Physics 195 / Applied Physics 195 — Assignment #5

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Date: Oct. 13, 2017
Due: 12:45pm + 10 min grace period, Oct. 25, 2017 at the dropbox outside Maxwell-Dworkin Room 131.

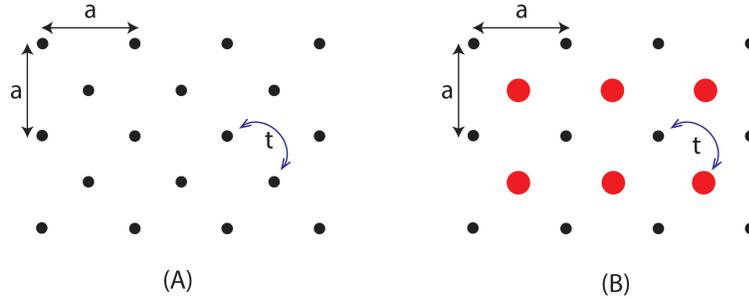**Problem 1 (150 pt): Electronic band structures of 2D crystals**

Figure 1: Problem 1

(a) Consider the 2D crystal of Fig. 1(A)—where atoms are represented by the solid black circles—under the tight binding approximation. Each atom has one valence electron. When the atom is isolated, the ground state energy of its valence electron is ϵ_0. The electron tunneling strength between ground states of any two nearest neighbor atoms is $t > 0$.

- Show the emergence of one electronic band and calculate its dispersion relation $\epsilon(\vec{k})$.

- Verify that $\epsilon(\vec{k} + \vec{G}) = \epsilon(\vec{k})$ for any arbitrary reciprocal lattice vector $\vec{G}$ (as discussed in class, this periodicity in the $\vec{k}$-space means that it is sufficient to consider $\epsilon(\vec{k})$ only within the 1st Brillouin zone).

- Draw the reciprocal lattice, 1st Brillouin zone, and single-electron energy contour map. Identify the Fermi surface and evaluate the Fermi energy ϵ_F. Argue that this crystal is a metal. Calculate the cohesive energy (electronic contribution).

(b) The 2D crystal of Fig. 1(B) is formed by periodically arranging two different types of atoms, shown as the solid black and red circles. This crystal can be described using the lattice-with-a-basis approach. Each atom has one valence electron. When the atom is isolated, the ground state energy of its valence electron is ϵ_A or ϵ_B, depending on the type of the atom (black or red). Under the tight binding approximation, the strength of electron tunneling between ground states of any two nearest neighbor atoms (which are necessarily the two different atom types) is $t > 0$.

- Show the emergence of two electronic bands, and calculate the dispersion relation $\epsilon(\vec{k})$ for each band.

- Verify that for each band $\epsilon(\vec{k} + \vec{G}) = \epsilon(\vec{k})$ for any arbitrary reciprocal lattice vector $\vec{G}$.

- Draw the reciprocal lattice, 1st Brillouin zone, and single-electron energy contour map (for both bands). Identify the electron-filled region in the $\vec{k}$-space. What is the size of the band gap? Argue that this crystal is an insulator (at $T = 0$ at least).

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Problem 2 (200 pt): Electronic band structure of graphene

Graphene is a 2D honeycomb net of carbon atoms [Fig. 2(a)]. Each carbon atom has four valence electrons. Three of them participate in covalent bonding—σ bonding—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.
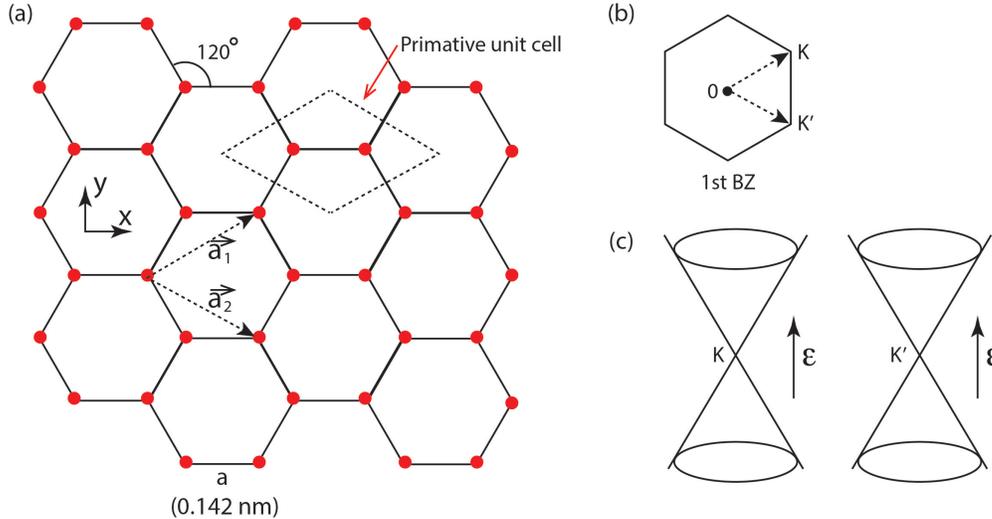

Figure 2: (a) Graphene crystal structure. (b) 1st Brillouin zone. (c) Energy dispersion around the Dirac points K and K'.

