PHYS*4150: Problem Set 5

Distributed: Friday March 15, 2019
Due: Friday March 29, 2019 at 10:30am

Problem 1 (10 pts): Weak periodic potential in 1D

For electron confined to one dimension, consider the application of a weak periodic potential given by the following series:

$$V(x) = V_1 \cos\frac{2\pi}{a}x + V_2 \cos\frac{4\pi}{a}x + V_3 \cos\frac{6\pi}{a}x + ... \tag{1}$$

Calculate the band gap at:

a) $k = \pi/a$ (Brillouin Zone boundary), between the first and second bands.

b) $k = 0$ (Brillouin Zone centre), between the second and third bands.

c) $k = -\pi/a$ (Brillouin Zone boundary), between the third and fourth bands.

Sketch the results on a reduced zone diagram (i.e. first Brillouin Zone).

Problem 2 (20 pts): Fermi surface in the NFEM

Consider a nearly free electron band and investigate the constant energy surface of $\varepsilon = 2.60\,\text{eV}$ above the bottom of the band. Suppose a Brillouin Zone face (Bragg plane) is normal to the $x-$direction at $\frac{1}{2}|\vec{\mathbf{G}}| = k_x = 0.78 \times 10^{10}\,\text{m}^{-1}$ and the band gap between the first and second bands is $0.150\,\text{eV}$ at that point. Assume the band gap is the result of a single Fourier component ($V_{\vec{\mathbf{G}}}$) of the weak potential $V(\mathbf{R})$.

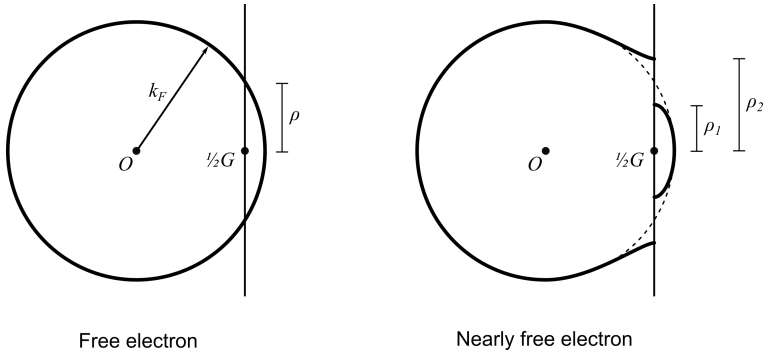

Figure 1: Constant energy surface in FEM and NFEM.

a) First assume the electron are absolutely free (FEM). Calculate the radius k_F of the constant energy sphere ($\varepsilon_F = 2.60\,\text{eV}$).

b) The intersection of this sphere with the Bragg plane forms a circle. Calculate the radius of this circle.

c) The weak potential $V(\mathbf{R})$ distorts the constant energy surface so it is no longer spherical. However, the intersection of the surface with the Bragg plane is still circular for each band. Find the radii of the two circles.

d) For what value of $V_{\vec{\mathbf{G}}}$ does the second band surface disappear?

Problem 3 (20 pts): Tight-binding model

For a tight-binding model that assumes that electrons can hop around a two-dimensional square lattice (with lattice constant a), if the electrons can only hop between nearest-neighbour sites, the energy dispersion relation is found to be:

$$\epsilon_{\mathbf{k}} = -2t\left[\cos k_x a + \cos k_y a\right], \tag{2}$$

where t is the hopping energy.

a) Plot the band structure in the first Brillouin Zone for the *lowest band only* along the path $\Gamma \to \mathrm{X} \to \mathrm{M} \to \Gamma$.

b) Plot the Fermi surface for $\epsilon_F = t$. This is equivalent to plotting the constant-energy surface $\epsilon = \epsilon_F$ where the energy is given by Eq. 2.

c) Find the general expression for the electron velocity in the $\Gamma \to \mathrm{M}$ direction. Evaluate it's magnitude and direction for an electron on the Fermi surface ($\epsilon_F = t$).

d) Explore how the Fermi surface changes as a function of changing ϵ_F. Plot the Fermi surface for value of $\epsilon_F = -3t$, $-t$, 0, t and $3t$.

