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The Transfer Matrix Method

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The scattering approach

Among the familiar examples of scattering phenomena, the most conspicuous are probably the dispersion of light and the partial transmission and reflection of electromagnetic waves by refractive media. In the quantum description of the electronic transport through a potential region $V(\mathbf{r})$, the macroscopic concepts of resistance and conductance entail also those of reflection and transmission amplitudes. The celebrated Landauer's approach to electronic transport [**?**], represents a remarkable example of an approach where this conception is neatly embodied. In this approach the conductance of any 1D elastically scattering system is written as

$$G = \frac{e^2}{\pi\hbar}\frac{tt^*}{rr^*} = \frac{e^2}{\pi\hbar}\frac{T}{R} \tag{2.1}$$

where t and r are the sample dependent scattering (transmission and reflection) amplitudes. A large number of derivations and debate papers have been published [**?**, **?**, **?**, **?**] on this formula and its generalization to multichannel 3D systems. In the next chapter, using the scattering matrix and the basic definitions that will be introduced here, we will discuss and derive the Landauer conductance formulas in a very simple and comprehensive way. The relations of these formulas (4.1) with the traditional linear response theory (LRT) has been object of great attention and controversy in the literature [?, ?]. In the linear response theory proposed by Kubo [**?**], the transport properties are studied following a different conception. These properties are treated as linear responses to external perturbations that drive the system out of equilibrium. There is a the large number of books and papers devoted to the LRT. This theory is beyond the scope of this book. The interested reader is referred, for instance, to [?, **?**].

To use the Landauer formulas to studying the electronic transport through a given sample, one needs to evaluate the corresponding transmission and reflection amplitudes. To calculate these backward and forward scattering probabilities, one needs to solve the Maxwell and the Schrödinger equations.

To accomplish this aim, the scattering approach plays a complementary role that, in some cases, may be relevant and crucial.

Studying transport processes, the transfer matrix and the conceptual structure of the scattering theory appears naturally as the appropriate one to deal with the Maxwell and Schrödinger equations. In this book we present well-known and new results of the scattering theory applied to transmission phenomena in open systems. It is also the purpose of this book to show that the transfer matrix technique can advantageously be used to study stationary properties of electromagnetic waves and quantum particles, properties relevant in the theoretical analysis of optoelectronic phenomena. We will show that the transfer matrix technique is a powerful tool in the theoretical analysis of the transport properties of ordered and disordered systems and for the precise evaluations of fundamental quantities, like the eigenvalues and eigenfunctions of quantum particles in simple potential regions $V(\mathbf{r})$ or more complex systems like the superlattice structures with arbitrary single-cell potential profiles.

We will introduce in this chapter the general framework of the scattering theory in a comprehensive albeit not so formal presentation. Excellent and mathematically more rigorous presentations can be found in the literature, for instance in [**?**, **?**]. Although we will devote some chapters to study electromagnetic waves and electromagnetic pulses through optical media, the general discussions and derivations will refer mostly to quantum particles and the Schrödinger equation.

In transport processes it is important to establish the geometry and the direction along which the electronic motion takes place. Most of the transport processes of interest occur along a given direction, which we will call, unless a magnetic field is present, the z axis or, when appropriate, the growing direction.

The theoretical procedures to solve the Schrödinger equation of specific open and closed systems bear some general and common characteristics. We will review here those mathematical and physical basic properties that will be used throughout this book.

Usually when the transport processes occur through devices with large cross sections, it is common to argue the invariance under transverse translation transformations. In those cases, the number of propagating modes and the density of transverse states is so large that one can safely decouple the transverse from the longitudinal dynamics, and work in the one-dimensional (1D) approximation. In other cases, when the transverse dimensions $w_x \simeq w_y = w$ and the Fermi energy E are small, such that the number of propagating modes $N \propto mw^2E/\pi\hbar^2$ is small, it is in principle feasible and possible to carry out a multi-mode or multichannel analysis.

We will try to use a unified notation for one-channel (1D) and N-channel systems. To fix the notation we will introduce and recall well-known expressions and definitions of fundamental quantities in the scattering theory.

2.0.1 Wave vectors in 1D one-channel systems

If we are dealing with a one-channel 1D system, we have generally to solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\varphi(z) + V(z)\varphi(z) = E\varphi(z). \tag{2.2}$$

for all values of z where the system is defined. The solution of this equation is feasible when the potential is constant, or sectionally constant, while the solution may be slightly or perhaps much more involved when $V(z)$ is a non-constant function. As mentioned in the introduction, the potential functions in most of the actual devices are stepwise constants. In others not, but one can use the semiclassical Wenzel-Kramers-Brillouin (WKB) approximation in the transfer matrix representation (see chapter **??**). In the case of sectionally-constant potential systems like in figure **??**, one has to consider a partition $z_0, z_1, z_2..., z_n$ of the z axis, according with the potential discontinuities,with $z_0 = 0$ and $z_n = L$. The Schrödinger equation is then solved for each constant-potential region. For open and non biased system the potential at $z < 0$ and $z > L$ is usually taken as $V(z) = 0$ and $V(z) = \infty$ for closed or bounded systems. As long as the potential functions and the boundary conditions are not specified, the solutions for $0 < z < L$ are unknown.

In the leads ($z < 0$ and $z > L$), where the Schrödinger equation can be written as

$$\frac{d^2}{dz^2}\varphi(z) + k^2\varphi(z) = 0, \quad \text{with} \quad k^2 = \frac{2mE}{\hbar^2}, \tag{2.3}$$

the solutions are the right (+) and left (-) moving plane waves

$$\varphi^{\pm}(z) = Ae^{\pm ikz}. \tag{2.4}$$

The normalization constants will usually be absorbed by the coefficients of the linear combinations. Hence, the wave functions at z_l and z_r (at the left and right hand sides), will be written in the 1D case as

$$\varphi(z_l) = a\,\varphi^+(z_l) + b\,\varphi^-(z_l) = a\,e^{ikz_l} + b\,e^{-ikz_l} \tag{2.5}$$

$$\varphi(z_r) = c\,\varphi^+(z_r) + d\,\varphi^-(z_r) = c\,e^{ikz_r} + d\,e^{-ikz_r} \tag{2.6}$$

In the scattering theory, the wave vectors more that the wave functions are used. For example, to deal with the scattering matrix we need to define two-points incoming and outgoing wave vectors like

$$\phi^i(z_l, z_r) = \begin{pmatrix} a\,\varphi^+(z_l) \\ d\,\varphi^-(z_r) \end{pmatrix} \quad \text{and} \quad \phi^o(z_l, z_r) = \begin{pmatrix} c\,\varphi^+(z_r) \\ b\,\varphi^-(z_l) \end{pmatrix}, \tag{2.7}$$

and for the transfer matrix M we need to define one point wave vectors like

$$\phi(z_l) = \begin{pmatrix} a\,\varphi^+(z_l) \\ b\,\varphi^-(z_l) \end{pmatrix} \quad \text{and} \quad \phi(z_r) = \begin{pmatrix} c\,\varphi^+(z_r) \\ d\,\varphi^-(z_r) \end{pmatrix}. \tag{2.8}$$

2.0.2 Wave vectors in 3D N-channel systems

Suppose now that we are interested in describing the transport properties through a potential region $V(x,y,z)$ laterally bounded by infinite hard walls, with z, extending from z_l to z_r, and $0 \leq x \leq w_x, 0 \leq y \leq w_y$ in the transversal direction.

In the leads, outside the scattering potential region, i.e. for $z < z_l$ and $z > z_r$ where $V(x,y,z) = 0$, the Schrödinger equation separates into transverse and longitudinal variables. The wave functions $\phi_j(x,y)$ satisfying the equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi_j(x,y) + k_{Tj}^2\phi_j(x,y) = 0, \tag{2.9}$$

with boundary conditions $\phi_j(0,y) = \phi_j(w_x,y) = \phi_j(x,0) = \varphi_j(x,w_y) = 0$, form a complete set of functions in the transverse variables x and y. In this equation $k_{Tj}^2 = \pi^2 j^2/w_y^2$ is the quantized transverse-motion momentum. We will use below the wave functions $\phi_j(x,y)$ to expand the 3D wave function $\varphi(x,y,z)$.

In the leads, the wave functions $\varphi_j(z)$ satisfy the homogeneous equation

$$\frac{d^2}{dz^2}\varphi_j(z) + (k^2 - k_{Tj}^2)\varphi_j(z) = 0, \tag{2.10}$$

with $k^2 = 2mE/\hbar^2$ the Fermi wave number. For $k_j^2 = k^2 - k_{Tj}^2 > 0$, the solutions are running waves and are referred to as propagating modes or open channels. In this case the wave functions at z_l and z_r (at the left and right hand sides), are the linear combinations

$$\varphi(z_l) = \sum_j^N \left[a_j\,\varphi_j^+(z_l) + b_j\,\varphi_j^-(z_l)\right] = \sum_j^N \left[a_j\,e^{ik_jz_l} + b_j\,e^{-ik_jz_l}\right], \tag{2.11}$$

$$\varphi(z_r) = \sum_j^N \left[c_j\,\varphi_j^+(z_r) + d_j\,\varphi_j^-(z_r)\right] = \sum_j^N \left[c_j\,e^{ik_jz_r} + d_j\,e^{-ik_jz_r}\right], \tag{2.12}$$

that generalize those defined in Eqs. (2.5) and (2.6). When $k_j^2 = k^2 - k_{Tj}^2 < 0$, the solutions decay exponentially and are referred to as closed channels or evanescent modes.

In some cases it is convenient and necessary to use normalized plane waves. In those cases we will use the plane waves

$$\varphi_j^{\pm}(z) = \frac{e^{\pm ik_jz}}{\sqrt{\hbar k_j/m^*}}, \tag{2.13}$$

normalized to unit particle current in the propagating mode j.

