

# 1 Transfer Matrix

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In this chapter we introduce and discuss a mathematical method for the analysis of the wave propagation in one-dimensional systems. The method uses the transfer matrix and is commonly known as the *transfer matrix* method [7, 29].

The transfer matrix method can be used for the analysis of the wave propagation of quantum particles, such as electrons [29, 46, 49, 81, 82, 115–117, 124, 103, 108, 131, 129, 141] and of electromagnetic [39, 123, 124], acoustic, and elastic waves. Once this technique is developed for one type of wave, it can easily be applied to any other wave problem.

First we will treat the scattering from an arbitrary one-dimensional potential. Usually, one writes the amplitudes of the waves to the left side of the potential in terms of those on the right side. This defines the *transfer matrix*  $\mathbf{M}$ . Since we work in a one-dimensional system, the wave in both the left and right sides of the potential has two components, one moving to the right and one moving to the left. Therefore, the transfer matrix  $\mathbf{M}$  is a  $2 \times 2$  matrix. The  $2 \times 2$  *scattering matrix*  $\mathbf{S}$  will also be introduced; it describes the outgoing waves in terms of the ingoing waves. The relationship between the transfer and scattering matrices will be introduced. Time-reversal invariance and conservation of the current density impose strong conditions on the form of the transfer matrix  $\mathbf{M}$ , regardless of the specific form of the potential. Through the transfer matrix formalism, the transmission and reflection amplitudes can easily be defined and evaluated. Both traveling and standing (bound) waves will be examined.

Once the transfer matrix is calculated for one potential, it can be easily extended to calculate analytically the transfer matrix for  $N$  identical potentials [39, 165]. As the number of potentials increases, the traveling waves give rise to pass bands, while the standing or bound waves give rise to gaps in the energy spectrum of the system.

The appearance of bands and gaps is a common characteristic of wave propagation in periodic media. Bands and gaps appear in electronic systems [1, 3, 4, 11, 17, 23, 30], photonic crystals (electromagnetic waves) [33–36, 39], phononic crystals (acoustic waves), and left-handed materials. The transfer matrix formalism is also very useful in calculating reflection and transmission properties of disordered random systems [49, 59, 89, 90, 103, 108, 124, 129].

## 1.1 A Scattering Experiment

Perhaps the simplest problem in quantum mechanics is the one-dimensional propagation of an electron in the presence of a localized potential. The motion of a quantum particle of mass  $m$  in the presence of a potential  $V(x)$  in one dimension is governed by Schrödinger's equation [7, 25, 30]

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + [V(x) - E] \Psi(x) = 0. \quad (1.1)$$

Here,  $\Psi(x)$  is the *wave function* and  $E$  the energy of the electron.

In the absence of a potential, the electron is a wave that travels along in a particular direction. In the presence of a potential, we would like to know how the propagation of the electron changes. Can the electron reflect back? Can the electron pass through the potential? These questions illustrate some quantum effects not present in classical physics.

For simplicity, we assume that the potential  $V(x)$  is nonzero only inside a finite region,

$$V(x) = \begin{cases} V(x) & \text{for } 0 \leq x \leq \ell, \\ 0 & \text{for } x < 0 \text{ and } x > \ell. \end{cases} \quad (1.2)$$

An electron approaches the sample represented by the potential  $V(x)$  from either the left or the right side of the potential and is scattered by the sample. Scattering means that the electron is either reflected back or transmitted through the sample. We can measure the transmission and reflection amplitudes,  $t$  and  $r$ , respectively (they will be defined later), and from  $t$  and  $r$  we can extract information about the physical properties of the sample.

We assume that Schrödinger's equation outside the potential region is known and that it can be written as a superposition of plane waves:

$$\begin{aligned} \Psi_L(x) &= \Psi_L^+(x) + \Psi_L^-(x), \quad x \leq 0, \\ \Psi_R(x) &= \Psi_R^+(x) + \Psi_R^-(x), \quad x \geq \ell. \end{aligned} \quad (1.3)$$

Here, the subscripts L (Left) and R (Right) indicate the position of the particle with respect to the potential region, and the superscripts + (–) determine the direction of propagation: + means that the electron propagates in the positive direction (from left to right) and – means that the electron moves from right to left (see figure 1.1). Thus,  $\Psi_L^+(x)$  is the wave function of the electron left of the sample, propagating to the right; hence it is approaching the sample. We call  $\Psi_L^+(x)$  the *incident* wave, in contrast to  $\Psi_L^-(x)$ , which is the wave function of the electron propagating away from the sample toward the left side.

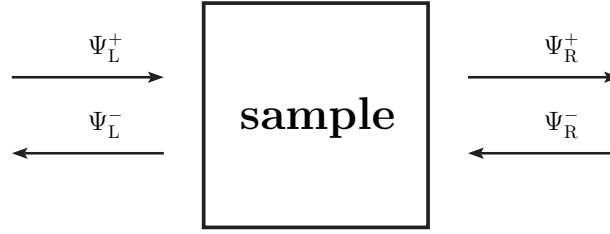


FIGURE 1.1. A typical scattering experiment. Incident waves  $\Psi_L^+(x)$  and  $\Psi_R^-(x)$  are scattered by the sample, characterized by the potential  $V(x)$ . Outgoing waves  $\Psi_L^-(x)$  and  $\Psi_R^+(x)$  consist of waves transmitted through the sample as well as waves reflected from the sample. Outside the sample, the wave function can be expressed as a superposition of plane waves given by equations (1.3) and (1.4).

The components of the wave function can be expressed as

$$\begin{aligned} \Psi_L^+(x) &= Ae^{+iqx}, & \Psi_L^-(x) &= Be^{-iqx}, \\ \Psi_R^+(x) &= Ce^{+iqx}, & \Psi_R^-(x) &= De^{-iqx}. \end{aligned} \quad (1.4)$$

Here,  $q$  is the *wave vector* related to the energy,  $E$  of the electron through the *dispersion relation*

$$E = E(q). \quad (1.5)$$

The dispersion relation (1.5) determines the physical properties of the electron in the region outside the sample ( $x < 0$  and  $x > \ell$ ). We will call these regions *leads*. To guarantee the plane wave propagation of the particle, i.e., equation (1.4), we require that both leads are translationally invariant. In the simplest cases, we will represent both leads as free space. Then  $q = k$  and  $k$  is related to the energy of the free particle,

$$E = \frac{\hbar^2 k^2}{2m}. \quad (1.6)$$

More general realizations of leads, for instance consisting of periodic media, will be discussed later. In this book, we assign  $k$  to the free-particle wave vector and use  $q$  for more general cases.

## 1.2 Scattering Matrix and Transfer Matrix

The general solution  $\Psi(x)$  of the Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + [V(x) - E] \Psi(x) = 0 \quad (1.7)$$

must be a continuous function of the position  $x$ . The same must be true for the first derivative  $\partial \Psi(x)/\partial x$ . In particular, the requirement of the continuity of the wave function

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and its derivative at the boundaries of the potential  $V(x)$  gives

$$\Psi_L(x=0^-) = \Phi(x=0^+), \quad \left. \frac{\partial \Psi_L(x)}{\partial x} \right|_{x=0^-} = \left. \frac{\partial \Phi(x)}{\partial x} \right|_{x=0^+} \quad (1.8)$$

on the left boundary of the sample, and

$$\Psi_R(x=\ell^+) = \Phi(x=\ell^-), \quad \left. \frac{\partial \Psi_R(x)}{\partial x} \right|_{x=\ell^+} = \left. \frac{\partial \Phi(x)}{\partial x} \right|_{x=\ell^-} \quad (1.9)$$

on the right boundary. Here,  $\Phi(x)$  is the solution of Schrödinger's equation *inside* the potential region  $0 \leq x \leq \ell$ . Generally,  $\Phi(x)$  cannot be expressed as a simple superposition of propagating waves.

We can, in principle, solve Schrödinger's equation (1.7) and find explicit expressions for the wave functions for any position  $x$ , including the region of the scattering potential. However, this is possible only in very few special cases, since the Schrödinger equation is not analytically solvable for a general form of the potential  $V(x)$ . In many cases, however, it is sufficient to know only the form of the wave function *outside* the potential region. This problem is much easier, since the wave function consists only of a superposition of plane waves, as discussed in equations (1.3) and (1.4). However, we need to estimate the coefficients  $A$ – $D$ , defined in equation (1.4). This can be done if we know the right-hand sides of the four equations (1.8) and (1.9). Thus, the wave function outside the sample is fully determined by the four parameters that describe the scattering properties of the sample.

