Chapter 2

Electron transport in nanowires

In order to describe electron transport properties in nanowires, simple classical concepts of conductance like Ohm's law are no longer applicable. In this chapter we describe the basic principles of the electronic transport through nanowires. The first section will focus on metallic conductors in general. Further on, the effect of the dimensionality of the sample on the conductance is discussed and an expression for the conductance through a ballistic system is derived. In the final part, the tunneling current, which is a purely quantum mechanical phenomenon, is explained.

2.1 Conductors in general

A conducting material like a metal contains electric charges, which are free to move throughout the lattice. Each atom in a metal contributes at least one free electron to the lattice; these electrons are delocalized and the wave function is nonzero throughout the whole lattice. The typical electronic band structure of metals is responsible for the fact that metals are good conductors. The Fermi energy, which is the highest energy electrons can have at zero temperature and in equilibrium, is situated inside one of its energy bands. For electrical conduction, it is necessary to have empty, unoccupied electron states directly above the Fermi energy.

Classically, the conductance G of a metal is characterized by Ohm's law. According to his law, the current I through a conductor is determined by the potential difference V and the resistance R (Ohm's law: $V = IR$). The resistance R of a metallic wire, is defined by:

$$R = \rho \frac{L}{A} = \frac{1}{G} \tag{2.1}$$

with L the length and A the cross-section of the wire. The resistivity ρ is a material constant which for gold is approximately $2 \cdot 10^{-8}$ Ohm m. The conductance G, i.e. the reciprocal of resistance, of a metallic wire depends on both the cross-section and the length. However, this simple description yields only for macroscopic conductors. When the cross-section of the wire tends to zero, for example if the dimensions of the wire approach the dimensions of single atoms, one would expect the resistance to become infinite. In reality, the resistance of very thin wires is quantized. In order to describe electron transport through these mesoscopic systems, one often makes a distinction between different transport regimes. The specific transport mechanism depends on different length scales. In the next section, we will discuss these length scales. Section 2.3 explains the differences between the distinct transport regimes.

2.2.4 Phase coherence length

The phase coherence length l_φ is a measure of the distance that an electron can travel before its phase is randomized. Usually, this does not happen during elastic scattering events. On the other hand, inelastic scattering events do randomize the phase of the electron wave. Therefore, l_i and l_φ are often mixed up.

2.3 Different transport regimes

As introduced above, electron transport can occur in two different regimes: the diffusive regime and the ballistic regime. If the electrons are scattered often during their way through the system, they are called to behave diffusively. On the other hand, if the electrons can traverse the system without scattering even once, the system is considered ballistic. The cross-over between diffusive and ballistic transport is set by the elastic mean free path l_e. For the case that the elastic mean free path l_e is smaller than the dimensions of the system, many scattering events occur, and the system thus behaves diffusively. In contrast, if l_e is larger than the dimensions of the system the regime is called ballistic.

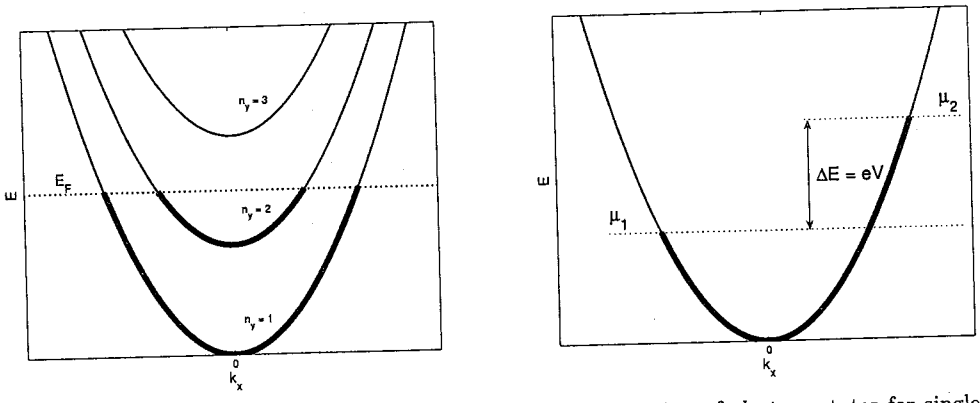
Second, a distinction can be made between the classical and the quantum diffusive regime. If the electrons scatter such that the phase is strongly destroyed over short time intervals (i.e. the phase coherence length is smaller than the size of the system) it is called the classical diffusive regime. Conversely, if the phase information is conserved during many scattering events the regime is called quantum diffusive and quantum effects due to the wave nature of the electrons can be expected. The transport in the ballistic regime can either be regarded as classical or quantum depending relation between the Fermi wave length λ_F and the size of the system L. An overview of the different electron transport regimes is given in Table 2.1.

