

QUANTUM TRANSPORT

1. Introduction

The description of electronic conduction implies two levels which seem at first sight disconnected : one is microscopic and the other is macroscopic.

The microscopic level:

From the birth of quantum mechanics, a description on the atomic scale gave rise to a classification of the conductors in metals, insulators or semiconductors. One can divide the propagation of electronic waves through the atomic lattice in eigenmodes (Bloch waves) which in turn gather up in energybands. The Pauli principle applied to the filling of the states brings the definition of a Fermi energy around which the propagation of the electron is described by an effective Hamiltonian $\hbar^2 k^2 / 2m^*$ where m^* is a positive or negative band mass, possibly anisotropic (tensor), related to the band curvature of the considered energy domain and k the wavevector of the Bloch wave.

The macroscopic level:

The conductor is characterized by a σ *local* conductivity, i.e. defined everywhere. From this, one defines a conductance $G = \sigma \Sigma / L$ (Σ is the cross section and L is the length). Ohm's law applies and, with Kirchhoff's laws, one gets relations between current and voltage. The macroscopic parameter σ is related to microscopic quantities through the Drude's formula: $\sigma = ne^2 \tau / m^*$ where n is the electronic density and τ is an average relaxation time. Conductivity can be derived through a semi-classical linear response theory (Boltzmann) where one establishes a current density \vec{j} in response to a local electric field \vec{E} . The time τ is introduced phenomenologically or can be derived from microscopic considerations, using, e.g. the Fermi golden rule. In the case where τ represents the inelastic scattering time of electrons weakly coupled with their environment (phonons, photons, etc.) the Fermi golden rule works well. In the case where τ represents the inelastic scattering time of electrons with several impurities or on an extended potential, one needs to go beyond a perturbative approach. On the other hand, conductivity becomes *non local* on this length scale for two reasons. First, it makes sense only if one considers many elastic scattering lengths so that one obtains a statistical average and, in the case of an extended potential, only if one considers the whole potential. Then, there is a characteristic length ℓ_φ called *quantum coherence length*, below which every possible electronic paths interfere in a quantum manner. This means that the system cannot be cut in subsets, or, more precisely, although such a cutting is theoretically possible with some precautions, the result of observables for any measure makes no sense below ℓ_φ .

The mesoscopic scale: Thus a complete description of electronic transport brings the mesoscopic length ℓ_φ inbetween quantum and classical descriptions. There is a

general approach of the quantum theory of linear response, called the Kubo approach, which allows to describe completely the electronic transport and to establish exact relations between different physical quantities, as for instance a relation between the conductivity coefficients and the correlation function of the current fluctuations. To use it, one must in general solve the Hamiltonian on the scale ℓ_φ . However, it appears that the Kubo formalism is not intuitive for simple transport problems on the scale ℓ_φ , as those we are going to consider. We shall rather present an approach developed during the last fifteen years, which, thanks to interactions between theory and microfabrication technology, allowed to check these concepts at the scale ℓ_φ . This is the *quantum scattering theory*, also called the Landauer approach. There is a demonstration which shows the equivalence of this approach with the one of Kubo.

On the scale ℓ_φ , the local conductivity σ makes no sense; however one can define a conductance G . It connects the current I going through the mesoscopic conductor placed between two macroscopic areas separated by ℓ_φ , to the electrochemical potential difference $\Delta\mu = eV$ applied between those two areas: $I = (e/h)T\Delta\mu = (e^2/h)TV$. This is the Landauer formula. $T = \sum_n T_n$ is the sum of the transmission coefficients of the electronic waves propagating through the mesoscopic conductor. The more the conductor is transmitting, the more it is conducting. Being careful, one can use all the intuition acquired on wave propagation, like in wave optics, for instance, and foresee the conductance by considering the conductor as an electronic wave guide (regardless of its complexity). The quantity $e^2/h = 1/(25812.8056\Omega)$ is the quantum of conductance.

Typical values for ℓ_φ are 10 to 30 nm for metals or doped semiconductors at room temperature. At low temperatures (lower than 1 Kelvin), in rather clean metals, ℓ_φ reaches the micron and even, exceptionally and at lower temperatures, a hundred of microns for some copper monocrystals. For two-dimensional metals realised in semiconductors, ℓ_φ reaches typically 10 μm .

