Assignment 6: Solution

1. In class, we derived the relationship $v_k = \frac{V_k}{N}$ where v_k is the volume of a point in k-space, V_k is the volume of the first Brillouin zone and N is the total number of unit cells in the solid's volume. Show that v_k is also equal to $\frac{(2\pi)^3}{\Omega}$ where Ω is the volume of the unit cell in direct space. Hence the number of k points in the first Brillouin zone (FBZ) does not change by the imposition of a periodic potential.

   Solution:

   We know that the value of the FBZ is

$$\mathrm{V}_k = \vec{a}^* \cdot \vec{b}^* \times \vec{c}^*. \tag{1}$$

$$\begin{aligned} \vec{a}^* &= \frac{2\pi}{\Omega}\vec{b} \times \vec{c} \\ \vec{b}^* &= \frac{2\pi}{\Omega}\vec{c} \times \vec{a} \\ \vec{c}^* &= \frac{2\pi}{\Omega}\vec{a} \times \vec{b} \end{aligned} \tag{2}$$

   where, $\Omega = \vec{a} \cdot \vec{b} \times \vec{c}.$

   Solving for V_k

$$\vec{a}^* \cdot \vec{b}^* \times \vec{c}^* = \frac{(2\pi)^3}{\Omega^3}(\vec{b} \times \vec{c}) \cdot ((\vec{c} \times \vec{a}) \times (\vec{a} \times \vec{b})) \tag{3}$$

   Let's say $(\vec{c} \times \vec{a}) = \vec{F}$ and use the vector identity $\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B})$,

to show

$$\begin{aligned}(\vec{c}\times\vec{a})\times(\vec{a}\times\vec{b}) &= \vec{F}\times(\vec{a}\times\vec{b}) \\ &= \vec{a}(\vec{F}\cdot\vec{b}) - \vec{b}(\vec{F}\cdot\vec{a}) \\ &= \vec{a}((\vec{c}\times\vec{a})\cdot\vec{b}) - \vec{b}((\vec{c}\times\vec{a})\cdot\vec{a})\end{aligned} \tag{4}$$

The second term in the last expression is zero giving,

$$\begin{aligned}(\vec{c}\times\vec{a})\times(\vec{a}\times\vec{b}) &= \vec{F}\times(\vec{a}\times\vec{b}) \\ &= \vec{a}(\vec{a}\cdot\vec{b}\times\vec{c}) \\ &= \vec{a}((\vec{c}\times\vec{a}).\vec{b}) \\ &= \Omega\vec{a}\end{aligned} \tag{5}$$

Therefore Equation 2 becomes,

$$\begin{aligned}V_k &= \frac{(2\pi)^3}{\Omega^3}(\vec{b}\times\vec{c})\cdot(\Omega\vec{a}) \\ &= \frac{(2\pi)^3}{\Omega^2}\Omega \\ &= \frac{(2\pi)^3}{\Omega}\end{aligned} \tag{6}$$

Now V_k is equal to value of the first BZ and Ω is equal to volume of the unit cell in the direct space. Thus we get

$$\begin{aligned}\mathrm{v}_k &= \frac{\mathrm{V}_k}{N} \\ &= \frac{(2\pi)^3}{N\Omega}\end{aligned} \tag{7}$$

$$\mathrm{v}_k = \frac{(2\pi)^3}{\mathrm{V}_{\mathrm{solid}}} \tag{8}$$

The volume of a k-point is $(2\pi)^3/\mathrm{V}_{solid}$. The periodic potential does not change the structure of the k-point.

2. Show that for a Bloch function in 1D

$$\psi_{kn}(x) = e^{ikx}u_{kn}(x), \tag{9}$$

the following Schrodinger equation holds for u_{kn}:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\hbar}{m}kp_x + V(x)\right]u_{kn}(x) = \left(\varepsilon_n(k) - \frac{\hbar^2k^2}{2m}\right)u_{kn}(x). \tag{10}$$

Solution:

One dimensional Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{kn}(x) + V(x)\psi_{kn}(x) = \varepsilon_n(k)\psi_{kn}(x). \tag{11}$$

