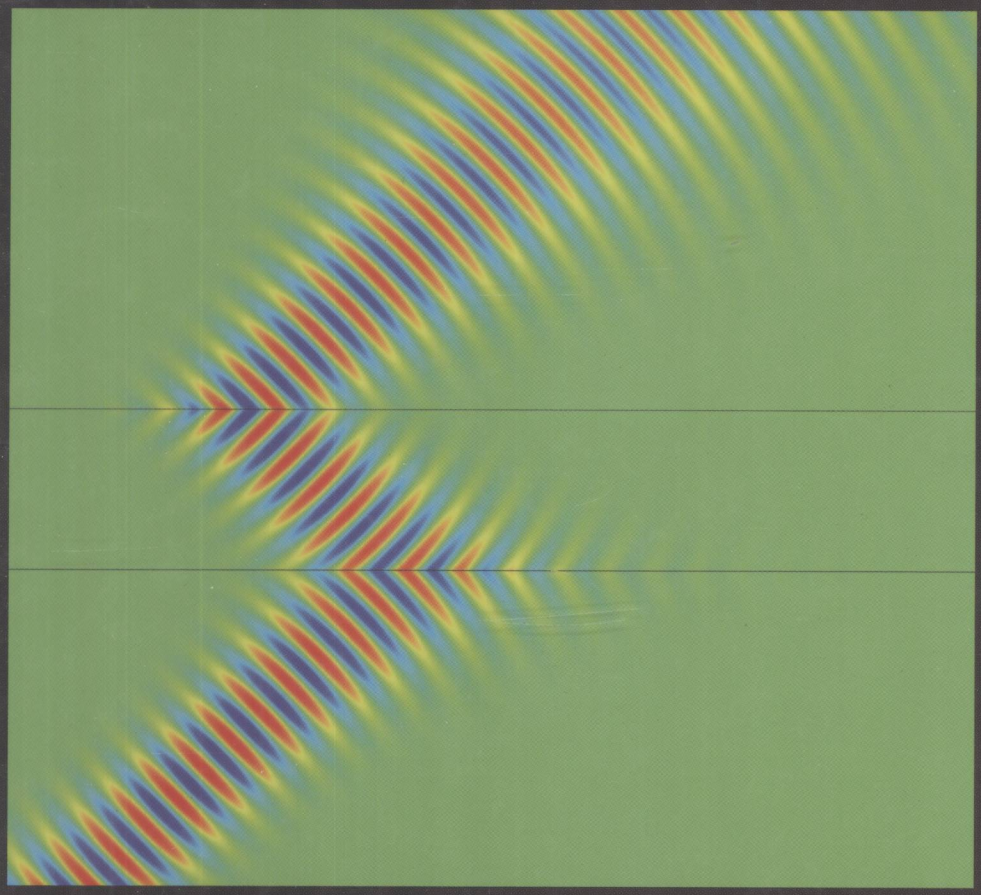
Peter **Markoš** • Costas M. **Soukoulis**



WAVE PROPAGATION

FROM **ELECTRONS** TO **PHOTONIC CRYSTALS** AND **LEFT-HANDED MATERIALS**

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Preface

This volume is intended to serve as a general text on wave propagation for senior undergraduates and first-year graduate students in physics, applied physics, engineering, materials sciences, optics, and other related scientific disciplines. We also hope that it will be useful for the many scientists working in different areas of wave propagation.

The importance of waves in our everyday life can hardly be overestimated. Waves are everywhere. Most of the information we receive comes to us in the form of waves. We see and hear through waves. We transmit and receive information through waves. We rely on waves to bring us music, television, Email, and wireless communications. We can cook with waves, talk to each other, and see things because of waves. Waves are also used in medicine; and in industry to examine objects, such as planes, for cracks and stress. Waves in periodic media usually exhibit some common characteristics. The most important is the possible appearance of stop bands (also called gaps) separating pass bands (also called bands). This means that the frequency axis may be divided into alternating regions of gaps and bands.

Although matrices and matrix properties are important parts of the physics and engineering curriculum, transfer matrices are rarely discussed in standard undergraduate textbooks. In this text, we introduce the transfer matrix formalism that can be used to study any one-dimensional wave propagation problem. The transfer matrix formalism will be used to solve problems about the propagation of electrons in potential barriers and wells, as well as some concerning the propagation of electromagnetic waves in photonic crystals and left-handed materials.

Chapter 1 introduces the transfer matrix method. The transfer matrix, as well as the scattering matrix, is defined. Through the transfer matrix formalism, the transmission

and reflection amplitudes can be easily defined and evaluated. Both traveling and standing (bound) waves are examined.