In general, linear relations between outgoing and incoming waves can be written as

$$\begin{pmatrix} \Psi_L^-(x=0) \\ \Psi_R^+(x=\ell) \end{pmatrix} = \mathbf{S} \begin{pmatrix} \Psi_L^+(x=0) \\ \Psi_R^-(x=\ell) \end{pmatrix}, \quad (1.10)$$

where the matrix  $\mathbf{S}$ ,

$$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}, \quad (1.11)$$

is called the *scattering matrix*. By definition, the matrix  $\mathbf{S}$  relates the *outgoing* waves to the *incoming* waves as shown in figure 1.1. Its elements completely characterize the scattering and transmission properties of the one-dimensional potential  $V(x)$ .

We can also define the *transfer matrix*  $\mathbf{M}$  by the relation

$$\begin{pmatrix} \Psi_R^+(x=\ell) \\ \Psi_R^-(x=\ell) \end{pmatrix} = \mathbf{M} \begin{pmatrix} \Psi_L^+(x=0) \\ \Psi_L^-(x=0) \end{pmatrix}. \quad (1.12)$$

The matrix  $\mathbf{M}$  expresses the coefficients of the wave function on the *right-hand* side of the sample in terms of the coefficients of the wave function on the *left-hand* side.

While the representation in terms of the scattering matrix  $\mathbf{S}$  can be easily generalized to three-dimensional systems, the transfer matrix approach is more appropriate for the

analysis of one-dimensional systems and will be used frequently in the following chapters. On the other hand, physical properties of the scattering are formulated more easily by the  $\mathbf{S}$  matrix.

By comparing the linear equations (1.10) and (1.12), it is easy to express the elements of the transfer matrix  $\mathbf{M}$  in terms of the elements of the scattering matrix  $\mathbf{S}$  (see problem 1.1):

$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} S_{21} - \frac{S_{22} S_{11}}{S_{12}} & \frac{S_{22}}{S_{12}} \\ -\frac{S_{11}}{S_{12}} & \frac{1}{S_{12}} \end{pmatrix}. \quad (1.13)$$

Equivalently, we can express the elements of the scattering matrix  $\mathbf{S}$  in terms of the elements of the transfer matrix:

$$\mathbf{S} = \begin{pmatrix} -\frac{M_{21}}{M_{22}} & \frac{1}{M_{22}} \\ M_{11} - \frac{M_{12} M_{21}}{M_{22}} & \frac{M_{12}}{M_{22}} \end{pmatrix}. \quad (1.14)$$

The scattering matrix  $\mathbf{S}$  contains four complex parameters. In general, the matrix  $\mathbf{S}$  is fully determined by eight real parameters. However, when solving a given physical problem, we can use its *physical symmetries* to reduce the number of independent parameters. Two symmetries—conservation of the current density and time-reversal symmetry—will be discussed in the following sections.

### 1.2.1 Conservation of the Current Density

For the time-independent problems discussed in this chapter, the total number of particles in the potential region,

$$\int_0^\ell \Psi^* \Psi \, dx, \quad (1.15)$$

is constant. For this case, in section 1.5.1 we derive the result that the current density entering the sample from one side must be equal to the current density that leaves the sample on the other side:

$$j(x=0) = j(x=\ell). \quad (1.16)$$

We remind the reader that the current density  $j(x)$  is defined as

$$j(x) = \frac{\hbar i}{2m} \left[ \Psi(x) \frac{\partial \Psi^*(x)}{\partial x} - \Psi^*(x) \frac{\partial \Psi(x)}{\partial x} \right]. \quad (1.17)$$

Using the definition of the current density, equation (1.17) and the expression for the current density for a plane wave,  $j = (\hbar q/m)|\Psi|^2$ , derived later in section 1.5.1, we can express the current density on both sides of the sample [equation (1.16)] as

$$j_L = \frac{\hbar q}{m} (|\Psi_L^+|^2 - |\Psi_L^-|^2) = \frac{\hbar q}{m} (|\Psi_R^+|^2 - |\Psi_R^-|^2) = j_R, \quad (1.18)$$

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which are equal in magnitude, according to equation (1.16). Note that the current does not depend on  $x$ . Equation (1.18) can be rewritten in a more convenient form as

$$|\Psi_L^-|^2 + |\Psi_R^+|^2 = |\Psi_L^+|^2 + |\Psi_R^-|^2, \quad (1.19)$$

or, in vector notation

$$(\Psi_L^{-*} \ \Psi_R^{+*}) \begin{pmatrix} \Psi_L^- \\ \Psi_R^+ \end{pmatrix} = (\Psi_L^{+*} \ \Psi_R^{-*}) \begin{pmatrix} \Psi_L^+ \\ \Psi_R^- \end{pmatrix}, \quad (1.20)$$

where  $\Psi^*$  is the complex conjugate of  $\Psi$ .

Now we use equation (1.10), which relates the outgoing waves  $\Psi_L^-$  and  $\Psi_R^+$  with the incoming waves  $\Psi_L^+$  and  $\Psi_R^-$ . For complex conjugate waves, the relation (1.10) reads

$$(\Psi_L^{-*} \ \Psi_R^{+*}) = (\Psi_L^{+*} \ \Psi_R^{-*}) \mathbf{S}^\dagger, \quad (1.21)$$

where the conjugate matrix  $\mathbf{S}^\dagger$  is defined in appendix A as the matrix

$$\mathbf{S}^\dagger = \begin{pmatrix} S_{11}^* & S_{21}^* \\ S_{12}^* & S_{22}^* \end{pmatrix}. \quad (1.22)$$

Inserting (1.10) and (1.21) into equation (1.20), we obtain the identity

$$(\Psi_L^{+*} \ \Psi_R^{-*}) \mathbf{S}^\dagger \mathbf{S} \begin{pmatrix} \Psi_L^+ \\ \Psi_R^- \end{pmatrix} = (\Psi_L^{+*} \ \Psi_R^{-*}) \begin{pmatrix} \Psi_L^+ \\ \Psi_R^- \end{pmatrix}. \quad (1.23)$$

The relation (1.23) must be valid for any incoming wave. This can be guaranteed only if the scattering matrix satisfies the relation

$$\mathbf{S}^\dagger \mathbf{S} = \mathbf{1}, \quad (1.24)$$

which means that the scattering matrix is *unitary*.

The explicit form of equation (1.24) is given by

$$\begin{pmatrix} S_{11}^* & S_{21}^* \\ S_{12}^* & S_{22}^* \end{pmatrix} \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.25)$$

After matrix multiplication, we obtain the following relationships between the matrix elements of the scattering matrix:

$$\begin{aligned} |S_{11}|^2 + |S_{21}|^2 &= 1, & |S_{22}|^2 + |S_{12}|^2 &= 1, \\ S_{11}^* S_{12} + S_{21}^* S_{22} &= 0, & S_{12}^* S_{11} + S_{22}^* S_{21} &= 0. \end{aligned} \quad (1.26)$$

Note, from equation (1.24) it follows also (see problem 1.2) that

$$|\det \mathbf{S}| = 1. \quad (1.27)$$

Equation (1.24) can be also written as

$$\mathbf{S}^\dagger = \mathbf{S}^{-1}. \quad (1.28)$$

Using the expression for the inverse matrix, given by equation (A.9) we obtain

$$\begin{pmatrix} S_{11}^* & S_{21}^* \\ S_{12}^* & S_{22}^* \end{pmatrix} = \frac{1}{\det \mathbf{S}} \begin{pmatrix} S_{22} & -S_{21} \\ -S_{12} & S_{11} \end{pmatrix}. \quad (1.29)$$

Comparison of the matrix elements of equation (1.29) gives some additional useful relationships for the matrix elements of the scattering matrix:

$$|S_{11}| = |S_{22}|. \quad (1.30)$$

Then, from the third and fourth equations (1.26) we obtain that

$$|S_{12}| = |S_{21}|. \quad (1.31)$$

The conservation of the current density also introduces a relationship between the elements of the transfer matrix  $\mathbf{M}$ . We can derive them beginning with equation (1.18), describing the conservation of the current density,

$$|\Psi_L^+|^2 - |\Psi_L^-|^2 = |\Psi_R^+|^2 - |\Psi_R^-|^2. \quad (1.32)$$

It is easy to verify that equation (1.32) can be rewritten in the vector form as

$$(\Psi_L^{+*} \ \Psi_L^{-*}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix} = (\Psi_R^{+*} \ \Psi_R^{-*}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \Psi_R^+ \\ \Psi_R^- \end{pmatrix}. \quad (1.33)$$

Now we use the definition of the transfer matrix, equation (1.12), and its conjugate form

$$(\Psi_R^{+*} \ \Psi_R^{-*}) = (\Psi_L^{+*} \ \Psi_L^{-*}) \mathbf{M}^\dagger \quad (1.34)$$

to obtain

$$(\Psi_L^{+*} \ \Psi_L^{-*}) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix} = (\Psi_L^{+*} \ \Psi_L^{-*}) \mathbf{M}^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathbf{M} \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix}. \quad (1.35)$$

Since this relation should hold for any wave function  $\Psi_L^+$  and  $\Psi_L^-$ , we obtain the relationship [29, 103, 108, 129, 141]

$$\mathbf{M}^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathbf{M} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.36)$$

The explicit form of equation (1.36) is given by

$$\begin{pmatrix} M_{11}^* & M_{21}^* \\ M_{12}^* & M_{22}^* \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (1.37)$$

which means that the elements of the transfer matrix satisfy the following relations:

$$\begin{aligned} |M_{11}|^2 - |M_{21}|^2 &= 1, & |M_{22}|^2 - |M_{12}|^2 &= 1, \\ M_{11}^* M_{12} - M_{21}^* M_{22} &= 0, & M_{12}^* M_{11} - M_{22}^* M_{21} &= 0. \end{aligned} \quad (1.38)$$

### 1.2.2 Time-Reversal Symmetry

Physical systems that are symmetric with respect to an inversion of time possess another symmetry which further reduces the number of independent parameters of the matrices  $\mathbf{S}$  and  $\mathbf{M}$ .

