PHZ6426: Fall 2013
Problem set # 5: Nearly-free-electron and tight-binding models: Solutions
due Wednesday, 11/13 at the time of the class

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Please help your instructor by doing your work neatly. **Every (algebraic) final result must be sup**

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P1 [20 points] Consider a 1D electron system subject to a weak periodic potential

$$U(x) = U_0 \left[\cos^4 \frac{\pi x}{a} - \frac{3}{8} \right],$$

Find and plot the dispersions of energy bands in the first Brillouin zone. Plot the energies in units of $\hbar^2\pi^2/2ma^2$, the wave numbers in units of $1/a$, and assume that $U_0 = 0.1$ in these units.

Solution

Using the trigonometric identity $\cos^2 x = (1 + \cos(2x))/2$, the potential can be re-written as

$$U(x) = U_0 \left(\frac{1}{2} \cos \frac{2\pi x}{a} + \frac{1}{8} \cos \frac{4\pi x}{a} \right) = U_0 \left(\frac{1}{4} e^{2i\pi x/a} + \frac{1}{16} e^{4\pi i x/a} + \text{c.c.} \right)$$

There are two non-zero harmonics with amplitudes $u_{\pm 1} = U_0/4$ and $u_{\pm 2} = U_0/16$ with wavenumbers $q = \pm 2\pi/a$ and $q = \pm 4\pi/a$. Scattering at harmonic with $q = \pm 2\pi/a$ lifts denegeracy of the free-electron states with energies $\varepsilon_1 = \hbar^2 k^2/2m$ and $\varepsilon_2 = \hbar^2(k \mp 2\pi/a)^2/2m$. The degeneracy points are $k = \pm\pi/a$. The energy levels near these points are given by

$$\varepsilon = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \sqrt{\frac{(\varepsilon_1 - \varepsilon_2)^2}{4} + \left(\frac{U_0}{4} \right)^2}.$$

Likewise, scattering at harmonic with $q = \pm 4\pi/a$ lifts denegeracy of the free-electron states with energies $\varepsilon_1 = \hbar^2 k^2/2m$ and $\varepsilon_3 = \hbar^2(k \mp 4\pi/a)^2/2m$. The degeneracy points are $k = \pm 2\pi/a$. The energy levels near these points are given by

$$\varepsilon = \frac{\varepsilon_1 + \varepsilon_3}{2} \pm \sqrt{\frac{(\varepsilon_1 - \varepsilon_3)^2}{4} + \left(\frac{U_0}{16} \right)^2}.$$

P2 [20 points] Consider 2D electrons subject to a weak periodic potential

$$U(x,y) = U_0 \left(\cos \frac{2\pi x}{a} + \cos \frac{2\pi y}{a} \right).$$

a) [8 points] Find the energy bands near the edges of the first Brillouin zone. (Hint: the edges of the Brillouin zone are the Bragg planes where the eigenstates are doubly degenerate.) Plot the bands and isoenergetic surfaces.

Solution The non-zero harmonics of the potential have wavenumbers $(\pm b, q_y = 0)$ and $(q_x = 0, q_y = \pm b)$, where $b = 2\pi/a$, with amplitudes $U_0/2$. Consider one of the edges, e.g., $k_x = \pi/a$; by symmetry, the energy spectrum will be the same at other edges. The two free-electron states with energies $\varepsilon^0_{k_x,k_y} = \hbar^2 \left(k_x^2 + k_y^2\right)/2m$ and $\varepsilon^0_{k_x-2\pi/a,k_y} = \hbar^2 \left((k_x - 2\pi/a)^2 + k_y^2\right)/2m$ are degenerate at this edge. The energy levels near the edge are given by

$$\varepsilon = \frac{\varepsilon^0_{k_x,k_y} + \varepsilon^0_{k_x-2\pi/a,k_y}}{2} \pm \sqrt{\frac{\left(\varepsilon^0_{k_x,k_y} - \varepsilon^0_{k_x-2\pi/a,k_y}\right)^2}{4} + \left(\frac{U_0}{2}\right)^2}.$$

b) [12 points] Repeat the analysis of part a) for regions near the corners of the first Brillouin zone, where there are four degenerate eigenstates.