Table 2.1: Different transport regimes.

	Classic	**Quantum**
Diffusive	$\lambda_F, l_i, l_e \ll L$	$\lambda_F, l_e \ll L, l_i,$
Ballistic	$\lambda_F \ll L < l_i, l_e$	$\lambda_F, L < l_e < l_i$

2.4 Quantized conductance

For this thesis, the most important transport regime is the quantum ballistic regime. We will therefore derive a formalism which describes the conductance in a quantum ballistic system, called the Landauer-Büttiker formalism. The electrons in such a system behave quantum ballistically and the different length scales are related as: $\lambda_F, L < l_e < l_i$. In order to derive an expression for the conductance of a nanowire, one first needs to know its dimensionality and the density of states.



(a) Occupation of electron states for multiple energy modes n_y

(b) Occupation of electron states for single conducting mode with applied bias voltage

Figure 2.2: Dispersion relations. (a) Conductance through narrow channels is quantized and scales with the integer number of occupied modes n_y. (b) Biased electron system with $\Delta E = \mu_2 - \mu_1$. Electrons with an energy between μ_1 and μ_2 contribute to the transport for a single mode. These electrons can only have positive wave numbers k_x.

the Fermi energy. It is of importance to realize that the energy level splitting is strongly dependent on the confinement ($\Delta E \propto 1/W^2$).
We will now derive an expression for the density of states. The density of states per unit length scale in 1D k-space can be written as follows:

$$D_{1D}(k) \equiv \frac{1}{L}\frac{dN}{dk} = \frac{1}{L}\frac{1}{\Delta k} = \frac{g_s}{\pi} \tag{2.9}$$

with N the total number of occupied states, $\Delta k = \pi/L$ the spacing between two successive k-values and g_s the spin-degeneracy. An expression for the 1D density of state in energy space can be found from $k = \sqrt{(2m/\hbar)E}$, leading to:

$$D_{1D}(E) \equiv \frac{1}{L}\frac{dN}{dE} = \frac{1}{L}\frac{dN}{dk}\frac{dk}{dE} = \frac{g_s}{\pi}\sqrt{\frac{m}{2\hbar^2 E}} \tag{2.10}$$

2.4.2 Conductance through ballistic channels

The energy of each electron is now characterized by the quantum numbers n_y and k_x, the former being discrete and the latter continuous. The product of the density of states and the velocity of the electrons integrated over energy gives the net particle current that flows within a single mode n_y:

$$J_{n_y} = \frac{1}{2}\int_{\mu_1}^{\mu_2} v_{n_y}(E) D_{1D}(E) dE \tag{2.11}$$

where v_{n_y} is the particle velocity and μ_1, μ_1 the electrochemical potentials of the reservoirs 1 and 2, respectively. The factor 1/2 is introduced because only electrons with a positive k-vector are taken into account, as depicted in Fig. 2.2(b). The total particle current can

