

### 1.3 Scattering matrix and Landauer formula

In two previous Sections, we studied electron transport in idealized waveguides with or without potential barrier. They do not only illustrate concepts of quantum transport, they also model concrete experimental situations. A waveguide with no potential barrier models a QPC, a constriction created by gates in 2DEG. A waveguide with potential barrier models electron propagation through an insulating layer between two metals.

Real nanostructures can be made in a variety of ways, and can be more complicated. Modern fabrication technology allows for making sophisticated semiconductor heterostructures, combining and shaping different metals, using nanotubes, molecules and even single atoms as elements of an electron transport circuit. Various means can be used to control the transport properties of a fabricated nanostructure. It is only possible to describe all this in a single book because all these systems do obey the general laws of quantum transport that we formulate in this Section.

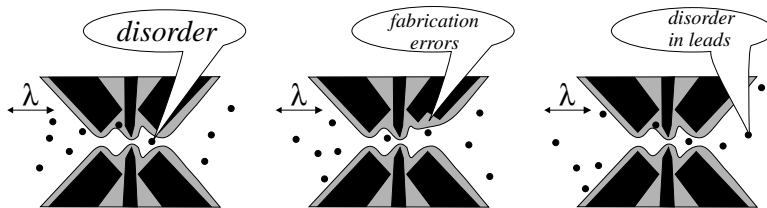


Fig. 1.12. Nanostructures of an identical design are never identical.

There is a common feature of all fabrication methods: Two nanostructures that are intended to be identical, that is, are made with the same design and technology, are *never* identical. Beside the artificial features brought by design, there is also *disorder* originating from defects of different kind inevitably present in the structure. The position of and/or potential created by such defect is random and in most cases can be neither controlled nor measured. It is unlikely that this situation changes with further technological developments: Even if one achieves a perfect control of every atom in a nanostructure, one would not be able to control all the atoms in the macroscopic contact leads, those can not be separated from the nanostructure. The defects scatter electrons thus affecting the transport properties. Conductance of the structure is thus

random depending on a specific realization of disorder in the structure and in the leads: Formidal number of uncontrollable parameters.

Fortunately, transport properties of any nanostructure can be expressed through a smaller set of parameters. The condition for this is that electrons traverse the structure without elergy loss, so that they experience only elastic scattering. These conditions for a given structure are always achieved at sufficiently low temperature and voltage applied. The scattering is characterized by a *scattering matrix* that contains information about electron wavefunctions far from the structure. The transport is described by a set of *transmission eigenvalues* derived from this scattering matrix. A great deal of literature on quantum transport, and a great deal of this book, is in fact devoted to evaluation of the transmission eigenvalues and establishing their general properties. In this Section, we derive the relation between conductance and transmission eigenvalues and thus demonstrate that understanding of transmission properties of a system authomatically means understanding of its transport properties.

*Scattering matrix.* We have mentioned in Section 1.2 that any nanostructure taking part in quantum transport is a part of an electric circuit: It is connected to several *reservoirs* which are in thermal equilibrium and are characterized by a fixed voltage. In this Section, we only consider the case when there are two reservoirs (to be referred as left and right). Generalization to many reservoirs is given in Section 1.5. Somewhere

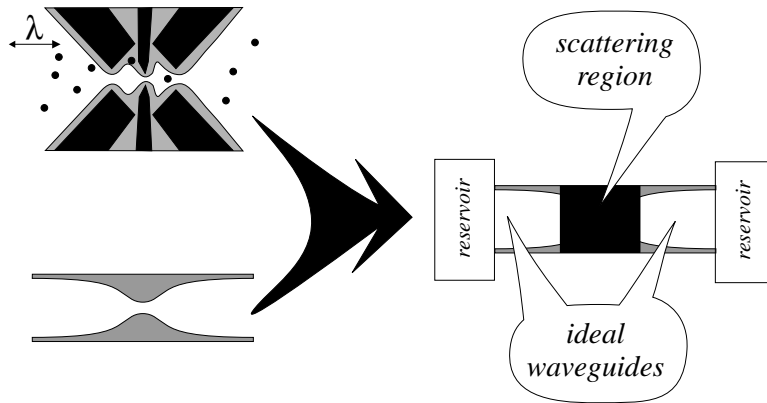


Fig. 1.13. Scattering approach to quantum transport. Ideal waveguides and reservoirs brought from QPC plus scattering in between form an adequate model of transport in any nanostructure.