Solution The basis must now include four degenerate states with energies $\varepsilon^0_{k_x,k_y}$, $\varepsilon^0_{k_x-b,k_y}$, $\varepsilon^0_{k_x-b,k_y-q_y}$, and $\varepsilon^0_{k_x-b,k_y-b}$. Using the fact the only non-zero harmonics of the periodic potential are $U_{q_x=\pm b,0} = U_{q_x=0,q_y=\pm b} = U_0/2$, we obtain equations for the weighing factors of the four degenerate states [cf. Eq. (9.19) in *AM*]:

$$\begin{aligned}
(\varepsilon - \varepsilon^0_{k_x,k_y}) c_{k_x,k_y} &= \frac{U}{2}(c_{k_x-b,k_y} + c_{k_x,k_y-b}) \\
(\varepsilon - \varepsilon^0_{k_x-b,k_y}) c_{k_x-b,k_y} &= \frac{U}{2}(c_{k_x,k_y} + c_{k_x-b,k_y-b}) \\
(\varepsilon - \varepsilon^0_{k_x,k_y-b}) c_{k_x,k_y-b} &= \frac{U}{2}(c_{k_x,k_y} + c_{k_x-b,k_y-b}) \\
(\varepsilon - \varepsilon^0_{k_x-b,k_y-b}) c_{k_x-b,k_y-b} &= \frac{U}{2}(c_{k_x-b,k_y} + c_{k_x,k_y-b}). \qquad (1)
\end{aligned}$$

Inverting the matrix and measuring the wavenumbers in units of $1/a$ and energies in units of $\hbar^2/2ma^2$, we obtain for the four energy levels

$$\begin{aligned}
\varepsilon_1 &= E_0 + R_+ \\
\varepsilon_2 &= E_0 - R_+ \\
\varepsilon_3 &= E_0 + R_- \\
\varepsilon_4 &= E_0 - R_-
\end{aligned}$$

where

$$\begin{aligned}
E_0 &= k_x^2 + k_y^2 - 2\pi(k_x + k_y) + 4\pi^2 \\
R_\pm &= \frac{1}{2}\left[4U_0^2 + 32\pi^2(k_x^2 + k_y^2 - 2\pi(k_x + k_y) + 2\pi^2) \pm 4\sqrt{(U_0^2 + 16\pi^2(\pi - k_x)^2)(U_0^2 + 16\pi^2(\pi - k_y)^2)}\right]^{1/2}
\end{aligned}$$

P3 [20 points] The Kronig-Penney model allows one to consider both the nearly-free-electron and tight-binding limits. Previously, we focused on the latter. Now, consider the (repulsive) Dirac-Kronig-Penney model, which, as we showed earlier, gives the following implicit equation for the energy bands:

$$\cos ka = \cos qa + u \frac{\sin qa}{qa}, \qquad (2)$$

where $q = \sqrt{2mE}/\hbar$ and $u = mU_0 a/\hbar^2 > 0$. Assuming that $u \ll 1$, find the solution of Eq. (2) near the Bragg points $k \approx \pm\pi/a, \pm 2\pi/a \ldots$. (Reminder: the $\approx$ sign means that k is close yet not equal to the wavenumber of the Bragg point.) Compare your result with that of the nearly-free-electron model.

Solution

The maximum value of the r.h.s. of Eq. (2) ($= 1 + u$) occurs at $q = 0$. The minimum value occurs near $qa = \pi$. To see this, substitute $qa = \pi + \delta$ and expand the r.h.s. to second order in δ:

$$R \equiv \cos qa + u\frac{\sin qa}{qa} = -1 + \frac{\delta^2}{2} - \frac{u\delta}{\pi} + \ldots$$

$\partial R/\partial\delta = 0$ gives $\delta = u/\pi$, and the minimum value of R is $R_{\min} = -1 - u^2/2\pi^2 < -1$. Since $\cos k \geq -1$, Eq. (2) has no soluton in the region around the minimum of R, where $R_{\min} \leq R \leq -1$. This region corresponds to a gap in the energy spectrum.

To find the energy levels near the gap, substitute $ka = \pi + p$ into Eq. (2) and expand $\cos ka$ in p as $\cos(\pi + p) = -1 + p^2/2$. The resulting equation

$$\delta^2 - \frac{2}{\pi}u\delta - p^2 = 0$$

has two roots

$$\delta_\pm = \frac{u}{\pi} \pm \sqrt{p^2 + \left(\frac{u}{\pi}\right)^2}.$$

Returning to the original variables, we obtain for the energy levels

$$\begin{aligned} E_\pm &= \frac{\pi^2\hbar^2}{2ma^2}\left[1 + \frac{u}{\pi^2} \pm \sqrt{\left(\frac{ka}{\pi} - 1\right)^2 + \left(\frac{u}{\pi^2}\right)^2}\right]^2. \\ &\approx \frac{\pi^2\hbar^2}{2ma^2}\left[1 + \frac{2u}{\pi^2} \pm 2\sqrt{\left(\frac{ka}{\pi} - 1\right)^2 + \left(\frac{u}{\pi^2}\right)^2}\right], \end{aligned} \tag{3}$$

where the last line is valid to first order in u.

