PHYSICS 152B/232
Spring 2017
Homework Assignment #2 Solutions

[1] Consider a tight-binding model of monovalent atoms on a two-dimensional rectangular lattice with primitive direct lattice vectors $\boldsymbol{a}_1 = a_x\,\hat{\boldsymbol{x}}$ and $\boldsymbol{a}_2 = a_y\,\hat{\boldsymbol{y}}$ and hopping integrals $t_{x,y}$.

(a) Assuming $a_x > a_y$, which of $t_{x,y}$ do you expect to be largest? Why?

(b) Find the dispersion relation $E(\boldsymbol{k})$.

(c) Sketch the Fermi surface within the Brillouin zone.

Solution :

(a) The hopping integrals are due to the overlaps of exponentially localized atomic wavefunctions. Therefore $a_x > a_y$ entails $t_x < t_y$.

(b) The dispersion is

$$E(k_x, k_y) = -2t_x\cos(k_x a_x) - 2t_y\cos(k_y a_y) \quad .$$

(c) See Fig. 1. Define the energies $B \equiv 2t_x + 2t_y$ and $\Delta \equiv -2t_x + 2t_y$, which are both positive. Then for $E(\boldsymbol{k}) \in (-B, -\Delta)$, the equal energy surfaces are closed contractable ellipse-like curves shown in blue. For $E(\boldsymbol{k}) \in (\Delta, B)$, the Fermi surfaces are closed ellipse-like curves shown in red. Recall that the Brillouin zone is topologically a torus, so the red curves are indeed closed and contractable. The solid and dashed black curves, respectively, lie at energies $\mp\Delta$. For monovalent atoms, there is one electron per cell, and by symmetry the Fermi energy lies at $\varepsilon_{\rm F} = 0$, and therefore resembles one of the green curves which are closed but not contractable since they wind around the Brillouin zone torus.

[2] Consider the one-dimensional Bloch oscillations discussed in §1.6.3 of the Lecture Notes. Setting $k(0) = 0$, show that a Taylor expansion of the motion $x(t)$ agrees with the ballistic result to order t^2, if the ballistic mass is taken to be the effective mass m^* at $k = 0$.

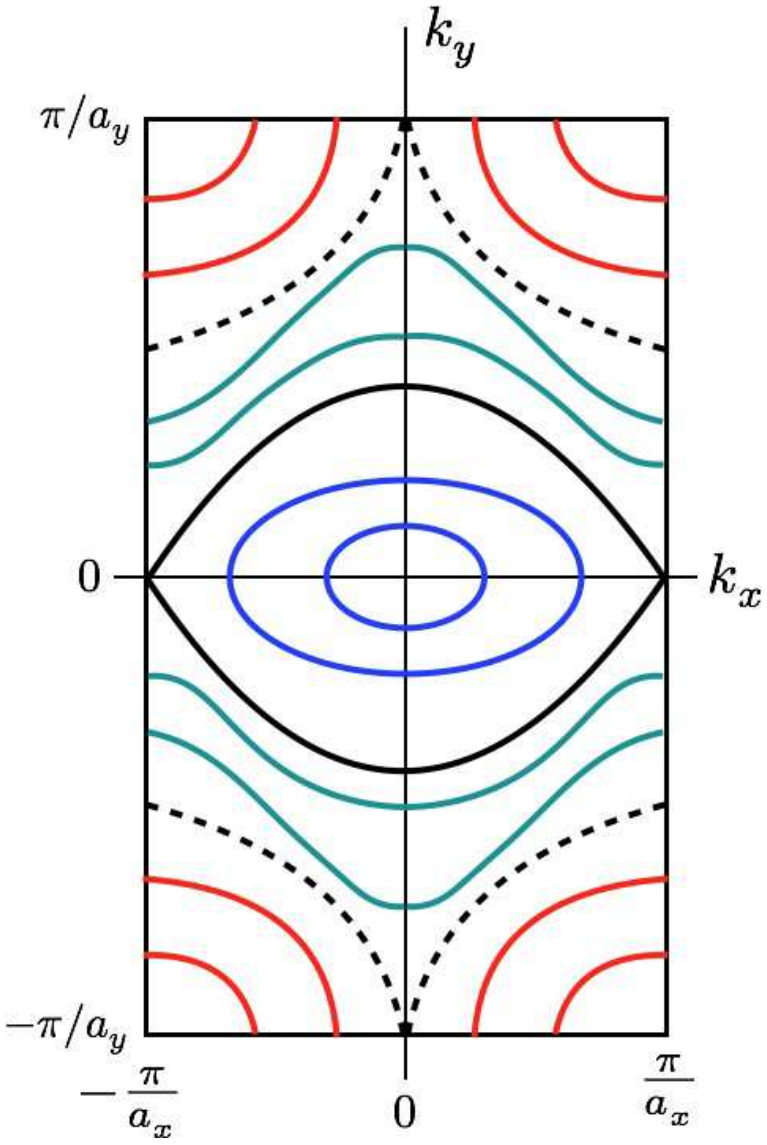

Figure 1: Equal energy surfaces for the function $E(k_x, k_y)$ in problem 1. The Fermi surface is topologically among the family of green curves. See text for description.