If the system possesses time-reversal symmetry and if  $\Psi(x)$  is a solution of Schrödinger's equation, then its complex conjugate  $\Psi^*(x)$  is also a solution. In our special case, the wave functions *outside* the potential region are expressed as plane waves given by equations (1.3) and (1.4). The complex conjugate of the wave

$$\phi(x) = e^{iqx} \quad (1.39)$$

is the wave

$$\phi^*(x) = e^{-iqx}, \quad (1.40)$$

which propagates in the opposite direction. This means that, after time reversal, we have the same physical system as before, but the incoming waves are  $\Psi_L^{-*}$  and  $\Psi_R^{+*}$  and the outgoing waves are  $\Psi_L^{+*}$  and  $\Psi_R^{-*}$ . Since the scattering matrix  $\mathbf{S}$  relates *any* incoming waves to the outgoing waves, we obtain

$$\begin{pmatrix} \Psi_L^{+*} \\ \Psi_R^{-*} \end{pmatrix} = \mathbf{S} \begin{pmatrix} \Psi_L^{-*} \\ \Psi_R^{+*} \end{pmatrix}. \quad (1.41)$$

On the other hand, the complex conjugate of equation (1.10) reads

$$\begin{pmatrix} \Psi_L^{-*} \\ \Psi_R^{+*} \end{pmatrix} = \mathbf{S}^* \begin{pmatrix} \Psi_L^{+*} \\ \Psi_R^{-*} \end{pmatrix}. \quad (1.42)$$

Now, inserting equation (1.42) into equation (1.41), we obtain

$$\begin{pmatrix} \Psi_L^{+*} \\ \Psi_R^{-*} \end{pmatrix} = \mathbf{S}\mathbf{S}^* \begin{pmatrix} \Psi_L^{+*} \\ \Psi_R^{-*} \end{pmatrix}. \quad (1.43)$$

Since relation (1.43) must hold for any incoming waves, we conclude that

$$\mathbf{S}\mathbf{S}^* = \mathbf{S}^*\mathbf{S} = \mathbf{1}. \quad (1.44)$$

This condition, in conjunction with the unitary relation, equation (1.24), implies that the scattering matrix  $\mathbf{S}$  must be symmetric. Indeed, in terms of matrix elements, the



condition (1.44) reads

$$\begin{aligned} |S_{11}|^2 + S_{12}^* S_{21} &= 1, & |S_{22}|^2 + S_{21}^* S_{12} &= 1, \\ S_{11}^* S_{12} + S_{12}^* S_{22} &= 0, & S_{21}^* S_{11} + S_{22}^* S_{21} &= 0. \end{aligned} \quad (1.45)$$

Comparison of the third equation of (1.26),  $S_{11}^* S_{12} + S_{22} S_{21}^* = 0$ , with the third equation of (1.45) shows that the scattering matrix  $\mathbf{S}$  is a symmetric matrix when the system possesses both time-reversal symmetry and conservation of current density,

$$S_{12} = S_{21}. \quad (1.46)$$

Time-reversal symmetry also implies that

$$\begin{pmatrix} \Psi_{\mathbf{R}}^{-*} \\ \Psi_{\mathbf{R}}^{+*} \end{pmatrix} = \mathbf{M} \begin{pmatrix} \Psi_{\mathbf{L}}^{-*} \\ \Psi_{\mathbf{L}}^{+*} \end{pmatrix}. \quad (1.47)$$

The above equation follows from the definition of the transfer matrix  $\mathbf{M}$  given by equation (1.12). Indeed, the wave  $\Psi_{\mathbf{R}}^{-*}$  now plays the role of the *incoming* wave and the wave  $\Psi_{\mathbf{R}}^{+*}$  is the *outgoing* wave, while  $\Psi_{\mathbf{L}}^{-*}$  is the incoming wave and  $\Psi_{\mathbf{L}}^{+*}$  is the outgoing wave. Equation (1.47) can be written as

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \Psi_{\mathbf{R}}^{+*} \\ \Psi_{\mathbf{R}}^{-*} \end{pmatrix} = \mathbf{M} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \Psi_{\mathbf{L}}^{+*} \\ \Psi_{\mathbf{L}}^{-*} \end{pmatrix}. \quad (1.48)$$

On the other hand, the complex conjugate of the relation (1.12) reads

$$\begin{pmatrix} \Psi_{\mathbf{R}}^{+*} \\ \Psi_{\mathbf{R}}^{-*} \end{pmatrix} = \mathbf{M}^* \begin{pmatrix} \Psi_{\mathbf{L}}^{+*} \\ \Psi_{\mathbf{L}}^{-*} \end{pmatrix}. \quad (1.49)$$

Comparison of the last two equations shows that, in the case of time-reversal symmetry, the transfer matrix satisfies the relationship

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathbf{M} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \mathbf{M}^*. \quad (1.50)$$

With the use of symmetry (1.50), we obtain that *for systems with time-reversal symmetry*, the transfer matrix  $\mathbf{M}$ , has the form

$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{12}^* & M_{11}^* \end{pmatrix} \quad (1.51)$$

[29, 103, 108, 129, 141]. We also have from the expression (1.13) that  $\det \mathbf{M} = S_{21}/S_{12}$ . With the use of equation (1.46), we obtain, for the case of time-reversal symmetry, that

$$\det \mathbf{M} = 1. \quad (1.52)$$

From equation (1.51) it also follows that  $\text{Tr } \mathbf{M} = M_{11} + M_{22} = M_{11} + M_{11}^*$  is a real number when time-reversal symmetry is preserved.

By applying both the requirement for conservation of probability flux and time-reversal symmetry, we reduce the number of independent elements of the transfer matrix to three. Indeed,  $\mathbf{M}$  is given by two *complex* numbers  $M_{11}$  and  $M_{12}$ , or by four real numbers, which determine the real and imaginary parts of  $M_{11}$  and  $M_{12}$ . These four numbers are not independent, because of the constraint  $\det \mathbf{M} = 1$ .

### 1.3 Transmission and Reflection Amplitudes

To find the physical meaning of the elements of the scattering matrix  $\mathbf{S}$ , we return to the scattering experiment described in section 1.1. Consider a particle approaching the sample from the right. As no particle is coming from the left, we have

$$\Psi_L^+ = 0. \quad (1.53)$$

We also normalize the incoming wave to unity,

$$|\Psi_R^-|^2 = 1. \quad (1.54)$$

From equation (1.10), we obtain that the transmitted wave  $\Psi_L^-(x)$  is given by

$$\Psi_L^-(x=0) = S_{12} \Psi_R^-(x=\ell) \quad (1.55)$$

and the reflected wave  $\Psi_L^+(x+\ell)$  is given by

$$\Psi_R^+(x=\ell) = S_{22} \Psi_R^-(x=\ell). \quad (1.56)$$

We call  $S_{12}$  the *transmission amplitude*  $t$  and  $S_{22}$  the *reflection amplitude*  $r$ :

$$t = S_{12}, \quad r = S_{22}. \quad (1.57)$$

In the same way, we consider scattering of the particle coming from the left side of the potential. We obtain  $r' = S_{11}$  as the reflection amplitude, and  $t' = S_{21}$  as the transmission amplitude from left to the right. Finally, in terms of transmission and reflection amplitudes, we can write the scattering matrix  $\mathbf{S}$  in the form

$$\mathbf{s} = \begin{pmatrix} r' & t \\ t' & r \end{pmatrix}. \quad (1.58)$$

Using the relationship between scattering and transfer matrices, equation (1.13), we can express the transfer matrix in the form

$$\mathbf{M} = \begin{pmatrix} t' - \frac{rr'}{t} & \frac{r}{t} \\ -\frac{r'}{t} & \frac{1}{t} \end{pmatrix}. \quad (1.59)$$

For further applications, it is useful to write the transfer matrix in the form

$$\mathbf{M} = \begin{pmatrix} t' - rt^{-1}r' & rt^{-1} \\ -t^{-1}r' & t^{-1} \end{pmatrix} \quad (1.60)$$

(problem 1.3). The order of terms in expression (1.60) is important for the analysis of scattering on many scattering centers as well as for generalization of the transfer matrix to many-channel problems, discussed in section 1.5.3.