Problem 4 (35 pts): Vibrations in a square lattice

Consider a two-dimensional square lattice as shown in Figure 2. This problem will explore *transverse* vibrational modes of this lattice, i.e. vibrations for which the atomic motion is perpendicular to the atomic plane.

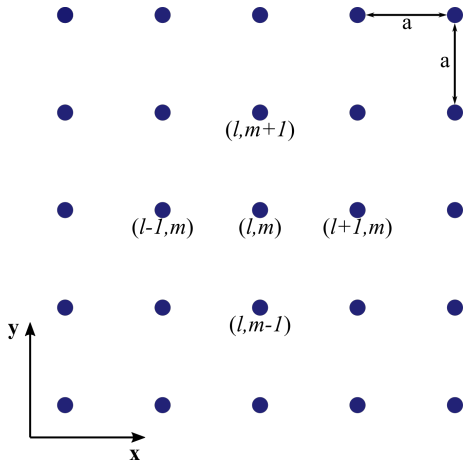

Figure 2: 2D square lattice showing points near atom l, m.

The lattice has N rows and N columns of identical atoms at positions given by $\mathbf{R} = la\hat{x} + ma\hat{y}$, where a is the lattice constant (and distance between nearest neighbour atoms), and l, m are integers. Let $u_{l,m}$ denote the displacement of atom l, m in the direction normal to the lattice plane. Assume each atom has mass M, and the force constant between nearest neighbours is K.

a) Construct an expression for the harmonic potential energy U^{harm} starting from A&M equation 22.9:

$$U^{harm} = \frac{1}{4} \sum_{\mathbf{R},\mathbf{R}'} \sum_{\mu,\nu=x,y,z} \left[u_\mu(\mathbf{R}) - u_\mu(\mathbf{R}')\right] \phi_{\mu,\nu}(\mathbf{R} - \mathbf{R}') \left[u_\nu(\mathbf{R}) - u_\nu(\mathbf{R}')\right], \tag{3}$$

$$\phi_{\mu,\nu}(r) = \frac{\partial^2 \phi(r)}{\partial r_\mu \partial r_\nu}. \tag{4}$$

b) Show that the equation of motion for this system is given by:

$$M\ddot{u}_{l,m} = K\left[(u_{l+1,m} + u_{l-1,m} - 2u_{l,m}) + (u_{l,m+1} + u_{l,m-1} - 2u_{l,m})\right]. \tag{5}$$

To do this, use the expression:

$$M\ddot{u}_{l,m} = -\frac{\partial U^{harm}}{\partial u_{l,m}}. \tag{6}$$

Convince yourself that this is just a generalized form of Newton's force law: $F = ma$.

c) Identify each force term on the right of Eq. 5, i.e., if you started simply from Newton's law what is the source of each force. Be careful to note the direction of each force.

d) Assume solutions of the form $u_{l,m} \propto \exp\{\mathrm{i}(k_x la + k_y ma - \omega t)\}$ to show that the dispersion relation for this system is:

$$M\omega^2 = 2K(2 - \cos k_x a - \cos k_y a). \tag{7}$$

e) Show that the region of **k**-space for which independent solutions exist may be taken as a square with side $2\pi/a$, which is the first Brillouin Zone of the square lattice.

f) Sketch separately the dispersion curves ω vs **k** along the directions [1,0] (i.e. $k = k_x$, $k_y = 0$), and [1,1] (i.e. $k_x = k_y$), up to the first Brillouin Zone boundary.

g) For $ka << 1$, show

$$\omega = \sqrt{\frac{K}{M}} a(k_x^2 + k_y^2)^{1/2} = \sqrt{\frac{K}{M}} ka. \tag{8}$$

Notice that this result shows that in the limit $ka << 1$, the phase velocity ($v_p = \omega/k$) is equal to the group velocity ($v_g = \frac{\partial \omega}{\partial k}$).