Exercise 2.1

Speed of electrons. Estimate the average random speed of an electron gas in a semiconductor at 300 K.

Note: The free electron mass $m_e = 9.10938356 \times 10^{-31}$ kg.

Solution

According to the kinetic theory of gas, the average kinetic energy of an electron is $\frac{3}{2}k_BT$, which also equals to $\frac{1}{2}m_e\overline{v}^2$. This leads to

$$\overline{v} = \sqrt{\frac{3k_BT}{m_e}} = \sqrt{\frac{3 \times 1.38064852 \times 10^{-23} \times 300}{9.10938356 \times 10^{-31}}} \approx 116793\,\mathrm{m/s}.$$

Exercise 2.2

*Transmission electron microscope.*Electron beams are used to study the atomic structure of crystals, as in the transmission electron microscope (TEM). The resolution of the microscope depends on the energy of the electrons, which determines the corresponding wavelength of the electrons. The minimum focal point of the electron beam depends on its wavelength. Determine the electron wavelength if they have an energy of:

a) 100 keV

b) 1 MeV

Solution

For a material wave, the de Broglie wavelength is the wavelength, , associated with a massive particle (i.e., a particle with mass, as opposed to a massless particle) and is related to its momentum, p by the following relation:

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

Further, energy of particle with mass m(for electron $m = 9.1 \times 10^{-31} kg$) moving with speed v, is given by:

$$E = \frac{p^2}{2m}$$

$$p = \sqrt{2mE}$$

$$\lambda = \frac{h}{\sqrt{2mE}}$$

The wavelength is inversely proportional to the square-root of the particle energy. It can be calculated that the wavelength corresponding to an electron with 1 eV energy is 1.228 nm.

a) for 100 keV

$$\lambda = \frac{1.288\ nm}{\sqrt{10^5}} = 3.883\ pm$$

b) for 1 MeV

$$\lambda = \frac{1.288\ nm}{\sqrt{10^6}} = 1.228\ pm$$

Exercise 2.3

Electron energy states in a potential wire. Determine (a)the energy levels of an electron in a two-dimensional square box of length D, assuming an infinitely high potential barrier around the box, (b) the allowable energy levels for D = 5 nm, and (c) the degeneracy of the first four energy levels.

Solution

Similar to 1-D potential well in L4, we can use separation of variable technique to obtain the solution for 2-D potential well. We use the following form variable separation:

$$\psi(x, y, t) = X(x)Y(y)T(t)$$

On substitution in the Schrodinger equation, we can obtain the time invariant equation as below:

$$-\frac{\bar{h}^2}{2m}\left[Y\frac{\partial^2 X}{\partial x^2} + X\frac{\partial^2 Y}{\partial y^2}\right] + (U - E)XY = 0$$

For regions inside the box, where $U = 0$, i.e, for $0 < x < D$ and $0 < y < D$, we have the governing equation as:

$$-\frac{\bar{h}^2}{2m}\left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}\right] - E = 0$$

and for regions outside the box, where the potential is infinite, we have: $XY = 0$, or the wave function ψ must vanish. The continuity of the wave function states that the probability density of finding the matter cannot be double valued at the same location. Hence by the continuity of the wave function at the interface, we must have:

$$X = 0 \ at \ x = 0 \ and \ x = D$$

$$Y = 0 \ at \ y = 0 \ and \ y = D$$

By simple mathematical manipulation we can convert the governing equation with partial derivatives into equations with ordinary derivatives, as follows:

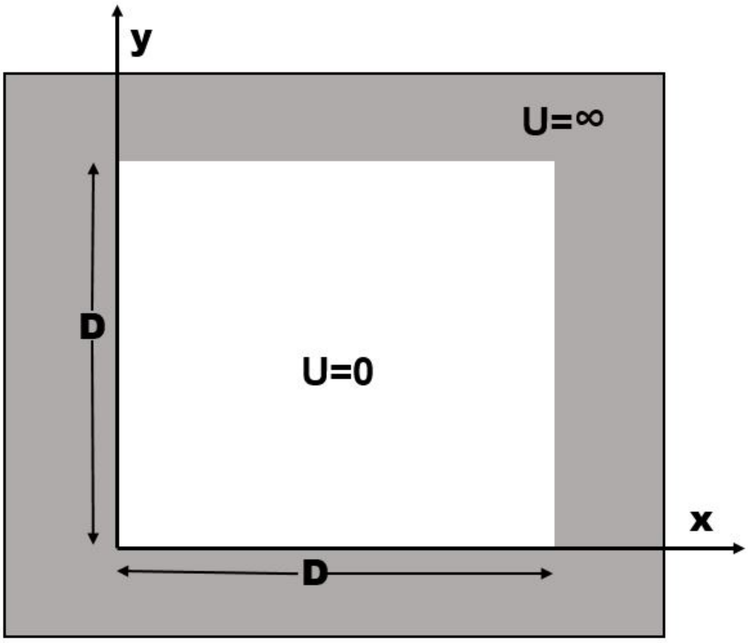

Figure 1: Representation of a square potential well of size D with infinite potential barrier.