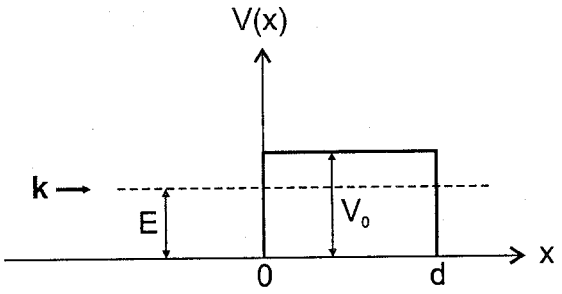


Figure 2.3: Square potential of width d and height V_0. An electron comes in from the left with a wave vector k and an energy E.

electrons cannot cross the gap, because they do not have sufficient energy to overcome the barrier. However, quantum mechanics allows these electrons to travel through the barrier, a phenomenon which is called tunneling. A schematic drawing of the energy band diagram for such a system is shown in Fig. 2.4(a).
In the remaining of this section, an expression for the transmission of electron waves through a simple barrier will be derived. The simplest barrier one could consider is a square potential as displayed in Fig. 2.3:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } 0 < x < d \\ 0 & \text{for } x > d \end{cases}$$

The one-dimensional time-independent Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \tag{2.17}$$

Considering only $0 < E < V_0$ and using:

$$k = \frac{\sqrt{2mE}}{\hbar}, \qquad k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

one finds three solutions to the Schrödinger equation, at the left of the barrier, in the barrier and at the right of the barrier:

$$\psi(x) = \begin{cases} e^{ikx} + (t_1 - 1)e^{-ikx} & \text{for } x < 0 \\ t_1 e^{-k'd}[e^{-k'(x-d)} + (t_2 - 1)e^{k'(x-d)}] & \text{for } 0 < x < d \\ t_1 t_2 e^{-k'd} e^{ik(x-d)} & \text{for } x > d \end{cases}$$

where t_1 and t_2 are the amplitude transmission coefficients for the transmission at 0 and at d, respectively. By satisfying the boundary conditions for continuity of $d\psi/dx$ and ψ at $x = 0$ and $x = d$ one finds:

$$t_1 = \frac{2k}{k + ik'}, \qquad t_2 = \frac{2ik'}{k + ik'}$$

The total transmission probability T can now be evaluated:

$$T = \left|t_1 t_2 e^{-k'd}\right|^2 = \frac{16E(V_0 - E)}{V_0^2} exp\left(\frac{-2d}{\hbar}\sqrt{2m(V_0 - E)}\right) \tag{2.18}$$

as illustrated in Fig. 2.4(b). The wave function of the electrodes in this region are determined by the superposition of the incoming and reflected waves at the interfaces. This leads to periodic maxima in the transmission coefficient as a function of the applied bias voltage, called Gundlach oscillations [5]. The shape of the barrier is conserved by keeping the electric field F constant. Hence, we can write the expression for the differential conductance as function of bias voltage, as obtained by Kolesnychenko *et al.* [6]:

$$\frac{dI}{dV} \sim A(V)cos(\zeta(V)) \tag{2.21}$$

where the argument ζ is given by:

$$\zeta(V) = \frac{4\sqrt{2m}}{3\hbar}\frac{(eV-\phi_2)^{3/2}}{eF} \tag{2.22}$$

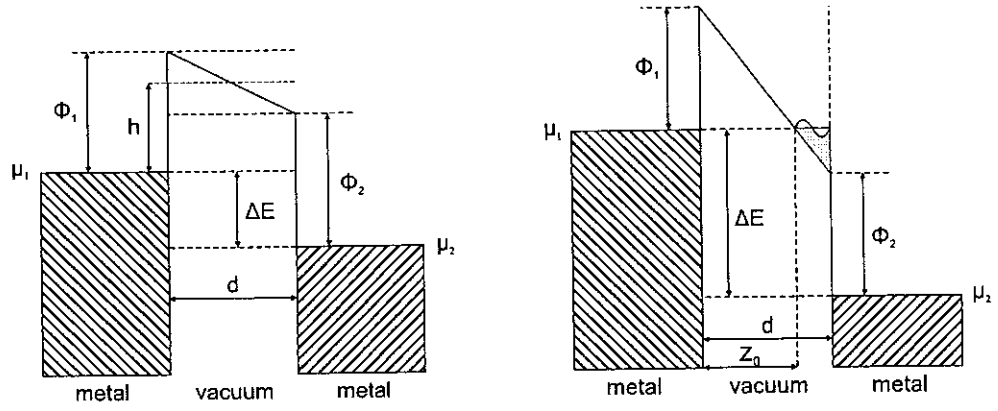
and F is the electric-field strength in the vacuum gap. The differential conductance has a maximum when the argument ζ equals $2\pi n$. The bias voltage V as a function of peak number n can then be written as:

$$eV = \phi_2 + \left(\frac{3\pi\hbar}{2\sqrt{2m}}\right)^{2/3} F^{2/3}n^{2/3} \tag{2.23}$$

From a plot of V versus $n^{2/3}$ one obtains the work function ϕ_2 as the intercept at the voltage axis and the electric-field strength F from the slope of the curve. The distance between the contacts will be related to the electric-field F. An expression for the distance d between the electrodes can be found:

$$d = \frac{1}{eF}(eV + \Delta\phi) \tag{2.24}$$

where $\Delta\phi$ is the difference in work function between the two contacts. The fact that both the work function and information about the distance d can be obtained from a differential conductance measurement makes this a powerful method for calibrating break junction devices. Also, since this method provide us with information about the work function of the metal, we can investigate if impurities are present on the metal surface.



(a) Normal tunneling (b) Fowler-Nordheim tunneling

Figure 2.4: Energy band diagrams for two metal surfaces separated by a small vacuum gap of distance d. The work functions of both metals are represented by Φ_1 and Φ_2 for the left and the right metal, respectively. The difference in electrochemical potentials between μ_1 and μ_2 is equal to the bias voltage ($\Delta E = \mu_1 - \mu_2 = eV$). (a) For small bias voltages one can approximate the triangular shaped barrier by a square potential of height h. (b) If $\Delta E = eV$ exceeds the work function of the metal, part of barrier region becomes classically accessible, which leads to periodic maxima in the transmission coefficient. Standing waves between the classical turning point z_0 and the right electrode result in an oscillating dependence of the tunneling probability.

When a small bias voltage is applied, the shape of the barrier does not rigorously change and the conductance for a single mode of the junction can be approximated by:

$$G \propto \frac{2e^2}{h} T = exp\left(\frac{-2d}{\hbar}\sqrt{2m(\phi - \frac{eV}{2})}\right) \tag{2.19}$$

where ϕ the work function of the material. The factor $1/2$ in $eV/2$ comes from the fact that the real barrier is approximated by a square potential. For triangular shaped barriers one can define an average barrier height h (illustrated in Fig. 2.4(a)), which is exactly half of the maximum barrier height. Assuming $eV/2 \ll \phi$ leads to a simplified expression for the conductance of a tunnel junction:

$$G \propto e^{-2\kappa d} \tag{2.20}$$

where $\kappa = \sqrt{2m\phi}/\hbar$.

2.6 Gundlach oscillations

A common problem encountered with the break junction geometry, is the lack of information about the electrode separation. Fortunately, since the invention of the break junction technique several calibration methods are developed. One of the calibration techniques is based on field-emission resonance, i.e. tunneling in the Fowler-Nordheim regime [4]. Fowler-Nordheim tunneling is a special type of tunneling and occurs when the applied voltage V exceeds the work function ϕ of the material. Part of the barrier region now becomes classically accessible,

then be calculated by summing over all occupied modes n_y:

$$J(\mu) = \sum_{n_y=1}^{N_{ymax}} \frac{1}{2} \int_{\mu_1}^{\mu_2} v_{n_y}(E) D_{1D}(E) dE = \sum_{n_y=1}^{N_{ymax}} \frac{1}{2} \int_{\mu_1}^{\mu_2} \sqrt{\frac{m}{2\hbar^2 E}} \sqrt{\frac{2E}{m^*}} \frac{g_s}{\pi} dE \tag{2.12}$$

with $N_{y_{max}}$ the highest occupied mode. Due to the fact that electrons can have two spin directions, each state can be occupied twice, leading to $g_s = 2$. Thus, for a single mode n_y the particle current becomes:

$$J_{n_y} = \frac{2}{2\pi\hbar}(\mu_2 - \mu_1) = \frac{2}{h}(\Delta\mu) \tag{2.13}$$