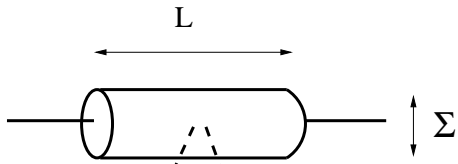
The quantum scattering theory gave a number of results. Some of them are presented here:

- *Resistivity of metals at low temperatures*: weak localization (increase of resistance due to reinforcement of electronic waves backscattering through quantum coherence), universal conductance fluctuations (interferences between electronic waves give rise to small irregular but reproducible variations, of the order e^2/h , when a parameter like the magnetic field is varied).
- *Violation of Ohm's law below ℓ_φ* : non additivity of resistances, (apparently) negative resistances. (Above ℓ_φ resistances are classically added and thus the mesoscopic approach includes in itself the macroscopic description).
- *Interferences of electronic waves*: a mode transmission represents the square of a transmission amplitude. Therefore, when electrons take two paths with a probability amplitude $a_1 = |a_1|e^{i\varphi_1}$ and $a_2 = |a_2|e^{i\varphi_2}$ respectively, the total transmission $T = |a_1 + a_2|^2$ exhibits oscillations with a phase difference of $\varphi_1 - \varphi_2$.

- *Conductance quantization:* in narrow conductors of width similar to the electronic wave length, the number of transmitted modes can be selectively controlled. According to Landauer formula, the conductance shows quantized steps of e^2/h . Further in the lesson, the relation between these steps and the metrological quantization of conductance in the quantum Hall regime will be shown.
- *Resonant tunnel effect:* electrons propagating between two barriers exhibit interferences, which lead to a resonance in the conductance when they are constructive. This is the corresponding electronic system for the Fabry-Perrot resonator in optics. Devices based on this effect are usually realised in electronics.
- *Tunnel spectroscopy:* quantum boxes are submicronic dots for electrons. They can be seen as artificial atoms. In the Landauer approach, the resonant tunnel effect allows to interpret the tunnel spectroscopy of these objects in a simple way.
- *The so called proximity effects,* where superconductivity contaminates a normal metal in an hybrid normal-supraconductor junction, have been reviewed using the Landauer approach. Many effects have been explained and new ones have been unveiled.

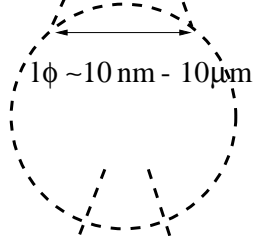
The list seems rather long (even if incomplete). During the lessons, several of these subjects will be explained more into details. Electronic interactions will also be considered. If one compares the interaction energy $\sim e^2/4\pi\epsilon\epsilon_0 a$ of electrons in a metal for instance, it is of the same order as the quantum kinetic energy $\sim \hbar^2/m^*a^2$ (a is here the average distance between the electrons). In fact, there is simply a small miracle which makes that in more than two dimensions, excitations which carry current in a metal are quasiparticles with properties similar to those of quasi-independent electrons (they can be seen as real electrons surrounded by a neutral cloud of screening charges which reduce the long range Coulomb interaction).

However, in low dimensions, the effect of interactions becomes crucial. In the case of a metal dot or a quantum box sufficiently isolated (zero dimension), interactions give rise to the Coulomb blockade phenomenon. The arrival and departure of electrons from the quantum dot change the neutrality and cost an energy $e^2/2C$ where C is the capacitance of the quantum dot. This effect arises in some mesoscopic systems and leads to the observation of charge quantization, which has been used to built up electrometers having a sensitivity up to $10^{-5}e$. An application in fundamental metrology is in process and indirect applications of this effect are already used to realize memories for microchips.



