Density of states

The density of states (DOS) is the number of states at a particular energy level that electrons are allowed to occupy, i.e. the number of electron states per unit volume per unit energy.

the wavenumber, k_x

$k_x = \frac{n\,\pi}{L_x}$, $n = 1,2,3, \ldots.$

This analysis can now be repeated in the *y* and *z*-direction. Each possible solution then corresponds to a cube in *k*-space with size *n*π/*L* as indicated in Figure 16.

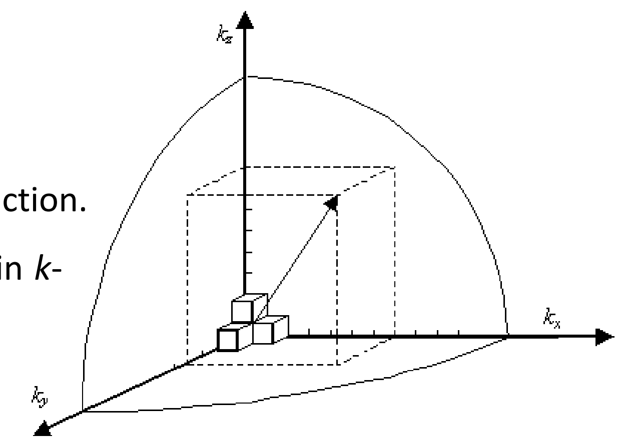

Figure 16.

The k-space volume of single state cube in k-space:

$V_{single-state} = k_x k_y k_z$

$V_{single-state} = \left(\frac{\pi}{L_x}\right)\left(\frac{\pi}{L_y}\right)\left(\frac{\pi}{L_z}\right) = \left(\frac{\pi^3}{V}\right) = \left(\frac{\pi^3}{L^3}\right)$

the k-space volume of a sphere in k-space:

$$V_{sphere} = \frac{4\pi k^3}{3}$$

Number of filled states in a sphere: $N = \frac{V_{sphere}}{V_{single-state}} \times 2 \times \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2}\right)$

A factor of (2) is added to account for the two possible electron spins of each solution

Correction factor in counting identical states +/-n_x, +/-n_y, +/-n_z

$$N = \frac{\frac{4}{3}\pi\, k^3}{\frac{\pi^3}{L^3}} \times 2 \times \left(\frac{1}{8}\right) = \frac{L^3 k^3}{3\,\pi^2}$$

The density per unit energy is then obtained using the chain rule:

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{L^3}{\pi^2}k^2\frac{dk}{dE}$$

The kinetic energy *E* of a particle with mass *m** is related to the wavenumber, *k*, by:

$$E(k) = \frac{\hbar^2 k^2}{2m^*}, \text{ providing } \frac{dk}{dE} = \frac{m^*}{\hbar^2 k} \text{ and } k = \frac{\sqrt{2m^* E}}{\hbar}$$

And the density of states per unit volume and per unit energy, g(E), becomes:

$$g(E) = \frac{1}{L^3}\frac{dN}{dE} = \frac{8\pi\sqrt{2}}{h^3} m^{*3/2} \sqrt{E}, \text{for } E \geq 0$$

The same analysis also applies to electrons in a semiconductor. The minimum energy of the electron is the energy at the bottom of the conduction band, E_c, so that the density of states for electrons in the conduction band is given by:

$$g_c(E) = \frac{8\pi\sqrt{2}}{h^3} m^{*3/2} \sqrt{E - E_c}, \text{for } E \geq E_c$$

$$g_c(E) = 0, \text{for } E < E_c$$

Example: Calculate the number of states per unit energy in a 100 by 100 by 10 nm piece of silicon ($m^* = 1.08\, m_o$) 100 meV above the conduction band edge. Write the result in units of eV^{-1}.