Some times the spin degrees of freedom have to be considered explicitly. In those cases the number N of channels factorize as $N = \mathcal{N}s$, with s the number of spin projections, and the wave functions are written as

$$\varphi(z) = \sum_{j,\sigma}^{\mathcal{N},s} a_{j\sigma}\varphi^{+}_{j\sigma}(z) + \sum_{j,\sigma}^{\mathcal{N},s} b_{j\sigma}\varphi^{-}_{j\sigma}(z) \tag{2.14}$$

For the sake of an easy notation, that usually helps to visualize better the physical relations, we shall omit the spin index. It will be used in chapter **??** where the spin degree of freedom is relevant.

For the purpose of using a unified notation, the two-points and one point wave vectors (see Eqs. (2.7) and (2.8)) are written now as

$$\phi^{i}(z_l, z_r) = \begin{pmatrix} \phi^{i}(z_l) \\ \phi^{i}(z_r) \end{pmatrix}, \qquad \phi^{o}(z_l, z_r) = \begin{pmatrix} \phi^{o}(z_r) \\ \phi^{o}(z_l) \end{pmatrix}, \tag{2.15}$$

and

$$\phi(z_l) = \begin{pmatrix} \phi^{+}(z_l) \\ \phi^{-}(z_l) \end{pmatrix}, \qquad \phi(z_r) = \begin{pmatrix} \phi^{+}(z_r) \\ \phi^{-}(z_r) \end{pmatrix}. \tag{2.16}$$

Here $\phi^{+}(z_s)$ and $\phi^{-}(z_s)$, with $s = l, r$, are the N-dimensional right and left moving wave vectors

$$\phi^{+}(z_l) = \begin{pmatrix} a_1\varphi^{+}_1(z_l) \\ a_2\varphi^{+}_2(z_l) \\ \dots \\ a_N\varphi^{+}_N(z_l) \end{pmatrix} = \phi^{i}(z_l), \qquad \phi^{-}(z_l) = \begin{pmatrix} b_1\varphi^{-}_1(z_l) \\ b_2\varphi^{-}_2(z_l) \\ \dots \\ b_N\varphi^{-}_N(z_l) \end{pmatrix} = \phi^{o}(z_l), \tag{2.17}$$

and

$$\phi^{+}(z_r) = \begin{pmatrix} c_1\varphi^{+}_1(z_r) \\ c_2\varphi^{+}_2(z_r) \\ \dots \\ c_N\varphi^{+}_N(z_r) \end{pmatrix} = \phi^{o}(z_r), \qquad \phi^{-}(z_r) = \begin{pmatrix} d_1\varphi^{-}_1(z_r) \\ d_2\varphi^{-}_2(z_r) \\ \dots \\ d_N\varphi^{-}_N(z_r) \end{pmatrix} = \phi^{i}(z_r) \tag{2.18}$$

All these vectors were defined in terms of the plane wave solutions at the leads. Although these vectors will in the next sections allow us to introduce the scattering and transfer matrices and some important relations, the main problem, that of solving the Schrödinger equation for specific scattering regions, remains open and will partially be addressed in this book.

Before concluding this part, let us come back to the beginning, where we introduced the transverse solutions $\varphi_j(x, y)$ in the leads of a laterally bounded potential $V(x, y, z)$. We mentioned there that the 2D functions $\varphi_j(x, y)$ will be used to expand 3D functions. In fact,, we can use this complete set of functions to expand the 3D wave function $\varphi(x, y, z)$ in the scattering region, i.e. for $z_l < z < z_r$, as

$$\varphi(x, y, z) = \sum_{j} \phi_j(x, y)\varphi_j(z) \quad \text{for} \quad z_l < z < z_r. \tag{2.19}$$

It is worth noticing that for this expansion one has, at least, two choices: either one uses always the same trigonometric functions satisfying Eq. (2.9) or alternatively one uses at each point z_p of the scattering region, when available, the exact transverse solutions $\phi_j(x, y, z_p)$. In any case one has to deal at the end with an infinite system of coupled equations.

To make the discussion easier, we will consider from now on only two-dimensional systems, ignoring the x-direction, and for the expansion purpose of $\phi_j(x, y, z_p)$ only the first choice. The second choice will be mentioned latter when discussing electronic transport in the presence of a transverse electric field. In the first choice we have $\phi_j(y) = \sqrt{2/w_y}\sin \pi j y/w_y$. Substituting the expanded wave function into the Schrödinger equation, we obtain the system of coupled equations

$$\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\varphi_j(z) - \sum_i V_{ij}(z)\varphi_i(z) + (k^2 - k_{Tj}^2)\varphi_j(z) = \tag{2.20}$$

where V_{ij} are the coupling matrix elements

$$V_{ij}(z) = \frac{2}{w_y}\int_0^{w_y} dy V(y, z)\phi_i(y)\phi_j(y) \qquad i, j = 1, 2, ... \tag{2.21}$$

This set of coupled equations is infinite, therefore impossible to solve in general. Thus, it is natural to cut at a finite fixed number N, which we call the channels' number that, depending on the Fermi energy, may include only open channels or open plus some closed channels. We will show here that using the transfer matrix method the coupled equations can, for some systems, be tackled and the wave functions $\varphi_j(z)$ determined.

Even though in this book we will be basically concerned with transfer matrices, the relation of the transfer matrix elements with the scattering amplitudes is an essential relation. Studying the transport processes, the scattering amplitudes are important quantities, and they will be obtained from the transfer matrices. To understand the relation of the transfer matrix with the scattering amplitudes we shall introduce some definitions and basic properties of the scattering matrix.

2.1 The scattering matrix and some basic properties

We know that when a flux of quantum particles approach a potential region, like in figure 2.1, part of the incoming flux is reflected while the other part passes through. In the scattering approach, the reflection and the transmission amplitudes, r and t, are fundamental physical quantities. These amplitudes are fully determined by the incoming flux, the potential function and the boundary conditions. We will schematically indicate how these amplitudes are defined. Since the scattering matrix is usually defined in terms of incoming and outgoing functions we will rename, temporally, the right and left moving modes as incoming or outgoing waves, depending on whether they are approaching or leaving the scattering region. This means that a wave function written as

$$\varphi(z) = a\varphi^+(z) + b\varphi^-(z). \tag{2.22}$$

can also be written as

$$\varphi(z) = \varphi^i(z) + \varphi^o(z). \tag{2.23}$$

In fact, if we have a scattering process like the one shown in figure 2.1,

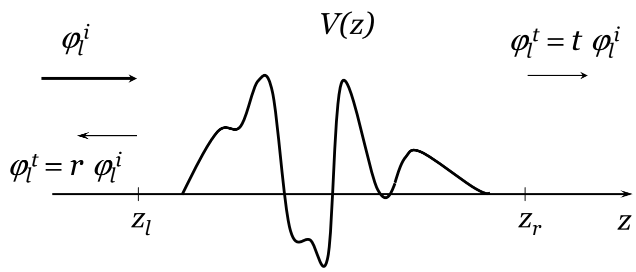

Fig. 2.1. The incoming wave from the left is partially transmitted and partially reflected. The scattering amplitudes are t and r respectively

the incoming wave approaches from the left and the outgoing waves are the reflected and the transmitted ones. Hence, the wave functions at z_l and at z_r can be written as

$$\varphi(z_l) = \varphi_l^i(z_l) + \varphi_l^r(z_l), \tag{2.24}$$

and

$$\varphi(z_r) = \varphi_l^t(z_r). \tag{2.25}$$

The relation of the incoming, reflected and transmitted wave functions with those introduced before is the following

$$\varphi_l^i(z_l) = a\ \varphi^+(z_l) \tag{2.26}$$
$$\varphi_l^r(z_l) = b\ \varphi^-(z_l) \tag{2.27}$$
$$\varphi_l^t(z_r) = c\ \varphi^+(z_r) \tag{2.28}$$

The reflection and transmission amplitudes r an t are defined such that

$$\varphi_l^r(z_l) = r\ \varphi_l^i(z_l) \tag{2.29}$$
$$\varphi_l^t(z_r) = t\ \varphi_l^i(z_l), \tag{2.30}$$

It is clear that to determine r and t using these relations, we have still to obtain the coefficients a, b and c. This is possible only when the Schrödinger

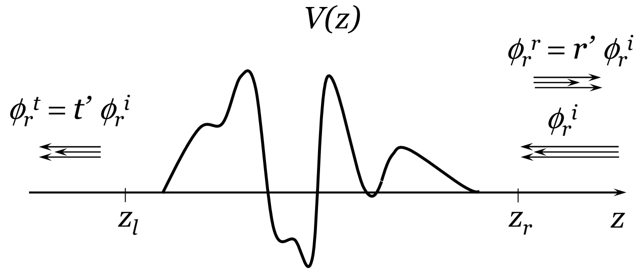

Fig. 2.2. N-propagating modes coming from the right are partially transmitted and partially reflected. The scattering amplitudes are t' and r' respectively

equation, at the interaction region, is solved and all the boundary conditions fulfilled.