between the reservoirs there is *scattering region* – the nanostructure proper. Let us start from the assumption that we use formulating a model for QPC: Ideal waveguides connect the reservoirs and the scattering region (Fig. 1.13). This is convenient since the scattering only takes place in a finite region, the reservoirs being far from this region. The wave functions may have very complicated form in the scattering region, but in the waveguides they are always combinations of plane waves. Left and right waveguides do not have to have the same axis and the same cross-section. This is why it is convenient to introduce the separate coordinates  $x_L < 0, y_L, z_L$  and  $x_R > 0, y_R, z_R$  for the left and right waveguides, respectively. Generally, a wavefunction at fixed energy  $E$  can be presented as a linear combination of the plane waves,

$$\psi(x_L, y_L, z_L) = \sum_n \frac{1}{\sqrt{2\pi\hbar v_n}} \Phi_n(y_L, z_L) \left[ a_{Ln} e^{ik_x^{(n)} x_L} + b_{Ln} e^{-ik_x^{(n)} x_L} \right], \quad (1.31)$$

and

$$\psi(x_R, y_R, z_R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m}} \Phi_m(y_R, z_R) \left[ a_{Rm} e^{-ik_x^{(m)} x_R} + b_{Rm} e^{ik_x^{(m)} x_R} \right]. \quad (1.32)$$

Here we label the transport channels in the left and right waveguides by the indices  $n$  and  $m$ , respectively. The corresponding transverse wavefunctions are  $\Phi_n$  and  $\Phi_m$ , and energies of the transverse motion are  $E_n, E_m$ . For any transport channel  $n$  or  $m$ , be it in the left or in the right waveguide, the energy  $E$  fixes the value of the wavevector  $k_x^{(n)} = \sqrt{2m(E - E_n)/\hbar}$ . Transport is due to propagating, not evanescent waves, and  $k_x^{(n)}$  has to be real. Then, only a finite number of open channels,  $N_L$  to the left and  $N_R$  to the right, exists at a fixed energy  $E$ . We explicitly wrote the square roots of velocities  $v_n$  in each channel. This is to assure that the current density does not contain these factors and is expressed in terms of  $a_{Ln}, b_{Ln}$  or  $a_{Rm}, b_{Rm}$  only.

In Eqs. (1.31), (1.32) the coefficients  $a_{Ln}, a_{Rm}$  are the amplitudes of the waves coming from the reservoirs, and  $b_{Ln}, b_{Rm}$  are the amplitudes of the waves transmitted through or reflected back from the scattering region. These coefficients are therefore not independent: The amplitude of the wave reflected from the obstacle linearly depends on the amplitudes of incoming waves in all the channels,

$$b_{\alpha l} = \sum_{\beta=L,R} \sum_{l'} s_{\alpha l, \beta l'} a_{\beta l'}, \quad \beta = L, R, \quad l = n, m. \quad (1.33)$$

The proportionality coefficients are combined into a  $(N_L + N_R) \times (N_L + N_R)$  scattering matrix  $\hat{s}$ . It has the following block structure,

$$\hat{s} = \begin{pmatrix} \hat{s}_{LL} & \hat{s}_{LR} \\ \hat{s}_{RL} & \hat{s}_{RR} \end{pmatrix} \equiv \begin{pmatrix} \hat{r} & \hat{t}' \\ \hat{t} & \hat{r}' \end{pmatrix}. \quad (1.34)$$

The  $N_L \times N_L$  reflection matrix  $\hat{r}$  describes the reflection of the waves

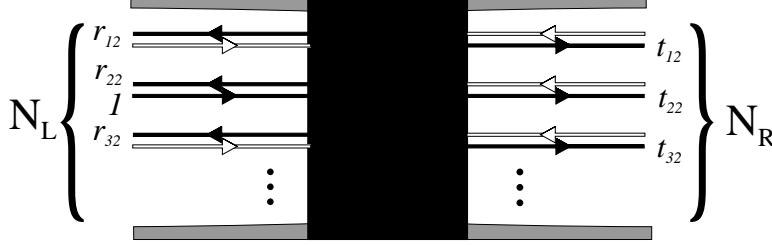


Fig. 1.14. Structure of two-terminal scattering matrix. We show reflection and transmission amplitudes of the electron wave coming from the left in the second transport channel,  $n = 2$ .