The difference in electrochemical potential between the two contacts is given by $\Delta\mu = -eV_{bias}$ and each particle has charge $q = -e$. Putting that in, one finds for the charge current for all occupied modes:

$$I = \sum_{n_y=1}^{N_{ymax}} -eJ_{n_y} = -N_{y_{max}} \frac{2e}{h}(\Delta\mu) = N_{y_{max}} \frac{2e^2}{h} V_{bias} \tag{2.14}$$

This result can be expressed in terms of conductance:

$$G = N_{y_{max}} \frac{2e^2}{h} \tag{2.15}$$

Expression 2.15 is the well-known result for the two-terminal conductance of a very narrow ballistic channel. It shows that conductance is quantized and scales with the integer number of occupied modes. The highest occupied mode can be estimated from $N_{y_{max}} \approx 2W/\lambda_F$. Obviously, real ballistic channels are not fully ideal in the sense that every electron emitted from the reservoir 1 will end up in reservoir 2. One can therefore generalize expression 2.15 to obtain the famous Landauer-Büttiker formula:

$$G = N_{y_{max}} \frac{2e^2}{h} \sum_{n_y=1}^{N_{ymax}} T_n \tag{2.16}$$

where T_n is called the transmission probability, meaning the probability for a wave to reach the other side of the system. The existence of quantized conductance was demonstrated for the first time by van Wees *et al.* in 1988 [2].

It is important to realize that nanowires are in principle three-dimensional structures. Although the derivation of the quantized conductance expression 2.16 is done for a two-dimensional system with a quantization in the y-direction, it is easy to see that quantization in two directions (y and z) gives also a limited number of electron transport modes [3].

2.5 Tunneling

Section 2.4 discussed the conductance of systems which are confined in one or two directions, thereby creating an effective one-dimensional conductance channel. What would happen if a barrier is introduced in such a channel, or in other words, what would happen if we break the nanowire but still keep the two ends of the wire near to each other? Classically,

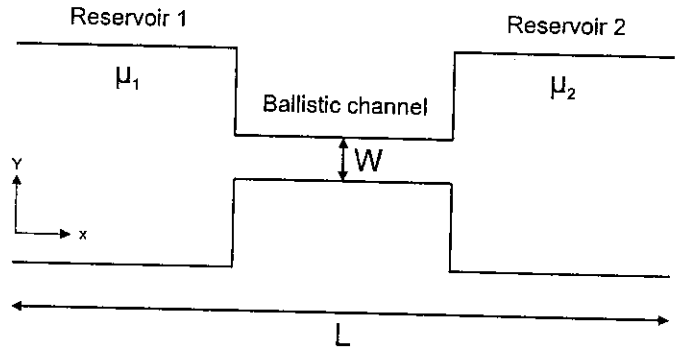


Figure 2.1: Typical 2D ballistic channel of length L and width W. The electrons traversing this channel are only confined in the y-direction. The ballistic channel is connected on both sides to a reservoir with electrochemical potentials μ_1 and μ_2. .

