Advanced Condensed Matter Physics
Homework Assignment 2

Due date February, February 17, 2012

1. Electrons on a chain. As we discussed in class, the spectrum of one-electron energies in an atomic chain is $\varepsilon(k) = -2t\cos ka$, where k is the wavenumber, a is the lattice spacing, and t is a tunneling amplitude. This result is valid in the tight-binding limit, where electrons tunnel weakly between adjacent atoms. We will discuss the field theories appropriate for different fillings of the band. Ignore the electron spin.

It is convenient to work in the grand canonical ensemble. In practice, this means measuring the energy of an electron from the Fermi level, or the chemical potential μ at finite temperatures. The tight-binding Hamiltonian acts on the Wannier states $|x\rangle = |0\rangle$, $|\pm a\rangle$, $|\pm 2a\rangle \ldots$ as follows:

$$H|x\rangle = -\mu|x\rangle - t|x-a\rangle - t|x+a\rangle.$$

A state with lattice momentum (wavenumber) k is

$$|k\rangle = N^{-1/2}\sum_x e^{ikx}|x\rangle,$$

where N is the number of sites in the chain and $L = Na$ is its length. For periodic boundary conditions, the allowed lattice momenta are $k = 2\pi n/L$, where n is an integer. An arbitrary state $|\psi\rangle$ can be written in the Wannier basis:

$$|\psi\rangle = \sum_x c_x|x\rangle.$$

(a) At low electron concentrations, the chemical potential is at the bottom of the band, $\mu = -2t$, and low-energy states have momenta close to 0. Their Wannier coefficients $c_x = \langle x|k\rangle = N^{-1/2}e^{ikx}$ vary slowly with x. The same is true for any superposition of low-energy states. In this case, the discrete coefficients c_x can be well approximated by a smooth function, $c_x \approx \psi(x)$. The Hamiltonian $\mathcal{H}$ for this wavefunction can be obtained by expanding

$$\begin{aligned}\mathcal{H}\psi(x) &= \langle x|H|\psi\rangle = \langle x|H\sum_{x'}\psi(x')|x'\rangle = \langle x|\sum_{x'}\psi(x')\left(2t|x'\rangle - t|x'-a\rangle - t|x'+a\rangle\right)\\ &= 2t\psi(x) - t\psi(x+a) - t\psi(x-a).\end{aligned}$$

Expand ψ to the lowest nontrivial order to show that the effective Hamiltonian is that of a non-relativistic particle, $\mathcal{H} = -\hbar^2\partial_x^2/2m$.

(b) When the band is half-filled, $\mu = 0$, low-energy states are found near the Fermi momenta $k_R = \pi/2a$ and $k_L = -\pi/2a$. The Wannier coefficients c_x of the states $|k_R\rangle$ and $|k_L\rangle$ vary quickly, with a phase shift of $\pm\pi/2$ between adjacent sites, which means that they are not a smooth function of the coordinate. The same is true for other low-energy states nearby. We may nonetheless represent an arbitrary low-energy state $|\psi\rangle$ in terms of two smooth functions, $\psi_L(x)$ and $\psi_R(x)$:

$$|\psi\rangle = \sum_x \psi_R(x)e^{ik_Rx}|x\rangle + \psi_L(x)e^{ik_Lx}|x\rangle.$$

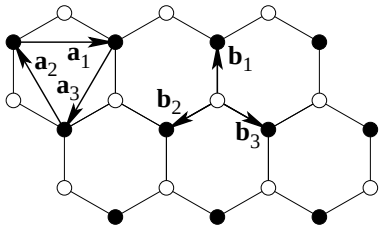
For example, $\psi_R(x) = N^{-1/2}$ and $\psi_L(x) = 0$ for $|k_R\rangle$. Use the same method as in part (a) to derive an effective Hamiltonian,

$$\mathcal{H}\begin{pmatrix}\psi_R\\ \psi_L\end{pmatrix} = \begin{pmatrix}-i\hbar c\,\partial_x & 0\\ 0 & i\hbar c\,\partial_x\end{pmatrix}\begin{pmatrix}\psi_R\\ \psi_L\end{pmatrix}.$$

The resulting energy-momentum relation is that of relativistic massless particles, $\varepsilon(p) = \pm pc$. What is the "speed of light" c?