The *transmission (reflection) coefficients* are defined, respectively, as the probability that the particle is transmitted (reflected):

$$T = |t|^2 \quad \text{and} \quad R = |r|^2. \quad (1.61)$$

Using the symmetry properties of the scattering matrix, equations (1.30) and (1.31), we have

$$|r| = |r'| \quad \text{and} \quad |t| = |t'|. \quad (1.62)$$

Conservation of the current density, equations (1.26), gives

$$|t|^2 + |r|^2 = 1 \quad \text{and} \quad |t'|^2 + |r'|^2 = 1. \quad (1.63)$$

Equations (1.63) have a simple physical interpretation. When the sample contains no losses and no sources, then the electron can be either reflected back or transmitted through the sample.

Now we use the definition (1.58) and rewrite the third equations (1.26),  $S_{11}^* S_{12} + S_{21}^* S_{22} = 0$ , in the form

$$\frac{r}{t} = -\left(\frac{r'}{t'}\right)^*. \quad (1.64)$$

This helps us to express

$$M_{11} = t' - \frac{r}{t}r' = t' + \frac{|r'|^2}{(t')^*} = \frac{1}{(t')^*} (|t'|^2 + |r'|^2) = \frac{1}{(t')^*}, \quad (1.65)$$

and we can write the transfer matrix, given by equation (1.59) in the more symmetric form

$$\mathbf{M} = \begin{pmatrix} (t')^{*-1} & rt^{-1} \\ -t^{-1}r' & t^{-1} \end{pmatrix}. \quad (1.66)$$

When scattering is symmetric with respect to time inversion, we have also

$$t = t' \quad (1.67)$$

[see equation (1.46)]. It is also evident that for no scattering potential,  $V(x) \equiv 0$ , we have  $T = 1$  and  $R = 0$ .

## 1.4 Properties of the Transfer Matrix

The transfer matrix enables us to study the properties of the sample through scattering experiments. Far from the sample, we prepare a plane wave with a given wave vector  $q$  and measure how this wave transmits through the potential. Of course, the transmission coefficient  $T$ , the reflection coefficient  $R$ , as well as all elements of matrices  $\mathbf{S}$  and  $\mathbf{M}$  are functions of  $q$ . Thus, we discover the properties of the system from its scattering response. It is evident that both the transmission and the reflection depend on the energy  $E = E(q)$  of the incoming particle. In particular,

$$t = t(q) \quad \text{and} \quad r = r(q). \quad (1.68)$$

As will be shown in the next chapters, the transfer matrix is a very powerful method of analysis for one-dimensional systems.

The transfer matrix depends on the properties of the entire system represented by the potential  $V(x)$  and the two leads on the left and right sides of the potential. Any change in the physical properties of the leads (regions outside the sample) also changes the transfer matrix. We also must keep in mind that, when deriving the symmetry properties of the transfer matrix, we assumed that the leads at both sides of the sample are equal to each other. We will see that this condition is not always satisfied. Although the transfer matrix method works also in the case of different leads, some symmetry relations are not satisfied. For instance, the determinant of the transfer matrix  $\mathbf{M}$  can be different from one.

For completeness, we note there is also another definition of the transfer matrix used in the literature. It uses the linear relationship between coefficients  $A$ – $D$  defined in equation (1.4), instead of wave functions:

$$\begin{pmatrix} C \\ D \end{pmatrix} = \mathbf{T} \begin{pmatrix} A \\ B \end{pmatrix}. \quad (1.69)$$

By inserting the explicit expression for the wave functions, equation (1.4), into equation (1.12), we see that the transfer matrix  $\mathbf{M}$ , equation (1.12), is related to  $\mathbf{T}$  as

$$\mathbf{M} = \begin{pmatrix} e^{iq\ell} & 0 \\ 0 & e^{-iq\ell} \end{pmatrix} \mathbf{T}. \quad (1.70)$$

Note that, in the limit of zero potential  $V \equiv 0$ , the  $\mathbf{T}$  matrix is the unit matrix, while the matrix  $\mathbf{M}$  possesses the phase factors  $e^{\pm iq\ell}$ , which the particle gains as it moves between  $x = 0$  and  $x = \ell$ . In the following we will use the transfer matrix  $\mathbf{M}$ . All results can be easily reformulated in terms of the matrix  $\mathbf{T}$ . Of course, the transmission and reflection coefficients  $T$  and  $R$  are the same in both formulations, since the transfer matrices  $\mathbf{M}$  and  $\mathbf{T}$  differ from each other only in the phase.

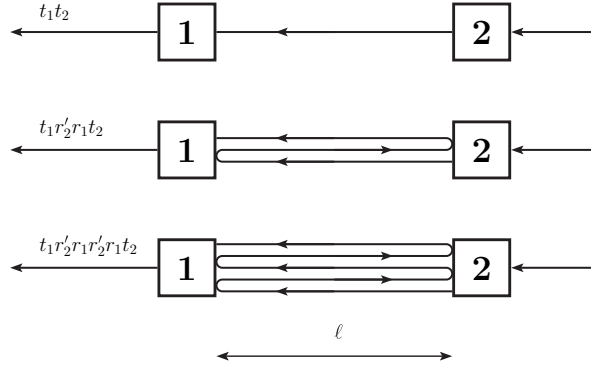


FIGURE 1.2. Schematic explanation of the calculation of the transmission through two barriers. A few paths with the electron scattered between the barriers are shown. To show different transmission paths, samples are separated by a distance  $\ell$ . We consider  $\ell \equiv 0$  in the text.

#### 1.4.1 Multiplication of Transfer Matrices

Consider a more complicated experiment in which the particle is scattered by two individual samples. The first sample is given by the potential  $V_1(x)$ , located at  $(a < x \leq b)$ , and the second sample is determined by the potential  $V_2(x)$ , located at  $(b \leq x < c)$ . The problem of transmission and reflection through such a system can be treated in two ways: either we can use the transfer matrices  $\mathbf{M}_1$  and  $\mathbf{M}_2$ , which determine the scattering properties of individual potentials  $V_1$  and  $V_2$ , or we can consider the potential  $V_{12}(x)$  defined on the interval  $a \leq x \leq c$  and use the corresponding transfer matrix  $\mathbf{M}_{12}$ . Physically, it is clear that the results obtained by these two methods must be the same. This indicates that the transfer matrix  $\mathbf{M}_{12}$  is completely determined by the elements of the transfer matrices  $\mathbf{M}_1$  and  $\mathbf{M}_2$ . To derive the relationship between the transfer matrices, we express the wave function in three regions:

$$\begin{aligned} \Psi_L(x) &= \Psi_L^+(x) + \Psi_L^-(x), & x \leq a, \\ \Psi(x=b) &= \Psi^+(b) + \Psi^-(b), & x \equiv b, \\ \Psi_R(x) &= \Psi_R^+(x) + \Psi_R^-(x), & x \geq c. \end{aligned} \quad (1.71)$$

Two samples are schematically shown in figure 1.2. Then, from the definition of the transfer matrix  $\mathbf{M}$ , equation (1.12), we have

$$\begin{pmatrix} \Psi^+(b) \\ \Psi^-(b) \end{pmatrix} = \mathbf{M}_1 \begin{pmatrix} \Psi_L^+(a) \\ \Psi_L^-(a) \end{pmatrix} \quad (1.72)$$

and

$$\begin{pmatrix} \Psi_R^+(c) \\ \Psi_R^-(c) \end{pmatrix} = \mathbf{M}_2 \begin{pmatrix} \Psi^+(b) \\ \Psi^-(b) \end{pmatrix}. \quad (1.73)$$

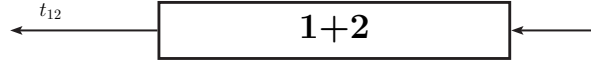


FIGURE 1.3. Transmission of the electron through the entire system consisting of two samples 1 + 2.

