8.231 Physics of Solids I — Fall 2017
Problem Set 6

Posted: Tuesday, Oct 17, 2017
***Due:* Tuesday, Oct 24, 2017**

Readings (Optional)

- A. C. Bleszynski-Jayich, W. E. Shanks, B. Peaudecerf, E. Ginossar, F. von Oppen, L. Glazman, and J. G. E. Harris, "Persistent Currents in Normal Metal Rings". *Science*. **326**, 272 (2009).

Note: Bonus problems are more challenging. It is fine you do not solve them. By solving them you can earn extra credits.

Problem 1

Nearly Free Electron Approximation in Two Dimensions

Consider an electron in a two-dimensional square lattice with lattice constant a. There is a weak periodic potential given by

$$U = -V_0 \left[\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right) \right]. \tag{1}$$

(a) In the small V_0 limit, solve the Schrödinger equation using nearly free electron approximation to calculate the energy $E(\mathbf{k})$ of the *lowest* energy band at the following $\mathbf{k} = (k_x, k_y)$ points: $(0,0)$, $(\pi/a, 0)$, $(0, \pi/a)$ and $(\pi/a, \pi/a)$. You only need to find $E(k)$ up to first order in V_0.

(b) Sketch a set of constant energy contours for the bands you obtained at $E = E_0/4$, $E_0/2$, $3E_0/4$, and E_0 where $E_0 \equiv \hbar^2\pi^2/(ma^2)$ for

1. Free electron (i.e. $V_0 = 0$);
2. Weak periodic potential (i.e. small V_0).

Note that energy contours should lie inside the Brillouin zone defined by $|k_x| < \pi/a$ and $|k_y| < \pi/a$.

Problem 2

Twisted Boundary Conditions

According to Bloch's theorem, the wavefunction of an electron moving in a periodic potential is of the form $|\psi_{\mathbf{k}}(\mathbf{r})\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} |u_{\mathbf{k}}(\mathbf{r})\rangle$, where $|u_{\mathbf{k}}(\mathbf{r})\rangle$ is periodic both in the unit cell and in $\mathbf{k}$. When counting the possible k-states, we usually assume periodic boundary condition (PBC): $|\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{L})\rangle = |\psi_{\mathbf{k}}(\mathbf{r})\rangle$. In this way,

$$e^{i\mathbf{k}\cdot\mathbf{L}} = 1 \Leftrightarrow \mathbf{k} = 2\pi \sum_{i=1}^{d} \frac{n_i}{L_i}\mathbf{a}_i,\ 0 \le n_i < L_i. \tag{2}$$

In general, the boundary condition can be twisted instead of periodic:

$$|\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{L})\rangle = e^{i\theta} |\psi_{\mathbf{k}}(\mathbf{r})\rangle . \tag{3}$$

Experimentally, these boundary conditions can be realized by threading the magnetic flux as a consequence of the Aharonov-Bohm effect (c.f. the optional reading material above).

In this problem, we study the consequences of anti-periodic boundary condition (APBC) when $\theta = \pi$ in Eq. (3). To be concrete, we consider a one-dimensional system whose energy dispersion is

$$E(k) = -\sqrt{A + B\cos(k)}. \tag{4}$$

Here $A > B > 0$. The first Brillouin zone is $k \in [-\pi, \pi]$. The spacing between the unit cell is taken to be $a = 1$ for convenience. (This is in fact the polyacetylene you have already computed in Problem 2 of Problem Set 4.) Assume there are L unit cells in total. For simplicity, assume there is no spin degeneracy so that each k-state can only admit one electron.

(a) What are the possible k values under APBC? Notice here $k \in [-\pi, \pi]$.

(b) Numerically compute the total energy difference per unit cell between PBC and APBC:

$$\Delta E \equiv \frac{1}{L} \left[\sum_{k \in \text{APBC } k\text{-states}} E(k) - \sum_{k \in \text{PBC } k\text{-states}} E(k) \right], \tag{5}$$

for

- Insulators, i.e., fully-filled band (#electrons $= L$).
- Metals, e.g. half-filled band (#electrons $= L/2$, you may assume L is even).

Show that ΔE decays exponentially with L for insulators and decays in power law for metals. This can be regarded as the "theorists' definitions" of insulators and metals.

(Hint: To show exponential decay, you may use semi-log plot. To show power law decay, you may use log-log plot.)

(c) (Bonus) Analytically prove the power law decay for metals, with whatever approximations you need as long as they are justified.

(d) (Bonus) Analytically prove the exponential decay for insulators, with whatever approximations you need as long as they are justified.

(Hint: Poisson summation formula may be useful:

$$\sum_{n=-\infty}^{\infty} \delta(x - nT) = \frac{1}{T} \sum_{k=-\infty}^{\infty} e^{2\pi i k x / T}. \tag{6}$$

Some knowledge of complex analysis may also be helpful.)