coming from the left. Thus,  $r_{nn'}$  is the amplitude of the following process: The electron coming from the left in the transverse channel  $n'$ , is reflected to the channel  $n$ . Consequently,  $|r_{nn'}|^2$  is the probability of this process. The  $N_R \times N_R$  reflection matrix  $\hat{r}'$  describe reflection of particles coming from the right. Finally,  $N_R \times N_L$  transmission matrix  $\hat{t}$  is responsible for the transmission through the scattering region. If magnetic field  $B$  is applied, the elements of the scattering matrix obey the following conditions,  $r_{nn'}(B) = r_{n'n}(-B)$ ,  $r'_{mm'}(B) = r'_{m'm}(-B)$ ,  $t_{mn}(B) = t'_{nm}(-B)$ . In particular, without the magnetic field the transmission matrix  $\hat{t}'$  in Eq. (1.34) is the transpose of the matrix  $t$ .

Any scattering matrix satisfies the unitarity condition,  $\hat{s}^\dagger \hat{s} = \hat{1}$ . The diagonal element of  $\hat{s}^\dagger \hat{s}$  is

$$(\hat{s}^\dagger \hat{s})_{nn} = \sum_{n'} |r_{nn'}|^2 + \sum_m |t_{mn}|^2 = 1, \quad (1.35)$$

since it represents a total probability of an electron in the channel  $n$  to be either reflected or transmitted, to any channel.

*Landauer formula.* We now turn to the calculation of current, with Eq. (1.17) as the starting point. Let us calculate the current through a cross-section located in the left waveguide. The electrons with  $k_x > 0$  originate from the left reservoir, and their filling factor is therefore  $f_L(E)$ . Now, the electrons with  $k_x < 0$  in a given channel  $n$  are coming from

the scattering region. A fraction of these electrons originate from the left reservoir and are reflected; they carry the filling factor  $f_L(E)$ . This fraction is determined by the probability to be reflected to the channel  $n$  from all possible starting channels  $n'$ ,  $R_n(E) = \sum_{n'} |r_{nn'}|^2$ . Other electrons are transmitted through the scattering region, their filling factor being  $f_R(E)$ . The resulting filling factor for  $k_x < 0$  is therefore  $R_n f_L(E) + (1 - R_n) f_R(E)$ . We write for the current

$$\begin{aligned} I &= 2_s e \sum_n \left\{ \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) f_L(E) \right. \\ &+ \left. \int_{-\infty}^0 \frac{dk_x}{2\pi} v_x(k_x) [R_n(E) f_L(E) + (1 - R_n(E)) f_R(E)] \right\} \quad (1.36) \\ &= 2_s e \sum_n \int_0^\infty \frac{dk_x}{2\pi} v_x(k_x) (1 - R_n(E)) [f_L(E) - f_R(E)]. \end{aligned}$$

To derive the last equation line, we have changed  $k_x \rightarrow -k_x$  in the second integral in Eq. (1.36). We use the unitarity relation (1.35) to prove that

$$1 - R_n = \sum_m |t_{mn}|^2 = (\hat{t}^\dagger \hat{t})_{nn}.$$

Now we repeat the trick of the previous Section changing variables from  $k_x$  to  $E$  and arrive at the following expression,

$$I = \frac{2_s e}{2\pi} \int_0^\infty dE \operatorname{Tr} [\hat{t}^\dagger \hat{t}] [f_L(E) - f_R(E)], \quad (1.37)$$

where we have used the short-hand notation

$$\operatorname{Tr} [\hat{t}^\dagger \hat{t}] = \sum_n (\hat{t}^\dagger \hat{t})_{nn}.$$

Alternatively, the trace can be presented as a sum of eigenvalues  $T_p$  of the Hermitian matrix  $\hat{t}^\dagger \hat{t}$ , *transmission eigenvalues*. Because of the unitarity of the scattering matrix,  $T_p$  are real numbers between zero and one.

The transmission eigenvalues depend on energy. However, in the linear regime, when the applied voltage is much smaller than the typical energy scale of this dependence, they can be evaluated at the Fermi surface, and we obtain the expression for conductance,

$$G = G_Q \sum_p T_p(E_F). \quad (1.38)$$

Calculation of current in the right waveguide gives the same result: Current is conserved.

Eq. (1.38) is known as the (two-terminal) *Landauer formula*.

