [Fig. 1(a)]. Show that $\vec{a}_1$ and $\vec{a}_2$ are given by:

$$\vec{a}_1 = \frac{3a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}; \tag{3}$$

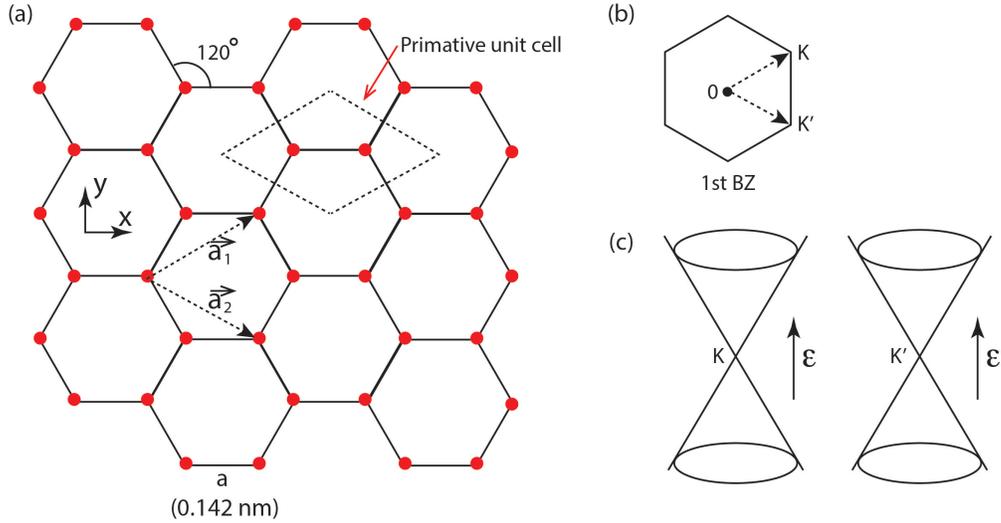$$\vec{a}_2 = \frac{3a}{2}\hat{x} - \frac{\sqrt{3}a}{2}\hat{y}. \tag{4}$$

Figure 1: (a) Honeycomb net of carbon atoms in graphene. (b) 1st Brillouin zone. (c) Energy dispersion around the Dirac points K and K'.

(b) Express the primitive lattice vectors $\vec{b}_1$ and $\vec{b}_2$ with which the reciprocal lattice can be spanned. Draw the 1st Brillouin zone, specifying characteristic dimensions. Show that the 1st Brillouin zone so drawn [Fig. 1(b)] is of hexagonal shape, just like the hexagons of the honeycomb direct lattice [Fig. 1(a)]; note from Figs. 1(a) and (b) that the 1st Brillouin zone hexagon is rotated from the hexagons of the honeycomb direct lattice.

(c) The 1st Brillouin zone has six corner points [Fig. 1(b)]. They can be classified into two groups of three equivalent points (the three points in each group are equivalent in that via translations by reciprocal lattice vectors from a point, you can arrive at any of the remaining two points). The two corner points K and K' of the 1st Brillouin zone [Fig. 1(b)] represent these two groups. Note that K and K' themselves are not equivalent; no translation by reciprocal lattice vectors can bring K to K' or K' to K. Show that these two corner points are located at:

$$\vec{K} = \frac{2\pi}{3a}\hat{k}_x + \frac{2\pi}{3a\sqrt{3}}\hat{k}_y; \tag{5}$$

$$\vec{K'} = \frac{2\pi}{3a}\hat{k}_x - \frac{2\pi}{3a\sqrt{3}}\hat{k}_y. \tag{6}$$