Since the honeycomb net is not a Bravais lattice, graphene should be described with the lattice-with-a-basis formalism [Lecture #6]. Following Homework #4, and with reference to Fig. 2(a), we here may use the hexagonal lattice spanned by the primitive vectors $\vec{a}_1$ and $\vec{a}_2$, where the lattice's primitive unit cell contains two carbon atoms. From Homework #4, we know that the 1st Brillouin zone is of hexagonal shape with six corner points [Fig. 2(b)]. These corner points 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. 2(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.

(a) By using the tight binding method for the π electron, whose energy eigenvalue in an isolated carbon atom is set at $\epsilon_0 = 0$, 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

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

(b) 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.

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

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

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

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

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. (3) 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. 2(c)] and the two bands $\epsilon_{+}(\vec{k})$ and $\epsilon_{-}(\vec{k})$ touch sharply at the Dirac points.

(d) Show that Eq. (3) may be re-written into

$$\epsilon_{\pm}(\vec{q}) \approx \pm \hbar v_F q \tag{4}$$

where v_F is the Fermi velocity. Estimate the value of the hopping strength t in eV, based on $v_F \sim 10^6$ m/s.

(**Remark**) In deriving Eq. (1), you must have used (effectively) a 2×2 tight-binding Hamiltonian matrix. We can readily simplify this effective Hamiltonian matrix near the Dirac points with 1st order approximation. Then of course, the near-Dirac-point energy dispersion, Eq. (4), directly results as the eigen energies of this near-Dirac-point Hamiltonian matrix. Now, this near-Dirac-point Hamiltonian has the form of the Weyl-Dirac Hamiltonian for a relativistic 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. (4), is reminiscent of the dispersion relation of relativistic massless particles.

(e) Imagine that the two carbon atoms in each primitive unit cell of the hexagonal lattice are now replaced by two different kinds of atoms, shown as red and sky blue solid circles in Fig. 3. Further assume that these two atoms have ground state energies of $\epsilon_{0,\text{red}} = \delta/2$ and $\epsilon_{0,\text{blue}} = -\delta/2$ (in contrast to the graphene case of $\epsilon_0 = 0$ for every carbon atom). On the other hand, use the same nearest-neighbor hopping parameter t as in graphene. Show that band gap now opens up near the K and K' points (what is the size of the gap?) and the energy dispersions exhibit approximately quadratic dependencies on q near these points.
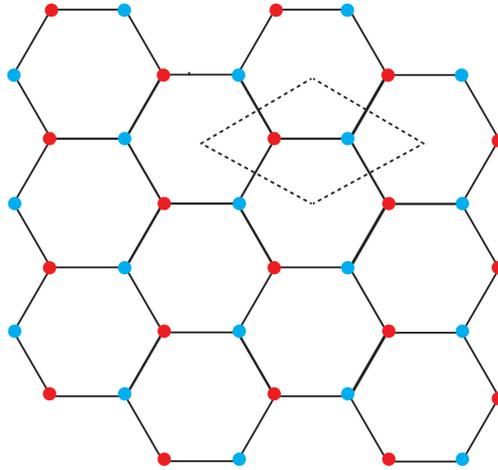

Figure 3: Two different types of atoms in the primitive unit cell of the hexagonal lattice.

Problem 3 (50 pt): Electronic s-band of BCC crystal

Show that under the tight-binding approximation the dispersion relation of the electronic s-band of the BCC crystal (one atom per primitive unit cell) is given by

$$\epsilon(\vec{k}) = \epsilon_0 - 8t \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \cos \frac{k_z a}{2}, \tag{5}$$

where ϵ_0 is the atomic s-level energy and $t > 0$ is the strength of electron hopping between the s levels of two nearest neighbor atoms. Now, if we consider the electron hopping (hopping strength: $t' > 0$) between the s levels of two next-to-nearest atoms as well, show that the electronic s-band dispersion relation is modified to

$$\epsilon(\vec{k}) = \epsilon_0 - 8t \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \cos \frac{k_z a}{2} - 2t'[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]. \tag{6}$$