By combining the equations (1.72) and (1.73), we obtain

$$\begin{pmatrix} \Psi_R^+(c) \\ \Psi_R^-(c) \end{pmatrix} = \mathbf{M}_2 \mathbf{M}_1 \begin{pmatrix} \Psi_L^+(a) \\ \Psi_R^-(a) \end{pmatrix}. \quad (1.74)$$

As discussed above, we can consider the whole system as represented by the transfer matrix  $\mathbf{M}_{12}$ . Then we can write

$$\begin{pmatrix} \Psi_R^+(c) \\ \Psi_R^-(c) \end{pmatrix} = \mathbf{M}_{12} \begin{pmatrix} \Psi_L^+(a) \\ \Psi_R^-(a) \end{pmatrix}. \quad (1.75)$$

A comparison of (1.74) with (1.75) gives the composition law

$$\mathbf{M}_{12} = \mathbf{M}_2 \mathbf{M}_1. \quad (1.76)$$

Since the matrix  $\mathbf{M}_{12}$  is the transfer matrix of the whole system, its matrix elements determine the transmission and the reflection amplitudes [equation (1.60)] for the entire system. This enables us to determine the transmission and the reflection amplitudes of the entire system (figure 1.3) in terms of elements of the transfer matrices of the system's constituents. For example, we can calculate the transmission amplitude  $t_{12}$  for an electron approaching the system from the *right*. Using the explicit form of the transfer matrix, equation (1.60),

$$\begin{aligned} \mathbf{M} &= \begin{pmatrix} t'_{12} - r_{12} t_{12}^{-1} r'_{12} & r_{12} t_{12}^{-1} \\ -t_{12}^{-1} r'_{12} & t_{12}^{-1} \end{pmatrix} \\ &= \begin{pmatrix} t'_2 - r_2 t_2^{-1} r'_2 & r_2 t_2^{-1} \\ -t_2^{-1} r'_2 & t_2^{-1} \end{pmatrix} \begin{pmatrix} t'_1 - r_1 t_1^{-1} r'_1 & r_1 t_1^{-1} \\ -t_1^{-1} r'_1 & t_1^{-1} \end{pmatrix}, \end{aligned} \quad (1.77)$$

we find by matrix multiplication that

$$t_{12}^{-1} = t_2^{-1} t_1^{-1} - t_2^{-1} r'_2 r_1 t_1^{-1}, \quad (1.78)$$

which can be written as

$$t_{12} = t_1 [1 - r'_2 r_1]^{-1} t_2. \quad (1.79)$$

The physical interpretation of formula (1.79) is more clear if we expand the right-hand side (r.h.s.) of equation (1.79) in terms of a power series:

$$t_{12} = t_1 [1 + r'_2 r_1 + r'_2 r_1 r'_2 r_1 + \dots] t_2. \quad (1.80)$$

Table 1.1. Physical meaning of the parameters of the scattering matrix,  $\mathbf{S}$  equation (1.58), and the transfer matrix,  $\mathbf{M}$  equation (1.60).

$t$	transmission of a wave propagating from right to left
$r$	reflection of a wave coming from right
$t'$	transmission of a wave propagating from left to right
$r'$	reflection of a wave coming from left

Then we see that transmission amplitude  $t_{12}$  is given by the sum of the contributions of all possible paths through the two potential regions,  $V_1$  and  $V_2$ . Three such paths are shown in figure 1.2. The first term in (1.80),  $t_1 t_2$ , represents the transmission through both the potentials. The second term  $t_1 r'_2 r_1 t_2$  corresponds to the path when an electron passes through the second sample ( $t_2$ ), is reflected back from the second sample ( $r_1$ ), and, after reflection from the second sample ( $r'_2$ ), finally passes through the first one ( $t_1$ ). Higher terms in the expansion (1.80) contain higher powers of  $(r'_2 r_1)^n = r'_2 r_1 r'_2 r_1 \dots$ . The  $n$ th term corresponds to a trajectory in which the electron is  $n$  times scattered between samples 1 and 2 before it passes through the second sample and escapes to the left.

In the same way, we can derive an expression for the reflection amplitude. From equation (1.77) we obtain that

$$\begin{aligned} -t_{12}^{-1} r'_{12} &= -t_2^{-1} r'_2 (t'_1 - r_1 t_1^{-1} r'_1) - t_2^{-1} t_1^{-1} r'_1 \\ &= -t_2^{-1} r'_2 t'_1 + t_2^{-1} [r'_2 r_1 - 1] t_1^{-1} r'_1. \end{aligned} \quad (1.81)$$

Now we multiply both sides of the last equations by  $-t_{12} = -t_1 [1 - r'_2 r_1]^{-1} t_2$  and obtain

$$r'_{12} = r'_1 + t_1 [1 - r'_2 r_1]^{-1} r'_2 t'_1. \quad (1.82)$$

We remind the reader that, in agreement with our convention (table 1.1),  $r'_{12}$  is the reflection amplitude for the particle which approaches the sample from the left and is reflected back to the left.

The reflection amplitude again contains contributions of an infinite number of trajectories. The first term in equation (1.82) is just the reflection from the first barrier. All subsequent terms represent trajectories in which the electron transmits through the first barrier, then is  $n$  times reflected between both barriers, and is finally transmitted through the first sample (with transmission amplitude  $t_1$ ) and leaves the system to the left.

Of special interest is the case when  $V_2(x) = 0$ . Then, the matrix  $\mathbf{M}_2$  is the diagonal matrix and

$$\mathbf{M}_{12} = \begin{pmatrix} e^{iq\ell} & 0 \\ 0 & e^{-iq\ell} \end{pmatrix} \mathbf{M}_1, \quad \ell = c - b, \quad (1.83)$$

and consequently

$$T_{12} = \frac{1}{|t_{12}|^2} = \frac{1}{|e^{iq\ell}t_1|^2} = \frac{1}{|t_1|^2} = T_1. \quad (1.84)$$

Also, it is evident that  $R_{12} = R_1$ . This important result is easy to understand physically, since any reflection can appear only in the region where the potential is nonzero. The transmission and reflection coefficients through the barrier are not changed if we add a free interval of any length to the barrier. However, we must keep in mind that addition of such an interval changes the *phases* of the transmission and reflection amplitudes.

The composition relationship (1.76) can be easily generalized for the case of  $N$  barriers, resulting in the transfer matrix  $\mathbf{M}$  given by

$$\mathbf{M} = \mathbf{M}_N \mathbf{M}_{N-1} \cdots \mathbf{M}_2 \mathbf{M}_1. \quad (1.85)$$

### 1.4.2 Propagating States

Consider a system with time-reversal symmetry. Then  $\det \mathbf{M} = 1$  and  $\text{Tr } \mathbf{M}$  is real. The two eigenvalues  $\lambda_1$  and  $\lambda_2$  of the transfer matrix are related by

$$\lambda_2 = \frac{1}{\lambda_1}. \quad (1.86)$$

We will distinguish two cases. In the first case  $|\lambda_1| = 1$ . Then  $\lambda_1$  can be written as

$$\lambda_1 = e^{iq\ell}, \quad (1.87)$$

with the wave vector  $q$  being real. As  $\lambda_2 = e^{-iq\ell}$ , we have  $\text{Tr } \mathbf{M} = \lambda_1 + 1/\lambda_1 = 2 \cos q\ell$ . Note that

$$|\text{Tr } \mathbf{M}| \leq 2. \quad (1.88)$$

In the second case, we have  $|\lambda_1| \neq 1$ . Then we have  $|\text{Tr } \mathbf{M}| = |\lambda_1 + \lambda_1^{-1}| = 2 \cosh \kappa\ell > 2$ . In this case, the amplitude of the transmitted wave decreases exponentially with increasing width of the potential barrier.

Thus, we conclude that equation (1.88) represents a sufficient condition for the existence of the propagating solution. Condition (1.88) is very useful in the analysis of complicated long systems. Following the composition rule (1.76) derived in section 1.4.1, we can calculate the transfer matrix as a product of transfer matrices of individual subsystems. Then, equation (1.88) allows us to determine unambiguously whether or not a given solution is propagating. In this way, we can estimate the entire spectrum of propagating solutions of the system.

### 1.4.3 Bound States

A one-dimensional potential well

$$V(x) < 0 \quad (1.89)$$



always has at least one bound state [11]. A bound state is characterized by a wave function that decays exponentially on both sides of the potential. We can use the transfer matrix to estimate the energy of the bound state.