Substituting ψ_{kn} from equation (8),

$$\begin{aligned}\varepsilon_n(k)e^{ikx}u_{kn} &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}(e^{ikx}u_{kn}) + V(e^{ikx}u_{kn}),\\ &= -\frac{\hbar^2}{2m}\frac{d}{dx}\left(e^{ikx}\frac{d}{dx}u_{kn} + ike^{ikx}u_{kn}\right) + V(e^{ikx}u_{kn}),\end{aligned}$$

$$\begin{aligned}\varepsilon_n(k)e^{ikx}u_{kn} &= -\frac{\hbar^2}{2m}\left(e^{ikx}\frac{d^2}{dx^2}u_{kn} + ike^{ikx}\frac{d}{dx}u_{kn} + ike^{ikx}\frac{d}{dx}u_{kn} - k^2e^{ikx}u_{kn}\right) \\ &\quad + V(e^{ikx}u_{kn}), \\ &= -\frac{\hbar^2}{2m}\left(e^{ikx}\frac{d^2}{dx^2}u_{kn} + i2ke^{ikx}\frac{d}{dx}u_{kn} - k^2e^{ikx}u_{kn}\right) + Ve^{ikx}u_{kn}, \\ &= \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u_{kn} + \frac{\hbar}{m}k(-i\hbar\frac{d}{dx})u_{kn} + \frac{\hbar^2k^2}{2m}u_{kn} + Vu_{kn}\right]e^{ikx}.\end{aligned}$$

Using definition of momentum operator along x, $p_x = -i\hbar\frac{d}{dx}$, we obtain

$$\varepsilon_n(k)u_{kn} = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u_{kn} + \frac{\hbar}{m}kp_xu_{kn} + \frac{\hbar^2k^2}{2m}u_{kn} + Vu_{kn}\right] \tag{12}$$

Upon the arranging this given the desired form of the Schrodinger equation for the periodic function $u_{kn}(x)$:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\hbar}{m}kp_x + V(x)\right]u_{kn}(x) = \left(\varepsilon_n(k) - \frac{\hbar^2k^2}{2m}\right)u_{kn}(x). \tag{13}$$

3. Consider a simple cubic lattice of a monovalent element. What is the radius of the Fermi sphere k_F relative to the size of the first Brillouin zone (FBZ), k_i? Will distortion of the spherical Fermi surface occur?

   Solution:

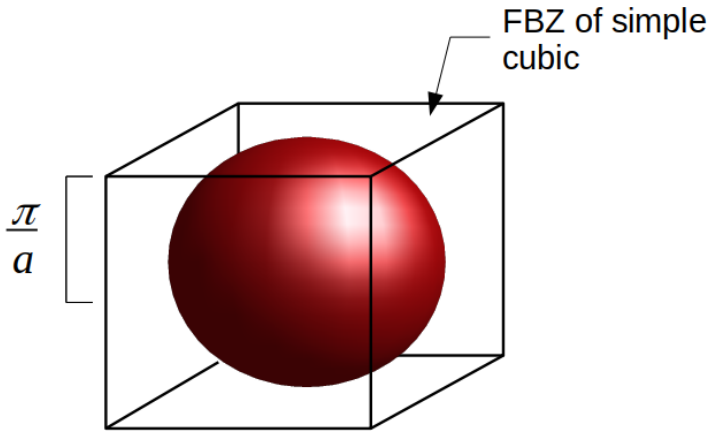
   The reciprocal lattice of a simple cubic lattice is also cubic with edge length $2\pi/a$. The minimum distance from the origin $(k_x, k_y, k_z) = 0$ to the nearest zone boundary

is π/a. Let $k_i = \pi/a$.

As $k_F = (3\pi^2 n)^{1/3}$ and $n = 1/a^3$, we have

$$\begin{aligned} \frac{k_F}{k_i} &= \left(\frac{3\pi^2}{a^3}\right)^{1/3} \frac{a}{\pi} \\ &= \left(\frac{3}{\pi}\right)^{1/3} = 0.9848. \end{aligned} \tag{14}$$

Yes, distortion of the spherical Fermi surface occur because the Fermi surface is close upto 98% to the boundaries. The diagram below shows the relation of the FBZ (cube) and the Fermi sphere is approximately shown below.



4. Consider a BCC monovalent metal. It's primitive lattice vectors are

$$\begin{aligned} \vec{a} &= \frac{a}{2}(1, 1, -1) \\ \vec{b} &= \frac{a}{2}(-1, 1, 1) \\ \vec{c} &= \frac{a}{2}(1, -1, 1) \end{aligned} \tag{15}$$

where $(1, 1, -1)$ represents the vector $\hat{i} + \hat{j} - \hat{k}$ and so on.