Generally, the scattering processes involve N-propagating modes, as well as incoming waves from the left and the right hand sides. Let us first generalize the previous equations and definition for scattering processes with N propagating modes. In this case the wave functions $\varphi_l^i(z_l)$, $\varphi_l^r(z_l)$ and $\varphi_l^t(z_l)$ in (2.26-2.28) become

$$\varphi_l^i(z_l) = \sum_j^N a_j \; \varphi_j^+(z_l) \tag{2.31}$$

$$\varphi_l^r(z_l) = \sum_j^N b_j \; \varphi_j^-(z_l) \tag{2.32}$$

$$\varphi_l^t(z_r) = \sum_j^N c_j \; \varphi_j^+(z_r) \tag{2.33}$$

To express the last two functions, i.e. $\varphi_l^r(z_l)$ and $\varphi_l^t(z_r)$, in terms of the incoming functions we need to introduce the following transformations

$$b_k \varphi_k^-(z_l) = \sum_j^N r_{kj} a_j \varphi_j^+(z_l), \tag{2.34}$$

$$c_k \varphi_k^+(z_r) = \sum_j^N t_{kj} a_j \varphi_j^+(z_l). \tag{2.35}$$

r_{kj} and t_{kj} represent the scattering amplitudes from channel j to channel k. Using these relations, we have

$$\varphi_l^r(z_l) = \sum_{k,j}^N r_{kj} a_j \varphi_j^+(z_l) \tag{2.36}$$

$$\varphi_l^t(z_r) = \sum_{k,j}^{N} t_{kj} a_j \varphi_j^+(z_l), \tag{2.37}$$

To visualize better the matrices r and t, let us define and recall the following vectors

$$\phi_l^i(z_l) = \begin{pmatrix} a_1\varphi_1^+(z_l) \\ a_2\varphi_2^+(z_l) \\ \cdots \\ a_N\varphi_N^+(z_l) \end{pmatrix} \quad \phi_l^r(z_l) = \begin{pmatrix} b_1\varphi_1^-(z_l) \\ b_2\varphi_2^-(z_l) \\ \cdots \\ b_N\varphi_N^-(z_l) \end{pmatrix} \quad \phi_l^t(z_r) = \begin{pmatrix} c_1\varphi_1^+(z_r) \\ c_2\varphi_2^+(z_r) \\ \cdots \\ c_N\varphi_N^+(z_r) \end{pmatrix} \tag{2.38}$$

and write the transformation relations (2.34) and (2.35) in the form

$$\phi_l^r(z_l) = r\,\phi_l^i(z_l) \qquad \text{and} \qquad \phi_l^t(z_r) = t\,\phi_l^i(z_l). \tag{2.39}$$

These relations generalize those in (2.29) and (2.30).

It is equally possible to have, like in figure 2.2, an incoming flux from the right. In this case, the reflected and transmitted wave vectors will be written as

$$\phi_r^r(z_r) = r'\,\phi_r^i(z_r) \qquad \text{and} \qquad \phi_r^t(z_l) = t'\,\phi_r^i(z_r), \tag{2.40}$$

with r' and t' the corresponding reflection and transmission amplitudes.

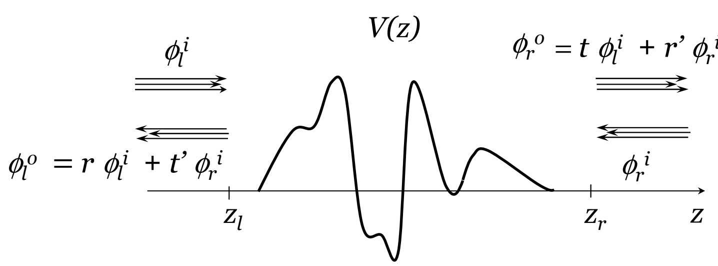

Fig. 2.3. The transmitted and reflected wave vectors give rise to the outgoing wave vectors at the left and right.

In the most general case, shown in figure 2.3, the incoming waves approach from the left and from the right. Both waves are reflected and transmitted. Thus the outgoing waves $\phi_l^o(z_l)$ and $\phi_r^o(z_r)$ are given by

$$\phi_l^o(z_l) = r\ \phi_l^i(z_l) + t'\ \phi_r^i(z_r), \tag{2.41}$$
$$\phi_r^o(z_r) = t\ \phi_l^i(z_l) + r'\ \phi_r^i(z_r). \tag{2.42}$$

Writing these equations in a matrix representation we have

$$\begin{pmatrix} \phi_l^o(z_l) \\ \phi_r^o(z_r) \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} \phi_l^i(z_l) \\ \phi_r^i(z_r) \end{pmatrix} \tag{2.43}$$

where the scattering matrix

$$S(z_r, z_l) = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \tag{2.44}$$

appeared naturally. This matrix contains the whole information of the scattering process in the potential region between z_l and z_r. Before introducing the transfer matrices we will briefly comment a couple of properties of the scattering matrix. Properties related with two important physical principles, the flux conservation and the time reversal invariance and with the composition rules of the S matrix in successive scattering processes.

2.1.1 Flux Conservation and Time Reversal Invariance

The flux conservation principle is also known as the probability conservation principle. This property implies that

$$\begin{pmatrix} \phi_l^i(z_l) \\ \phi_r^i(z_r) \end{pmatrix}^\dagger \begin{pmatrix} \phi_l^i(z_l) \\ \phi_r^i(z_r) \end{pmatrix} = \begin{pmatrix} \phi_l^o(z_l) \\ \phi_r^o(z_r) \end{pmatrix}^\dagger \begin{pmatrix} \phi_l^o(z_l) \\ \phi_r^o(z_r) \end{pmatrix} \tag{2.45}$$

$$= \begin{pmatrix} \phi_l^i(z_l) \\ \phi_r^i(z_r) \end{pmatrix}^\dagger S^\dagger S \begin{pmatrix} \phi_l^i(z_l) \\ \phi_r^i(z_r) \end{pmatrix} \tag{2.46}$$

Hence

$$S^\dagger S = S S^\dagger = I_{2N} \tag{2.47}$$

the scattering matrix is a unitary matrix. The matrix I_{2N} is the unit matrix

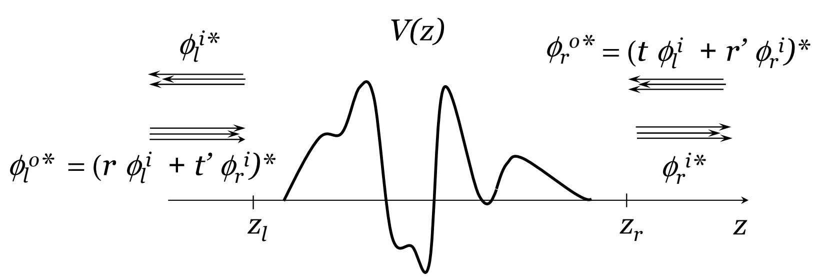

Fig. 2.4. The left and right moving waves are reverted by complex conjugation.

of dimension $2N \times 2N$. From this condition we have

$$\sum_j^N \left(|r_{ij}|^2 + |t_{ij}|^2\right) = \sum_j^N \left(R_{ij} + T_{ij}\right) = R_i + T_i = 1 \tag{2.48}$$

where R_{ij} and T_{ij} are the reflection and transmission coefficients from channel j to channel i. R_i and T_i are the total reflection and total transmission to channel i.

When the physical interactions are time reversal invariant the Hamiltonian is symmetric and belongs to the orthogonal universality class, named by the kind of matrix that diagonalizes the Hamiltonian. It is known that the complex conjugate of a propagating wave function is equivalent to time reversal operation. Therefore, under the time-reversal, the process of figure 2.3 transforms into the process shown in figure 2.4. If the system is time reversal invariant, the scattering matrix S should also fulfill the relation

$$\begin{pmatrix} \varphi_l^{i*}(z_l) \\ \varphi_r^{i*}(z_r) \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} \varphi_l^{o*}(z_l) \\ \varphi_r^{o*}(z_r) \end{pmatrix}. \tag{2.49}$$

Taking the complex conjugate of this equation, we have

$$\begin{pmatrix} \varphi_l^{i}(z_l) \\ \varphi_r^{i}(z_r) \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}^* \begin{pmatrix} \varphi_l^{o}(z_l) \\ \varphi_r^{o}(z_r) \end{pmatrix}. \tag{2.50}$$

From Eq. (2.43) we also have that

$$\begin{pmatrix} \varphi_l^{i}(z_l) \\ \varphi_r^{i}(z_r) \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}^{-1} \begin{pmatrix} \varphi_l^{o}(z_l) \\ \varphi_r^{o}(z_r) \end{pmatrix}. \tag{2.51}$$

This means that

$$S^* = S^{-1}. \tag{2.52}$$

Using the Flux Conservation requirement of Eq. (2.47) we conclude that, for time reversal invariant (TRI) systems, the scattering matrix is symmetric, i.e.

$$S = S^T. \tag{2.53}$$

Hence

$$r = r^T \qquad t' = t^T \qquad r' = r'^T \qquad . \tag{2.54}$$

The flux conservation and time reversal invariance requirements on the scattering matrix will be used at different points of this book. To illustrate with a simple example let us consider a 1D square barrier potential.