We have derived this relation assuming that the nanostructure is connected to ideal waveguides that support  $N_L$  and  $N_R$  transport channels. Now we can get rid of this unrealistic assumption repeating the reasoning we have used for the QPC. Let us unfold the waveguides so that their cross-sections become infinite: It should not change the transport properties of the nanostructure. The number of transport channels becomes infinite,  $N_L, N_R \rightarrow \infty$ . This means that there are infinitely many transmission eigenvalues. This also means that the total number of transport channels  $N_{L,R}$  is an "unphysical" quantity: It characterizes an auxiliary model rather than the nanostructure, and no transport property of a nanostructure would eventually depend on  $N_{L,R}$ †.

How to reconcile the finite conductance given by Eq. (1.38) with the infinite number of transmission eigenvalues? The implication is that infinitely many transmission eigenvalues are concentrated very close to zero transmission, so that they contribute neither to conductance nor to any other transport property.

To evaluate the transmission eigenvalues of a given nanostructure, one solves the Schrödinger equation in the scattering region and matches the two asymptotics (1.31), (1.32), extracting the scattering matrix. The solutions depend on all the details like location of gates and barriers and the given configuration of the disorder. Even for relatively simple systems, this is a time-consuming task, without much intellectual impact: A calculation for a given system does not give us an idea what the result would be if we add a gate or move a tunnel barrier. Moreover, the calculation will give a different result for a different configuration of disorder.

This makes it important to comprehend the general properties of transmission eigenvalues, those depending on the system design rather than on the details.

*One channel.* Let us start with a simple example: a scatterer that can transmit only one transport channel (for a given energy). All but one transmission eigenvalues are zero. The structure is thus characterized by a single transmission eigenvalue  $T$ . This is precisely the transmission coefficient we have discussed for the tunnel barrier in Section 1.1;  $R = 1 -$

† Confusingly enough, this "number of transport channels" is commonly used in literature to characterize the area of the (narrowest) cross-section of a nanostructure.

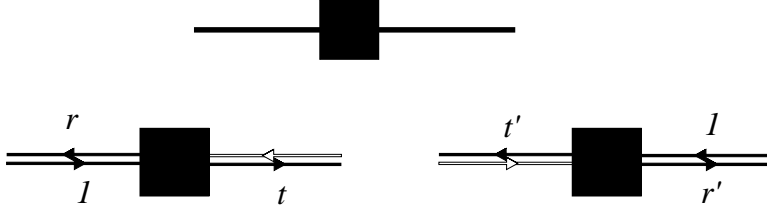


Fig. 1.15. One channel scatterer: notation, the transmission and reflection amplitudes of the waves coming from the left and from the right.

$T$  is the reflection coefficient. The scattering matrix is a  $2 \times 2$  matrix and contains more parameters, since in Eq. (1.34)  $r$ ,  $r'$ , and  $t$  are complex numbers, constrained by the conditions of unitarity (Fig. 1.15). There are three independent parameters  $T$ ,  $\theta$ , and  $\eta$ ,

$$\hat{s} = \begin{pmatrix} \sqrt{R}e^{i\theta} & \sqrt{T}e^{i\eta} \\ \sqrt{T}e^{i\eta} & -\sqrt{R}e^{i(2\eta-\theta)} \end{pmatrix}. \quad (1.39)$$

The phases  $\theta$  and  $\eta$  do not manifest itself in the transport in a single nanostructure of this type. As we show in Section ???, these phases are relevant if we combine two structures producing quantum interference effects.

For the ideal systems we considered previously — a rectangular potential barrier and a QPC — the scattering does not mix different transport channels. An electron in the channel  $n$  can be either reflected back and stay in the same channel, or be transmitted through the barrier and end up in an identical channel at the other side. Therefore the matrix of such an ideal system is *block-diagonal* — the matrices  $r$ ,  $r'$ ,  $t$ , and, importantly,  $t^\dagger t$  are diagonal. Thus, the transmission eigenvalues for these systems are just the transmission coefficients in the channels.