Recall the result of the NFE model (with diagonal matrix elements U_{11} and U_{22} equal to zero)

$$E_\pm = \frac{\varepsilon_k + \varepsilon_{k-2\pi/a} + U_{12}}{2} \pm \sqrt{\left(\frac{\varepsilon_k - \varepsilon_{k-2\pi/a}}{2}\right)^2 + U_{12}^2}, \tag{4}$$

where $\varepsilon_k = \hbar^2 k^2/2m$. The difference of the free-electron energies can be re-written as

$$\varepsilon_k - \varepsilon_{k-2\pi/a} = \frac{2\pi^2\hbar^2}{ma^2}\left(\frac{ka}{\pi} - 1\right),$$

while in their sum we can replace k by π/a:

$$\varepsilon_k + \varepsilon_{k-2\pi/a} = \frac{\hbar^2\pi^2}{ma^2}$$

Now it is obvious that the NFE result is equivalent to Eq. (4).

P4 [15 points] Find the dispersions of energy bands for *fcc* and *bcc* lattices taking into account hopping between the nearest and next-to-nearest neighbors.

Solution:

The tight binding dispersion relation is:

$$E_k = E_0 - t\sum_{\vec{R}_{nn}} e^{i\vec{k}\cdot\vec{R}_{nn}} - t'\sum_{\vec{R}_{nnn}} e^{i\vec{k}\cdot\vec{R}_{nnn}} \tag{5}$$

(a) case of *bcc*
8 n.n.:
$\frac{a}{2}(\pm1,+1,+1)$, $\frac{a}{2}(\pm1,+1,-1)$, $\frac{a}{2}(\pm1,-1,+1)$, $\frac{a}{2}(\pm1,-1,-1)$
6 n.n.n.:
$a(\pm1,0,0)$, $a(0,\pm1,0)$, $a(0,0,\pm1)$

$$\begin{aligned}\sum_{\vec{R}^{bcc}_{nn}} e^{i\vec{k}\cdot\vec{R}^{bcc}_{nn}} &= e^{(1/2)ia(+k_x+k_y+k_z)} + e^{(1/2)ia(-k_x+k_y+k_z)} \\ &+e^{(1/2)ia(+k_x+k_y-k_z)} + e^{(1/2)ia(-k_x+k_y-k_z)} \\ &+e^{(1/2)ia(+k_x-k_y+k_z)} + e^{(1/2)ia(-k_x-k_y+k_z)} \\ &+e^{(1/2)ia(+k_x-k_y-k_z)} + e^{(1/2)ia(-k_x-k_y-k_z)} \\ &= 2\cos[(a/2)(k_x+k_y+k_z)] + 2\cos[(a/2)(k_x-k_y+k_z)] \\ &+2\cos[(a/2)(k_x+k_y-k_z)] + 2\cos[(a/2)(k_x-k_y-k_z)] \\ &= 8\cos(k_xa/2)\cos(k_ya/2)\cos(k_ya/2)\end{aligned} \tag{6}$$

$$\begin{aligned}\sum_{\vec{R}^{bcc}_{nnn}} e^{i\vec{k}\cdot\vec{R}^{bcc}_{nnn}} &= e^{iak_x} + e^{-iak_x} + e^{iak_y} + e^{-iak_y} + e^{iak_z} + e^{-iak_z} \\ &= 2\cos(k_xa) + 2\cos(k_ya) + 2\cos(k_za)\end{aligned} \tag{7}$$

(b) case of *fcc*
12 n.n.:
$\frac{a}{2}(+1,0,\pm1)$, $\frac{a}{2}(0,+1,\pm1)$, $\frac{a}{2}(-1,0,\pm1)$, $\frac{a}{2}(0,-1,\pm1)$,
$\frac{a}{2}(+1,+1,0)$, $\frac{a}{2}(+1,-1,-)$, $\frac{a}{2}(-1,+1,0)$, $\frac{a}{2}(-1,-1,0)$;
6 n.n.n.:
$a(\pm1,0,0)$, $a(0,\pm1,0)$, $a(0,0,\pm1)$; (same as *bcc*)

$$\begin{aligned}\sum_{\vec{R}^{fcc}_{nn}} e^{i\vec{k}\cdot\vec{R}^{fcc}_{nn}} &= 2\cos[(a/2)(k_x+k_y)] + 2\cos[(a/2)(k_x-k_y)] \\ &+2\cos[(a/2)(k_x+k_z)] + 2\cos[(a/2)(k_x-k_z)] \\ &+2\cos[(a/2)(k_y+k_z)] + 2\cos[(a/2)(k_y-k_z)] \\ &= 4[\cos(k_xa/2)\cos(k_ya/2) + \cos(k_ya/2)\cos(k_za/2) + \cos(k_za/2)\cos(k_xa/2)]\end{aligned} \tag{8}$$

$$\sum_{\vec{R}^{fcc}_{nnn}} e^{i\vec{k}\cdot\vec{R}^{fcc}_{nnn}} = \sum_{\vec{R}^{bcc}_{nnn}} e^{i\vec{k}\cdot\vec{R}^{bcc}_{nnn}} \tag{9}$$