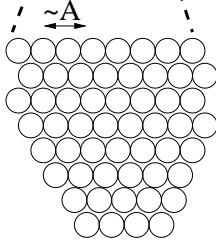
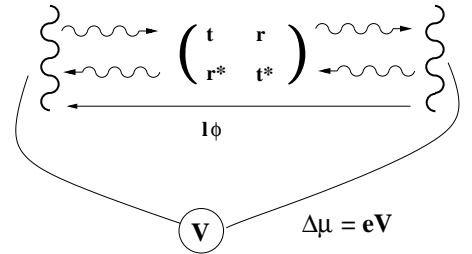
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$$G = \sigma(\Sigma / L)$$

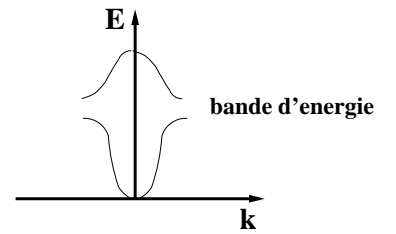


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$$G = (e/h) T \Delta\mu$$



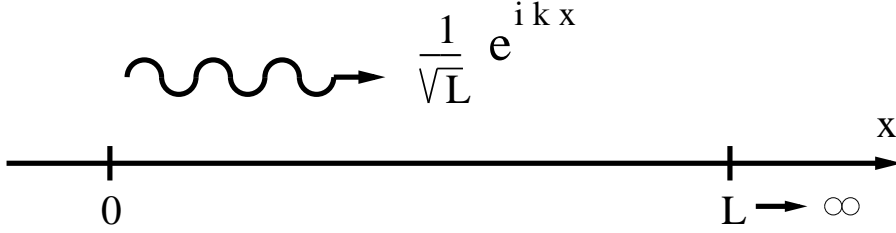
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2. The quantum of conductance

2.1. The current carried by one mode

Consider an ideal one-dimensional conducting wire of length L which tends to infinity. To simplify, spin degeneracy will be omitted in a first step.



An electron propagating from the left to the right is described by a wavefunction:

$$\varphi_k = \frac{1}{\sqrt{L}} \exp(ikx) \quad (1)$$

corresponding to an energy:

$$\varepsilon_k = \frac{\hbar^2}{2m} k^2 \quad (2)$$

The current carried by this mode is

$$i_k = \frac{e}{L} \langle \varphi_k | \hat{v} | \varphi_k \rangle = \frac{e}{L} \frac{\hbar k}{m} \quad (3)$$

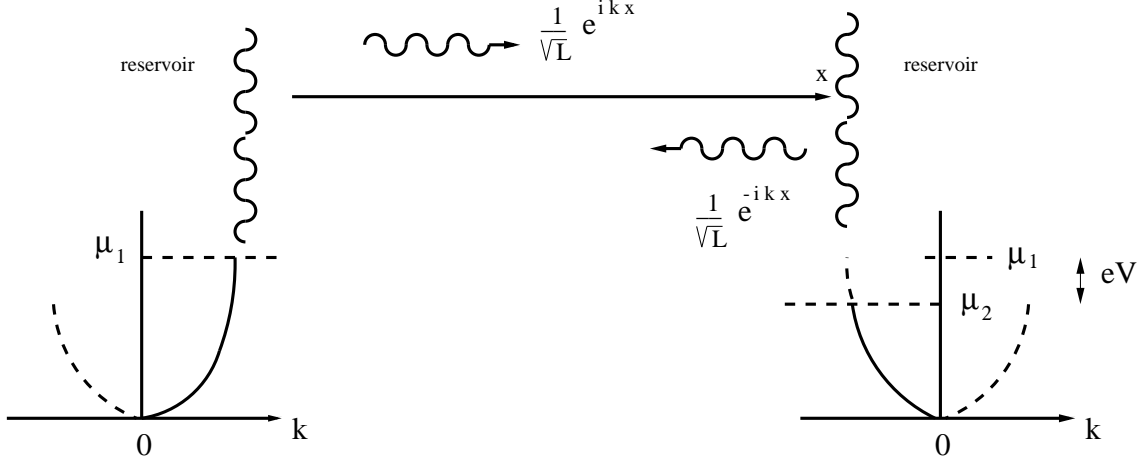
and the one carried by electrons having the energies $\varepsilon_k \in [E, E + \Delta E]$ and propagating to the right is:

$$\begin{aligned} I_{E, E+\Delta E} &= \frac{L}{2\pi} \int_{k(E)}^{k(E+\Delta E)} i_k dk = \frac{L}{2\pi} \int_E^{E+\Delta E} i_k \frac{dk}{d\varepsilon_k} d\varepsilon_k \\ &= \frac{e}{h} \Delta E \end{aligned} \quad (4)$$

Suppose now that the wire is connected on the left to a reservoir of electrons having a chemical potential μ_1 and emitting electrons to the right ($k > 0$) and that it is also connected on the right to a reservoir having a chemical potential $\mu_2 = \mu_1 - eV$ and emitting electrons to the left ($k < 0$).

