Landauer Büttiker Formalism

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Abstract

This is intended to be a very elementary introduction to the Landauer Büttiker Formalism. At first, basic concepts of electronic transport in mesoscopic structures are introduced, like transverse modes, reflectionless contacts and the ballistic conductor. The current per mode per energy is calculated and the value for the contact resistance derived. Then Landauer’s formula is proposed, including residual scatterer’s resistances. After investigating the question, where the voltage drop comes from, multiterminal devices are considered, proposing Büttiker’s multi-terminal formula, which is then applied to a simple three terminal device. The whole article is heavily based on [1].
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1 Symbols

<table>
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<th>Quantity</th>
<th>Größe</th>
<th>Symbol</th>
<th>SI-Unit</th>
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<tbody>
<tr>
<td>(2-D)Conductivity(^1)</td>
<td>(spezifische) Leitfähigkeit</td>
<td>(\sigma)</td>
<td>(\Omega^{-1} \cdot \text{m}^{-1})</td>
</tr>
<tr>
<td>(2-D)Resistivity(^1)</td>
<td>(spezifischer) Widerstand</td>
<td>(\rho)</td>
<td>(\Omega \cdot \text{m})</td>
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<tr>
<td>Conductance(^1)</td>
<td>Leitwert</td>
<td>(G)</td>
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<td>Widerstand</td>
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<td>(Leitungs-)bandunterkante</td>
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<td>Cutoff energy</td>
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<td>Stufenfunktion</td>
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<td>Effective mass</td>
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<tr>
<td>Width</td>
<td>Breite</td>
<td>(w)</td>
<td>m</td>
</tr>
<tr>
<td>Number of transverse modes</td>
<td>Anzahl transversaler Moden</td>
<td>(M)</td>
<td></td>
</tr>
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</table>

2 Ohmic Resistance Measurement

To start with, we consider a simple classical ohmic resistance measurement (fig. 1). The total resistance comprises of of several parts: The actual resistor, the wires, the instruments, the internal resistance of the battery...

\[
R_{\text{tot}} = R_U + R_I + R_0 + R_L \tag{1}
\]

But we won't worry 'bout all these details, so usually we calculate the resistor's resistance by calculating

\[
R_0 = \frac{U_R}{I} \tag{2}
\]

On the other hand, we know, that the resistance can be expressed by a specific, material dependent but geometry independent (2-D)resistivity \(\rho\), or, equivalently, it's (2-D)conductivity \(\sigma\), as:

\[
R_0 = G_0^{-1} = \frac{L}{\sigma w} \tag{3}
\]

\(^1\)Temparture dependent

Figure 1: Measuring the value of a resistance \(R_0\) is influenced by several sources of practical errors.
with $\sigma, w$ dimensions of the resistor. So what happens, if we tend this geometry towards zero? We would expect the resistance to become zero too:

$$\lim_{w,L \to 0} R_0 \neq 0$$ (wrong)

which is not observed experimentally. For the length $L$ going to zero and for small width $w$, we find a limiting value $\lim_{L \to 0} R_0 \to R_C(w)$, which does depend on the width. To find an explanation, we introduce several concepts.

3 Concepts

We treat the resistor as a conductor sandwiched between two contacts (fig. 2).

3.1 Transmission probability

Conductance should be related to the ease, with which electrons can pass a conductor, so we introduce the *transmission probability* $T$ as the probability for an electron to transmit through the conductor. Certainly, the reflection probability will be given by $1 - T$.

3.2 Ballistic conductor

A ballistic conductor is an ideal transmitting conductor without scatterers, having a transmission probability of $T = 1$.

3.3 Reflectionless contacts

An electron inside the conductor can exit “into a wide contact with negligible probability of reflection”. This is a quite good approximation, for the given case of a narrow conductor and almost infinitely wide contact, as we will see.
later. This assumption set us in the position to note, that the $+k$ states inside a ballistic conductor are populated by electron originating in the left contact only and vice versa.