(c) Still at half-filling, add a small perturbation in the form of a staggered potential, $+U$ on even sites and $-U$ on odd sites, or $Ue^{i\pi x/a}$. This wave has just the right wavenumber to scatter low-energy states near the right Fermi point into those near the left Fermi point, $k_R \to k_R - \pi/a = k_L$, and vice versa. Derive the new effective Hamiltonian and show that the particles acquire a mass, $\varepsilon(p) = \pm\sqrt{(mc^2)^2 + (pc)^2}$.

(d) Try a different perturbation, the Peierls distortion, in which atoms spontaneously shift alternatively left and right, so that the tunneling amplitude alternates between $t + \delta t$ and $t - \delta t$.



2. Electrons in graphene. Consider now atoms arranged in a honeycomb lattice, with lattice translations

$$\mathbf{a}_1 = (a, 0), \quad \mathbf{a}_2 = \left(-\frac{a}{2}, \frac{a\sqrt{3}}{2}\right), \quad \mathbf{a}_3 = \left(-\frac{a}{2}, -\frac{a\sqrt{3}}{2}\right).$$

It can be viewed as a superposition of two hexagonal sublattices, black and white. Nearest neighbors belong to different sublattices, with the shortest vectors connecting them

$$\mathbf{b}_1 = \left(0, \frac{a}{\sqrt{3}}\right), \quad \mathbf{b}_2 = \left(-\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right), \quad \mathbf{b}_3 = \left(-\frac{a}{2}, \frac{a}{2\sqrt{3}}\right).$$

The tight-binding Hamiltonian acts as follows:

$$H|\mathbf{r}, \circ\rangle = -t\sum_{i=1}^{3} |\mathbf{r} + \mathbf{b}_i, \bullet\rangle, \quad H|\mathbf{r}, \bullet\rangle = -t\sum_{i=1}^{3} |\mathbf{r} - \mathbf{b}_i, \circ\rangle.$$

(a) Show that this Hamiltonian has two energy bands symmetrically located around zero:

$$\varepsilon(\mathbf{k}) = \pm t \left| \sum_{i=1}^{3} \exp\left(i\mathbf{k}\cdot\mathbf{b}_i\right) \right|.$$

Thus at half-filling, the lower band is occupied, the upper band is empty, and the chemical potential $\mu = 0$. Examine the dispersions in your favorite plotting program.

(b) The two bands connect at two special wavevectors, $\mathbf{K} = (4\pi/3a, 0)$ and $-\mathbf{K}$, with the electron energies $\varepsilon(\mathbf{K}) = \varepsilon(-\mathbf{K}) = 0$. Low-energy electrons live near these "Dirac points." Because lattice momentum $\mathbf{K}$ is quite large, the Wannier coefficients of the states $|\mathbf{K}\rangle$ and $|-\mathbf{K}\rangle$ do not vary smoothly in space. Low-energy states can be parametrized in terms of $4 = 2 \times 2$ smooth wavefunctions (2 for each sublattice and 2 for each Dirac point):

$$|\psi\rangle = \sum_{\mathbf{r}\in\circ} \left[\psi_1(\mathbf{r})e^{i\mathbf{K}\cdot\mathbf{r}} + \psi_2(\mathbf{r})e^{-i\mathbf{K}\cdot\mathbf{r}}\right] |\mathbf{r}, \circ\rangle + \sum_{\mathbf{r}\in\bullet} \left[\psi_3(\mathbf{r})e^{i\mathbf{K}\cdot\mathbf{r}} + \psi_4(\mathbf{r})e^{-i\mathbf{K}\cdot\mathbf{r}}\right] |\mathbf{r}, \bullet\rangle.$$

Obtain an effective Hamiltonian for the 4-component vector $\psi_n(\mathbf{r})$ along the lines of Problem 1(b) and show that the resulting energy spectrum is $\varepsilon(p) = \pm cp$.