The total current I is:

$$\begin{aligned} I &= \frac{L}{2\pi} \int_0^{k(\mu_1)} i_k dk + \frac{L}{2\pi} \int_0^{k(\mu_2)} i_{-k} dk \quad \text{avec} \quad i_{\pm k} = \pm \frac{e}{L} \frac{\hbar k}{m} \\ &= \frac{e}{h} (\mu_1 - \mu_2) \\ &= \frac{e^2}{h} V \end{aligned} \quad (5)$$



The previous result is very fundamental: *the conductance associated to an electronic mode is exactly e^2/h* . This is the basis of the Landauer approach of quantum transport.

2.2. The current carried by many perfectly transmitted modes:

Consider a conductor of finite cross section. To simplify, one supposes that is a plane conductor where, in a band of width w , the electrons are confined by an abrupt wall.

A mode propagating to the right is defined by two indices: a wave vector k in the direction \hat{x} and an integer n which characterizes the confinement in the \hat{y} transversal direction. The energy and the wavefunction are respectively:

$$\varepsilon_{k,n} = \frac{\hbar^2}{2m} \left[\left(\frac{2n\pi}{w} \right)^2 + k^2 \right] \quad (6)$$

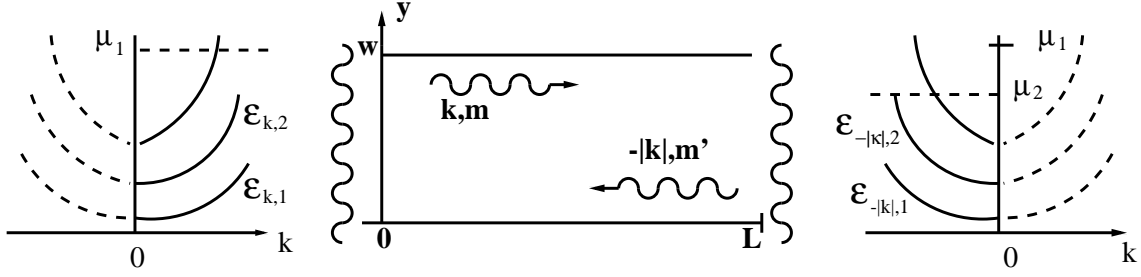
$$\varphi_{k,n} = \left(\frac{2}{Lw} \right)^{1/2} \sin \left(\frac{2\pi ny}{w} \right) \exp(ikx) \quad (7)$$

As previously, the elementary current is:

$$i_{k,n} = \frac{e}{L} \langle \varphi_{k,n} | \hat{v} | \varphi_{k,n} \rangle = \frac{e}{L} \frac{\hbar k}{m} \quad (8)$$

If now the conductor is placed inbetween two reservoirs having the chemical potential μ_1 and $\mu_2 = \mu_1 - eV$, with $eV \rightarrow 0$, the total current reads:

$$\begin{aligned} I &= \frac{L}{2\pi} \sum_n \left[\int_0^{k[\mu_1 - \frac{\hbar^2}{2m} (\frac{2\pi n}{w})^2]} i_k dk + \frac{L}{2\pi} \int_0^{k[\mu_2 - \frac{\hbar^2}{2m} (\frac{2\pi n}{w})^2]} i_{-k} dk \right] \\ &= \frac{e}{h} \sum_{n=1}^{N_{max}} eV \\ &= N_{max} \frac{e^2}{h} V \end{aligned} \quad (9)$$



where N_{max} corresponds to the last occupied subband, i.e.,

$$\frac{\hbar^2}{2m} \left(\frac{N_{max}\pi}{w} \right)^2 < \mu_1 \sim \mu_2 < \frac{\hbar^2}{2m} \left(\frac{(N_{max} + 1)\pi}{w} \right)^2.$$

Every occupied eigenmode contributes to the conductance with a quantity e^2/h . If there is spin degeneracy, the quantum of conductance associated to a mode will be doubled: $2e^2/h$.