### 3.4 Transverse modes

As we will see, electronic transport happens in discrete channels through a narrow conductor, which we call *transverse modes*. The electron dynamics in effective mass approximation inside the conductor is described by Schrödinger’s eigenvalue equation

$$
\left[ E_C + \frac{p^2}{2m^*} + V(x, y) \right] \psi(x, y, z) = E\psi(x, y, z)
$$

(4)

Here, $E_C$ is the conduction band edge of the (bulk) conductor material and $V(x, y)$ is a confining potential (fig. 3). Since the system is translational invariant in the $z$ direction, we choose a separating ansatz which yields:

$$
\psi(x, y, z) = \chi(x, y)\exp(ik_z z)
$$

$$
\Rightarrow \left[ \frac{p_x^2}{2m^*} + \frac{p_y^2}{2m^*} + V(x, y) \right] \chi_n(x, y) = \varepsilon_n \chi_n(x, y)
$$

$$
E_n(k_z) = E_C + \varepsilon_n + \frac{\hbar^2 k_z^2}{2m^*}
$$

The $\chi_n(x, y)$ are called *transverse modes* and $n$ is an index for the discrete spectrum. With this we can understand, why we can assume the contact to be reflectionless: An electron inside the conductor most probably will find an empty state in the contact when exiting, for we have almost infinitely many modes in a wide contact. For an electron in the contact, however, we have a different situation: To enter the conductor it must have exactly the correct energy corresponding to an empty transverse mode. Fig. 4 illustrates this matter. From now on we simply say $k := k_z$.

### 3.5 Distribution Function

We will assume the contacts to be in thermodynamical equilibrium, so the electrons simply are Fermi-distributed with some electrochemical potentials

![Figure 3: Lateral potential confining the width of a conductor.](image)
Figure 4: (4(a)): States in a conductor and contact. (4(b)): Schematic dispersion relations for some transverse modes.

\( \mu_1 \) and \( \mu_2 \):

- Left contact: \( f_1(E) \quad T=0K \quad \vartheta(\mu_1 - E) \) Fermi distribution
- Right contact: \( f_2(E) \quad T=0K \quad \vartheta(\mu_2 - E) \) Fermi distribution
- Conductor: 
  - \( +k \) states: \( f^+(E) = f_1(E) \quad T=0K \quad \vartheta(\mu_1 - E) \)
  - \( -k \) states: \( f^-(E) = f_2(E) \quad T=0K \quad \vartheta(\mu_2 - E) \)

### 3.6 Number of transverse modes

The effectively current carrying states are the states between \( \mu_1 \) and \( \mu_2 \) (fig. 5), so we only have to count the number of them and to calculate, which current is carried by each state. With cut-off energy \( \varepsilon_n = E_n(k = 0) \) for each transverse mode \( n \), the number of states that can be reached at an energy \( E \) is given by

\[
M(E) := \sum_n \vartheta(E - \varepsilon_n).
\]

Now we consider the \( +k \) states at first. Each mode \( n \) is occupied according to the left contact distribution function \( f_1(E) = f^+(E) \) and carries a current \( I_n^+ = Ne_{\text{eff}} \), where \( N = \frac{1}{L} \) is the
electron density for an electron inside a conductor of length \( L \) and \( v_{\text{eff}} \) is the effective velocity of the electrons. So we have:

\[
I_n^+ = \frac{e}{L} \sum_k \frac{\partial E}{\hbar \partial k} f^+(E(k)).
\]  

(5)

By using the formal transition \( \sum_k \rightarrow 2 \times \frac{L}{2\pi} \int dk \) this yields:

\[
I_n^+ = \frac{2e}{\hbar} \int_{\epsilon_n}^{\infty} f^+(E) dE.
\]

(6)

All modes together sum up to:

\[
I^+ = \frac{2e}{\hbar} \int_{-\infty}^{\infty} f^+(E)M(E) dE.
\]

(7)

Here \( \frac{2e}{\hbar} = 80 \text{ nA/meV} \) is the current per mode per energy. The same holds for the \(-k\) states.