The wave function of a bound state decreases exponentially for both  $x > \ell$  and  $x < 0$ :

$$\begin{aligned}\Psi_{\text{R}}^{+}(x) &\propto e^{-\kappa x}, & x > \ell, \\ \Psi_{\text{L}}^{-}(x) &\propto e^{+\kappa x}, & x < 0,\end{aligned}\tag{1.90}$$

where

$$q = i\kappa \quad \text{and} \quad \kappa > 0.\tag{1.91}$$

To avoid solutions that increase exponentially far from the sample, we require

$$\Psi_{\text{R}}^{-}(x) \equiv 0, \quad x > \ell,\tag{1.92}$$

and

$$\Psi_{\text{L}}^{+}(x) \equiv 0, \quad x < 0.\tag{1.93}$$

Inserting equations (1.92) and (1.93) into the transfer matrix equation (1.12), we obtain

$$\Psi_{\text{R}}^{-} = M_{21}\Psi_{\text{L}}^{+} + M_{22}\Psi_{\text{L}}^{-}.\tag{1.94}$$

We immediately obtain the result that, for the existence of a bound state, one needs to satisfy the following equation:

$$M_{22}(i\kappa) = 0 \quad \text{for} \quad \kappa > 0.\tag{1.95}$$

The solution  $\kappa_b = \kappa$  from equation (1.95) determines the energy  $E_b$  of the bound state, which is localized around the impurity. We will use this criterion to obtain different bound states for electrons and electromagnetic waves.

#### 1.4.4 Chebyshev's Identity

A special case of the multiplication law equation (1.85) is the case when all the potential barriers are equal:

$$\mathbf{M}_1 = \mathbf{M}_2 = \cdots = \mathbf{M}_N.\tag{1.96}$$

Then the resulting transfer matrix  $\mathbf{M}$  can be easily expressed in terms of the elements of the individual matrix  $\mathbf{M}_1$ , with the use of the Chebyshev identity [165].

Consider the transfer matrix  $\mathbf{M}$ ,

$$\mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.\tag{1.97}$$

The eigenvalues  $\lambda_1$  and  $\lambda_2$  of the matrix  $\mathbf{M}$  are

$$\lambda_1 = e^{iq\ell} \quad \text{and} \quad \lambda_2 = e^{-iq\ell}.\tag{1.98}$$

Chebyshev's identity states [39,165] that the  $N$ th power of the transfer matrix can be expressed as

$$\mathbf{M}^N = \begin{pmatrix} a & b \\ c & d \end{pmatrix}^N = \begin{pmatrix} aU_{N-1} - U_{N-2} & bU_{N-1} \\ cU_{N-1} & dU_{N-1} - U_{N-2} \end{pmatrix}. \quad (1.99)$$

Here, the function  $U_N = U_N(q)$  is defined as

$$U_N = \frac{\sin(N+1)q\ell}{\sin q\ell}, \quad (1.100)$$

and  $q\ell$  is given by the eigenvalues of the transfer matrix  $\mathbf{M}$ ,

$$\text{Tr } \mathbf{M} = \lambda_1 + \lambda_2 = 2 \cos q\ell. \quad (1.101)$$

All the above identities are valid in the case of real  $q$  (then  $|\lambda_1| = 1$ ) and in the case of complex  $q = i\kappa$  (then  $|\lambda_1| > 1$ ). A proof of Chebyshev's identity is given in section 1.5.2.

#### 1.4.5 Transmission through $N$ Identical Barriers

Chebyshev's identity allows us to derive a general expression for the transmission coefficient of  $N$  identical barriers. First, note that the transmission coefficient can be written as

$$T = |t|^2 = \frac{|t|^2}{|t|^2 + |r|^2} = \frac{1}{1 + \frac{|r|^2}{|t|^2}} \quad (1.102)$$

(we have used that  $|t|^2 + |r|^2 = 1$ ). Then, comparing the matrix elements of  $\mathbf{M}$  in equation (1.97) with the general expression of the transfer matrix in terms of transmission and reflection amplitudes, equation (1.60), we see that

$$M_{12} = \frac{r}{t}, \quad (1.103)$$

so that the transmission through a single barrier is

$$T_1 = \frac{1}{1 + |M_{12}|^2}. \quad (1.104)$$

Finally, from identity (1.99) we obtain the transmission for  $N$  identical barriers in the form

$$T_N = \frac{1}{1 + |M_{12}|^2 U_{N-1}^2}. \quad (1.105)$$

Using the explicit expressions for the function  $U_{N-1}$  [equation (1.100)] and for  $b$ , given by equation (1.103), we arrive at the general expression for the transmission of the particle through  $N$  identical barriers:

$$T_N = \frac{1}{1 + \left| \frac{r^2}{t^2} \right| \frac{\sin^2 Nq\ell}{\sin^2 q\ell}}, \quad (1.106)$$

where  $q\ell$  is given by equation (1.101).

Relationship (1.106) plays a crucial role in the analysis of transmission through periodic systems. We only need to calculate  $r/t$  for an individual potential and we immediately obtain, with the help of equation (1.106), the transmission coefficient for any number of barriers.

## 1.5 Supplementary Notes

### 1.5.1 Current Density

We derive in this section the equation for the conservation of the particle density and show that the requirement of constant particle density in a given volume leads to the conservation of the current density.

We first multiply both sides of the Schrödinger equation

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x)\Psi(x, t) \quad (1.107)$$

by the complex conjugate wave function  $\Psi^*$  and integrate both sides of the equation over  $x$  in the interval  $(x_a, x_b)$ :

$$i\hbar \int_{x_a}^{x_b} \Psi^* \frac{\partial \Psi}{\partial t} dx = -\frac{\hbar^2}{2m} \int_{x_a}^{x_b} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx + \int_{x_a}^{x_b} \Psi^* V(x)\Psi dx. \quad (1.108)$$

Then we consider the complex conjugate Schrödinger equation

$$-i\hbar \frac{\partial \Psi^*(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi^*(x, t)}{\partial x^2} + V^*(x)\Psi^*(x, t), \quad (1.109)$$

multiply it by  $\Psi$ , and again integrate from  $x_a$  to  $x_b$ ,

$$-i\hbar \int_{x_a}^{x_b} \Psi \frac{\partial \Psi^*}{\partial t} dx = -\frac{\hbar^2}{2m} \int_{x_a}^{x_b} \Psi \frac{\partial^2 \Psi^*}{\partial x^2} dx + \int_{x_a}^{x_b} \Psi V^*(x)\Psi^* dx. \quad (1.110)$$

Now we subtract equation (1.110) from equation (1.108):

$$i\hbar \int_{x_a}^{x_b} \left[ \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \right] dx = -\frac{\hbar^2}{2m} \int_{x_a}^{x_b} \left[ \Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \Psi \frac{\partial^2 \Psi^*}{\partial x^2} \right] dx + \int_{x_a}^{x_b} [\Psi^* V(x)\Psi - \Psi V^*(x)\Psi^*] dx. \quad (1.111)$$

Next, we use the following identities:

$$\Psi \frac{\partial \Psi^*}{\partial t} + \Psi^* \frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t} [\Psi^* \Psi] \quad (1.112)$$

and

$$\Psi \frac{\partial^2 \Psi^*}{\partial x^2} - \Psi^* \frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial}{\partial x} \left[ \Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x} \right] = \frac{2m}{\hbar i} \frac{\partial}{\partial x} j(x), \quad (1.113)$$

where  $j(x)$  is the current density at the point  $x$ :

$$j(x) = \frac{\hbar i}{2m} \left[ \Psi \frac{\partial \Psi^*}{\partial x} - \Psi^* \frac{\partial \Psi}{\partial x} \right]. \quad (1.114)$$

Finally, we use the identity

$$\int_{x_b}^{x_a} \frac{\partial j(x)}{\partial x} dx = j(x_b) - j(x_a). \quad (1.115)$$

Inserting relations (1.112)–(1.115) into equation (1.111), we obtain the final result

$$\begin{aligned} \frac{\partial}{\partial t} \int_{x_a}^{x_b} \Psi^* \Psi dx &= [j(x_b) - j(x_a)] \\ &+ \frac{1}{i\hbar} \int_{x_a}^{x_b} [\Psi^* V(x) \Psi - \Psi V^*(x) \Psi^*] dx. \end{aligned} \quad (1.116)$$

The physical interpretation of equation (1.116) is very simple: the term on the l.h.s. determines the change of the density of electrons in the region  $(x_a, x_b)$  versus time. This change is due either to the flux of the particle inside or outside the region (given by the first term on the r.h.s.), or to the creation (or annihilation) of particles inside the region (the last term on the r.h.s.). Note that the last term

$$\int_{x_a}^{x_b} [\Psi^* V(x) \Psi - \Psi V^*(x) \Psi^*] dx \quad (1.117)$$

is zero if the potential  $V(x)$  is real:

$$V(x) = V^*(x). \quad (1.118)$$

The case of complex potentials corresponds to systems with absorption or gain. In this book, we will treat only real potentials.