Solution:

$$g(E) = \frac{8\pi\sqrt{2}}{h^3} m^{*3/2} \sqrt{E - E_c}$$

$$= \frac{8\pi\sqrt{2}\,(1.08 \times 9.1 \times 10^{-31})^{3/2}}{(6.626 \times 10^{-34})^3} \sqrt{0.1 \times 1.6 \times 10^{-19}}$$

$$= 1.51 \times 10^{56}\ \mathrm{m^{-3} J^{-1}}$$

So that the total number of states per unit energy equals

$$g(E)V = 1.51 \times 10^{56} \times 10^{-22}\ \mathrm{J^{-1}} = 2.41 \times 10^{5}\ \mathrm{eV^{-1}}$$

For calculation the density of states for **2D structure** (i.e. quantum well) as shown in Figure 17, we can use a similar approach:

the k-space volume of single state cube in k-space:

$$V_{single-state} = \left(\frac{\pi}{L_x}\right)\left(\frac{\pi}{L_y}\right) = \left(\frac{\pi^2}{V}\right) = \left(\frac{\pi^2}{L^2}\right)$$

the k-space volume of a sphere in k-space:

$$V_{circle} = \pi\, k^2$$

The number of filled states in a sphere:

$$N = \frac{V_{circle}}{V_{single-state}} \times 2 \times \left(\frac{1}{2} \times \frac{1}{2}\right)$$

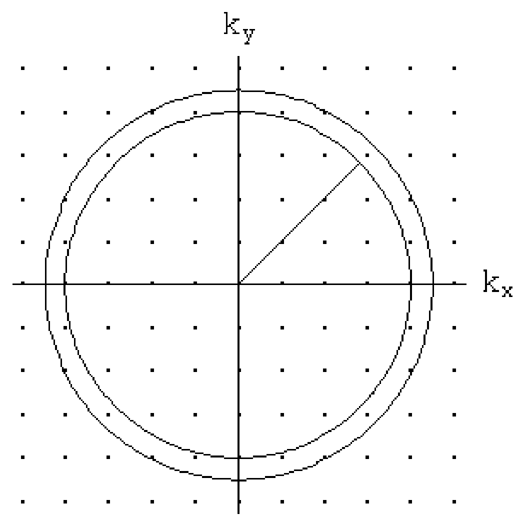

Figure 17.

$$N = \frac{\pi\, k^2}{\frac{\pi^2}{L^2}} \times 2 \times \left(\frac{1}{4}\right) = \frac{L^2 k^2}{2\pi}$$

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{L^2}{\pi} k \frac{dk}{dE} = \frac{L^2\, m^*}{\pi\, \hbar^2}$$

$$g(E) = \frac{1}{L^2} \times \frac{dN}{dE} = \frac{m^*}{\pi\, \hbar^2}$$

**The 2D density of states does not depend on energy.

For calculation the density of states for **1D structure** (i.e. quantum wire), we can use a similar approach:

k-space volume of single state cube in k-space: $V_{single-state} = \left(\frac{\pi}{L_x}\right) = \left(\frac{\pi}{V}\right) = \left(\frac{\pi}{L}\right)$

k-space volume of a sphere in k-space:

$$V_{line} = k$$

A number of filled states in a sphere:

$$N = \frac{V_{line}}{V_{single-state}} \times 2 \times \left(\frac{1}{2}\right)$$

$$N = \frac{k}{\frac{\pi}{L}} = \frac{k\,L}{\pi}$$

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{m^*\,L}{\hbar\,\pi\,\sqrt{2m^*\,E}}$$

$$g(E) = \frac{1}{L} \times \frac{dN}{dE} = \frac{1}{\hbar\,\pi}\,\sqrt{\frac{m}{2\,E}}$$

$$g(E) = \frac{1}{\hbar\,\pi}\,\sqrt{\frac{m}{2\,(E-E_C)}}$$

When considering the density of states for **<u>0D structure</u>** (i.e. quantum dot), no free motion is possible. Because there is no k-space to be filled with electron and all available states exist only at discrete energies, we describe the density of states for 0D with the delta function:

$$g(E) = 2\,\delta(E - E_c)$$

An example of the density of states in 3, 2 and 1 dimensions is shown in Figure 18. The figure shows the density of states per unit volume and energy for a 3-D semiconductor (blue curve), a 10 nm quantum well with infinite barriers (red curve) and a 10 nm by 10 nm quantum wire with infinite barriers (green curve). m^* / m_0 = 0.8.