### 3.7 Contact Resistance

Apply a low voltage \( U = (\mu_1 - \mu_2)/e \) to a ballistic conductor, such that \( M(E) = \text{const} = M \) for \( \mu_2 < E < \mu_1 \), which is referred to as transport at the Fermi edge. Then the current will be

\[
I = I^+ - I^- = \frac{2e}{\hbar} M(\mu_1 - \mu_2) = \frac{2e^2}{\hbar} M \frac{(\mu_1 - \mu_2)}{e}
\]

The conductance will be

\[
G_C = \frac{I}{U} = \frac{2e^2}{\hbar} M
\]

and the resistance (contact resistance) is

\[
G_C^{-1} = \frac{h}{2e^2 M} \approx \frac{12.9 \text{ k}\Omega}{M}
\]

These results have been confirmed experimentally (fig. 6).
Figure 6: Discrete conductance steps in a narrow conductor (adopted from: [1]).

4 Landauer Formula

A fully analogous treatment including a resident scatterer inside the conductor with transmission probability $T$ yield Landauer’s formula for the conductance of a mesoscopic conductor:

$$G_{\text{tot}} = \frac{2e^2}{h} MT$$  \hspace{1cm} \text{Landauer 1957}  \hspace{1cm} (8)

This formula includes:

- Contact resistance
- Discrete modes
- Ohm’s law

Ohm’s law is obtained considering the limiting case of a long conductor including many scatterers, which will not be derived here. The interested reader may be suggested to have a look in [1]. Finally we want to divide the resistance into two parts: The resistance originating in the transition to the contacts and the residual scatterer’s resistance:

$$G^{-1} = \frac{h}{2e^2 MT} = \frac{h}{2e^2 M} + \frac{h}{2e^2 M} \frac{1 - T}{T}$$  \hspace{1cm} (9)
5 Residual scatterer’s resistance on a microscopic scale

Distribution functions (T = 0 K):

To have a look at the distribution function for the electrons inside the conductor for temperature 0K, we first consider the +k states. Coming in from the left contact (XL), they are Fermi distributed according to the left contact electrochemical potential $\mu_1$ and move on to the scatterer (L). Here a fraction $T$ transmits the scatterer, the remaining part is reflected back to the left contact, so these electrons turn into $-k$ states. Directly after the scatterer (R) the +k states are highly nonequilibrium distributed. On their way to the right contact, however, they relaxate and form a new equilibrium Fermi distribution with some quasi-potential $F''$. The same holds for the $-k$ states originating in the right contact: First they are Fermi distributed according to the right contact electrochemical potential $\mu_2$, move on to the scatterer. Here, in principle a fraction $T$ is transmitted and the rest reflected, however to simplify the matter, we assume the scatterer to act only on the +k states, so all $-k$ states can transmit, which definitely is not quite correct. After passing the scatterer, the transmitted $-k$ states unify with the reflected +k states, that turned into $-k$ states and we again have a highly nonequilibrium...
distribution, which relaxes on its way to the left contact. A quasi Fermi-potential \( F' \) emerges.

In that simplified model the quasi-Fermi levels are given by:

\[
F' = \mu_2 + (1 - T)(\mu_1 - \mu_2) \tag{10}
\]

\[
F'' = \mu_2 + T(\mu_1 - \mu_2) \tag{11}
\]

Fig. 8 shows the electrochemical potentials for the two species across the conductor. Clearly we can see, that the voltage drop at the scatterer is:

+ \( k \) states \( eV^+_s = \mu_1 - F'' = (1 - T)\Delta\mu = eG_s^{-1}I \)

- \( k \) states \( eV^-_s = F' - \mu_2 = (1 - T)\Delta\mu = eG_s^{-1}I \)

whereas the voltage drop at the contacts is:

\[ eV_c = T(\mu_1 - \mu_2) = eG_c^{-1}I \]

according to eqn. 9.