2.4.1 Density of states

A nanowire can be described as a 2D ballistic channel of length L and width W, connected to two reservoirs with electrochemical potentials μ_1 and μ_2, respectively (illustrated in Fig. 2.1). The density of states, which is the number of electron states per unit energy range, in the channel can be calculated from the free electron gas approximation. For a two-dimensional system, the Schrödinger equation is given by:

$$\frac{\hbar}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)=E\psi(x,y) \tag{2.5}$$

with as a general solution the 2D wave function:

$$\psi(x,y)=e^{(k_x x+k_y y)} \tag{2.6}$$

For wave vectors $k^2=k_x^2+k_y^2$ and assuming a electron confinement in the y-direction one finds that the wave vector satisfies:

$$k^2=\left(\frac{n_x\pi}{L}\right)^2+\left(\frac{n_y\pi}{W}\right)^2 \tag{2.7}$$

with $n_x, n_y = 1, 2, 3, \ldots$ the available electron modes. Because electrons travelling in the x-direction are completely free, we can approximate k_x by setting $L=\infty$. Hence, k_x now becomes a continuum and the total energy of an electron inside the channel can now be written as:

$$E_n(k)=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2}{2m}\left(k_x^2+\left(\frac{n_y\pi}{W}\right)^2\right) \tag{2.8}$$

Expression 2.8 shows that the energy and wave vector of an electron are quantized in the y-direction, while being continuous in the x-direction. This means that the electron behaves one-dimensional, which makes it much easier to evaluate the net current through the channel. The relation between energy and wave vector is called the dispersion relation and is shown in Fig. 2.2(a). All available k-states are filled up to the Fermi energy, indicated by the thick line. For the case shown in Fig. 2.2(a) only the modes $n_y=1$ and $n_y=2$ are relevant modes for electron transport through the system, because there are free electron states right above

2.2 Characteristic length scales

The electronic properties of nanodevices are governed to a large extent by the size of the system. In other words, if the dimensions of the system in three directions are given by L_x, L_y and L_z, one can determine the dimensionality of the system by a comparing the different lengths with other length scales, such as the Fermi wave length, the elastic mean free path, the inelastic mean free path and the phase coherence length. In general, a conducting system can be classified as a three-, two- or one-dimensional system. The relevant length scales are described below.

2.2.1 Fermi wave length

For electron transport in a metal only electrons with an energy close to the Fermi energy are important. The Fermi wave length is therefore a relevant length scale in nanoscale systems. The quantum mechanical wave character of the electrons becomes important when the electron wavelength is comparable with the size of the system. For an electron having mass m, kinetic energy E_{kin} and a velocity v, one can easily calculate its de Broglie wavelength λ:

$$E_{kin} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2} \tag{2.2}$$

Electrons at the Fermi energy will have the largest kinetic energy, equal to E_F. Therefore, the associated Fermi wave length λ_F is:

$$\lambda_F = \frac{h}{\sqrt{2mE_F}} \tag{2.3}$$

For simple metals, the Fermi wave length is $\lambda_F \sim 2 \cdot 10^{-10}$ m.

2.2.2 Elastic mean free path

Ideal solids consist of a perfect, regular lattice, having no irregularities which can destroy the symmetry of the crystal. In reality, perfect crystals do not exist and the lattice contains impurities and dislocations. Electrons travelling inside the solid do not have an infinite mean free path and scattering processes take place all the time. As a result, the elastic mean free path l_e, which is a measure for the distance between two elastic scattering events, has a finite value. If an electron scatters from a fault in the crystal (dislocations, impurities, walls), due to the large differences in masses of the electron and the ion, no energy will be transferred during the scattering event and the scattering is considered elastic. The elastic mean free path can be calculated from the time τ_e between two successive scattering events:

$$l_e = \tau_e v_F \tag{2.4}$$

where $v_F = \hbar k_F / m$ is the Fermi velocity.

2.2.3 Inelastic mean free path

Besides electron-impurity scattering, other relevant electron scattering events inside the crystal can occur. For example, moving electrons can excite lattice vibrations or electrons can scatter with other electrons, both resulting in an energy exchange between both scattering partners. Therefore, these scattering events are considered to be inelastic. The inelastic mean free path l_i is defined as the distance between two inelastic scattering events.