

Condensed Matter Physics

Homework Assignment 9

Due date Friday, November 5

1. Band structure of graphene: the tight-binding approximation.

In the atomic limit, the motion of a π electron in the graphene plane can be described as tunneling to a nearest site. The tunneling is described by the Hamiltonian

$$H|\mathbf{r}, \bullet\rangle = -\tau \sum_{n=1}^3 |\mathbf{r} + \delta_n, \circ\rangle,$$

$$H|\mathbf{r}, \circ\rangle = -\tau^* \sum_{n=1}^3 |\mathbf{r} - \delta_n, \bullet\rangle,$$

where \bullet and \circ denote the two sublattices (Fig. 1) and τ is the “hopping amplitude”.

(a) With the aid of the Fourier transform,

$$|\mathbf{k}, \bullet\rangle = \sum_{\mathbf{r} \in \bullet} e^{i\mathbf{k} \cdot \mathbf{r}} |\mathbf{r}, \bullet\rangle, \quad |\mathbf{k}, \circ\rangle = \sum_{\mathbf{r} \in \circ} e^{i\mathbf{k} \cdot \mathbf{r}} |\mathbf{r}, \circ\rangle,$$

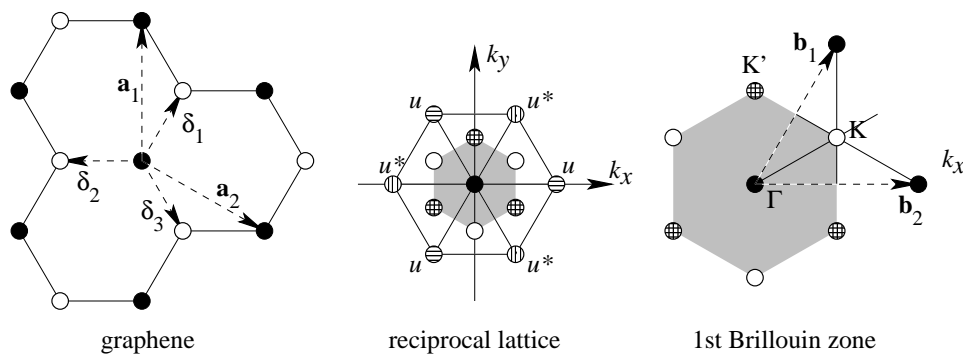


Figure 1: Graphene and part of its reciprocal lattice.

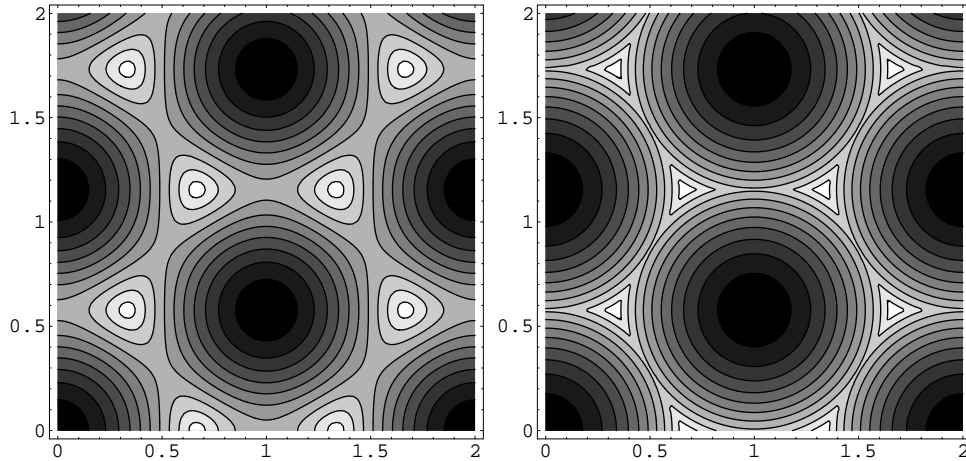


Figure 2: Contour plots of energy dispersions $E(k_x, k_y)$. Lighter regions correspond to higher energies. Left: the lower band $E_{\mathbf{k}}$ in the tight-binding approximation. Right: the free-electron band $\hbar^2|\mathbf{k}|^2/2m$ and its shadows $\hbar^2|\mathbf{k} - \mathbf{G}|^2/2m$ shifted by vectors of the reciprocal lattice \mathbf{G} .

obtain the Hamiltonian in momentum basis:

$$\begin{aligned} H|\mathbf{k}, \bullet\rangle &= -\tau_{\mathbf{k}}|\mathbf{k}, \circ\rangle, \\ H|\mathbf{k}, \circ\rangle &= -\tau_{\mathbf{k}}^*|\mathbf{k}, \bullet\rangle, \end{aligned}$$

where $\tau_{\mathbf{k}} = \tau \sum_{n=1}^3 e^{-i\mathbf{k}\cdot\delta_n}$.

(b) Find the eigenvalues $E(\mathbf{k})$ of the hopping Hamiltonian. Show that the upper and lower bands are degenerate at the corners of the Brillouin zone $\mathbf{k}_K = (0, -4\pi/3a)$ and $\mathbf{k}_{K'} = (0, 4\pi/3a)$.

