Pedro Pereyra P

The Transfer Matrix Method

SPIN Springer's internal project number, if known

– Application to transport and optical properties of solids –

February 2, 2010

Springer
Berlin Heidelberg New York
Hong Kong London
Milan Paris Tokyo

4

Conductance an optical response in the scattering approach

The transport processes and propagation of classical and quantum waves, the relevant physical quantities may conveniently be described, depending on the nature of the specific physical process, in terms of either the scattering or the transfer matrix elements. S-matrices, which relate the incoming wave functions with the outgoing ones, have been widely used to describe electromagnetic and elastic waves; they are also valuable for a broad class of problems in low and high energy physics. The transfer matrices M, which relate the wave vector on one side of the system with that on the other, are widely used in different fields of physics and engineering. In solid state physics, transfer-matrix methods have been extensively applied to study electron energy bands in ordered and disordered systems-6 as well as to establish general criteria for the existence of energy gaps in the spectrum of arbitrary one-dimensional atomic chains, especially in connection with delta- function potentials.7-9 In Landauers scattering approach to electronic transport processes, con- ductance properties of mesoscopic multichannel disordered conductors are analyzed through transfer matrix ensembles.-4

We have already mentioned the relevance of the Landauer conductance formula in the scattering approach to electronic transport [?]. The formal representation of resistance and conductance in terms of transmission and reflection coefficients has been a propitious idea in the quantum description of the conduction properties of ordered and disordered samples. The astonishing simplicity of the Landauer formula and its profound implications on the description of a physical phenomenon that was thought extremely complex, lead to careful derivations where not only the physical conditions of applicability were search, punctilious derivations were also accomplished. Derivations where the role of measuring probes and charge carrier reservoirs, as well as differences between electrostatic and electrochemical potentials, were taken into account [?, ?, ?, ?]. We will show here that the simple one-channel and multichannel Landauer formulas deserve also simple derivations. We will see that if one follows the simple and sensitive reasoning that guided Rolf Landauer to conceive the way in which a piece of an electronic circuit, the sample

or potential region, behaves or modifies the transport phenomena, one can easily derive the well known Landauer formulas.

4.0.1 The one-channel 1D Landauer conductance. For phase coherent systems

In 1957, Rolf Landauer suggested to view the conduction in a 1D system as a transmission problem such that

$$G = \frac{e^2}{\pi\hbar}\frac{T}{R}. \tag{4.1}$$

The eventual divergency of the conductance, when the transmission coefficient $T \to 1$, was largely discussed and new formulas free of divergencies were search. The physical connection between G and T was to some extent well accepted, but the presence or not of the reflection coefficient has been finally ascribed to the probes position, in the leads or the reservoir, when the sample conductance is measured.

Let us suppose that we have the system shown in figure **??** where a conducting sample is connected to leads and the incident particles come only from the left hand side. The partial elastic reflection and transmission of particles by the scattering sample leads, in general, to different particle densities at the left and right of the system. At the left, for samples at low temperature where the phase coherence is kept, i.e. for non disordered samples, the particle's density is

$$n_l = |\varphi_i + \varphi_r|^2 = |1 + r|^2|\varphi_i|^2 = \big(1 + |r|^2 + 2\Re e[r]\big)|\varphi_i|^2 \tag{4.2}$$

while the particle's density at the right is

$$n_r = |\varphi_t|^2 = |t|^2|\varphi_i|^2. \tag{4.3}$$

The induced density difference is then

$$\delta n = n_l - n_r == \big(1 + |r|^2 - |t|^2 + 2\xi\big)|\varphi_i|^2 = 2\big(R + \xi\big)|\varphi_i|^2 \tag{4.4}$$

where we have used that $R+T = 1$ and defined $\xi = \Re e[r]$. As the temperature grows or the sample disordered grows, and the phase coherence is lost, $\xi \to 0$. Since

$$\delta n = \frac{dn}{dE}\delta E = \mathcal{D}(E)\delta E \tag{4.5}$$

an electrostatic potential difference ($\delta E = e\delta V$) given by

$$\delta V = \frac{2\big(R + \xi\big)|\varphi_i|^2}{e\mathcal{D}(E)} \tag{4.6}$$

is induced. Here the density of states is $\mathcal{D}(E) = 1/\pi\hbar v_i$. We known that in a system like this, the current densities at the left and right are the same. The current density on the right is

$$\boldsymbol{j}_t = |\varphi_t|^2 \frac{\hbar \boldsymbol{k}_i}{m} = |t|^2 |\varphi_i|^2 v_i \hat{\mathbf{z}} \tag{4.7}$$

Thus, the electric current is

$$I = eT|\varphi_i|^2 v_i \tag{4.8}$$

Using these results one easily obtains the conductance

$$G = \frac{I}{\delta V} = \frac{e^2}{2\pi\hbar}\frac{T}{R+\xi} = \frac{e^2}{2\pi\hbar}\frac{T}{R}\big(1 - \frac{\xi}{R} + ...\big) \tag{4.9}$$

Which leading term is precisely the one channel 1D Landauer conductance in the case of no spin degeneration.