2.1.2 Composition rules of S in successive scattering processes

In transport and conduction problems the propagating particles suffer, generally, successive scattering processes. Suppose that we have the potential function as in figure 2.5. For each of the two potential barriers we can identified the incoming and outgoing vectors and establish the following relations

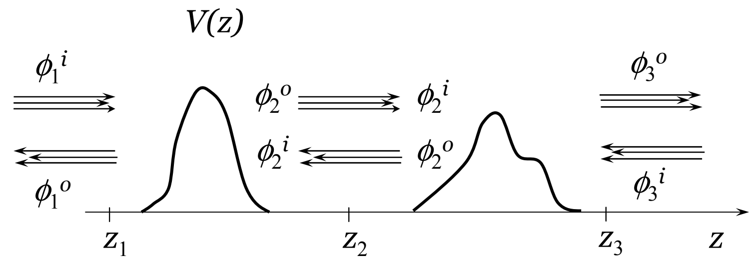

Fig. 2.5. incoming and outgoing functions in the scattering process by a square barrier potential.

$$\begin{pmatrix} \phi_1^o(z_1) \\ \phi_2^o(z_2) \end{pmatrix} = \begin{pmatrix} r_1 & t_1' \\ t_1 & r_1' \end{pmatrix} \begin{pmatrix} \phi_1^i(z_1) \\ \phi_2^i(z_2) \end{pmatrix} = S_1 \begin{pmatrix} \phi_1^i(z_1) \\ \phi_2^i(z_2) \end{pmatrix} \tag{2.55}$$

$$\begin{pmatrix} \phi_2^i(z_2) \\ \phi_3^o(z_3) \end{pmatrix} = \begin{pmatrix} r_2 & t_2' \\ t_2 & r_2' \end{pmatrix} \begin{pmatrix} \phi_2^o(z_2) \\ \phi_3^i(z_3) \end{pmatrix} = S_2 \begin{pmatrix} \phi_2^o(z_2) \\ \phi_3^i(z_3) \end{pmatrix} \tag{2.56}$$

Notice that in order to refer to the same vectors in (2.55), we have changed in (2.56) the incoming and outgoing vectors at z_2 by the outgoing and incoming vectors at that point, respectively. The S matrix for the successive scattering processes is defined as

$$\begin{pmatrix} \phi_1^o(z_1) \\ \phi_3^o(z_3) \end{pmatrix} = S \begin{pmatrix} \phi_1^i(z_1) \\ \phi_3^i(z_3) \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} \phi_1^i(z_1) \\ \phi_3^i(z_3) \end{pmatrix} \tag{2.57}$$

The composition rule of the scattering matrices S_1 and S_2 to obtain the matrix S is rather involved. The successive scattering processes is physically similar to that of an electromagnetic wave through a planar slab (or thin film) bounded by two semi-infinite media. The electromagnetic waves are transmitted and reflected in each interface an infinity number of times. In fact for the calculation of the slab reflection and transmission coefficients, one the well-known method uses the Fresnel coefficients r_{f1} and t_{f1} and r_{f2} and t_{f2}, and the infinite summation such

$$t = t_{f2}e^{i\phi}t_{f1} + t_{f2}e^{i\phi}r_{f1}e^{i\phi}r_{f2}e^{i\phi}t_{f1} + t_f(e^{i\phi}r_{f1}e^{i\phi}r_{f2})^2e^{i\phi}t_f + \tag{2.58}$$

with $\phi = \boldsymbol{k} \cdot \boldsymbol{d}$ the phase that the EM wave gains when it moves across the slab. This sum converges to the well-known Airy formula

$$t = \frac{t_{f2}e^{i\phi}t_{f1}}{1 - e^{i\phi}r_{f1}e^{i\phi}r_{f2}} \tag{2.59}$$

If we expand the matrix equations in (2.55) and (2.56) and rewrite them to express $\phi_1^o(z_1)$ and $\phi_3^o(z_3)$ in terms of $\phi_1^i(z_1)$ and $\phi_3^i(z_3)$, we have after some algebra

$$\begin{aligned}\phi_1^o(z_1) &= \left(t_1'\frac{1}{I_N - r_2 r_1'} r_2 t_1 + r_1\right)\phi_1^i(z_1) + t_1'\frac{1}{I_N - r_2 r_1'} t_2' \phi_3^i(z_3) \\ \phi_3^o(z_3) &= t_2\frac{1}{I_N - r_1' r_2} t_1 \phi_1^i(z_1) + \left(t_2\frac{1}{I_N - r_1' r_2} r_1' t_2' + r_2'\right)\phi_3^i(z_3)\end{aligned} \quad (2.60)$$

Therefore

$$S = \begin{pmatrix} r_1 + t_1'\frac{1}{I_N - r_2 r_1'} r_2 t_1 & t_1'\frac{1}{I_N - r_2 r_1'} t_2' \\ t_2\frac{1}{I_N - r_1' r_2} t_1 & r_2' + t_2\frac{1}{I_N - r_1' r_2} r_1' t_2' \end{pmatrix} \quad (2.61)$$

As one could expect, the matrix elements of the composed S matrix correspond with the Airy formulae, in the limit $\phi \to 0$. Behind two successive scattering systems we have a complex physics underlying an infinite number of scattering processes. If we would increase the number of successive scattering centers, the mathematics will become not only involved but unmanageable. Below we will see that, in contradistinction, the transfer-matrix composition rules are extremely simple and appealing.

2.1.3 The S matrix of a 1D square barrier potential

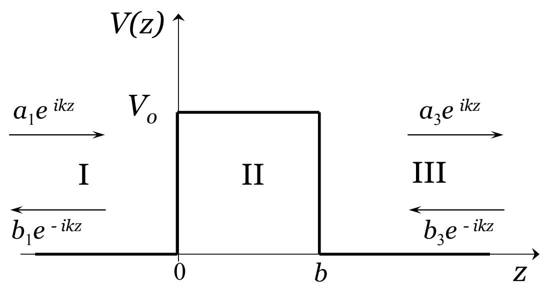

Fig. 2.6. incoming and outgoing functions in the scattering process by a square barrier potential.

In this book we are not concerned with direct calculations of scattering matrices. The complexity of composition rules of these matrices make them the less appropriate ones for the kind of systems of interest here. To illustrate an explicitly calculation of the S matrix, and to visualize some of its properties and relations with the transfer matrix, we shall however consider here a simple example: the square barrier potential. Let the square barrier shown in figure 2.6. The potential function is defined by

$$V(z) = \begin{cases} 0 & z \le 0, \ \ z \ge b \\ V_o & 0 < z < b \end{cases} \quad (2.62)$$

This potential function has been used for many years as a simple example of repulsive potential. It is clear that the constant potentials with sharp discontinuities were just an approximation, however, with the development of the epitaxial growing techniques, this kind of potentials with abrupt changes in the conduction band edge, become possible. If we have the structure $GaAs/Al_xGa_{1-x}As/GaAs$ with a layer $Ga_{1-x}Al_xAs$ of thickness b and $x \simeq 0.3$, the electrons feel a barrier like in figure 2.6, with $V_o \simeq 0.23$eV.

To obtain the scattering matrix of this system, we have to solve the Schrödinger equation for a given value of the energy E, which we will assume is smaller than V_o. The solutions in each of the three regions are:

$$\varphi_{\mathrm{I}}(z) = a_1 e^{ikz} + b_1 e^{-ikz} \qquad z \leq 0 \tag{2.63}$$

$$\varphi_{\mathrm{III}}(z) = a_3 e^{ikz} + b_3 e^{-ikz} \qquad z \geq b \tag{2.64}$$

with $k = \sqrt{2mE/\hbar^2}$ for regions I and III, and

$$\varphi_{\mathrm{II}}(z) = a_2 e^{qz} + b_2 e^{-qz} \qquad 0 < z < b \tag{2.65}$$

with $q = \sqrt{2m(V_o - E)/\hbar^2}$ for the second region II. The continuity conditions in $z = 0$ and $z = b$, give rise to the following equations

$$a_1 + b_1 = a_2 + b_2 \tag{2.66}$$
$$ik(a_1 - b_1) = q(a_2 - b_2). \tag{2.67}$$

and

$$a_2 e^{qb} + b_2 e^{-qb} = a_3 e^{ikb} + b_3 e^{-ikb} \tag{2.68}$$
$$q(a_2 e^{qb} - b_2 e^{-qb}) = ik(a_3 e^{ikb} - b_3 e^{-ikb}). \tag{2.69}$$

which for the purpose of finding the S-matrix can, after some algebra, be written in the form

$$\begin{aligned} Ab_1 + Ba_3 e^{ikb} &= Fa_1 + Gb_3 e^{-ikb} \\ Cb_1 + Da_3 e^{ikb} &= Ha_1 + Jb_3 e^{-ikb}. \end{aligned} \tag{2.70}$$

with

$$\begin{aligned} &A = H^* = i(k^2 + q^2)\sinh qb\,, && B = J = 2kq, \\ &C = F^* = 2kq\cosh qb + i(q^2 - k^2)\sinh qb\,, && D = G = 0. \end{aligned} \tag{2.71}$$

From these equations it is possible to express the outgoing wave functions b_1 and $a_3 e^{ikb}$ at $z = 0$ and $z = b$ as functions of the incoming waves in the matrix representation

$$\begin{pmatrix} A & B \\ C & 0 \end{pmatrix} \begin{pmatrix} b_1 \\ a_3 e^{ikb} \end{pmatrix} = \begin{pmatrix} C^* & 0 \\ A^* & B \end{pmatrix} \begin{pmatrix} a_1 \\ b_3 e^{-ikb} \end{pmatrix}. \tag{2.72}$$

Multiplying by the inverse of the left hand side matrix, this equation becomes

$$\begin{pmatrix} b_1 \\ a_3 e^{ikb} \end{pmatrix} = \frac{1}{C} \begin{pmatrix} A^* & B \\ B & -A \end{pmatrix} \begin{pmatrix} a_1 \\ b_3 e^{-ikb} \end{pmatrix}. \tag{2.73}$$

Therefore, the scattering matrix S_b of the square barrier potential is

$$S_b = \frac{1}{C} \begin{pmatrix} A^* & B \\ B & -A \end{pmatrix} = \begin{pmatrix} r_b & t'_b \\ t_b & r'_b \end{pmatrix} \tag{2.74}$$

It is easy to verify that

$$S_b S_b^\dagger = 1 \qquad \text{and} \qquad S_b = S_b^T \tag{2.75}$$

with reflection and transmission amplitudes

$$r_b = -\frac{i(k^2+q^2)\sinh qb}{2kq\cosh qb + i(q^2-k^2)\sinh qb} \tag{2.76}$$

$$t_b = \frac{2kq}{2kq\cosh qb - i(q^2-k^2)\sinh qb} \tag{2.77}$$

fulfilling the well known relation

$$|r_b|^2 + |t_b|^2 = 1. \tag{2.78}$$

2.2 The transfer matrix and some basic properties

Transfer matrices and their properties were used in the1950s to study electronic spectra and transport processes through ordered and disordered linear chains. [**?**, **?**] More recently, multichannel-transfer-matrix approaches became rather common in the scattering approach to quantum wires. [?] Two types of transfer matrices are most known: the transfer matrix W of the first kind, relating wave functions and their derivatives at two points or planes of the scattering region, and the transfer matrix M of the second kind, connecting state vectors at two points or planes of the scattering region. Transfer matrices of the first kind were used by James [?] and quite recurrently in 1D solid-state physics. [?] On the other hand, the transfer matrices of the second kind were used by Luttinger [**?**] and Borland, [**?**] who called them transformation matrices. Lately, these matrices appeared more frequently and came to be called also transfer matrices. A simple unitary transformation relate the transfer matrices of the first and second kind. We will mainly be concerned with the transfer matrices of the second kind, but in some cases, especially when the wave functions can not be written in the propagating modes representation, the transfer matrices of the first kind are very helpful.