P5 [25 points] Bilayer graphene consists of two graphene layers stacked on top of each other in a *Bernal* manner, i.e., such that only one of the two inequivalent lattice sites, e.g., A, has the nearest neighbor along the

vertical (see Fig. 1). The tight-binding Hamiltonian in the nearest-neighbor-hopping approximation reads

$$\hat{H} = -\gamma_0 \sum_{m,\mathbf{R},\mathbf{R}'} \hat{a}^\dagger_{m,\mathbf{R}} \hat{b}_{m,\mathbf{R}'} - \gamma_1 \sum_{\mathbf{R},\mathbf{R}'} \hat{a}^\dagger_{1,\mathbf{R}} \hat{a}_{2,\mathbf{R}'} + \text{H.c.} \tag{10}$$

where $\hat{a}_m$ and $\hat{b}_m$ with $m = 1, 2$ are the electron annihilation operators for sites A and B in the bottom (1) and top (2) planes, correspondingly, sum over $\mathbf{R}$ and $\mathbf{R}'$ includes only the nearest neighbors, and parameters γ_0 and γ_1 are real (FYI, $\gamma_0 \approx 3$ eV and $\gamma_1 \approx 0.4$ eV). The planes are separated by distance c (≈ 3Å). Find the energy spectrum for arbitrary $\mathbf{k}$ in the Brillouin zone. Plot the isonergetic contours. Analyze the spectrum near the K and K' points.

Solution

The unit cell of a graphene bilayer consists of four atoms. The electron state is a 4-spinor

$$|\psi\rangle = \begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ b_2 \end{pmatrix},$$

where $a_1 \dots b_2$ are the amplitudes of finding an electron on site $A_1 \dots B_2$. In basis of $|\psi\rangle$ states , the Hamiltonian can be written as a 4×4 matrix

$$\hat{H} = \begin{pmatrix} 0 & S & -\gamma_1 & 0 \\ S^* & 0 & 0 & 0 \\ -\gamma_1 & 0 & 0 & S \\ 0 & 0 & S^* & 0 \end{pmatrix}, \tag{11}$$

where S is the matrix element connecting A and B sites in the same plane. The top left and bottom right 2×2 blocks are the same as for a monolayer. Diagonalizing Hamiltonian in Eq. (11), we obtain for the energy levels

$$\varepsilon = \pm\sqrt{\frac{\gamma_1^2 + |S|^2}{2} \pm \sqrt{\frac{\gamma_1^4}{4} + \frac{\gamma_1^2 |S|^2}{2} - \frac{3}{4}|S|^4}}. \tag{12}$$

Recall that $|S| = (3/2)\gamma_0 a k \equiv \hbar v_F k$ near the K and K' points, where k is measured from either of these two points. In the low-energy limit $|S| \ll \gamma_1$, two out of the four branches in Eq. (12) approach finite value (equal to γ_1), whereas the other two vanish. Expanding these last two dispersions in Taylor series, we find

$$\varepsilon = \pm|S|^2/\gamma_1 = \pm(\hbar^2 v_F^2/\gamma_1)k^2 \equiv \pm\hbar^2 k^2/2m^*,$$

where $m^* \equiv \gamma_1/2v_F^2$. Therefore, the low energy excitations in bilayer graphene are massive electrons and holes. Degeneracy of the spectrum at K and K' points is not lifted by inter-layer coupling but the functional form of the dispersion around the degeneracy point is modified from linear to quadratic.

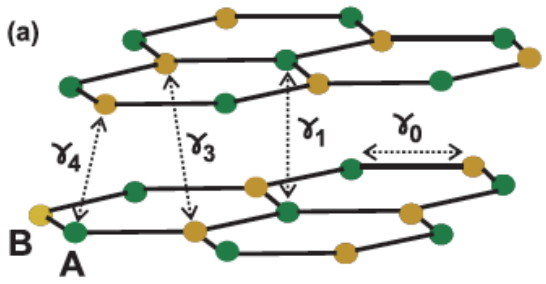

Figure 1: Crystal structure of bilayer graphene, from A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, A. K. Geim, Rev. Mod. Phys. **81**, 109 (2009).