Let us now suppose the N-channel case where r and t are $N \times N$ matrices. We can in this case start obtaining the electric current I. Because of flux conservation it is the same at the left and the right side of the scattering sample. The current density, in channel a, on the right hand side is

$$\boldsymbol{j}_{la}(z) = \sum_{b,c} \frac{i\hbar}{2m}\left(\varphi_{ic} t^T_{ca} \frac{\partial}{\partial z} t^*_{ab} \varphi^*_{ib} - \varphi^*_{ic} t^\dagger_{ca} \frac{\partial}{\partial z} t_{ab} \varphi_{ib}\right) \hat{\mathbf{z}} \tag{4.10}$$

$$j_{la}(z) = \frac{\hbar}{2m} \sum_{b,c} k_b \left(\varphi_{ic} t^T_{ca} t^*_{ab} \varphi^*_{ib} + \varphi^*_{ic} t^\dagger_{ca} t_{ab} \varphi_{ib}\right) \tag{4.11}$$

it is easy to show that the first and the second term are equal, thus

$$j_{la}(z) = \frac{\hbar}{m} \sum_{b,c} k_b \varphi_{ic} \varphi^*_{ib} t_{ac} t^*_{ab} \tag{4.12}$$

If we integrate, taking into account that the wave functions in the leads satisfy the normalization condition

$$\int \varphi^*_{ic}(z) \varphi_{ib}(z) dz = \frac{\delta_{bc}}{\hbar k_b/m}, \tag{4.13}$$

the current in channel a takes the form

$$I_a = e \sum_{b,c} \delta_{cb} t_{ac} t^*_{ab} = e \sum_b t_{ab} t^*_{ab} \tag{4.14}$$

and the total current becomes

$$I = e \sum_{ab} t_{ab} t^*_{ab} = e \mathrm{Tr}\, t t^\dagger \tag{4.15}$$

On the other hand we can evaluate the induced electrostatic potential from the particle densities difference. These densities at the left and right sides are

$$n_{la}(z) = \sum_{b,c} \varphi^*_{ic}(I_N + r)^\dagger_{ca}(I_N + r)_{ab}\varphi_{ib} \tag{4.16}$$

and

$$n_{ra}(z) = \sum_{b,c} \varphi^*_{ic} t^\dagger_{ca} t_{ab} \varphi_{ib} \tag{4.17}$$

After integration on z the induced particles density difference, in channel a, takes the form

$$\delta n_a = n_{la} - n_{ra} = \sum_b \frac{1}{v_b}\left[(I_N + r)_{ab}(I_N + r)^\dagger_{ba} - t_{ab}t^\dagger_{ba}\right] \tag{4.18}$$

Again, this change in the particle density can be written as

$$\delta n_a = \frac{dn_a}{dE}\delta E = \mathcal{D}_a(E) e\delta V = \frac{1}{\pi\hbar v_a} e\delta V, \tag{4.19}$$

and the total particle density difference will be

$$\sum_a \delta n_a = \sum_a \frac{1}{\pi\hbar v_a} e\delta V. \tag{4.20}$$

We can then write

$$\delta V = \frac{\pi\hbar \sum_{ab} v_b^{-1}\left[(I_N + r)_{ab}(I_N + r)^\dagger_{ba} - t_{ab}t^\dagger_{ba}\right]}{e\sum_a v_a^{-1}} \tag{4.21}$$

which in a more compact form is

$$\delta V = \frac{\pi\hbar \sum_b 2\, v_b^{-1}\big(R_{bb} + \Re e[r_b]\big)}{e\sum_a v_a^{-1}} \tag{4.22}$$

where $R_{bb} = \sum_a r^*_{ba} r_{ab} = 1 - T_{bb}$. Since $\Re e[r_b] \simeq \mathcal{O}(1/N)$ we have

$$\delta V = \frac{\pi\hbar \sum_b 2\, v_b^{-1} R_{bb}}{e\sum_a v_a^{-1}} \tag{4.23}$$

Therefore, we have the well known [**?**, **?**] multichannel conductance

$$G = \frac{e^2}{2\,\pi\hbar}\frac{\mathrm{Tr}\, tt^\dagger \sum_a v_a^{-1}}{\sum_b v_b^{-1} R_{bb}} \tag{4.24}$$

A factor 2 must be added when the system is spin degenerated.