$$\frac{1}{X}\frac{d^2 X}{dx^2} + k_x^2 = 0 \ , \ subject \ to \ X = 0 \ at \ x = 0 \ and \ D$$

$$\frac{1}{Y}\frac{d^2 Y}{dy^2} + k_y^2 = 0 \ , \ subject \ to \ Y = 0 \ at \ y = 0 \ and \ D$$

where k_x and k_y are independent of x and y and related by:

$$k_x^2 + k_y^2 = \frac{2m}{\bar{h}^2}E$$

Solving independently the two equations, we have:

$$X(x) = A_n sin(k_x x),\ for\ \ k_x = \frac{n\pi}{D}\ for\ n = 1, 2, 3...$$

$$Y(y) = B_l sin(k_y y),\ for\ \ k_y = \frac{l\pi}{D}\ for\ l = 1, 2, 3...$$

Therefore, the allowable energy levels depends on 2 quantum number and epsressed as:

$$E_{nl} = \frac{n^2\pi^2\bar{h}^2}{2mD^2} + \frac{l^2\pi^2\bar{h}^2}{2mD^2} = \frac{(n^2+l^2)\pi^2\bar{h}^2}{2mD^2}$$

The spatial component of the wave function is given as follows:

$$\psi_{nl} = C_{nl}\ sin\left(\frac{n\pi x}{D}\right) sin\left(\frac{l\pi y}{D}\right)$$

and C_{nl} is obtained using the normalization condition, as follows:

$$C_{nl} = \left[\int_0^D \int_0^D sin^2\left(\frac{n\pi x}{D}\right) sin^2\left(\frac{l\pi y}{D}\right)\ dxdy\right]^{-1/2} = \frac{2}{D}$$

b) The allowable energy level for $D = 500\ nm$, $m = 9.1 \times 10^{-31} kg$, $h = 6.626 \times 10^{-34}\ J.s$

$$E_{nl} = (n^2 + l^2) \times 2.412 \times 10^{-21} J = 0.0151(n^2 + l^2)\ eV$$

c) The different energy level corresponds different values of $(n^2 + l^2)$. The possible values are 2,5,8,10,13,18, and so on...

$$(n^2 + l^2) = 2\ for(n, l) =\ (1, 1)$$

$$(n^2 + l^2) = 5\ for(n, l) =\ (1, 2), (2, 1)$$

$$(n^2 + l^2) = 8\ for(n, l) =\ (2, 2)$$

$$(n^2 + l^2) = 10\ for(n, l) =\ (1, 3), (3, 1)$$

The degeneracy for the first four energy level are the number of possible quantum state for same energy level, which is **1,2,1,2** for the first four level respectively.

Exercise 2.4

*Electron density of states inside quantum wires.*Derive the expression for density of states inside a quantum wire and plot this expression for $L_x = L_y = 5\ nm$

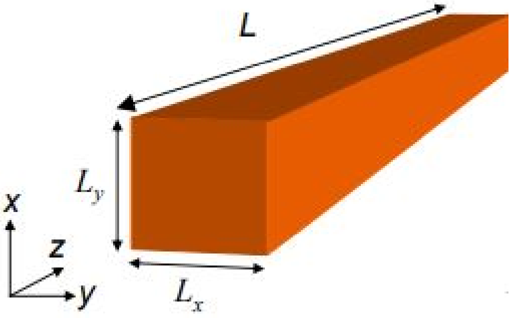

Figure 2: In a quantum wire, electron is free to move in one direction and confined in the other two directions.