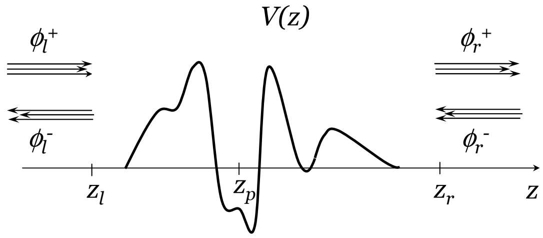

Fig. 2.7. The incoming and outgoing spin independent wave vectors. Here we use the simplified notation $\phi_l^{\pm}$ for $\phi^{\pm}(z_l)$ and $\phi_r^{\pm}$ for $\phi^{\pm}(z_r)$

It is worth noticing that the transfer matrix method is not an alternative method to solve differential equations. The transfer matrix plays a complementary role, it is useful to manage the continuity requirements, boundary conditions and obtaining relevant physical conditions and physical quantities. It will be seen, also, that the transfer matrix properties, properly used, enhance the power of some analytical calculations and, hence, of the numerical evaluation procedures.

Since the explicit form of the transfer matrix depends on the specific system at hand, we will present here just some general definitions. To give an example of the transfer matrix definition relating functions at two points of the z axis, we will use the wave functions shown in figure 2.7 at z_l and z_r, but it must be clear that the transfer matrices relate wave vectors at any two points of the z axis.

2.2.1 Definition of the transfer matrix M

While the scattering matrix relates incoming with outgoing wave vectors, the transfer matrix relates wave vectors at two points of the z axis. Suppose we have the wave functions $\varphi_j^{\pm}$ at z_l and z_r, of figure 2.7. As in Eq. (2.38) we can use them to write the N-dimensional, right and left moving wave vectors

$$\phi^+(z_l) = \begin{pmatrix} a_1\varphi_1^+(z_l) \\ a_2\varphi_2^+(z_l) \\ \ldots \\ a_N\varphi_N^+(z_l) \end{pmatrix} \quad \text{and} \quad \phi^-(z_l) = \begin{pmatrix} b_1\varphi_1^-(z_l) \\ b_2\varphi_2^-(z_l) \\ \ldots \\ b_N\varphi_N^-(z_l) \end{pmatrix} \tag{2.79}$$

at z_l and the right and left moving vectors

$$\phi^+(z_r) = \begin{pmatrix} c_1\varphi_1^+(z_r) \\ c_2\varphi_2^+(z_r) \\ \ldots \\ c_N\varphi_N^+(z_r) \end{pmatrix} \quad \text{and} \quad \phi^-(z_r) = \begin{pmatrix} d_1\varphi_1^-(z_r) \\ d_2\varphi_2^-(z_r) \\ \ldots \\ d_N\varphi_N^-(z_r) \end{pmatrix} \tag{2.80}$$

at z_r. With these vectors one can form the total wave vectors

$$\phi(z_l) = \begin{pmatrix} \phi^+(z_l) \\ \phi^-(z_l) \end{pmatrix} \qquad \text{and} \qquad \phi(z_r) = \begin{pmatrix} \phi^+(z_r) \\ \phi^-(z_r) \end{pmatrix} \tag{2.81}$$

at z_l and z_r. Once the Schrödinger equation has been solved and the continuity requirements satisfied, it is possible to show that two vectors like these are related to each other by a matrix, *the transfer matrix*. In this case by the transfer matrix $M(z_r, z_l)$ defined by

$$\phi(z_r) = M(z_r, z_l)\phi(z_l) \equiv \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \phi(z_l) \tag{2.82}$$

This type of relation can, certainly, be established for any two points of the growing direction. For this reason, if z_1 and z_2 are two points in the z axis of the system, we will always try to obtain the transfer matrix $M(z_2, z_1)$ such that

$$\phi(z_2) = M(z_2, z_1)\phi(z_1) \tag{2.83}$$

In the next chapters we will explicitly obtain transfer matrices for some basic potential profiles. A transfer matrix $M(z_2, z_1)$ relating wave vectors at at z_1 and z_2, behaves as a propagator of the physical information. In some way, the transfer matrix $M(z_2, z_1)$ transforms the physics at z_1 into the physics at z_2. The transfer matrix $M(z_r, z_l)$, defined here, like the scattering matrix $S(z_r, z_l)$ defined before, contains the whole information of the scattering process in the potential region between z_l and z_r. As will be shown in the next section there is a close relation between the transfer and the scattering matrix.

2.2.2 The scattering amplitudes and the transfer matrix elements

Based on the scattering and the transfer matrix definitions, one can easily find important and useful relations between the transfer matrix elements and the scattering amplitudes. Since

$$\begin{array}{ll} \phi_l^i(z_l) = \phi^+(z_l) & \phi_r^i(z_r) = \phi^-(z_r) \\ \phi_l^o(z_l) = \phi^-(z_l) & \phi_r^o(z_r) = \phi^+(z_r) \end{array} \tag{2.84}$$

we can write Eq. (2.82) as

$$\begin{pmatrix} \phi_r^o(z_r) \\ \phi_r^i(z_r) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} \phi_l^i(z_l) \\ \phi_l^o(z_l) \end{pmatrix} \tag{2.85}$$

From this relation and Eq. (2.43), that defines the scattering matrix, we easily obtain

$$\begin{aligned} (\alpha + \beta r - t)\varphi_l^i(x_1) &= (r' - \beta t')\varphi_r^i(x_2) \\ (\gamma + \delta r)\varphi_l^i(z_l) &= (1 - \delta t')\varphi_r^i(z_r). \end{aligned} \tag{2.86}$$

Since the incoming amplitudes, $\varphi_l^i(z_l)$ and $\varphi_r^i(z_r)$, are arbitrarily and independently fixed, they are also linearly independent functions. All coefficients must vanish, i.e.

$$\begin{aligned} \alpha + \beta r - t &= 0, \\ r' - \beta t' &= 0, \\ \gamma + \delta r &= 0, \\ 1 - \delta t' &= 0. \end{aligned} \tag{2.87}$$

Hence

$$\begin{aligned} r &= -\frac{1}{\delta}\gamma\,, \qquad & t &= \alpha - \beta\frac{1}{\delta}\gamma\,, \\ r' &= \beta\frac{1}{\delta}\,, \qquad & t' &= \frac{1}{\delta}\,. \end{aligned} \tag{2.88}$$

These are very important relations. They show that one can immediately obtain the scattering amplitudes when the transfer matrix is known, and viceversa. Let us now see what kind of requirements result on the transfer matrix when flux conservation and time reversal invariance are imposed.

2.2.3 FC and TRI in the transfer matrix M

Suppose again that we have the spin independent scattering process shown in Figure 2.7. Independent of the specific potential and the solutions in that region, It is clear that the flux is conserved if the particle current density at z_l, given by [1]

$$\boldsymbol{J}_l = \frac{i\hbar}{2m}\left[\phi^T(z_l)\boldsymbol{\nabla}\phi^*(z_l) - \phi^\dagger(z_l)\boldsymbol{\nabla}\phi(z_l)\right], \tag{2.89}$$

is equal to the particle density at z_r, given by

$$\boldsymbol{J}_r = \frac{i\hbar}{2m}\left[\phi^T(z_r)\boldsymbol{\nabla}\phi^*(z_r) - \phi^\dagger(z_r)\boldsymbol{\nabla}\phi(z_r)\right], \tag{2.90}$$

In the leads, with

$$\Sigma_z K = \Sigma_z \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix} = \begin{pmatrix} I_N & 0 \\ 0 & -I_N \end{pmatrix} \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix} \quad \text{and} \quad k = \begin{pmatrix} k_1 & 0 & 0 & \dots & 0 \\ 0 & k_2 & 0 & \dots & 0 \\ & & & \dots & \\ 0 & 0 & 0 & \dots & k_N \end{pmatrix} \tag{2.91}$$

the flux condition becomes

$$\begin{aligned} -\phi^T(z_l)\Sigma_z K_l \phi^*(z_l) + \phi^\dagger(z_l)\Sigma_z K_l \phi(z_l) = &- \phi^T(z_r)\Sigma_z K_r \phi^*(z_r) \\ &+ \phi^\dagger(z_r)\Sigma_z K_r \phi(z_r) \end{aligned} \tag{2.92}$$

[1] ^{T} means transpose and † means the transpose conjugate

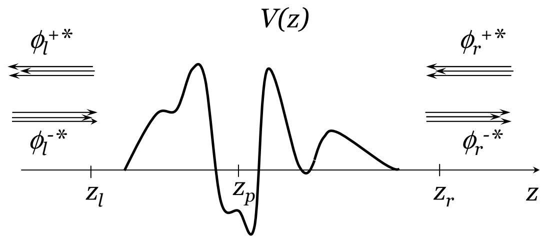

Fig. 2.8. The incoming and outgoing wave vectors.