6 Multiterminal Devices

Now we want to extend our investigations to multi-terminal devices, having more than 2 probes (or electrodes or contacts, generally terminals). Fig. 9
Figure 9: Conceptual idea of a multiterminal device with 4 terminals (contacts).

schematically shows a 4 terminal device with a scatterer inside the conductor. When treating such devices, we have to note, that there exist different problems, that may arise, some of which are sketched in fig. 10 So how do we

Figure 10: Different problems with multiterminal devices arise: (10(a)): The terminals may couple differently to different species of states (e.g. $+ - k$ states). (10(b)): Since the terminal are invasive by themselves, they may produce additional sources of scattering. (10(c)): A propagating wave may interfere with it’s own from a scatterer reflected part. This is a pure quantum-mechanical effect and the results of a measurement may depend on the exact location of the terminals.

have to treat such multi-terminal devices? It was Büttiker, who realized, that there is no principal difference between voltage probes and current probes, so we can simply extend the two terminal Landauer formula by summing over all probes:

$$I_p = \frac{2e}{\hbar} \sum_q \left( T_{q-p} \mu_p - T_{p-q} \mu_q \right)$$

(12)
Here $T_{q-p} := M_{q-p} T_{q-p}$ is the product of transmission probability $T$ from contact $p$ to contact $q$ and the number of transverse modes $M$ between them, and is called transmission function. Just let us rewrite this a little:

$$G_{pq} := \frac{2 e^2}{h} T_{pq}$$
$$V_q := \frac{\mu_q}{e}$$

with

$$\sum_q G_{qp} = \sum_q G_{pq}$$

$$I_p = \sum_q G_{pq} (V_p - V_q)$$

7 Three Terminal Device

![Figure 11: Conceptual idea of a 3 terminal-device.](image)

For a voltage contact $p$, we know that there is almost no current flowing, so we can write:

$$I_p = 0 \Rightarrow V_p = \frac{\sum_{q\neq p} G_{pq} V_q}{\sum_{q\neq p} G_{pq}}$$

As an example we will apply this result to a three terminal device as shown in fig. 11. Here the probe at potential $V_2$ may be the voltage probe and we just want to measure the resistance of that device. From eqn. 12 we can
write:

\[
\begin{pmatrix}
I_1 \\
I_2 \\
I_3
\end{pmatrix} =
\begin{pmatrix}
G_{11} (V_1 - V_1) + G_{12} (V_1 - V_2) + G_{13} (V_1 - V_3) \\
G_{21} (V_2 - V_1) + G_{22} (V_2 - V_2) + G_{23} (V_2 - V_3) \\
G_{31} (V_3 - V_1) + G_{32} (V_3 - V_2) + G_{33} (V_3 - V_3)
\end{pmatrix}
\]

\[
= \begin{bmatrix}
G_{12} + G_{13} & -G_{12} & -G_{13} \\
-G_{21} & G_{21} + G_{23} & -G_{23} \\
-G_{31} & -G_{32} & G_{31} + G_{32}
\end{bmatrix}
\begin{pmatrix}
V_1 \\
V_2 \\
V_3
\end{pmatrix}
\]

This can be reduced further. From Kirchhoff’s knot rule, we know, that
\[I_1 + I_2 + I_3 = 0\], so these three equations are not independent and we can only solve for \(I_1\) and \(I_2\). \(I_3\) then follows immediately. Secondly we can choose a reference potential without changing the physics behind it, so we choose \(V_3 = 0\) to simplify the matter. This yields:

\[
\Rightarrow \begin{pmatrix}
I_1 \\
I_2
\end{pmatrix} = \begin{bmatrix}
G_{12} + G_{13} & -G_{12} \\
-G_{21} & G_{21} + G_{23}
\end{bmatrix}^{-1}
\begin{pmatrix}
V_1 \\
V_2
\end{pmatrix}
\]

\[
\Leftrightarrow \begin{pmatrix}
V_1 \\
V_2
\end{pmatrix} = \begin{bmatrix}
R_{aa} & R_{ab} \\
R_{ba} & R_{bb}
\end{bmatrix} \begin{pmatrix}
I_1 \\
I_2
\end{pmatrix}
\]

and the resistance is given as

\[
R = \frac{V_2}{I_1} \bigg|_{I_2=0} = \frac{R_{ba} I_1 + R_{bb} I_2}{I_1} \bigg|_{I_2=0} = R_{ba}
\]

\(R\) can be obtained from the conductance coefficients \(G_{ij}\) and these can be obtained from the scattering matrix \(S_{lm}\), for which we have to solve the threedimensional problem quantummechanically, e.g. using Green’s function.
References