*Distribution of transmission eigenvalues.* The transmission eigenvalues  $T_p$  depend on disorder configuration and therefore are random (Fig. 1.16). We need a quantity that characterizes *design* of a nanostructure rather than a concrete disorder configuration. This is provided by the distribution function of transmission eigenvalues (transmission distribution)  $P(T)$ . Suppose we make an ensemble of nanostructures sharing an identical design and differing in disorder configurations. Each nanostructure provides a set of transmission eigenvalues. Let us concentrate on a narrow interval of transmissions from  $T$  to  $T + dT$ , count the number of transmission eigenvalues that fall into this interval, and divide this by the total number of nanostructures. In the limit of a big ensemble

ble, the result converges to  $P(T)dT$ . Mathematically, the transmission distribution is thus defined as follows,

$$P(T) = \left\langle \sum_p \delta(T - T_p(E)) \right\rangle. \quad (1.40)$$

The angular brackets in above relation mean the ensemble average, that is, the average over all formally identical nanostructures in the ensemble. The function  $P(T)$  facilitates evaluating other averages. The average of an arbitrary function of the transmission eigenvalues becomes

$$\left\langle \sum_p f(T_p) \right\rangle = \int_0^1 dT f(T)P(T). \quad (1.41)$$

In particular, one integrates  $TP(T)$  to obtain the average conductance  $\langle G \rangle$ .

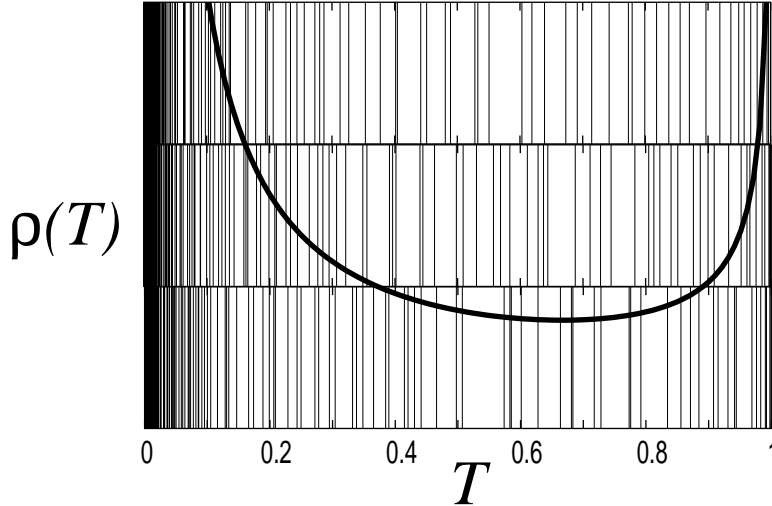


Fig. 1.16. Transmission eigenvalues. We show the transmission eigenvalues for three disorder realization of a diffusive conductor with nominal resistance of  $350\Omega$ . The transmission distribution (thick solid line) is given by Eq. 1.43.

What is the use of the above relation? If the average conductance of a nanostructure much exceeds the conductance quantum,  $\langle G \rangle \gg G_Q$ , the transmission eigenvalues are dense, the typical spacing between the eigenvalues being much less than one. This means that the sums over transmission eigenvalues can be replaced by the integrals according to



Eq. (1.41). The transport properties are thus *self-averaged* in this limit, their fluctuations being much smaller than the average values. The transport properties appear to be almost insensitive to a specific disorder configuration. The fluctuations of transport properties may become significant if  $\langle G \rangle \simeq G_Q$ , and the transmission eigenvalues are sparse.

A fair part of this book either quantifies the transmission distribution or makes use of it. In the rest of this Section, we provide examples of  $P(T)$  without quantifying it.

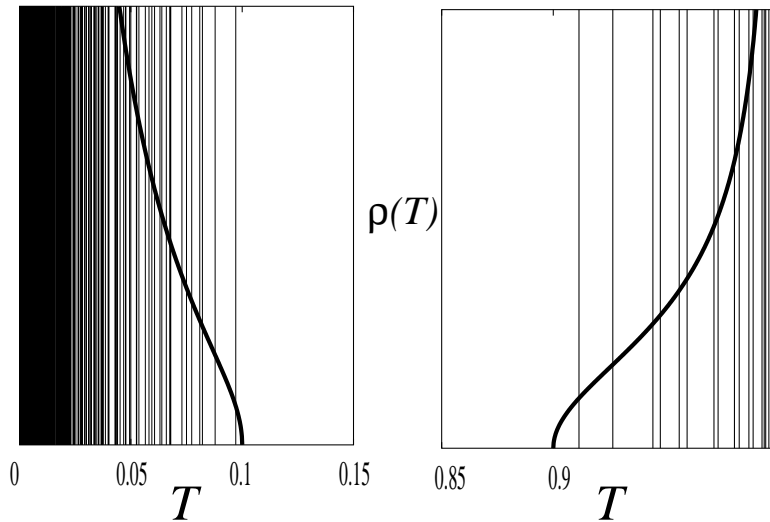


Fig. 1.17. Examples of transmission distribution. Left: tunnel junction in series with a diffusive conductor of a small resistance. Right: QPC with 20 open channels in series with a diffusive conductor.