The two terms on the left are equal and the same happens on the right. Using this and taking into account that $\Sigma_z K = K^{1/2}\Sigma_z K^{1/2}$, the flux condition can be written as

$$\phi^T(z_l)K_l^{1/2}\Sigma_z K_l^{1/2}\phi^*(z_l) = \phi^T(z_r)K_r^{1/2}\Sigma_z K_r^{1/2}\phi^*(z_r). \tag{2.93}$$

This is an important intermediate result that makes evident the implications that may have the normalization factor of the plane waves in the leads. If we would have considered the wave functions

$$\varphi_j(z) = \frac{1}{\sqrt{m/\hbar k_j}} e^{ik_j z}, \tag{2.94}$$

the factors $K^{1/2}$ will be canceled by the normalization constant and we will have

$$\phi^T(z_l)\Sigma_z\phi^*(z_l) = \phi^T(z_r)\Sigma_z\phi^*(z_r). \tag{2.95}$$

This point is particularly important when the kinetic energy on the left hand side is different to that on the right, as is the case for biased systems. Using the relation

$$\phi(z_r) = M(z_r, z_l)\phi(z_l) \tag{2.96}$$

on the right hand side of (2.95) we have

$$\phi^T(z_l)\Sigma_z\phi^*(z_l) = \phi^T(z_l)M^T\Sigma_z M^*\phi^*(z_l). \tag{2.97}$$

Thus, the flux conservation requirement on the transfer matrix is

$$M^\dagger\Sigma_z M = \Sigma_z. \tag{2.98}$$

It is worth noticing that we have consider the same masses m at the left and right. In the application to semiconductor structures, where it is common to assume the effective mass approximation, the masses could be different and mass factors m_r^*/m_l^* must be taken into account, properly.

Consider now the spin independent process of figure 2.8, which is the time reversed of the process shown in figure 2.7. The scattering process is said to be time reversal invariant if the transfer matrix M satisfying the relation

$$\begin{pmatrix} \phi^+(z_r) \\ \phi^-(z_r) \end{pmatrix} = M(z_r, z_l) \begin{pmatrix} \phi^+(z_l) \\ \phi^-(z_l) \end{pmatrix} \tag{2.99}$$

fulfills also the relation

$$\begin{pmatrix} \phi^{-*}(z_r) \\ \phi^{+*}(z_r) \end{pmatrix} = M(z_r, z_l) \begin{pmatrix} \phi^{-*}(z_l) \\ \phi^{+*}(z_l) \end{pmatrix} \tag{2.100}$$

taking the complex conjugate of this equation we have

$$\begin{pmatrix} \phi^-(z_r) \\ \phi^+(z_r) \end{pmatrix} = M^*(z_r, z_l) \begin{pmatrix} \phi^-(z_l) \\ \phi^+(z_l) \end{pmatrix}. \tag{2.101}$$

Since

$$\begin{pmatrix} \phi^-(z_r) \\ \phi^+(z_r) \end{pmatrix} = \begin{pmatrix} 0 & I_N \\ I_N & 0 \end{pmatrix} \begin{pmatrix} \phi^+(z_r) \\ \phi^-(z_r) \end{pmatrix} = \Sigma_x \begin{pmatrix} \phi^+(z_r) \\ \phi^-(z_r) \end{pmatrix}, \tag{2.102}$$

equation (2.101) can be written in the form

$$\Sigma_x \begin{pmatrix} \phi^+(z_r) \\ \phi^-(z_r) \end{pmatrix} = M^*(z_r, z_l)\Sigma_x \begin{pmatrix} \phi^+(z_l) \\ \phi^-(z_l) \end{pmatrix}. \tag{2.103}$$

that transforms into

$$\begin{pmatrix} \phi^+(z_r) \\ \phi^-(z_r) \end{pmatrix} = \Sigma_x M^*(z_r, z_l)\Sigma_x \begin{pmatrix} \phi^+(z_l) \\ \phi^-(z_l) \end{pmatrix}. \tag{2.104}$$

Hence the time reversal invariance property implies the condition

$$M = \Sigma_x M^* \Sigma_x \tag{2.105}$$

If the transfer matrix is written in terms of the matrix blocks α, β, γ and δ, this time reversal invariance condition takes the form

$$\begin{aligned} \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha^* & \beta^* \\ \gamma^* & \delta^* \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \delta^* & \gamma^* \\ \beta^* & \alpha^* \end{pmatrix}. \end{aligned} \tag{2.106}$$

Therefore, the transfer matrix of a TRI, spin independent, scattering process has the structure

$$M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \tag{2.107}$$

Combining the FC and TRI conditions (2.98) and (2.105) we have

$$M^T \mathcal{F} M = \mathcal{F} \qquad \text{with} \qquad \mathcal{F} = \Sigma_z \Sigma_x = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}. \tag{2.108}$$

which define the symplectic group $Sp(2N, \mathcal{C})$ with $N(2N+1)$ free parameters. In some cases like in the multichannel approach to disordered conductors, other representations of the transfer matrix can be useful. We will refer to this issue in the next sections, especially for the orthogonal and the symplectic universality classes.

2.2.4 Other consequences of FC and TRI

Since $t' = 1/\alpha^*$ and $t' = t^T$, for TRI systems, it is clear that $t = 1/\alpha^\dagger$. We will show now that using the FC and TRI requirements one can derive, in general, the relation $t = 1/\alpha^\dagger$ as well as that $\det M = 1$.

The flux conservation requirement for TRI systems written in the form

$$\begin{pmatrix} \alpha^\dagger & \beta^T \\ \beta^\dagger & \alpha^T \end{pmatrix} \begin{pmatrix} I_N & 0 \\ 0 & -I_N \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} = \begin{pmatrix} I_N & 0 \\ 0 & -I_N \end{pmatrix} \tag{2.109}$$

implies the condition

$$\begin{pmatrix} \alpha^\dagger\alpha - \beta^T\beta^* & \alpha^\dagger\beta - \beta^T\alpha^* \\ \beta^\dagger\alpha - \alpha^T\beta^* & \beta^\dagger\beta - \alpha^T\alpha^* \end{pmatrix} = \begin{pmatrix} I_N & 0 \\ 0 & -I_N \end{pmatrix}, \tag{2.110}$$

which means that

$$\begin{aligned} \alpha^\dagger\alpha - \beta^T\beta^* &= I_N \\ \alpha^\dagger\beta - \beta^T\alpha^* &= 0. \end{aligned} \tag{2.111}$$

The second of this equations leads to

$$\frac{1}{\alpha^\dagger}\beta^T = \beta\frac{1}{\alpha^*}. \tag{2.112}$$

If we now recall that

$$t = \alpha - \beta\frac{1}{\alpha^*}\beta^*, \tag{2.113}$$

and use the previous relation, we obtain

$$t = \alpha - \frac{1}{\alpha^\dagger}\beta^T\beta^* = \frac{1}{\alpha^\dagger}\left(\alpha^\dagger\alpha - \beta^T\beta^*\right). \tag{2.114}$$

Thus

$$t = \frac{1}{\alpha^\dagger}. \tag{2.115}$$

To show that $\det M = 1$ we use the following identity

$$M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} = \begin{pmatrix} \alpha & 0 \\ \beta^* & \alpha^* \end{pmatrix} \begin{pmatrix} I_N & \alpha^{-1}\beta \\ 0 & I_N - \alpha^{*-1}\beta^*\alpha^{-1}\beta \end{pmatrix} \tag{2.116}$$

Since

$$\det M = \det \begin{pmatrix} \alpha & 0 \\ \beta^* & \alpha^* \end{pmatrix} \det \begin{pmatrix} I_N & \alpha^{-1}\beta \\ 0 & I_N - \alpha^{*-1}\beta^*\alpha^{-1}\beta \end{pmatrix} \tag{2.117}$$

and

$$\det \begin{pmatrix} A & 0 \\ C & D \end{pmatrix} = \det(AD) = \det A \det D, \tag{2.118}$$

we have

$$\det M = \det(\alpha\alpha^*) \det(I_N - \alpha^{*-1}\beta^*\alpha^{-1}\beta). \tag{2.119}$$

This equation, using (2.114) and (2.115), can also be written as

$$\det M = \det(\alpha) \det(\alpha^* - \beta^*\alpha^{-1}\beta) = \det(\alpha) \det(t^*). \tag{2.120}$$

Thus

$$\det M = \det(\alpha) \det\left(\frac{1}{\alpha^T}\right) = 1. \tag{2.121}$$

2.2.5 The composition rule of the M matrices

At variance of the involved composition rules for the S-matrices, the transfer matrix composition rules are extremely simple. If we have the successive potential regions of figure 2.9, which correspond to figure 2.5, in each region we have the transfer matrix relations

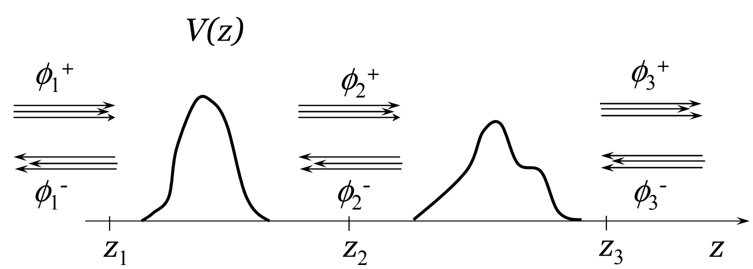

Fig. 2.9. The right and left moving wave vectors in two successive potential regions.

