Movement of electrons in nanostructures 2-D electron gas, quantum wire and quantum dot

Dr. Miklós Berta

bertam@sze.hu

2024. március 18.

SZÉCHENYI ISTVÁN EGYETEM
SZE - GYŐR

Fizika és Kémia Tanszék

Consider a crystal lattice with all dimensions much smaller than the electron free path in this crystal lattice, and let there be electrons with energy above the Fermi level (electrons moving freely in the crystal lattice). Then the electron moves in the grid without any collisions (ballistic conductor).

$$L_x, L_y, L_z << l_{free} \sim \mu\text{m},$$

$$E_e > E_F$$

In such a lattice, the time-independent Schrödinger equation of „free" electrons:

$$\Big\{ -\frac{\hbar^2}{2m_e}\Delta \Big\}\psi(x,y,z) = E\psi(x,y,z)$$

Let us search for the solution in the following form:

$$\psi(x,y,z) = \varphi(x).\chi(y).\kappa(z).$$

After the previous substitution, the original dynamic equation breaks into 3 independent equations:

$$\frac{\partial^2 \varphi(x)}{\partial x^2} + k_x^2 \varphi(x) = 0, \; ahol \; k_x^2 = \frac{2m_e E_x}{\hbar^2}$$

$$\frac{\partial^2 \chi(y)}{\partial y^2} + k_y^2 \chi(y) = 0, \; ahol \; k_y^2 = \frac{2m_e E_y}{\hbar^2}$$

$$\frac{\partial^2 \kappa(z)}{\partial z^2} + k_z^2 \kappa(z) = 0, \; ahol \; k_z^2 = \frac{2m_e E_z}{\hbar^2}.$$

These are the equations of motion of the electron enclosed in a one-dimensional box (or on the one-dimensional string) in each direction.

So:

$$k_x = n_x \frac{\pi}{L_x},\ k_y = n_y \frac{\pi}{L_y},\ k_z = n_z \frac{\pi}{L_z},$$

$$n_x = 1, 2, 3, ...,\ n_y = 1, 2, 3, ...,\ n_z = 1, 2, 3, ...\ .$$

$$E = E_x + E_y + E_z = \frac{\pi^2 \hbar^2}{2m_e}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

2-D electron gas, or 2DEG

Let's assume that the 3-D box can be designed in such a way that $L_z \sim 10^{-10}$ m, i.e. approximately the diameter of 1 atom, while $L_x,\ L_y > Lz$.
Then, the energy of the energy level with the lowest energy in the z direction is:

$$E_z^{(min)} \sim 30 \text{ eV}.$$

As long as the total energy of the electron is less than this value, movement in the z direction is not possible, the set of free electrons behaves as a 2-D electron gas (2DEG)! (Movement in the z direction is „frozen”.)
In the 2DEG, the „free” electrons have an energy directly above the Fermi energy level.

Quantum- or nanowire

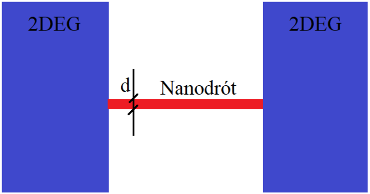
Let's reduce the size of the 2DEG in the y direction so that $L_x >> L_y$, then we get a quantum or nanowire. Such a structure is a 1-D nanostructure.

In the case of a nanowire, the parameter L_y is denoted by d and is called the diameter of the nanowire!

The energy levels of the electrons in the nanowire are:

$$E_{1D} = \frac{\pi^2 \hbar^2}{2m_e} \left(\frac{n_{1D}^2}{d^2} \right).$$

Next, we examine the following layout!



Let's choose the diameter d_0 of the nanowire as small as the energy of the lowest energy level of the electrons in the nanowire ($n_{1D} = 1$) is greater than the energy of the conduction electrons in the 2DEG.

$$E_{1D}^{(1)} = \frac{\pi^2 \hbar^2}{2m_e} \left(\frac{1}{d_0^2} \right) > E_{2DEF}^{F}$$

If we connect a voltage between the two ends of the nanowire in this case, no electric current will flow through the nanowire either. All „conducting channels" are closed!

Let's choose the value of the nanowire's diameter d_1 enough high to be the energy of the lowest energy level of the electrons in the nanowire ($n_{1D} = 1$) smaller than the energy of the conduction electrons in 2DEG, but for the $n_{1D} = 2$ level's the energy is greater than the energy of the conduction electrons in 2DEG.

$$E_{1D}^{(1)} = \frac{\pi^2 \hbar^2}{2m_e}\left(\frac{1^2}{d_1^2}\right) < E_{2DEF}^{F} < E_{1D}^{(2)} = \frac{\pi^2 \hbar^2}{2m_e}\left(\frac{2^2}{d_1^2}\right)$$

If a voltage is then applied between the two ends of the nanowire, an electric current flows through the nanowire. The „conducting channel" characterized by the quantum number $n_{1D} = 1$ is „opened"!

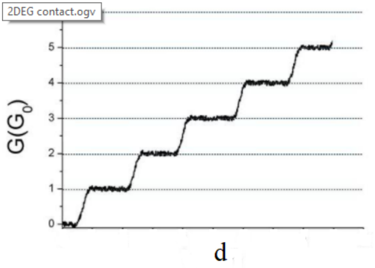
It is clearl that by increasing the nanowire's diameter the other „conducting channels" can also be „opened"!

The conductivity of the nanowire changes by discrete values (in quanta) when the diameter of the wire is changed. With more detailed calculations, it can be shown that the quantum of electrical conductivity is:

$$G_0 = \frac{2e^2}{h} = 82 \cdot 10^{-6}\,\mathrm{S}.$$

The corresponding electrical resistance is:

$$R_0 = \frac{1}{G_0} = 12,2\,\mathrm{k\Omega}.$$



Quantum dot, or q-dot

If $L_x \sim L_y \sim \mathbf{nm}$, then we are talking about a quantum dot (nanostructure with zero dimension).
The values of the energy levels of the electron in the quantum dot are proportional to the square of the quantum numbers, similarly to the energy levels of the electron in the atom, but their value can be fine-tuned with the dimensions L_x, L_y! – ARTIFICIAL ATOM

$$E = E_x + E_y = \frac{\pi^2 \hbar^2}{2m_e}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right)$$

Thank you!