(d) By using the tight binding approximation for the π electron, whose energy in a carbon atom is set at $\epsilon_0 = 0$ (this is no more than an uninteresting shift of the energy reference point), and by considering only the nearest neighbor electron hopping with a strength of $t > 0$, show that there are two π bands, whose dispersion relations are given by

$$\epsilon_{\pm}(\vec{k}) = \pm t\sqrt{1 + 4\cos\frac{3k_x a}{2}\cos\frac{\sqrt{3}k_y a}{2} + 4\cos^2\frac{\sqrt{3}k_y a}{2}}. \tag{7}$$

(e) Plot the energy dispersion $\epsilon(\vec{k})$ three-dimensionally. Feel free to use any tool of your choice; the main purpose here is to quickly visualize the bands. Show from the plot that the two bands $\epsilon_+(\vec{k})$ and $\epsilon_-(\vec{k})$ meet (sharply touch) at each of the 6 corner points of the 1st Brillouin zone, where $\epsilon_{\pm}(\vec{k}) = 0$. Also explicitly show $\epsilon_{\pm}(\vec{k}) = 0$ for $\vec{k} = \vec{K}$ and $\vec{k} = \vec{K'}$ by calculation. Points $\vec{K}$ and $\vec{K'}$ are called Dirac points. Note that there is no band gap. Discuss how these two bands are filled at $T = 0$ with π electrons.

(f) Show that near the dirac point $\vec{K}$, the energy dispersion $\epsilon_{\pm}(\vec{k})$ can be approximated as

$$\epsilon_{\pm}(\vec{k}) \approx \pm\frac{3at}{2}|\vec{k} - \vec{K}|, \tag{8}$$

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which, with $\vec{q} \equiv \vec{k} - \vec{K}$ and $q \equiv |\vec{q}|$, can be simplified into

$$\epsilon_\pm(\vec{q}) \approx \pm\frac{3at}{2}q. \tag{9}$$

Note that this Dirac-point energy dispersion is very different from the quadratic free electron energy dispersion $\hbar^2 k^2/(2m)$. Show that Eq. (9) holds also for the other Dirac point $\vec{K}'$, with $\vec{q} = \vec{k} - \vec{K}'$. In sum, near each of the Dirac points at the corners of the 1st Brillouin zone, the electronic bands $\epsilon_\pm(\vec{k})$ assume conical shapes [Fig. 1(c)] and the two bands $\epsilon_+(\vec{k})$ and $\epsilon_-(\vec{k})$ touch sharply at the Dirac points.

(g) As we briefly discussed in Lecture #10 (and as we will go more deeply into in the next lecture), the electron velocity $\vec{v}$ in a crystal is given by $(1/\hbar)\nabla_{\vec{k}}\epsilon(\vec{k})$. Show that near the Dirac points, the magnitude of the electron velocity is given by $3at/(2\hbar)$. Since this constant velocity (independent of energy or of $\vec{k}$) is the velocity at the Fermi level as well, we may as well write $v_F = 3at/(2\hbar)$. This constant (Fermi) velocity near the Dirac points makes a striking contrast to the free electron case, where the (Fermi) velocity varies with energy or $\vec{k}$. Using v_F, which has been demonstrated to be $\sim 10^6$ m/s, we can re-write the electronic energy dispersion of Eq. (9) into

$$\epsilon_\pm(\vec{q}) \approx \pm\hbar v_F q. \tag{10}$$

Remark: In deriving Eq. (7), you must have used (effectively) a 2×2 tight-binding Hamiltonian matrix. We can readily simplify this Hamiltonian matrix near the Dirac points with 1st order approximation. Then of course, the near-Dirac-point energy dispersion, Eq. (10), directly results as the eigen energies of this near-Dirac-point Hamiltonian matrix. Now, in a formal analogy, this near-Dirac-point Hamiltonian has exactly the same form as the Hamiltonian of an ultra-relativistic or massless particle of spin 1/2 (*e.g.*, neutrino), with the velocity of light c replaced with the Fermi velocity v_F. In fact, the near-Dirac-point energy dispersion, Eq. (10), is pleasantly reminiscent of the dispersion relation of ultra relativistic or massless particles.