$$\begin{pmatrix} \phi^+(z_2) \\ \phi^-(z_2) \end{pmatrix} = \begin{pmatrix} \alpha_1 & \beta_1 \\ \gamma_1 & \delta_1 \end{pmatrix} \begin{pmatrix} \phi^+(z_1) \\ \phi^-(z_1) \end{pmatrix} = M_1(z_2, z_1) \begin{pmatrix} \phi^+(z_1) \\ \phi^-(z_1) \end{pmatrix} \quad (2.122)$$

$$\begin{pmatrix} \phi^+(z_3) \\ \phi^-(z_3) \end{pmatrix} = \begin{pmatrix} \alpha_2 & \beta_2 \\ \gamma_2 & \delta_2 \end{pmatrix} \begin{pmatrix} \phi^+(z_2) \\ \phi^-(z_2) \end{pmatrix} = M_2(z_3, z_2) \begin{pmatrix} \phi^+(z_2) \\ \phi^-(z_2) \end{pmatrix} \quad (2.123)$$

while the transfer matrix M for the successive potential regions is

$$\begin{pmatrix} \phi^+(z_3) \\ \phi^-(z_3) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} \phi^+(z_1) \\ \phi^-(z_1) \end{pmatrix} = M(z_3, z_1) \begin{pmatrix} \phi^+(z_1) \\ \phi^-(z_1) \end{pmatrix} \quad (2.124)$$

It is clear from these relations that

$$M(z_3, z_1) = M_2(z_3, z_2) M_1(z_2, z_1) \quad (2.125)$$

This simple composition rule, known also as the multiplicative property of transfer matrices, contrasts with the complexity of the corresponding rule for the S matrices. Once the transfer matrix of the composed system is obtained one can easily obtain the reflection and transmission amplitudes. Let us verify this.To simplify the expressions let us suppose that the interactions in each of the potential regions is TRI. In this case

$$M = \begin{pmatrix} \alpha_2 & \beta_2 \\ \beta_2^* & \alpha_2* \end{pmatrix} \begin{pmatrix} \alpha_1 & \beta_1 \\ \beta_1^* & \alpha_1* \end{pmatrix} = \begin{pmatrix} \alpha_2\alpha_1 + \beta_2\beta_1^* & \alpha_2\beta_1 + \beta_2\alpha_1^* \\ \beta_2^*\alpha_1 + \alpha_2^*\beta_1^* & \beta_2^*\beta_1 + \alpha_2^*\alpha_1^* \end{pmatrix}. \quad (2.126)$$

We have seen that

$$\beta = r' \frac{1}{t'}\,, \qquad \alpha^* = \frac{1}{t'} = \frac{1}{t^T}\,, \qquad \beta^* = -\frac{1}{t'} r \quad (2.127)$$

The transmission amplitude t of the two successive processes is then

$$t = \frac{1}{(\alpha_2\alpha_1 + \beta_2\beta_1^*)^\dagger} = \frac{1}{\alpha_1^\dagger\alpha_2^\dagger + \beta_1^T\beta_2^\dagger} \quad (2.128)$$

If we use the previous relations and that the reflection amplitudes for TRI systems are symmetric, we have

$$t = \frac{1}{\frac{1}{t_1}\frac{1}{t_2} - \left(\frac{1}{t_1'}\right)^T {r_1'}^T r_2^T \left(\frac{1}{t_2'}\right)^T}. \quad (2.129)$$

Hence

$$t = t_2 \frac{1}{I_N - r_1' r_2} t_1, \quad (2.130)$$

as in (2.61). To study the conduction and stationary properties of more complicated structures, we will generally deal with transfer matrices. The physical expressions will be written in terms of the transfer matrix elements.

2.2.6 The M matrix for the 1D square barrier potential

In the next chapters and throughout the book we will systematically use a procedure that makes easier to obtain transfer matrices for systems with more than two discontinuity points. To obtain the square barrier transfer matrix M_b we can use the continuity conditions in (2.67) and (2.69) derived before. If we write those equations in the form

$$\begin{aligned} Ba_3e^{ikb} - Gb_3e^{-ikb} &= Fa_1 - Ab_1 \\ Da_3e^{ikb} - Jb_3e^{-ikb} &= Ha_1 - Cb_1. \end{aligned} \tag{2.131}$$

with

$$\begin{aligned} A = H^* &= i(k^2+q^2)\sinh qb\ , \qquad & B = J = 2kq, \\ C = F^* &= 2kq\cosh qb + i(q^2-k^2)\sinh qb\ , \qquad & D = G = 0, \end{aligned} \tag{2.132}$$

it is possible to express the wave functions at $z = b$ in terms of the wave functions at $z = 0$ as follows

$$\begin{pmatrix} a_3e^{ikb} \\ b_3e^{-ikb} \end{pmatrix} = \frac{1}{2kq}\begin{pmatrix} F & H \\ H^* & F^* \end{pmatrix}\begin{pmatrix} a_1 \\ b_1 \end{pmatrix}. \tag{2.133}$$

Thus, the square barrier transfer matrix is

$$M_b = \begin{pmatrix} \cosh qb + i\frac{(k^2-q^2)}{2kq}\sinh qb & -i\frac{(k^2+q^2)}{2kq}\sinh qb \\ i\frac{(k^2+q^2)}{2kq}\sinh qb & \cosh qb - i\frac{(k^2-q^2)}{2kq}\sinh qb \end{pmatrix} = \begin{pmatrix} \alpha_b & \beta_b \\ \beta_b^* & \alpha_b^* \end{pmatrix}. \tag{2.134}$$

and since $t_b = 1/\alpha_b^\dagger$, we obtain again the square barrier transmission amplitude

$$t_b = \frac{2kq}{2kq\cosh qb - i(q^2-k^2)\sinh qb}. \tag{2.135}$$

2.2.7 Definition of the transfer matrix W

Let us now introduce the transfer matrix W of the first kind. As will be seen here, the use of this matrix is much more convenient for an important class of problems, especially those involving external fields. Consider again the spin independent scattering process of figure 2.7, with solutions at z_l and at z_r given by

$$\varphi_j(z_l) = a_j\varphi_j^+(z_l) + b_j\varphi_j^-(z_l) \tag{2.136}$$

and

$$\varphi_j(z_r) = c_j\varphi_j^+(z_r) + d_j\varphi_j^-(z_r), \tag{2.137}$$

respectively. With these functions and their derivatives $\varphi_j'(z_l)$ and $\varphi_j'(z_r)$, we can form the vectors

$$\Phi(z_l) = \begin{pmatrix} \varphi_1(z_l) \\ \cdots \\ \varphi_N(z_l) \\ \varphi_1'(z_l) \\ \cdots \\ \varphi_N'(z_l) \end{pmatrix} \qquad \text{and} \qquad \Phi(z_r) = \begin{pmatrix} \varphi_1(z_r) \\ \cdots \\ \varphi_N(z_r) \\ \varphi_1'(z_r) \\ \cdots \\ \varphi_N'(z_r) \end{pmatrix} \tag{2.138}$$

These kind of vectors can be defined at any two points z_1 and z_2. The matrix $W(z_r, z_l)$ that satisfies the relation

$$\Phi(z_r) = W(z_r, z_l)\Phi(z_l) = \begin{pmatrix} \theta & \mu \\ \nu & \chi \end{pmatrix} \Phi(z_l), \tag{2.139}$$

is the transfer matrix of the first kind that connects wave functions and their derivatives at z_l and at z_r. In general, one can define a transfer matrix $W(z_2, z_1)$, for any two points z_1 and z_2 of the z axis of the system, such that

$$\Phi(z_2) = W(z_2, z_1)\Phi(z_1). \tag{2.140}$$

2.2.8 FC and TRI and the transfer matrix W

Using the wave vectors $\phi^{\pm}(z_l)$ and $\phi^{\pm}(z_r)$ defined before, in the simplified notation $\phi_l^{\pm}$ and $\phi_r^{\pm}$, we can write the vectors $\Phi(z)$ at z_l and z_r as

$$\Phi(z_l) = \begin{pmatrix} \phi_l^+ + \phi_l^- \\ \phi_l^{+\prime} + \phi_l^{-\prime} \end{pmatrix} \qquad \text{and} \qquad \Phi(z_r) = \begin{pmatrix} \phi_r^+ + \phi_r^- \\ \phi_r^{+\prime} + \phi_r^{-\prime} \end{pmatrix}, \tag{2.141}$$

and the current densities $\boldsymbol{J}(z)$ as

$$\begin{aligned} \boldsymbol{J}_l &= \frac{i\hbar}{2m}\left[(\phi_l^+ + \phi_l^-)^T \boldsymbol{\nabla}(\phi_l^+ + \phi_l^-)^* - (\phi_l^+ + \phi_l^-)^\dagger \boldsymbol{\nabla}(\phi_l^+ + \phi_l^-)\right] \\ &= \frac{i\hbar}{2m}\left[\Phi^T(z_l)\begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}\Phi^*(z_l)\right]\hat{\mathbf{z}}, \end{aligned} \tag{2.142}$$

and

$$\begin{aligned} \boldsymbol{J}_r &= \frac{i\hbar}{2m}\left[(\phi_r^+ + \phi_r^-)^T \boldsymbol{\nabla}(\phi_r^+ + \phi_r^-)^* - (\phi_r^+ + \phi_r^-)^\dagger \boldsymbol{\nabla}(\phi_r^+ + \phi_r^-)\right] \\ &= \frac{i\hbar}{2m}\left[\Phi^T(z_r)\begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}\Phi^*(z_r)\right]\hat{\mathbf{z}}. \end{aligned} \tag{2.143}$$

Therefore, the flux conservation requirement implies the condition

$$W^T \Sigma_y W = \Sigma_y. \tag{2.144}$$

Being Σ_y the Pauli matrix σ_y of dimension $2N \times 2N$. We shall now see what condition results for W from time reversal invariance. Consider again that the same matrix $W(z_r, z_l)$ that relates $\Phi(z_l)$ with $\Phi(z_l)$ in figure 2.7, relates also the vectors

$$\Phi^*(z_l) = \begin{pmatrix} \phi_l^+ + \phi_l^- \\ \phi_l^{+\prime} + \phi_l^{-\prime} \end{pmatrix}^* \qquad \text{and} \qquad \Phi^*(z_r) = \begin{pmatrix} \phi_r^+ + \phi_r^- \\ \phi_r^{+\prime} + \phi_r^{-\prime} \end{pmatrix}^*, \tag{2.145}$$

in figure 2.8. It is clear then that for TRI systems the transfer matrix W is real, i.e.

$$W = W^*. \tag{2.146}$$

The transfer matrices satisfying (2.144) and (2.146) belong to the non-compact real symplectic Lie group $sp(2N, R)$ with $N(2N+1)$ free parameters.