REMARK: If one knows how to construct such a conductor, being a real waveguide for electrons, and if one varies the chemical potential, one expects to see a step in the conductance each time a new subband is occupied. The *conductance “counts” the number of transmitted modes*. Such conductors exist: the quantum dots. You will see this during the exercises.

3. The Landauer formula

3.1. Diffusion of an electron by a localized potential

3.1.1. Reminder:

Conservation of the probability current. For a conservative system (Hamiltonian $H = |\vec{p}|^2/2m + V(\vec{r})$ time independent) the probability current is defined as

$$j(\vec{r}) = \frac{1}{2m} \left\{ \varphi^* (-i\hbar \vec{\nabla} \varphi) + (i\hbar \vec{\nabla} \varphi^*) \varphi \right\} \quad (10)$$

so that

$$\text{div}(j(\vec{r})) = 0. \quad (11)$$

As one can see

$$\begin{aligned} \text{div} \left\{ \varphi^* (-i\hbar \vec{\nabla} \varphi) + (i\hbar \vec{\nabla} \varphi^*) \varphi \right\} = \\ \left\{ \vec{\nabla} \varphi^* (-i\hbar \vec{\nabla} \varphi) + (i\hbar \vec{\nabla} \varphi^*) \vec{\nabla} \varphi - \varphi^* (i\hbar \Delta \varphi) + (i\hbar \Delta \varphi^*) \varphi \right\} = 0 \end{aligned} \quad (12)$$

using the fact that $\varphi^* \Delta \varphi = (2m/\hbar^2)(E - V(\vec{r}))\varphi^* \varphi$. Notice that if the spatial dependence of the wavefunction is a real function, then $j(\vec{r}) = \vec{0}$. This is the case, for instance, of a vanishing wave $\sim \exp(-\kappa x)$ or a stationary wave $\sim \cos(kx)$. On the other hand $j(\vec{r}) \neq \vec{0}$ for a progressive wave like $\exp(ikx)$.

Consider now the following example of a localized potential. For $\varepsilon > U$, an incoming wave from the left $\exp(ik_g x)$ is at the same time reflected to the left as $\exp(-ik_g x)$ and transmitted to the right as $\exp(ik_d x)$. Since the current is conserved, $j_d = j_g$, one should think on the *probability current amplitudes* rather than on the probability amplitudes. Thus we will consider an unit incoming current from which we will deduce the reflection r and transmission t amplitudes.

$$\varphi_g(x) = \left(\frac{m}{\hbar k_g}\right)^{1/2} \left(e^{ik_g x} + r e^{-ik_g x}\right) \quad \text{for } x \leq 0 \quad \text{and} \quad \varepsilon = \frac{\hbar^2}{2m} k_g^2, \quad (13)$$

$$\varphi_d(x) = \left(\frac{m}{\hbar k_d}\right)^{1/2} t e^{ik_d x} \quad \text{for } x \geq 0 \quad \text{and} \quad \varepsilon - U = \frac{\hbar^2}{2m} k_d^2. \quad (14)$$

Rewriting continuity for the probability current amplitude and its derivative, one gets:

$$1 + r = t \left(\frac{k_g}{k_d}\right)^{1/2} \quad (15)$$

$$1 - r = t \left(\frac{k_d}{k_g}\right)^{1/2} \quad (16)$$

and defining $\eta = k_d/k_g$ the expressions for the transmitted and reflected amplitudes read

$$t = \frac{2\eta^{1/2}}{1 + \eta} \quad r = \frac{1 - \eta}{1 + \eta} \quad (17)$$

Again for energies $\varepsilon > U$, one can consider an incoming wave from the right with unit probability current amplitude which is reflected to the right with an amplitude r' and transmitted to the left with an amplitude t' :

$$\varphi'_d(x) = \left(\frac{m}{\hbar k_d}\right)^{1/2} \left(e^{ik_d x} + r' e^{-ik_d x}\right) \quad \text{for } x \leq 0 \quad \text{and} \quad \varepsilon - U = \frac{\hbar^2}{2m} k_d^2, \quad (18)$$

$$\varphi'_g(x) = \left(\frac{m}{\hbar k_g}\right)^{1/2} t' e^{ik_g x} \quad \text{for } x \geq 0 \quad \text{and} \quad \varepsilon = \frac{\hbar^2}{2m} k_g^2. \quad (19)$$