(c) Investigate the shape of the spectrum $E(\mathbf{k})$ near the corners of the Brillouin zone. To do so, expand $E(\mathbf{k})$ in powers of $\mathbf{q} = \mathbf{k} - \mathbf{k}_K$. (Alternatively, you might expand the hopping Hamiltonian. Doing so will yield massless Dirac fermions near each corner.) The spectrum is presented in the left panel of Fig. 2.

2. Band structure of graphene: nearly free electrons. (You might find it helpful to read Chapter 9 in *Ashcroft and Mermin*.)

Note that the free-electron dispersions (right panel of Fig. 2) already bear strong resemblance to the tight-binding spectrum (left panel), with the exception of the boundaries and especially the corners of the Brillouin

zone. Scattering from the periodic potential of the ion cores will modify the spectrum precisely at these lines and points.

(a) Demonstrate that *three* free-electron bands,

$$E_0(\mathbf{k}) = \frac{\hbar^2 |\mathbf{k}|^2}{2m}, \quad E_1(\mathbf{k}) = \frac{\hbar^2 |\mathbf{k} - \mathbf{b}_1|^2}{2m}, \quad E_2(\mathbf{k}) = \frac{\hbar^2 |\mathbf{k} - \mathbf{b}_2|^2}{2m},$$

intersect at point K (Fig. 1).

(b) Choose one of the black sites as the origin $\mathbf{r} = 0$. Then the potential $V_\bullet(\mathbf{r})$ created by ions of the black sublattice is an even function, $V_\bullet(\mathbf{r}) = V_\bullet(-\mathbf{r})$. Show that its Fourier transform $v(\mathbf{k})$ is a real number.

We will only need the value of $v_\bullet(\mathbf{k})$ for the six vectors of the reciprocal lattice closest to the origin Γ (Fig. 1). Sixfold rotational symmetry of the black sublattice guarantees that the value v_\bullet will be the same for all six points. We will use v_\bullet as a phenomenological parameter characterizing the strength of scattering. For definiteness, take $v_\bullet < 0$ (attraction).

(c) The potential of the white sublattice

$$V_\circ(\mathbf{r}) = V_\bullet(\mathbf{r} - \delta_1) = V_\bullet(\mathbf{r} - \delta_2) = V_\bullet(\mathbf{r} - \delta_3)$$

is *not* invariant under the inversion $\mathbf{r} \rightarrow -\mathbf{r}$. Therefore its Fourier transform will be a complex number. Show that it equals

$$v_\circ = v_\bullet e^{\pm 2\pi i/3}$$

for the six reciprocal lattice points closest to Γ . Verify that the total is

$$u = v_\bullet + v_\circ = v_\bullet e^{\pm \pi i/3}.$$

(d) Analyze how the scattering potential lifts the triple degeneracy of the main and shadow bands at the point \mathbf{k}_K . Approximate the Hilbert space by the three states $|\mathbf{k}\rangle$, $|\mathbf{k} - \mathbf{b}_1\rangle$ and $|\mathbf{k} - \mathbf{b}_2\rangle$. Show that, in the basis of these states, the Hamiltonian is

$$H = \begin{pmatrix} E_0 & u & u^* \\ u^* & E_0 & u \\ u & u^* & E_0 \end{pmatrix}$$

to the first order in the periodic potential u .

(e) Find its eigenvalues and show that two of them are degenerate, as in the tight-binding approximation.

(f)* Determine the spectrum near the degeneracy point.

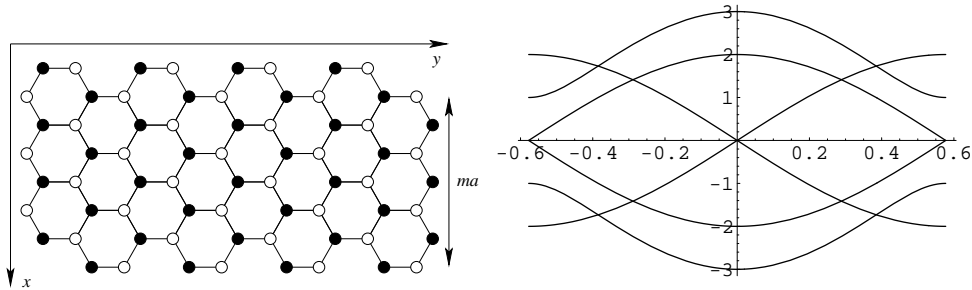


Figure 3: Left: a “zigzag” nanotube is made by gluing together the upper and lower edges of a graphene strip. Right: energy bands for $m = 3$.

3*. Nanotubes.

Cut a graphene strip of width ma and roll it up into a nanotube (Fig. 3). This introduces periodic boundary conditions along the x direction and makes k_x quantized in the units $2\pi/ma$. Although the energy spectrum $E(k_x, k_y)$ remains unchanged, the two-dimensional bands are replaced with $2m$ one-dimensional bands—two for each allowed value of k_x . Fig. 3 shows the bands for $m = 3$.

- (a) Determine how many bands will be filled and how many empty.
- (b) Determine for which widths m the Fermi energy does *not* lie in the energy gap.