(a) Show that the reciprocal lattice vectors are:

$$\begin{aligned} \vec{a^*} &= \frac{2\pi}{a}(1, 1, 0) \\ \vec{b^*} &= \frac{2\pi}{a}(0, 1, 1) \\ \vec{c^*} &= \frac{2\pi}{a}(1, 0, 1). \end{aligned} \tag{16}$$

Solution:

Take $\vec{a}, \vec{b}, \vec{c}$, as the direct lattice primitive basis vectors of the face centered cubic lattice, which are:

$$\begin{aligned} \vec{a} &= \frac{a}{2}(1, 1, -1) \\ \vec{b} &= \frac{a}{2}(-1, 1, 1) \\ \vec{c} &= \frac{a}{2}(1, -1, 1) \end{aligned} \tag{17}$$

Take $\vec{a}^*, \vec{b}^*, \vec{c}^*$, as the basis vectors in reciprocal space. To find these basis vectors we can use the following equations with $\Omega = \vec{a}.\vec{b} \times \vec{c}$

$$\begin{aligned} \vec{a^*} &= 2\pi \frac{\vec{b} \times \vec{c}}{\Omega} \\ \vec{b^*} &= 2\pi \frac{\vec{c} \times \vec{a}}{\Omega} \\ \vec{c^*} &= 2\pi \frac{\vec{a} \times \vec{b}}{\Omega} \end{aligned} \tag{18}$$

Now,

$$\vec{a}.(\vec{b}\times\vec{c}) = \frac{a^3}{8}\begin{vmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^3}{4}. \tag{19}$$

$$\vec{a^*} = \frac{8\pi}{a^3}.\frac{a^2}{4}\begin{vmatrix} \hat{i} & \hat{k} & \hat{k} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{2\pi}{a}(1,1,0) \tag{20}$$

Similarly,

$$\begin{aligned} \vec{b^*} &= \frac{2\pi}{a}(0,1,1) \\ \vec{c^*} &= \frac{2\pi}{a}(1,0,1) \end{aligned} \tag{21}$$

These vectors define a primitive cell in the reciprocal space, indicating an FCC reciprocal lattice.

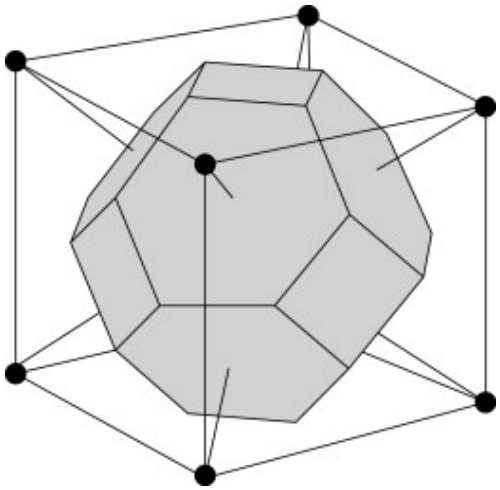
(b) Construct the first Brillouin zone and show that a dodecahedron (with 12 sides) is formed. Where are the 12 planes in terms of k_x, k_y and k_z?

Solution:

We construct a Wigner Seitz cell. The boundary planes bisect $\pm\vec{a^*}, \pm\vec{b^*}, \pm\vec{c^*}$ at $(k_x, k_y, k_z) = (\pm1, \pm1, 0), (\pm1, 0, \pm1), (0, \pm1, \pm1)$. These are 12 planes.

(c) What is the minimum distance from the origin of the k-space to the nearest zone boundary? Show that the distance is $k_i = \frac{\sqrt{2}\pi}{a}$.

Solution:



The minimum distance of any one such plane (e.g. $(\pm 1, \pm 1, 0) = (k_x, k_y, k_z)$) from the origin is

$$k_i = \frac{\pi}{a}\sqrt{(\pm 1)^2 + (\pm 1)^2} = \frac{\pi\sqrt{2}}{a}. \tag{22}$$

(d) What is the number of electrons per unit volume (n)? Find $k_F = (3\pi^2 n)^{\frac{1}{3}}$ where k_F shows the size of the Fermi sphere.