Let us start with a QPC and consider energy at which a finite number  $N_{open}$  of transport channels are open ( $T = 1$ ). An infinite number of channels are closed ( $T = 0$ ). The corresponding transmission distribution consists of two delta-functional peaks,

$$P(T) = N_{open}\delta(1 - T) + \infty \delta(T).$$

Closed channels do not play any role in transport, and the part with the open channels leads to the expression for the conductance,  $G = G_Q N_{open}$  we have already seen. We will ignore the part proportional to  $\delta(T)$  and write for a clean QPC

$$P_{QPC}(T) = N_{open}\delta(1 - T). \quad (1.42)$$

The transmission eigenvalues in a clean QPC are highly degenerate. If we add a small number of defects to the QPC, this degeneracy is lifted. The scattering at the defects mixes the channels: An incident electron in the open channel  $n$  which without scattering would pass the constriction, can now be reflected to any channel  $n'$ , or be transmitted to an arbitrary channel  $m$ . These processes modify the transmission matrix, and, consequently, the transmission eigenvalues. If such channel mixing is weak so that the probabilities to scatter from open channels are small, we expect that all transmission eigenvalues remain close to 1. The role of disorder is thus to lift the degeneracy (see Fig. 1.17). This regime is realized when the contribution of disorder to the total conductance of the system is sufficiently small, the resistance  $R$  due to defects being much smaller than the resistance of the QPC. At further increase of resistance  $R$  to values of the order of  $1/G_{QPC}$  the transmission eigenvalues are spread over the whole interval  $0 < T < 1$ .

A complementary example is a *tunnel junction*. Let us take a sufficiently wide ideal potential barrier at an energy much below the top energy of the barrier. All the transmission coefficients are guaranteed to be small,  $T \ll 1$ . If the channels do not mix, the transmission eigenvalues are just these coefficients and the transmission distribution concentrates near  $T = 0$ . If we add some defects next to the barrier, the channels mix. Some electrons after being reflected from the barrier are reflected by defects back to the barrier. They just get the "second chance" to tunnel through. Because of this, some transmission eigenvalues grow with increasing the defect resistance  $R$ . Similarly to QPC, the transmission eigenvalues are spread over the whole interval  $0 < T < 1$  if  $R$  is comparable with the resistance of the tunnel junction.

Let us add more defects. At some stage, the resistance due to the defects dominate the total resistance. At this point, we can forget about a QPC or a tunnel junction present in the structure. The electron that traverses the scattering region experiences many scattering events at the defects. Its motion is highly random. This corresponds to *diffusion* provided the conductance of the structure still exceeds much the conductance quantum. The transmission distribution in a diffusive structure appears to be universal — not depending of the details of the structure design (Fig. 1.16),

$$\rho = \frac{\langle G \rangle}{2G_Q} \frac{1}{T\sqrt{1-T}} \quad (1.43)$$

The integral of the transmission distribution over  $T$  gives the total num-

ber of transport channels. This integral diverges for the bimodal distribution (1.43) indicating an infinite number of channels that may take part in diffusive transport.

#### Advanced Material

*Q. The derivation of the Landauer formula you present is difficult to generalize in order to treat the current fluctuations. Is there a different formulation, more suitable for this purpose?*

*A.* We treat current fluctuations (noise) in the next Section. Here we present the operator formulation of the scattering approach and re-derive the Landauer formula. We follow the derivation of Ref. [4].

An arbitrary wavefunction in the left waveguide is represented as a sum of plane waves (1.31). These plain waves, however, do not form a basis, since they only represent asymptotic expressions of wavefunctions, which have complicated form in the scattering region and do not have to be orthogonal. What does form a basis is a set of *scattering states* — the states which originate from the reservoirs as plane waves and then are partially transmitted through the barrier and partially reflected back. The scattering state originated from the left reservoir has the form

$$\begin{aligned} \psi_{Ln}(x_L, y_L, z_L) &= \frac{1}{\sqrt{2\pi\hbar v_n(E)}} \Phi_n(y_L, z_L) e^{ik_x^{(n)} x_L} \\ &+ \sum_{n'} \frac{1}{\sqrt{2\pi\hbar v_{n'}(E)}} r_{n'n}(E) \Phi_{n'}(y_L, z_L) e^{-ik_x^{(n')} x_L}, \end{aligned} \quad (1.44)$$

in the left waveguide, and

$$\psi_{Ln}(x_R, y_R, z_R) = \sum_m \frac{1}{\sqrt{2\pi\hbar v_m(E)}} t_{mn}(E) \Phi_m(y_R, z_R) e^{-ik_x^{(m)} x_R} \quad (1.45)$$

in the right waveguide. Analogously, there are scattering states  $\psi_{Rm}$  originating from the right reservoir. All these states are orthogonal and complete and thus form a basis.