Solution

We know from the lecture, that the dispersion relation for an electron in bulk crystal is given by:

$$E(k_x, k_y, k_z) = \frac{\bar{h}^2}{2m^*}(k_x^2 + k_y^2 + k_z^2) = \frac{\bar{h}^2}{2m^*}k^2$$

where m^* is the effective mass of the electron and k is the wave-vector.
However, in a quantum wire, as shown in the figure 2 the energy is discrete due to imposed constraint in the x and y directions.Hence k_x and k_y can take values as follows:

$$k_x = \frac{n\pi}{L_x}\ and\ k_y = \frac{l\pi}{L_y}\ where,\ n, l\ = (0, 1, 2, 3, ...)$$

$$E(k_z, n, l) = \frac{\bar{h}^2}{2m^*}k_z^2 + \frac{\bar{h}^2\pi^2}{2m^*}\left[\left(\frac{n}{L_x}\right)^2 + \left(\frac{l}{L_y}\right)^2\right]$$

$$E_{nl} = \frac{\bar{h}^2\pi^2}{2m^*}\left[\left(\frac{n}{L_x}\right)^2 + \left(\frac{l}{L_y}\right)^2\right]$$

For each pair of value (n, l) we have certain value for E_{nl} which corresponds to different energy mode

For each combination we calculate the number of states between k_z and $k_z + dk_z$

$$N = 2\frac{dk_z}{2\pi/L}$$

The factor of 2 comes because each quantum state can gave positive and negative spin. By defintion, density of state is per unit length(for 1-D), per unit wave-vector. Therefore,

$$D(k) = \frac{1}{\pi}$$

The density of state as a function of E can be obtained by substituting the expression for E and also using the following relation:

$$D(k)dk = D(E)dE$$

$$\frac{dE}{dk} = \frac{\bar{h}^2}{m^*}k$$

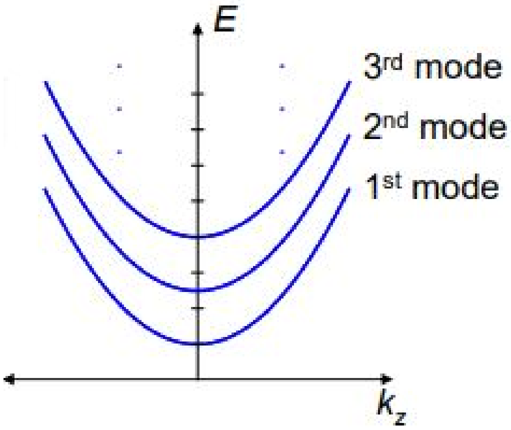

Figure 3: Different modes of energy for (n, l) pairs. It is effectively shifting the energy E upwards by E_{nl}

$$D(E) = D(k) \times \left(\frac{dE}{dk}\right)^{-1} = \sqrt{\frac{m^*}{2\pi^2\bar{h}^2}}(E - E_{nl})^{-1/2}$$

To plot the expression, it is important to understand that for each pair of n and l(i.e, for each mode), the energy E cannot be greater than E_{nl}. Thus for each combinations of n and l, we first obtain E_{nl} and then plot $D(E)\ vs\ E$ starting from previous value of E_{nl} to the current value of E_{nl}. We thus obtain a plot similar to figure 4.

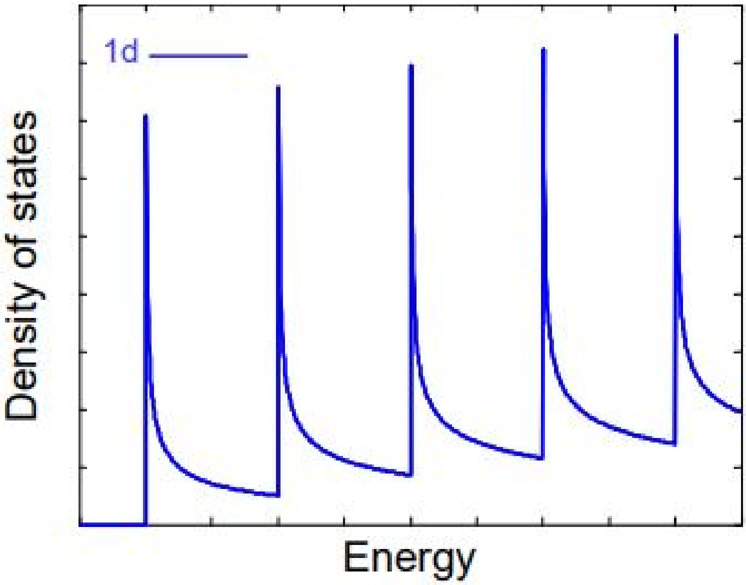

Figure 4: Density of states for a quantum wire.

Note: Comment on the contrasting difference in the plot for quantum wire(1-D) compared to bulk Crystal(3-D) which is parabolic and quantum well(2-D) for which the plot is step function. Can you guess or mathematically establish what will be the nature of plot for a quantum dot(0-D)?
Density of states is just a mathematical convenience, but what physical picture can we draw from these curves??