Solution:

For body centered cubic lattice, we have two atoms per unit cell (one electron per unit cell). So,

$$n = \frac{2}{a^3}. \tag{23}$$

$$\begin{aligned} k_F &= (3\pi^2 n)^{\frac{1}{3}} \\ &= \left(3\pi^2 \frac{2}{a^3}\right)^{\frac{1}{3}} = \frac{(6\pi^2)^{\frac{1}{3}}}{a} \end{aligned} \tag{24}$$

(e) Find $\frac{k_F}{k_i}$. How far or close to the zone boundaries does the Fermi surface extend?

Solution:

From part (c) and (d),

$$\begin{aligned}\frac{k_F}{k_i} &= \frac{(6\pi^2)^{\frac{1}{3}}/a}{\pi\sqrt{2}/a} \\ &= \frac{(6\pi^2)^{\frac{1}{3}}}{\pi\sqrt{2}} \\ &= \left(\frac{6\pi^2}{\pi^3}\right)^{\frac{1}{3}} \frac{1}{\sqrt{2}} \\ &= \left(\frac{6}{\pi}\right)^{\frac{1}{3}} \frac{1}{\sqrt{2}} = 0.88\end{aligned} \tag{25}$$

So, the Fermi surface extents to about 88% of the zone boundaries.

(f) Repeat all the above calculations for a monovalent FCC metal. Which of the FCC or BCC lattices is more likely to have a distorted Fermi sphere?

Solution:

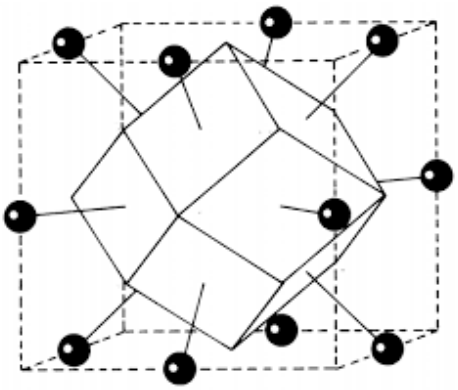
Primitive lattice vectors of FCC lattice are

$$\begin{aligned}\vec{a} &= \frac{a}{2}(0,1,1) \\ \vec{b} &= \frac{a}{2}(1,0,1) \\ \vec{c} &= \frac{a}{2}(1,1,0)\end{aligned} \tag{26}$$

And reciprocal lattice vector are

$$\begin{aligned}\vec{a^*} &= \frac{2\pi}{a}(-1,1,1)\\ \vec{b^*} &= \frac{2\pi}{a}(1,-1,1)\\ \vec{c^*} &= \frac{2\pi}{a}(1,1,-1).\end{aligned} \tag{27}$$

The boundary planes bisect $\pm\vec{a}^*, \pm\vec{b}^*, \pm\vec{c}^*$ at $(k_x, k_y, k_z) = (\pm 1, \pm 1, \pm 1)$.



The Minimum distance of any one such plane from the origin is

$$k_i = \frac{\pi}{a}\sqrt{(\pm 1)^2 + (\pm 1)^2 + (\pm 1)^2} = \frac{\pi\sqrt{3}}{a}. \tag{28}$$

For face centered cubic lattice, we have four monovalent atoms per unit cell (four electrons per unit cell). So,

$$n = \frac{4}{a^3}. \tag{29}$$

$$\begin{aligned} k_F &= (3\pi^2 n)^{\frac{1}{3}} \\ &= \left(3\pi^2 \frac{4}{a^3}\right)^{\frac{1}{3}} = \frac{(12\pi^2)^{\frac{1}{3}}}{a} \end{aligned} \tag{30}$$

From equation (26) and (28),

$$\begin{aligned} \frac{k_F}{k_i} &= \frac{(12\pi^2)^{\frac{1}{3}}/a}{\pi\sqrt{3}/a} \\ &= \frac{(12\pi^2)^{\frac{1}{3}}}{\pi\sqrt{3}} \\ &= \left(\frac{12\pi^2}{\pi^3}\right)^{\frac{1}{3}} \frac{1}{\sqrt{3}} \\ &= \left(\frac{12}{\pi}\right)^{\frac{1}{3}} \frac{1}{\sqrt{3}} = 0.903 \end{aligned} \tag{31}$$

So, the Fermi surface extents to about 90.3% of the zone boundaries.

Fermi surface for FCC monovalent extends more toward boundaries than BCC so it will undergo a greater degree of distortion.