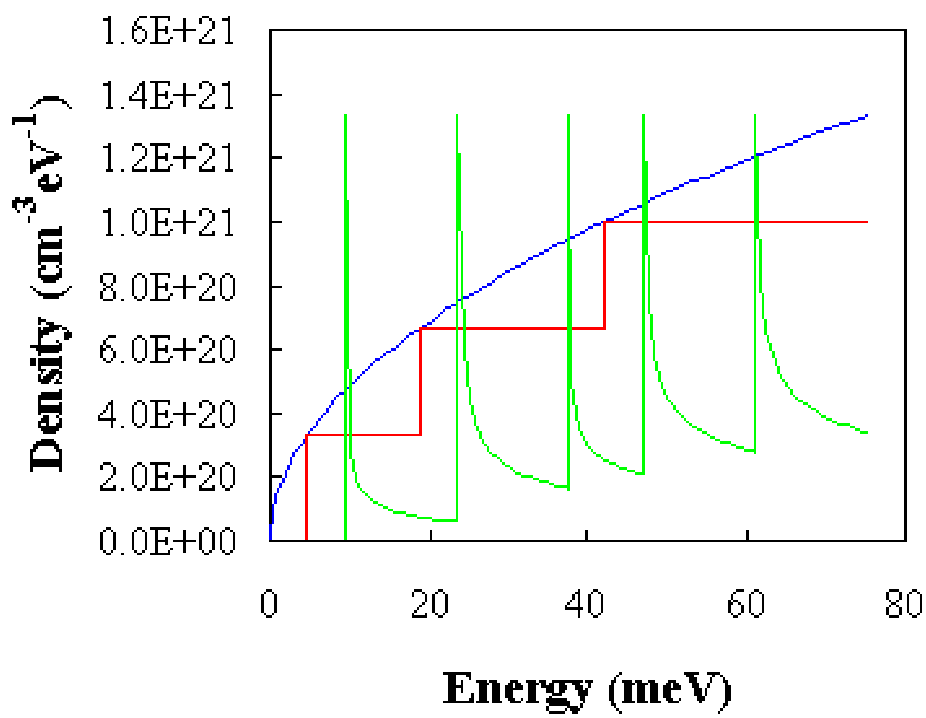

Figure 18.

Figure 19 shows the DOS as a function of energy for each structure

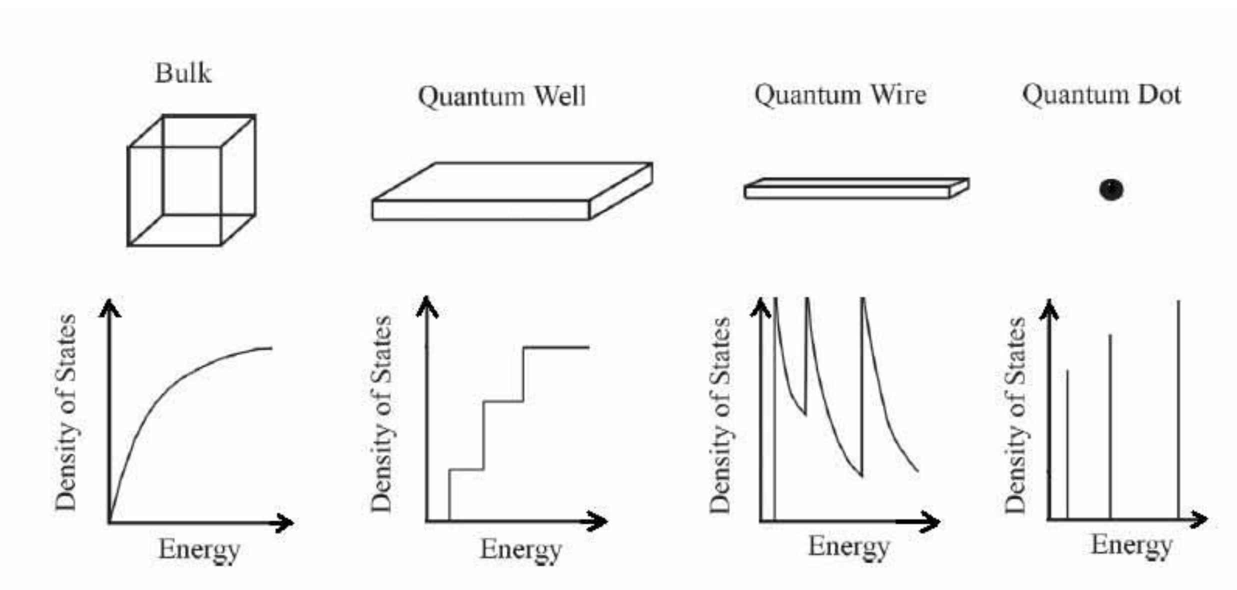

Figure 19.