Advanced Solid State Physics: Problems

I. 1. ELECTRONIC STRUCTURE OF GRAPHENE

Graphene is a monolayer of graphite. It has a honeycomb lattice. Recently, it drew a lot of attention since the properties of electrons in graphene resemble those of Dirac fermions in quantum electrodynamics.

(a) Identify the periods for graphene lattice. How many atoms there are per unit cell?

(b) Assume a tight-binding Hamiltonian, $\hat{H}\psi_i = -\sum_j t\psi_j$, where the summation is performed over all sites j adjacent to i, diagonalize it for two sublattices and find the energy spectrum.

(c) Find the periods for the reciprocal lattice. What is the unit cell of the reciprocal lattice? Construct the Brillouin zone – an equivalent representation of unique k-points – by drawing plains separating nearest sites of the reciprocal lattice.

(d) Check that the energy turns to zero at the corners of the Brillouine zone.

(e) Expand the energy spectrum in the vicinity of these points and find the linear spectrum.

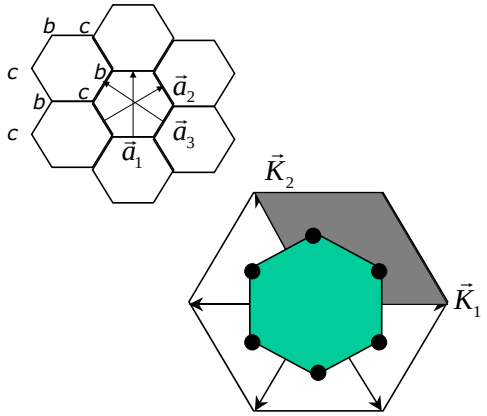

FIG. 1: *Top*: honeycomb graphene lattice. The two sublattices are marked b and c. The three shortest latice periods are shown; we choose $\vec{a}_1$ and $\vec{a}_2$ as the basic periods. *Bottom*: reciprocal lattice. The reciprocal lattice unit cell is shown as a shaded rhombic area; the Brillouin zone is a shaded hexagon. Energy nodes are shown as filled circles.

(a) Let us orient the lattice so that two of the sides of each hexagon – a unit cell – are directed along x-axis (Fig. 1). We can then translate a lattice in three directions such that it repeats itself. These three periods are

$$\begin{aligned} \vec{a}_1 &= a(0, \sqrt{3}) \\ \vec{a}_2 &= a(3/2, \sqrt{3}/2) \\ \vec{a}_3 &= a(-3/2, \sqrt{3}/2) \ . \end{aligned}$$

Any linear combination of these three periods is also a lattice period. However, for a two-dimensional lattice, three lattice periods are too much. There must be only two independent lattice periods. Indeed, we have, for instance, $\vec{a}_3 = \vec{a}_1 - \vec{a}_2$. This means we can just choose two of them – for instance, $\vec{a}_1$ and $\vec{a}_2$.

A unit cell contains six atoms (in each corner of the hexagon), but each atom is shared by three hexagons, hence two atoms per unit cell. We thus have two sublattices, shown on Fig. 1 as b and c.

(b) Assume that the wave function in graphene is a plane wave, with values different at two sublattices. It is best represented as the two-component wave function,

$$\psi(\vec{r}) = \begin{pmatrix} \psi_b \\ \psi_c \end{pmatrix} = \begin{pmatrix} u_b \\ u_c \end{pmatrix} e^{ik_x x + ik_y y} \ .$$

Note that each atom in the sublattice b has three nearest neighbors, each of them belongs to the sublattice c. The Schrödinger equation for such an atom looks like

$$Eu_b = -t\left\{e^{-ik_x a} + e^{ik_y\sqrt{3}a/2+ik_x a/2} + e^{-ik_y\sqrt{3}a/2+ik_x a/2}\right\}u_c \ .$$

In the same way,

$$Eu_c = -t\left\{e^{ik_x a} + e^{ik_y\sqrt{3}a/2-ik_x a/2} + e^{-ik_y\sqrt{3}a/2-ik_x a/2}\right\}u_b \ .$$

These two linear homogeneous equations for two variables u_b and u_c only have non-trivial solution when the following condition is satisfied,

$$E = t\sqrt{1 + 4\cos^2\frac{\sqrt{3}k_y a}{2} + 4\cos\frac{\sqrt{3}k_y a}{2}\cos\frac{3k_x a}{2}} \ , \tag{1}$$

that gives the energy spectrum in graphene in the tight-binding approximation.

(c) Each vector of the reciprocal lattice, $\vec{K}$, obeys the conditions $\vec{K}\vec{a}_1 = 2\pi n_1$ and $\vec{K}\vec{a}_2 = 2\pi n_2$, with integers n_1 and n_2. This provides the parametrization

$$\vec{K} = \frac{2\pi}{3a}(2n_2 - n_1, \sqrt{3}n_1) \ .$$

The shortest vectors correspond to the values $(0, \pm 1)$, $(\pm 1, 0)$, $(1, 1)$, and $(-1, -1)$. We choose two of them as the reciprocal lattice unit vectors, $\vec{K}_1 = (2\pi/3a)(2, 0)$ and $\vec{K}_2 = (2\pi/2a)(-1, \sqrt{3})$. The reciprocal lattice unit cell is a rhombus formed by these two vectors (Fig. 1): It contains all non-equivalent points in the reciprocal space. Equivalent are the points separated by a period of the reciprocal lattice.

It is usually more convenient, however, to choose the set of non-equivalent points differently — to construct a *Brillouin zone*. For this purpose, we take the origin of the resiprocal lattice and draw all six shortest lattice periods. Their ends define a hexagon that contains three unit cells. Then we take the middle of each vectors and put lines perpendicular to the vectors. These lines form another hexagon, which is a Brillouin zone (BZ). The volume of BZ equals to the volume of a unit cell, and one can check that BZ contains all non-equivalent points of the reciprocal space.

(d) The corners of BZ have the following coordinates:

$$\frac{4\pi}{3\sqrt{3}a}(0, \pm 1); \quad \frac{2\pi}{3\sqrt{3}a}(\pm\sqrt{3}, \pm 1)$$

It is straigthforward to check that the energy at all these points turns to zero. Note that despite the fact that we found six points each of them is shared by three BZ's, or three unit cells. Thus, we only have two non-equivalent K-points. Let us choose $\vec{K}_0 = (2\pi/3a)(1, \pm 1/\sqrt{3})$. Note that none of them is a reciprocal lattice period.

(e) Now we expand the energy in the vicinity of the nodes. We write $\vec{K} = \vec{K}_0 + \vec{q}$ and assume that q is small, $q_x a, q_y a \ll 1$. Expanding

$$\begin{aligned}\cos\frac{3k_x a}{2} &= -1 + \frac{9(q_x a)^2}{8} \ ; \\ \cos\frac{\sqrt{3}k_y a}{2} &= \frac{1}{2} \mp \frac{3q_y a}{4} - \frac{3(q_y a)^2}{16} \ ,\end{aligned}$$

we find that constant and linear terms cancel, and the energy has a *linear dispersion*

$$E = \frac{3t}{2}\sqrt{q_x^2 + q_y^2} \ . \tag{2}$$