Exercise 2.5

Unit cell in real and reciprocal space. A body-centered cubic lattice has the following primitive translation vector:

$$\boldsymbol{a_1} = \frac{1}{2}a(-\hat{x} + \hat{y} + \hat{z})$$
$$\boldsymbol{a_2} = \frac{1}{2}a(\hat{x} - \hat{y} + \hat{z})$$
$$\boldsymbol{a_3} = \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z})$$

a) Construct the Wigner-Seitz cell in real space.

b) Find out the corresponding primitive translation vector in the reciprocal space and prove that the reciprocal lattice is an fcc structure.

c) Sketch the Wigner-Seitz cell in the reciprocal space, that is, the first Brillouin zone.

Solution

a) To construct a Wigner-Seitz cell, one need to draw lines connecting one lattice point to all its nearby lattice points, and bisect each line with a plane. The Wigner-Seitz cell is the smallest polyhedron enclosed with these planes. Figure 5 is an example to this construction principle applied to 2D lattice. Figure 6 is the Wigner-Setiz cell of bcc lattice.

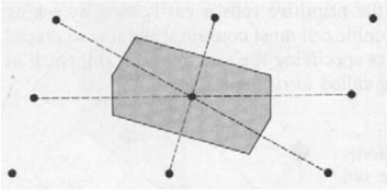

Figure 5: A Wigner-Seitz cell in 2D Bravais lattice.

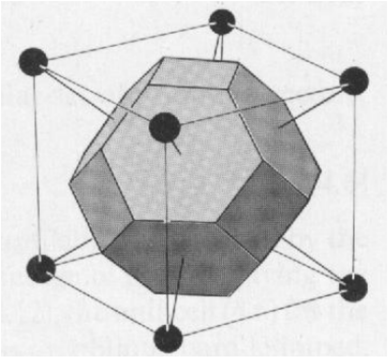

Figure 6: The Wigner-Seitz cell of bcc lattice.

The Wigner-Setiz cell of bcc lattice is made of hexagonal and square faces. Hexagonal faces are the bisection plane between center point and vertices and square faces are the plane between center point to another center points of nearest conventional unit cells of bcc lattice.

b) Primitive translation vector $\boldsymbol{b_1}$,$\boldsymbol{b_2}$ and $\boldsymbol{b_3}$ in the reciprocal space can be obtained through the relations with the primitive translation vectors in real space:

$$\boldsymbol{b_1} = 2\pi \frac{(\boldsymbol{a_2} \times \boldsymbol{a_3})}{(\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3})}$$

$$\boldsymbol{b_2} = 2\pi \frac{(\boldsymbol{a_3} \times \boldsymbol{a_1})}{(\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3})}$$

$$\boldsymbol{b_3} = 2\pi \frac{(\boldsymbol{a_1} \times \boldsymbol{a_2})}{(\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3})}$$

where $(\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3})$ is the volume of the primitive unit cell of bcc, which is $\frac{1}{2}a^3$.

Inserting real space primitive vectors to each relations, we get :

$$\boldsymbol{b_1} = 2\pi \frac{(\boldsymbol{a_2} \times \boldsymbol{a_3})}{(\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3})} = 2\pi \frac{(\frac{1}{4}a^2 - \frac{1}{4}a^2)\hat{x} + (\frac{1}{4}a^2 + \frac{1}{4}a^2)\hat{y} + (\frac{1}{4}a^2 + \frac{1}{4}a^2)\hat{z}}{\frac{1}{2}a^3} = \frac{2\pi}{a}(\hat{y} + \hat{z})$$

$$\boldsymbol{b_2} = \frac{2\pi}{a}(\hat{x} + \hat{z})$$

$$\boldsymbol{b_3} = \frac{2\pi}{a}(\hat{x} + \hat{y})$$

It is straightforward to see that $\boldsymbol{b_1}$,$\boldsymbol{b_2}$ and $\boldsymbol{b_3}$ are the primitive translation vector of fcc. Therefore, the reciprocal lattice of bcc with the lattice parameter of a in real space is fcc lattice with the lattice parameter of $\frac{4\pi}{a}$.

c) Figure 7 shows the Wigner-Seitz cell of fcc lattice which is constructed by the same method described in a).

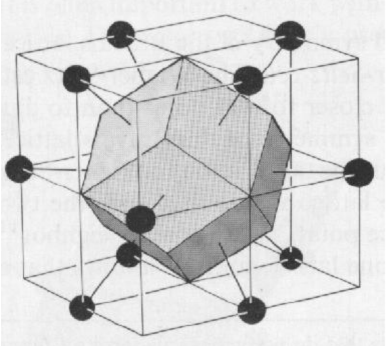

Figure 7: The Wigner-Seitz cell of fcc lattice.

**Above figures are taken from the reference book : Solid State Physics, Ashcroft and Mermin.*