If the last term in equation (1.116) is zero, then equation (1.116) reduces to

$$\frac{\partial}{\partial t} \int_{x_a}^{x_b} \Psi^* \Psi dx = j(x_b) - j(x_a). \quad (1.119)$$

Since we study only time-independent problems in this book, the density of particles in any region  $(x_a, x_b)$  does not change in time. Therefore the left-hand side of equation (1.116) is zero:

$$\frac{\partial}{\partial t} \int_{x_a}^{x_b} \Psi^* \Psi dx = 0. \quad (1.120)$$

This means that the number of particles in the region  $(x_a, x_b)$  does not change with time. equation (1.116) reduces to

$$j(x_a) = j(x_b), \quad (1.121)$$

which represents the conservation of the flux: if the number of particles inside a given region is constant, then the current flowing inward to this region must be equal to the current flowing outward.

Finally, we can express the current density for the case of a plane wave,

$$\Psi(x) = Ae^{ikx}. \quad (1.122)$$

Inserting this into equation (1.114), we obtain the result that the current density of a plane wave is

$$j = \frac{\hbar k}{m} |\Psi|^2 = \frac{\hbar k}{m} |A|^2. \quad (1.123)$$

The current density is proportional to the wave vector  $k$  (the velocity of the particle) and to the probability density  $|\Psi|^2$ . Note that the current  $j$  indeed does not depend on  $x$ .

### 1.5.2 Proof of the Chebyshev Identity

The Chebyshev identity is used in section 1.4.4 to derive useful relations for the matrix elements of the  $N$ th power of the transfer matrix  $\mathbf{M}$ . The Chebyshev identity is formulated as follows:

Consider a matrix  $\mathbf{M}$

$$\mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \quad (1.124)$$

Its eigenvalues  $\lambda_1$  and  $\lambda_2$  are given by

$$\lambda_1 = e^{iq\ell} \quad \text{and} \quad \lambda_2 = e^{-iq\ell}. \quad (1.125)$$

The  $N$ th power of the matrix  $\mathbf{M}$  can be expressed as

$$\mathbf{M}^N = \begin{pmatrix} a & b \\ c & d \end{pmatrix}^N = \begin{pmatrix} aU_{N-1} - U_{N-2} & bU_{N-1} \\ cU_{N-1} & dU_{N-1} - U_{N-2} \end{pmatrix}. \quad (1.126)$$

Here, the function  $U_N = U_N(q)$  is defined as

$$U_N = \frac{\sin(N+1)q\ell}{\sin q\ell}, \quad (1.127)$$

where  $q\ell$  is given by the eigenvalues of the transfer matrix  $\mathbf{M}$  [equation (1.87)], and satisfies the relation

$$\text{Tr } \mathbf{M} = \lambda_1 + \lambda_2 = 2 \cos q\ell. \quad (1.128)$$

All the above identities are valid when  $q$  is real (then  $|\lambda_1| = 1$ ) and when  $q$  is complex (then  $|\lambda_1| > 1$ ).

We will prove the Chebyshev identity given by equation (1.126), by mathematical induction.

First, note that the identity (1.126) is satisfied for  $N = 1$ . Indeed, from equation (1.127) we have  $U_0 \equiv 1$  and  $U_{-1} \equiv 0$ .

Next, assume that the identity (1.126) is valid for some  $N \geq 1$ . We show that then it is valid also for  $N + 1$ . To do so, we express

$$\begin{aligned} \mathbf{M}^{N+1} &= \mathbf{M}\mathbf{M}^N = \mathbf{M} \begin{pmatrix} aU_{N-1} - U_{N-2} & bU_{N-1} \\ cU_{N-1} & dU_{N-1} - U_{N-2} \end{pmatrix} \\ &= \begin{pmatrix} (a^2 + bc)U_{N-1} - aU_{N-2} & b[(a+d)U_{N-1} - U_{N-2}] \\ c[(a+d)U_{N-1} - U_{N-2}] & (d^2 + bc)U_{N-1} - dU_{N-2} \end{pmatrix}. \end{aligned} \quad (1.129)$$

We calculate the matrix element  $(M^{N+1})_{11}$ :

$$\begin{aligned} (a^2 + bc)U_{N-1} - aU_{N-2} &= [a(a+d) - ad + bc]U_{N-1} - aU_{N-1} \\ &= a[(a+d)U_{N-1} - U_{N-2}] - U_{N-1} \\ &= aU_n - U_{N-1}, \end{aligned} \quad (1.130)$$

where we have used the fact that  $a + d = 2 \cos q\ell$  and  $ad - bc = \det \mathbf{M} = 1$ . We also used the identity

$$U_N \equiv 2 \cos q\ell U_{N-1} - U_{N-2}, \quad (1.131)$$

which can be verified with the use of the trigonometric relations (the proof is given in problem 1.4). All the other matrix elements of the matrix  $\mathbf{M}$  can be calculated in the same way. Finally, we derive

$$\mathbf{M}^{N+1} = \begin{pmatrix} aU_N - U_{N-1} & bU_N \\ cU_N & dU_N - U_{N-1} \end{pmatrix}, \quad (1.132)$$

which is the relation obtained from (1.126) by the substitution  $N \rightarrow N + 1$ .

Starting with  $N = 1$ , we have just proven that relation (1.126) holds also for  $N = 2$ . Then, starting with  $N = 2$ , we find that (1.126) holds also for  $N = 3$ . By induction, we conclude that (1.126) is valid for any integer  $N$ .

#### *Another Proof of the Chebyshev Identity*

Another way to prove the Chebyshev identity (1.126) is the following. To get the  $N$ th power of the matrix  $\mathbf{A}$ , we first find its eigenvalues and eigenvectors. We write

$$\mathbf{M} = \mathbf{R} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \mathbf{L} \quad (1.133)$$

where  $\lambda_1$  and  $\lambda_2$  are eigenvalues, and  $\mathbf{L}$  ( $\mathbf{R}$ ) is the matrix of left (right) eigenvectors, respectively. They can be found with the help of the formulas given below in appendix A.

Then it is easy to find that

$$\mathbf{M}^N = \mathbf{R} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \mathbf{L} \mathbf{R} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \mathbf{L} \cdots = \mathbf{R} \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} \mathbf{L}, \quad (1.134)$$

since  $\mathbf{L}\mathbf{R} = 1$ . Next, one easily finds that

$$\lambda_{1,2} = e^{\pm iq\ell} \quad (1.135)$$

with  $q$  given by (1.101). After some algebra (do it!), one finds that  $\mathbf{M}^N$  is given by equation (1.99).

### 1.5.3 Quasi-One-Dimensional Systems

The transfer matrix can be easily generalized for the case of *quasi-one-dimensional* systems, which are finite in the direction perpendicular to the direction of propagation of the particle, and infinite in the  $x$  direction [29, 47, 103, 52, 115, 131, 118]. A particle propagates along the  $x$  direction, but, due to the finite size of the system in the transverse direction, it possess also transverse momentum  $k_{\perp}$ . The energy of the particle is then

$$E = \frac{\hbar^2}{2m} [k_{\parallel}^2 + k_{\perp}^2]. \quad (1.136)$$

In the one-dimensional case  $k_{\perp} \equiv 0$  and  $k = \sqrt{k_{\parallel}^2 + k_{\perp}^2} = k_{\parallel}$ . In quasi-one-dimensional systems, different values of  $k_{\perp}$  are allowed, as determined by the structure of the system. If there are  $N$  allowed values of  $k_{\perp n}$ ,  $n = 1, 2, \dots, N$ , then the functions  $\Psi_{\perp}^{+}(x)$  and  $\Psi_{\perp}^{-}(x)$  consist of superpositions of  $N$  plane waves,

$$\begin{aligned} \Psi_{\perp}^{+}(x) &= \sum_{n=1}^N A_n(z) e^{+ik_{\perp n}x}, \\ \Psi_{\perp}^{-}(x) &= \sum_{n=1}^N B_n(z) e^{-ik_{\perp n}x}. \end{aligned} \quad (1.137)$$

The right wave function  $\Psi_{\perp}^{+}(x)$  and  $\Psi_{\perp}^{-}(x)$  can be expressed in a similar way. The wave vectors  $k_{\perp n}$  are given by the boundary conditions in the transverse direction. Together with the energy  $E$  they determine the  $n$ th value of  $k_{\parallel}$ .

We can introduce the  $N \times N$  matrices of the transmission amplitudes  $t$  and  $t'$ . Their matrix elements  $t_{nm}$  and  $t'_{nm}$  give the transmission amplitude of the process in which an electron passes through the sample from the channel  $n$  on the left side of the sample to the channel  $m$  on the right side of the sample. In the same way, we introduce  $N \times N$  matrices of the reflection amplitudes  $r$  and  $r'$ . Then the transfer matrix can be expressed as a  $2N \times 2N$  matrix,

$$\mathbf{M} = \begin{pmatrix} t' - r t^{-1} r' & r t^{-1} \\ -t^{-1} r' & t^{-1} \end{pmatrix}. \quad (1.138)$$

Note that  $\mathbf{M}$  is formally identical to the one-dimensional transfer matrix given by equation (1.60). However, in this case we have to take care about the order of the matrices in the matrix products. For instance,  $r t^{-1} \neq t^{-1} r$ , since  $r$  and  $t$  are noncommutative matrices.

