Low-dimensional structures.

We have looked in some details into the electronic properties of bulk semiconductors. We shall now consider the effects of reduced dimensionality of the behaviour of charge carriers in materials. From a point of view of charge carriers low dimensionality would impact their behaviour when the size of a structure (device) in one of the dimensions becomes comparable to some sort of relevan parameters. Such parameter is taken to be the size of an exciton in a semiconductor – exciton *Bohr radius*.

Bohr radius:

$a_B = \dfrac{4\pi\hbar^2\varepsilon_0}{m_e e^2} =$ 5.3 x 10^{-11} m (or 0.53 Å),

exciton *Bohr radius*:

$$a_{ex} = \frac{a_B \varepsilon}{m^*/m_e}$$

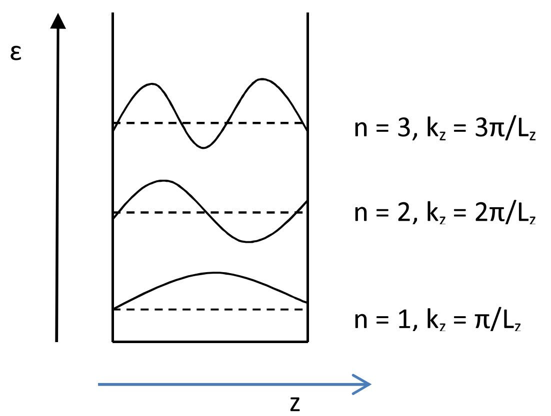
And clearly depends on specific semiconductors. For example, in bulk silicon $\varepsilon = 11.9, m_e^* = 0.26 m_e, m_h^* = 0.36 m_e \;\rightarrow m^* = \frac{m_e^* \times m_h^*}{m_e^* + m_h^*} = 0.15 m_e \rightarrow a_{ex} = 4.2$ nm.

Charge carriers can be confined in one, two or three dimensions. The table below shows various degrees of confinement and descriptions of the corresponding structures.

Confinement	Dimentionality	Structure
1D	2D	Quantum well
2D	1D	Quantum wire
3D	0D	Quantum dot

Electron states in confined structures

We have seen in the previous lectures that electron band structure diagrams can serve as a efficient and informative tool to understand the behaviour of charge carriers and therefore macroscopic properties (conductivity, band gaps, mobility, charge carrier concentration etc.) relevant to the device applications. We shall therefore consider below the effect of quantum confinement on the electronic structure of materials. Let's first consider the behaviour of electron in the confined direction in a *quantum well*. The possible energy states in the confined directions will depend on the boundary conditions which the structure imposes on the electron wave function. Let's make a simple assumption that the electron moves in a constant potential within the structure and is subject to an infinite potential barrier at each side. The wave function is then zero everywhere on the barrier:



Hence:

$$k_z = \frac{n\pi}{L_z}, \varepsilon_z = \frac{(\hbar k_z)^2}{2m^*} = n^2 \frac{(\hbar\pi)^2}{2m^* L_z^2}$$

Now, the motion in *x* and *y* directions is a free one and hence we can write the total kinetic energy as:

$$\varepsilon_n = n^2 \frac{(\hbar\pi)^2}{2m^* L_z^2} + \frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2\right), n = 1,2,3, \ldots$$

For the density of states (g(ε), another important concept we considered earlier) we will have:

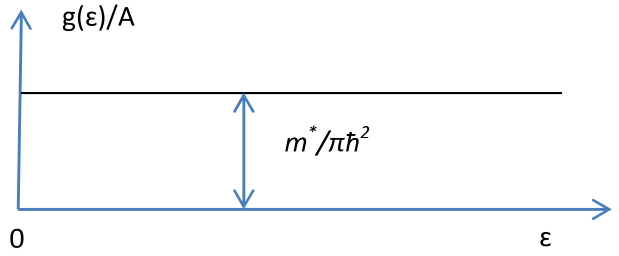
$$g(\varepsilon) = g(|k|)\frac{dk}{d\varepsilon} \times 2 \ (2\ is\ for\ spin)$$

where $g(|k|)$ is the density of states in *k*-space for a specific *k* and $\frac{dk}{d\varepsilon}$ can be obtained from the dispersion curve, which within effective mass approximation is a quadratic one: $\varepsilon = \frac{\hbar^2 k^2}{2m^*}$. Therefore

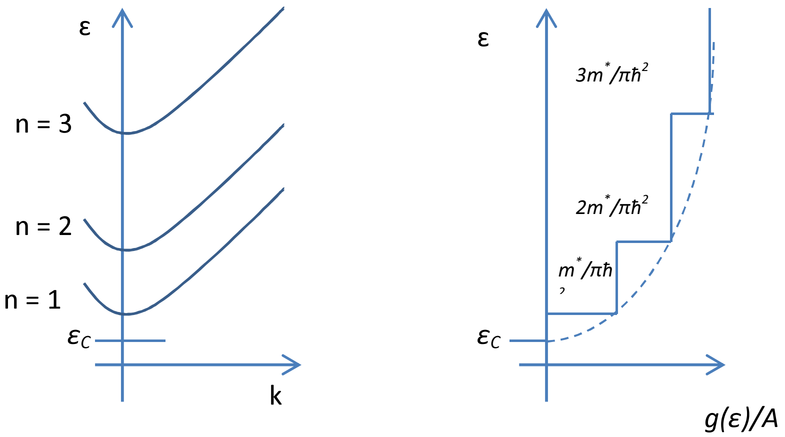
$$k = \sqrt{\frac{2m^*\varepsilon}{\hbar^2}} \Rightarrow \frac{dk}{d\varepsilon} = \sqrt{\frac{m^*}{2\hbar^2}}\ \varepsilon^{-1/2}$$