For each of these states, we can introduce creation and annihilation operators. Let us introduce the creation operators  $\hat{a}_{Ln}^\dagger(E)$  and  $\hat{a}_{Rm}^\dagger$  which create electrons in the scattering states with the energy  $E$ , originating from the left reservoir in the transport channel  $n$ , and from the right reservoir in the transport channel  $m$ , respectively. The conjugated operators  $\hat{a}_{Ln}(E)$  and  $\hat{a}_{Rm}$  annihilate particles in the same states. The operators  $\hat{a}^\dagger$ ,  $\hat{a}$  refer to a basis and therefore are sufficient for the quantum-mechanical description of the system.

However, for convenience we introduce another set of operators. The operator  $\hat{b}_{Ln}^\dagger(E)$  creates an electron with the energy  $E$  in the transport channel  $n$  in the left waveguide moving to the left. A similar creation operator for right-movers in the right waveguide is  $\hat{b}_{Rm}^\dagger(E)$ , and the annihilation operators are  $\hat{b}_{Ln}(E)$  and  $\hat{b}_{Rm}(E)$ . These operators are linearly related to the set  $\hat{a}$  via the scattering matrix,

$$\begin{aligned}\hat{b}_{\alpha l}(E) &= \sum_{\beta=L,R} \sum_{l'} s_{\alpha l, \beta l'}(E) \hat{a}_{\beta l'}(E); \\ \hat{b}_{\alpha l}^\dagger(E) &= \sum_{\beta=L,R} \sum_{l'} s_{\beta l', \alpha l}^\dagger(E) \hat{a}_{\beta l'}^\dagger(E), \quad \alpha = L, R, \quad l = n, m.\end{aligned}\tag{1.46}$$

Since electrons are fermions, the operators  $\hat{a}$  obey anticommutation relations,

$$\begin{aligned}\hat{a}_{\alpha l}^\dagger(E) \hat{a}_{\beta l'}(E') + \hat{a}_{\beta l'}(E') \hat{a}_{\alpha l}^\dagger(E) &= \delta_{\alpha\beta} \delta_{ll'} \delta(E - E'); \\ \hat{a}_{\alpha l}(E) \hat{a}_{\beta l'}(E') + \hat{a}_{\beta l'}(E') \hat{a}_{\alpha l}(E) &= 0; \\ \hat{a}_{\alpha l}^\dagger(E) \hat{a}_{\beta l'}^\dagger(E') + \hat{a}_{\beta l'}^\dagger(E') \hat{a}_{\alpha l}^\dagger(E) &= 0.\end{aligned}\tag{1.47}$$

The relations (1.47) take place since the scattering states form a basis. In the same way, the states describing left-moving electrons in the left waveguide and right-moving electrons in the right waveguide, also form a basis, and similar relations hold between the operators  $\hat{b}$  and  $\hat{b}^\dagger$ . However, the operators  $\hat{a}$  and  $\hat{b}$  do not obey such relations, as evident from Eq. (1.46).

Now we consider the quantum-mechanical averages of the products of creation and annihilation operators. Since the right-moving particles in the left waveguide originate from the left reservoir, and we have

$$\left\langle \hat{a}_{\alpha l}^\dagger(E) \hat{a}_{\beta l'}(E') \right\rangle = \delta_{\alpha\beta} \delta_{ll'} \delta(E - E') f_\alpha(E), \quad \alpha = L, R.\tag{1.48}$$

The average product of two creation or two annihilation operators is always zero.