2.2.9 The relations of W with M, and the scattering amplitudes

Based on the transfer matrix definitions

$$\phi(z_2) = M(z_2, z_1)\phi(z_1) \quad \text{with} \quad \phi(z) = \begin{pmatrix} \phi^+(z) \\ \phi^-(z) \end{pmatrix} \tag{2.147}$$

and

$$\Phi(z_2) = W(z_2, z_1)\Phi(z_1) \quad \text{with} \quad \Phi(z) = \begin{pmatrix} \phi^+(z) + \phi^-(z) \\ \phi^{+\prime}(z) + \phi^{-\prime}(z) \end{pmatrix} \tag{2.148}$$

we can establish the relation between these matrices. Let us assume that the points z_1 and z_2 of the last equation are points in the left and right hand side leads, moreover, it is might be important to consider the wave functions in the leads with the normalization factor $1/\sqrt{m/\hbar k_j}$, for which the currents become momentum independent. In that case, using

$$\Phi(z) = \begin{pmatrix} K^{-1/2} & K^{-1/2} \\ iK^{1/2} & -iK^{1/2} \end{pmatrix} \begin{pmatrix} \phi^+(z) \\ \phi^-(z) \end{pmatrix}. \tag{2.149}$$

we can write equation (2.150) in the form

$$\begin{pmatrix} K_2^{-1/2} & K_2^{-1/2} \\ iK_2^{1/2} & -iK_2^{1/2} \end{pmatrix} \begin{pmatrix} \phi^+(z_2) \\ \phi^-(z_2) \end{pmatrix} = W(z_2, z_1) \begin{pmatrix} K_1^{-1/2} & K_1^{-1/2} \\ iK_1^{1/2} & -iK_1^{1/2} \end{pmatrix} \begin{pmatrix} \phi^+(z_1) \\ \phi^-(z_1) \end{pmatrix}. \tag{2.150}$$

Since

$$\begin{pmatrix} K_2^{-1/2} & K_2^{-1/2} \\ iK_2^{1/2} & -iK_2^{1/2} \end{pmatrix}^{-1} = \frac{1}{2} \begin{pmatrix} K_2^{1/2} & -iK_2^{-1} \\ K_2^{1/2} & iK_2^{-1} \end{pmatrix}, \tag{2.151}$$

it is clear that

$$M(z_2, z_1) = \frac{1}{2} \begin{pmatrix} K_2^{1/2} & -iK_2^{-1} \\ K_2^{1/2} & iK_2^{-1} \end{pmatrix} W(z_2, z_1) \begin{pmatrix} K_1^{-1/2} & K_1^{-1/2} \\ iK_1^{1/2} & -iK_1^{1/2} \end{pmatrix} \tag{2.152}$$

Given this relation and assuming that

$$W(z_2, z_1) = \begin{pmatrix} \theta & \mu \\ \nu & \chi \end{pmatrix}, \tag{2.153}$$

one can straightforwardly obtain the scattering amplitudes

$$t = \frac{2}{K_2^{1/2} \left[\theta + K_2^{-1}\chi K_1 + i(\mu K_1 - K_2^{-1}\nu)\right] K_1^{-1/2}} \tag{2.154}$$

and

$$r = -tK_2^{1/2} \left[\theta - K_2^{-1}\chi K_1 + i(\mu K_1 + K_2^{-1}\nu)\right] K_1^{-1/2}. \tag{2.155}$$

2.2.10 The W matrix for the 1D square barrier potential

To obtain the transfer matrix W_b for the square barrier potential we use the continuity conditions

$$\begin{pmatrix} \varphi_{\mathrm{II}}(0^+) \\ \varphi'_{\mathrm{II}}(0^+) \end{pmatrix} = \begin{pmatrix} \varphi_{\mathrm{I}}(0^-) \\ \varphi'_{\mathrm{I}}(0^-) \end{pmatrix} \tag{2.156}$$

at the left side of the barrier, where $z = 0$, and

$$\begin{pmatrix} \varphi_{\mathrm{II}}(b^+) \\ \varphi'_{\mathrm{II}}(b^+) \end{pmatrix} = \begin{pmatrix} \varphi_{\mathrm{III}}(b^-) \\ \varphi'_{\mathrm{III}}(b^-) \end{pmatrix} \tag{2.157}$$

at $z = b$ on the right hand side of the barrier. To determine the transfer matrix $W(b, 0)$ connecting the wave vectors and their derivatives at the left and right of the square barrier, it is convenient to rewrite the previous equations as follows:

$$\begin{pmatrix} \varphi_2^+(0) & \varphi_2^-(0) \\ \varphi'^+_2(0) & \varphi'^-_2(0) \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} \varphi_{\mathrm{I}}(0) \\ \varphi'_{\mathrm{I}}(0) \end{pmatrix} \tag{2.158}$$

and

$$\begin{pmatrix} \varphi_2^+(b) & \varphi_2^-(b) \\ \varphi'^+_2(b) & \varphi'^-_2(b) \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} \begin{pmatrix} \varphi_{\mathrm{II}}(b) \\ \varphi'_{\mathrm{II}}(b) \end{pmatrix} = \begin{pmatrix} \varphi_{\mathrm{III}}(b) \\ \varphi'_{\mathrm{III}}(b) \end{pmatrix}. \tag{2.159}$$

To simplify the notation we have dropped the signs + and − for the coordinates. If we multiply equation (2.158) by the inverse of the matrix on the left, and substitute the coefficients vector in the last equation, we have

$$\begin{pmatrix} \varphi_{\rm III}(b) \\ \varphi'_{\rm III}(b) \end{pmatrix} = \begin{pmatrix} \varphi_2^+(b) & \varphi_2^-(b) \\ \varphi'^+_2(b) & \varphi'^-_2(b) \end{pmatrix} \begin{pmatrix} \varphi_2^+(0) & \varphi_2^-(0) \\ \varphi'^+_2(0) & \varphi'^-_2(0) \end{pmatrix}^{-1} \begin{pmatrix} \varphi_{\rm I}(0) \\ \varphi'_{\rm I}(0) \end{pmatrix} \tag{2.160}$$

This means that the transfer matrix $W_b \equiv W(b,0)$ is

$$W_b = \begin{pmatrix} \varphi_2^+(b) & \varphi_2^-(b) \\ \varphi'^+_2(b) & \varphi'^-_2(b) \end{pmatrix} \begin{pmatrix} \varphi_2^+(0) & \varphi_2^-(0) \\ \varphi'^+_2(0) & \varphi'^-_2(0) \end{pmatrix}^{-1} \tag{2.161}$$

Taking into account the explicit functions $\varphi_i^\pm(0)$ and $\varphi_i^\pm(b)$ obtained in (2.64), we have

$$W_b = \begin{pmatrix} e^{qb} & e^{-qb} \\ qe^{qb} & qe^{-qb} \end{pmatrix} \frac{1}{2q} \begin{pmatrix} q & 1 \\ q & -1 \end{pmatrix}^{-1} \tag{2.162}$$

which becomes

$$W_b = \begin{pmatrix} \cosh qb & \frac{1}{q}\sinh qb \\ q\sinh qb & \cosh qb \end{pmatrix} = \begin{pmatrix} \theta_b & \mu_b \\ \nu_b & \chi_b \end{pmatrix} \tag{2.163}$$

It is easy to establish the relation with the transfer matrix M_b. Since

$$\begin{pmatrix} \varphi_{\rm I}(0) \\ \varphi'_{\rm I}(0) \end{pmatrix} = \begin{pmatrix} k^{-1/2} & k^{-1/2} \\ ik^{1/2} & -ik^{1/2} \end{pmatrix} \begin{pmatrix} \varphi_1^+(0) \\ \varphi_1^-(0) \end{pmatrix} \tag{2.164}$$

and

$$\begin{pmatrix} \varphi_{\rm III}(b) \\ \varphi'_{\rm III}(b) \end{pmatrix} = \begin{pmatrix} k^{-1/2} & k^{-1/2} \\ ik^{1/2} & -ik^{1/2} \end{pmatrix} \begin{pmatrix} \varphi_3^+(b) \\ \varphi_3^-(b) \end{pmatrix}, \tag{2.165}$$

it is clear that

$$M_b = \frac{1}{2} \begin{pmatrix} k^{1/2} & -ik^{-1/2} \\ k^{1/2} & ik^{-1/2} \end{pmatrix} W_b \begin{pmatrix} k^{-1/2} & k^{-1/2} \\ ik^{1/2} & -ik^{1/2} \end{pmatrix} \tag{2.166}$$

This relation is a particular case of the general relation obtained in the last section. After multiplying, we obtain the transfer matrix M_b derived before, for the square barrier potential.

In this chapter we have introduced basic definitions of physical and mathematical quantities that will be used throughout this book. In the next chapter we will discuss briefly the fundamental physical quantities, for transport and optoelectronic processes, in the scattering approach language.

24H. M. James, Phys. Rev. 76, 1602 1949!. 25P. Erdos and R. C. Herndon, Adv. Phys. 31, 63 1982!. 26P. A. Mello, P. Pereyra, and N. Kumar, Ann. Phys. N.Y.! 181, 290 1988!; E. Merzbacher, Quantum Mechanics Wiley, New York, 1970!. 27 J. M. Luttinger, Philips Res. Rep. 6, 303 1951!. 28R. E. Borland, Proc. R. Soc. London, Ser. A 84, 926 1961!.