For a quantum well we will have for two dimensions where the movement is not restricted:

$g(|k|) = \frac{A}{(2\pi)^2} 2\pi|k|$ and $g(\varepsilon) = \frac{A}{(2\pi)^2} 2\pi \sqrt{\frac{2m^*\varepsilon}{\hbar^2}} \sqrt{\frac{m^*}{2\hbar^2}}\ \varepsilon^{-1/2} \times 2 = \frac{Am^*}{\pi\hbar^2}$



Now if we factor in the possible states in a potential well, then for the bottom of the conduction band we get:



We note that no states at all at the bottom of the conduction band corresponding to the bulk semiconductor. The density of states is a step-like function of energy. There will be a similar effect for holes in the valence band, and the effective band gap will be significantly greater than bulk band gap.

Quantum wire

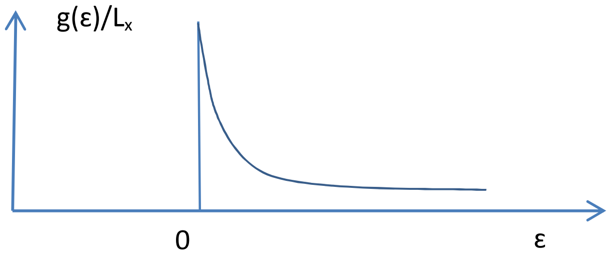
The confinement now is in two directions (let's say *z* and *y*) and hence we have:

$$\varepsilon_{nl} = \frac{(\hbar\pi)^2}{2m^*}\left(\frac{n^2}{L_z^2} + \frac{l^2}{L_y^2}\right) + \frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2\right), n, l = 1,2,3, \ldots$$

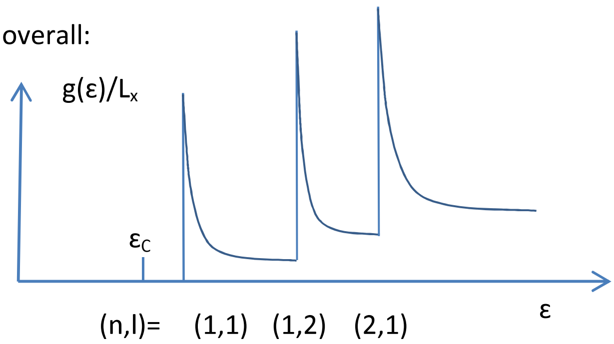
Now let's see the effect of this onto the density of states:

$$g(|k|) = \frac{L_x}{2\pi} \; and \; g(\varepsilon) = \frac{L_x}{2\pi}\sqrt{\frac{m^*}{2\hbar^2}}\,\varepsilon^{-1/2} \times 2$$

Giving for free direction:



Giving overall:



For $L_z \neq L_y$. If $L_z = L_y$ then peaks (1,2) and (2,1) coincide and we have a case of *degeneracy* and the peak will be double size of non-degenerate ones (e.g. (1,1)). In the case of quantum wire we again have enlarged band gap.

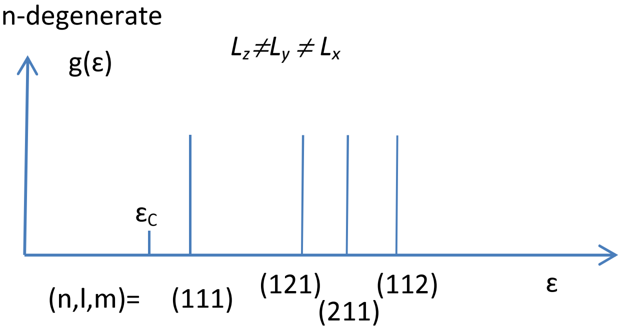
Quantum dot

The confinement now is in all directions and hence we have:

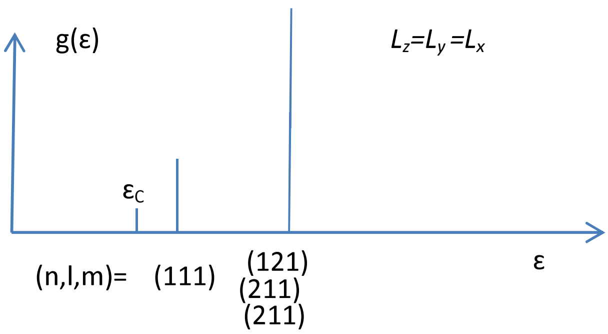
$$\varepsilon_{nlm} = \frac{(\hbar\pi)^2}{2m^*}\left(\frac{n^2}{L_z^2} + \frac{l^2}{L_y^2} + \frac{m^2}{L_x^2}\right), n, l, m = 1,2,3, \ldots$$

and both energy levels and the density of states are discrete-like:

non-degenerate



degenerate



The same will apply for the valence band. We can relate the band gap to the particle size assuming average dimension of *d*. The lowest energy state in the conduction band is then:

$$\varepsilon_e = \frac{3(\hbar\pi)^2}{2m_e^* d^2}$$

and in the valence band is:

$$\varepsilon_h = \frac{3(\hbar\pi)^2}{2m_h^* d^2}$$

giving:

$$\varepsilon_g = \varepsilon_g^{bulk} + \varepsilon_e + \varepsilon_h = \varepsilon_g^{bulk} + \frac{3(\hbar\pi)^2}{2d^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)$$