Solution :

According to §1.6.3 of the Lecture Notes, if $E(k) = -2\beta\cos(ka)$, and setting $k(0) = 0$, the motion of a Bloch wavepacket is given by

$$x(t) = x(0) - \frac{2\beta}{eE}\left[\cos\left(\frac{eaEt}{\hbar}\right) - 1\right] = \frac{\beta eEa^2t^2}{\hbar^2} = \frac{F}{2m^*}\,t^2 \quad ,$$

with $F = -eE$ the force on the electron. The relation between β and m^* is obtained from $E(k) = -2\beta + \beta a^2k^2 + \mathcal{O}(k^4)$, whence we identify $\beta = \hbar^2/2m^*a^2$.

[**3**] Make a sketch of the extended Brillouin zones like in Fig. 2.2 of the Lecture Notes, but for the triangular lattice. Then make plots the free electron Fermi surface for valences $Z = 2$ and $Z = 3$, such as in Fig. 2.3.

Solution :

See Fig. 2. For $Z = 2$ the free electron Fermi sphere extends into the second Brillouin zone, and for $Z = 3$ it extends into the third Brillouin zone!

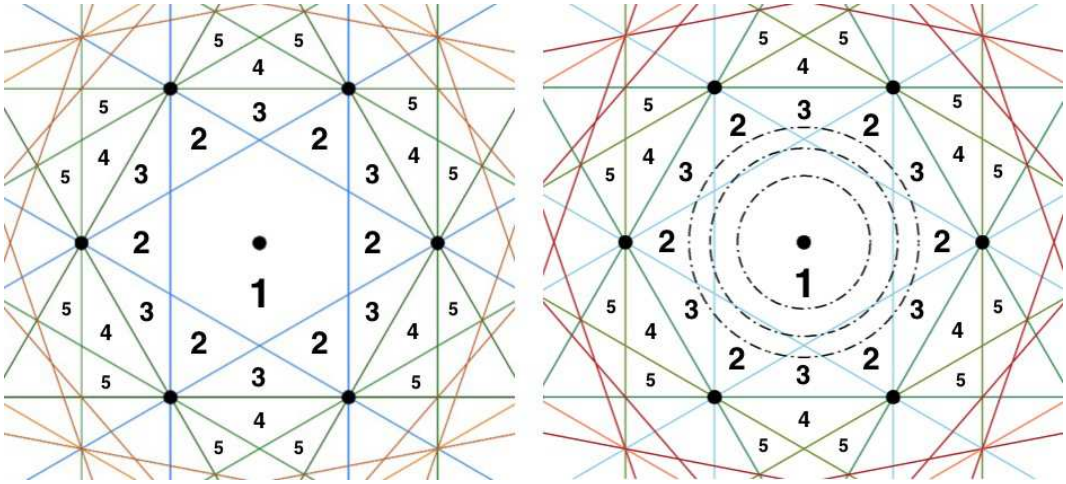

Figure 2: Left: Brillouin zones for the triangular lattice structure. Right: The concentric circles correspond to electron fillings of $Z = 1$, $Z = 2$, and $Z = 3$ per unit cell.

[**4**] Suppose, in the vicinity of the Γ point for some material, the electron dispersion is of the form $E(\boldsymbol{k}) = \frac{1}{2}(m^*)^{-1}_{\mu\nu}\, k^\mu\, k^\nu$, where m^* is the effective mass tensor. Find an expression for the low-temperature molar heat capacity in terms of density n and temperature T. Your expression should involve the tensor m^* in some way.

Solution :

The heat capacity is $C_V = V\gamma T$, where $\gamma = \frac{1}{3}\pi^2 k_{\rm B}^2\, g(\varepsilon_{\rm F})$. The density of states at the Fermi energy is $g(\varepsilon_{\rm F}) = mk_{\rm F}/\pi^2\hbar^2$ for free electrons (spin degeneracy included). For a general quadratic dispersion, we can choose our Cartesian axes to align with the principal axes of the effective mass tensor $m^*_{\alpha\beta}$. These axes are necessarily orthogonal because the effective mass tensor is symmetric. Along principal axes, the conduction band dispersion is given by $E(\boldsymbol{k}) = \frac{\hbar^2 k_x^2}{2m_x^*} + \frac{\hbar^2 k_y^2}{2m_y^*} + \frac{\hbar^2 k_z^2}{2m_z^*}$, and we may rescale each k_α in the DOS integral by $\sqrt{m^*_\alpha}$, yielding

$$g(\varepsilon_{\rm F}) = \frac{\det{}^{1/3}(m^*)\,(3\pi^2 n)^{1/3}}{\pi^2\hbar^2} \quad .$$