One finds then:

$$t' = t \quad \text{et} \quad r' = -r.$$

This simple example allows us to introduce the *diffusion matrix* S which connects the probability current amplitudes incoming in the region responsible for diffusion (here the potential step) with the outgoing probability current amplitudes, or in other words which connects the incoming waves with the outgoing transmitted or reflected waves.

$$\begin{pmatrix} \varphi_g^s \\ \varphi_d^s \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} \varphi_g^e \\ \varphi_d^e \end{pmatrix} \quad (20)$$

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = \begin{pmatrix} r & t \\ t & -r \end{pmatrix}. \quad (21)$$

An important property of S is its *unitarity* which results from the current conservation. Actually:

$$|\varphi_g^s|^2 + |\varphi_d^s|^2 = (\varphi_g^s \quad \varphi_d^s) \begin{pmatrix} \varphi_g^s \\ \varphi_d^s \end{pmatrix} \quad (22)$$

$$= ((\varphi_g^e \quad \varphi_d^e) S^\dagger) \left(S \begin{pmatrix} \varphi_g^e \\ \varphi_d^e \end{pmatrix} \right) \quad (23)$$

$$= |\varphi_g^e|^2 + |\varphi_d^e|^2 \quad (24)$$

if

$$S^\dagger S = 1$$

This implies the relations:

$$|r|^2 + |t|^2 = |r'|^2 + |t'|^2 = 1 \quad (25)$$

$$r^* t' + t^* r' = 0 \quad (26)$$

which can be easily verified with the particular example considered here. Two important quantities appear:

$$T = |t|^2 \quad \text{transmission} \quad (27)$$

$$R = |r|^2 \quad \text{reflection} \quad (28)$$

$$R + T = 1 \quad (29)$$

which represent the transmission and reflection *probabilities*. One can directly measure these quantities in a transport experiment.

Before going further, consider the case of the vanishing wave on the right for $0 \leq \varepsilon < U$. Defining $\eta = \kappa_d/\kappa_g$ where $U - \varepsilon = \hbar^2 \kappa_d^2/2m$ one finds easily

$$f = \frac{1 - i\eta}{1 + i\eta} = \exp(-i\delta) \quad (30)$$

The wave is completely reflected $|r|^2 = R = 1$. One notices the dephasing δ , so that $\tan(\delta/2) = \kappa_d/\kappa_g$, which corresponds to the delay that the wave took during “visiting” virtually the region to the right.

3.1.2. Conductance at zero temperature:

Lets compute the conductance within the same example and the zero temperature limit. Only the energies greater than U will interfere since in the other case the wave is completely reflected. It is supposed that the electrons emitted from the left come from a reservoir with a chemical potential $\mu_g > U$. This means that the incoming waves from the left, with energy $0 \leq \varepsilon \leq \mu_g$, are each one occupied with

one electron. In the same way, it is supposed that on the right side the wire is in equilibrium with a reservoir with chemical potential $\mu_d > U$. The incoming waves from the right, with energy $U \leq \varepsilon \leq \mu_d$, are each one occupied with one electron. This results in chemical potential difference of $\mu_g - \mu_d = eV$. To compute the total current, it is enough to consider for instance the case $x > 0$.

The current from the left is:

$$i_g = \frac{e}{h} \int_U^{\mu_g} d\varepsilon |t(\varepsilon)|^2 \quad (31)$$

and that from the right:

$$i_d = \frac{e}{h} \int_U^{\mu_d} d\varepsilon - \frac{e}{h} \int_U^{\mu_d} d\varepsilon |r(\varepsilon)|^2 \quad (32)$$

Therefore the total current is $I = i_g - i_d$:

$$I = \frac{e}{h} \int_{\mu_d}^{\mu_g} d\varepsilon |t(\varepsilon)|^2 \quad (33)$$

For $V \rightarrow 0$ one defines the conductance $G = I/V$:

$$G = |t(\varepsilon_F)|^2 \frac{e^2}{h} \quad (34)$$

is the Landauer formula. The *conductance is the transmission*.

Exercixe: verify directly that for the case $x < 0$ one gets the same result.