The transmission coefficient  $T$  is given as

$$T = \text{Tr } t^\dagger t = \sum_{nm} t_{nm}^* t_{nm} \quad (1.139)$$

where  $t$  is the  $N \times N$  transmission matrix. More detailed information about the transmission properties of the system can be obtained if one measures also the following transmission parameters [83, 151, 156]:

$$T_{nm} = |t_{nm}|^2 \quad (1.140)$$

and

$$T_n = \sum_m T_{nm}. \quad (1.141)$$

The matrix elements  $T_{nm}$  define the transmission amplitude from the state with  $k_{\parallel n}$  to the state  $k_{\parallel m}$ . The transmission coefficient  $T_n$  is the transmission through the sample from the state  $n$  to all possible states  $m$  on the other side of the sample.

If there is no absorption in the system (the potential  $V$  is real) then the reflection  $R$  can be found from the conservation of the current density,

$$R = N - T \quad (1.142)$$

Note that relations (1.36) and (1.50) are valid also for the general case  $N > 1$ . The  $2 \times 2$  matrices

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (1.143)$$

are replaced by  $2N \times 2N$  matrices

$$\begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}, \quad (1.144)$$

where  $\mathbf{1}$  is a unity  $N \times N$  matrix.

## 1.6 Problems

### **Problems with Solutions**

#### *Problem 1.1*

Derive the relationships (1.13) and (1.14) between the transfer matrix and scattering matrix.

*Solution.* The matrix equations (1.11) and (1.12) can be written explicitly as

$$\Psi_L^- = S_{11} \Psi_L^+ + S_{12} \Psi_R^-, \quad \Psi_R^+ = S_{21} \Psi_L^+ + S_{22} \Psi_R^- \quad (1.145)$$



and

$$\Psi_R^+ = M_{11}\Psi_L^+ + M_{12}\Psi_L^-, \quad \Psi_R^- = M_{21}\Psi_L^+ + M_{22}\Psi_L^-. \quad (1.146)$$

We express  $\Psi_R^-$  from the first equation (1.145):

$$\Psi_R^- = \frac{1}{S_{12}}\Psi_L^- - \frac{S_{11}}{S_{12}}\Psi_L^+ \quad (1.147)$$

and insert it into the second equation (1.145). We obtain

$$\Psi_R^+ = \left[ S_{21} - \frac{S_{11}S_{22}}{S_{12}} \right] \Psi_L^+ + \frac{S_{22}}{S_{12}}\Psi_L^-. \quad (1.148)$$

Now, compare equations (1.146) with equations (1.147) and (1.148) and get

$$\begin{aligned} M_{11} &= S_{21} - \frac{S_{11}S_{22}}{S_{12}}, & M_{12} &= \frac{S_{22}}{S_{12}} \\ M_{21} &= -\frac{S_{11}}{S_{12}}, & M_{22} &= \frac{1}{S_{12}}. \end{aligned} \quad (1.149)$$

The relations (1.149) are equivalent to the matrix equation (1.13). In the same way, we can express elements of the scattering matrix  $\mathbf{S}$  in terms of elements of the transfer matrix  $\mathbf{M}$  to obtain expression (1.14).

*Problem 1.2*

Prove that  $|\det \mathbf{S}| = 1$  [equation (1.27)].

*Solution.* Since the determinant of the product of two matrices  $\mathbf{AB}$  equals the product of their determinants,

$$\det \mathbf{AB} = \det \mathbf{A} \det \mathbf{B}, \quad (1.150)$$

we have for a unitary matrix  $\mathbf{S}$  that

$$\det \mathbf{S} \det \mathbf{S}^\dagger = 1. \quad (1.151)$$

On the other hand,

$$\det \mathbf{S}^\dagger = S_{11}^* S_{22}^* - S_{12}^* S_{21}^* = [\det \mathbf{S}]^*. \quad (1.152)$$

By combining the previous equations we obtain

$$|\det \mathbf{S}| = 1. \quad (1.153)$$

*Problem 1.3*

Derive the expression (1.60) for the transfer matrix.

*Solution.* From the definition of the scattering matrix, equation (1.58), we have

$$\begin{pmatrix} \Psi_L^- \\ \Psi_R^+ \end{pmatrix} = \begin{pmatrix} r' & t \\ t' & r \end{pmatrix} \begin{pmatrix} \Psi_L^+ \\ \Psi_R^- \end{pmatrix}, \quad (1.154)$$

which can be written in the form

$$\Psi_L^- = r'\Psi_L^+ + t\Psi_R^-, \quad \Psi_R^+ = t'\Psi_L^+ + r\Psi_R^-. \quad (1.155)$$

From the first equation (1.155) we express  $\Psi_R^- = t^{-1}\Psi_L^- - t^{-1}r'\Psi_L^+$ . Inserting this expression into the second equation (1.155), we obtain

$$\begin{pmatrix} \Psi_R^+ \\ \Psi_R^- \end{pmatrix} = \begin{pmatrix} t' - rt^{-1}r' & rt^{-1} \\ -t^{-1}r' & t^{-1} \end{pmatrix} \begin{pmatrix} \Psi_L^+ \\ \Psi_L^- \end{pmatrix}. \quad (1.156)$$

Comparing this with the definition of transfer matrix, equation (1.12), we obtain expression (1.60).

#### Problem 1.4

Prove the identity (1.131).

*Solution.* To prove the relation (1.131), we start from the definition of the function  $U_N$ , given by equation (1.127), and use the relation  $\sin(x \pm y) = \sin x \cos y \pm \cos x \sin y$ . We obtain

$$U_N(q\ell) = \frac{\sin(N+1)q\ell}{\sin q\ell} = \frac{\sin Nq\ell \cos q\ell + \cos Nq\ell \sin q\ell}{\sin q\ell} \quad (1.157)$$

and

$$U_{N-2}(q\ell) = \frac{\sin(N-1)q\ell}{\sin q\ell} = \frac{\sin Nq\ell \cos q\ell - \cos Nq\ell \sin q\ell}{\sin q\ell}. \quad (1.158)$$

Now we sum both equations to obtain

$$U_N + U_{N-2} = \frac{2 \cos q\ell \sin Nq\ell}{\sin q\ell} = 2 \cos q\ell U_n, \quad (1.159)$$

which is already the required identity, equation (1.131).

### Problems without Solutions

#### Problem 1.5

We can also define the transfer matrix  $\tilde{\mathbf{M}}$  by the relation

$$\begin{pmatrix} \Psi_L^+(x) \\ \Psi_L^-(x) \end{pmatrix} = \tilde{\mathbf{M}} \begin{pmatrix} \Psi_R^+(x+\ell) \\ \Psi_R^-(x+\ell) \end{pmatrix}. \quad (1.160)$$

$\tilde{\mathbf{M}}$  expresses the wave function on the *left* side of the potential region in terms of the wave function on the *right* side. Show that  $\tilde{\mathbf{M}} = \mathbf{M}^{-1}$ . Derive the explicit form of the transfer matrix  $\tilde{\mathbf{M}}$ :

$$\tilde{\mathbf{M}} = \begin{pmatrix} \frac{1}{S_{21}} & -\frac{S_{22}}{S_{21}} \\ \frac{S_{11}}{S_{21}} & S_{12} - \frac{S_{11}S_{22}}{S_{21}} \end{pmatrix}. \quad (1.161)$$

*Problem 1.6*

Using the multiplication law for transfer matrices, equation (1.76), as well as the physical arguments explained in section 1.4.1, derive the composition laws for the transmission amplitude  $t'_{12}$  and reflection amplitude  $r_{12}$  of a system that consists of two samples.

*Problem 1.7*

Write the transmission and reflection amplitudes as follows:

$$t = |t|e^{i\phi_t}, \quad r = |r|e^{i\phi_r}. \quad (1.162)$$

In section 1.4.1 we showed that the addition of a free space to the sample does not change transmission and reflection coefficients [equations (1.83) and (1.84)]. Show how the additional free space influences the phases  $\phi_t$  and  $\phi_r$ . Analysis of the phases of the transmission and reflection amplitudes is very important for inverse problems (see, for instance, section 2.6).

*Problem 1.8*

Repeat the analysis of section 1.4.3 with  $\kappa < 0$ . Show that in this case the bound state is given as a solution of the equation

$$M_{11}(i\kappa) = 0 \quad \text{for } \kappa < 0. \quad (1.163)$$