Let us proceed by writing down the field operators  $\hat{\Psi}(\mathbf{r}, t)$  and  $\hat{\Psi}^\dagger(\mathbf{r}, t)$ , which annihilate and create the electron at a given point and time moment. In the left waveguide, we have

$$\begin{aligned}\hat{\Psi}(\mathbf{r}, t) &= \int dE e^{-iEt\hbar} \sum_n \frac{\Phi_n(y_L, z_L)}{\sqrt{2\pi\hbar v_n(E)}} \left[ \hat{a}_{Ln} e^{ik_x^{(n)} x_L} + \hat{b}_{Ln} e^{-ik_x^{(n)} x_L} \right]; \\ \hat{\Psi}^\dagger(\mathbf{r}, t) &= \int dE e^{iEt\hbar} \sum_n \frac{\Phi_n^*(y_L, z_L)}{\sqrt{2\pi\hbar v_n(E)}} \left[ \hat{a}_{Ln}^\dagger e^{-ik_x^{(n)} x_L} + \hat{b}_{Ln}^\dagger e^{ik_x^{(n)} x_L} \right].\end{aligned}$$

The basic course of quantum mechanics teaches us that if we know the

wavefunction of the system, we can write down the expression for the current density. Now, the formulae for the field operators enables us to write the operator of current in the left waveguide,

$$\hat{I}(x_L, t) = \frac{\hbar e}{2im} \int dy_L dz_L \left[ \hat{\Psi}^\dagger \frac{\partial}{\partial x_L} \hat{\Psi} - \left( \frac{\partial}{\partial x_L} \hat{\Psi}^\dagger \right) \hat{\Psi} \right]. \quad (1.49)$$

To calculate the average current, we only need to know the *time-averaged* current operator. To avoid dealing with ill-defined delta-functions, we perform the following trick. Imagine that all the quantities are periodic in time with the period  $\mathcal{T} \rightarrow \infty$ . The allowed values of energy are then found from the condition that the exponents of the type  $\exp(iEt)$  are also periodic, hence  $E = 2\pi q\hbar/\mathcal{T}$  with an integer  $q$ . Consequently, we replace  $\int dE$  by  $2\pi\hbar/\mathcal{T} \sum_n$ . Using

$$\left\langle e^{i(E-E')t} \right\rangle_t = \delta_{qq'},$$

where the angular brackets here denote the time-average. This means that in the expression for the current (1.49) both field operators must be evaluated at the same energy. We obtain

$$\left\langle \hat{I} \right\rangle_t = \frac{G_Q}{e} \left( \frac{2\pi\hbar}{\mathcal{T}} \right)^2 \sum_n \sum_E \left[ \hat{a}_{Ln}^\dagger(E) \hat{a}_{Ln}(E) - \hat{b}_{Ln}^\dagger(E) \hat{b}_{Ln}(E) \right]. \quad (1.50)$$

Eq. (1.50) has an easy interpretation: The current in the left waveguide is the number of particles moving to the right (represented by  $\hat{a}^\dagger \hat{a}$ ) minus the number of particles moving to the left ( $\hat{b}^\dagger \hat{b}$ ), summed over all channels and energies.

Eliminating  $\hat{b}$  in favour of  $\hat{a}$ , we write

$$\begin{aligned} \left\langle \hat{I} \right\rangle_t &= \frac{G_Q}{e} \left( \frac{2\pi\hbar}{\mathcal{T}} \right)^2 \sum_n \sum_{\alpha\beta, ll'} \sum_E \hat{a}_{\alpha l}^\dagger(E) \hat{a}_{\beta l'}(E) \\ &\times \left[ \delta_{\alpha L} \delta_{\beta L} \delta_{nl} \delta_{n'l'} - s_{\alpha l, Ln}^*(E) s_{Ln, \beta l'}(E) \right]. \end{aligned} \quad (1.51)$$

The last step is to perform the quantum-mechanical average of Eq. (1.51) and to find the average current. At first glance, this makes no sense, since according to Eq. (1.48) the average of the product of two operators taken at the same energy is infinite. However, for the discretized energies we have to replace the delta-function by the Kronecker delta-symbol,

$$\delta(E - E') \rightarrow \frac{\mathcal{T}}{2\pi\hbar} \delta_{qq'}.$$

This cancels one factor of  $\mathcal{T}$ . Now we can take the limit  $\mathcal{T} \rightarrow \infty$  and from the discrete sum come back to the integral over energies. Taking into account that the averaging procedure yields  $\alpha = \beta$ ,  $l = l'$ , and using the unitarity condition (1.35), we safely arrive to the Landauer formula Eq. (1.37).

*Q. Smth about the relation between scattering matrices and Green's functions.*

*A.*

*Q. Smth about recursive Green's functions?*

*A.*