In chapters 2 and 3, the transfer matrix method is used to calculate the transmission and reflection properties of rectangular potential wells and barriers, as well as δ-function potentials. This material can be found in any book of quantum mechanics, but the transfer matrix presentation is superior, since it can be easily extended to any number of potential barriers and wells. The ideas of resonant transmission, bound states, and bonding and antibonding states are introduced in these chapters too.

In chapter 4, the transfer matrix technique is applied to the Kronig-Penney model. The most common characteristic of periodic media, that of bands and gaps, is introduced in this chapter. The group and phase velocities, the density of states, and the effective mass are introduced and evaluated.

In chapters 5 and 6 the so-called tight binding model (or equivalently the linear combination of atomic orbitals) is introduced. The tight binding model is of central importance because it is the simplest example of wave propagation in periodic media. The transfer matrix method is used to calculate the transmission and reflection properties of a lattice of N identical atoms, as well as those with 2 or 4 atoms in the unit cell. The properties of an isolated impurity are also presented. The Brillouin zone and the Fermi energy are introduced, and metals and insulators are briefly examined.

In chapter 7, the transfer matrix formalism is used to study disordered or random systems. The transmission and reflection properties of random systems are presented. The ideas of localization and probability distributions are introduced. In one-dimensional disordered systems the eigenstates are always exponentially localized.

In chapter 8, a short introduction to the accuracy of different numerical methods is given.

In chapter 9, the transfer matrix method is used to calculate the transmission and reflection properties of EM waves for different interfaces. The interfaces examined are a dielectric to dielectric, a dielectric to metal, and a dielectric to left-handed material. The Brewster angle and evanescent waves are also discussed.

In chapter 10 the transmission and reflection properties of dielectric and metallic slabs are examined. For normal incidence, the transmission of EM waves through a dielectric slab is exactly equivalent to the problem of an electron propagating through a potential barrier. The ideas of Fabry-Pérot and resonant tunneling are introduced and discussed.

In chapter 11, the transfer matrix method is used to study surface waves at different interfaces, such as vacuum-metal, and vacuum–left-handed materials interfaces. A discussion of the experimental observation of surface waves is also given.

In chapter 12, resonant tunneling through double-layer structures of dielectrics and metals is examined. In chapter 13, photonic crystals are introduced and discussed. In addition, layered materials of metals and dielectrics and of metals and left-handed materials are examined. In chapter 14, the effective parameters of photonic crystals and left-handed materials are calculated.

Chapter 15 covers wave propagation in nonlinear structures. The ideas of bistability and gap solitons are introduced.

Chapter 16 is devoted to left-handed materials. Transmission through a left-handed slab is presented. The ideas of focusing of propagating waves, recovery of evanescent waves, and perfect lenses are discussed. A short history of the left-handed field is also presented.

Each chapter concludes with a number of problems. These consist of two types: Problems with Solutions, which are set as problems and not in the main text because they are more technical and might interfere with the flow of the material presented in the text, and Problems without Solutions, which are of medium difficulty and cover the entire chapter. All the problems are solvable on the basis of the material presented in the chapter and do not need any more advanced references.

We gratefully acknowledge fruitful discussions with our colleague and friend Thomas Koschny. A special thanks is given to Rebecca Shivvers, for her help in the first editing of this book.

P. Markoš and C. M. Soukoulis

Contents

1 Transfer Matrix

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* **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 **M** is a 2×2 matrix. The 2×2 *scattering matrix* **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 **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]

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

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,

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

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:

$$\begin{aligned} \Psi_{\rm L}(x) &= \Psi_{\rm L}^{+}(x)+\Psi_{\rm L}^{-}(x),\ x\le 0, \\ \Psi_{\rm R}(x) &= \Psi_{\rm R}^{+}(x)+\Psi_{\rm R}^{-}(x),\ x\ge \ell. \end{aligned} \tag{1.3}$$

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, $\Psi_{\rm L}^{+}(x)$ is the wave function of the electron left of the sample, propagating to the right; hence it is approaching the sample. We call $\Psi_{\rm L}^{+}(x)$ the *incident* wave, in contrast to $\Psi_{\rm L}^{-}(x)$, which is the wave function of the electron propagating away from the sample toward the left side.

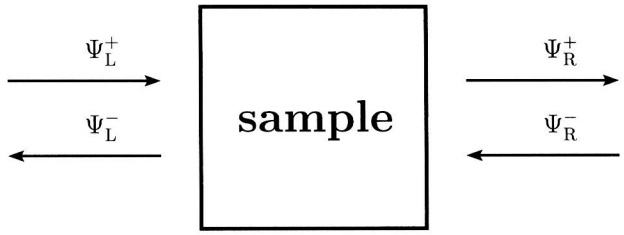

FIGURE 1.1. A typical scattering experiment. Incident waves $\Psi_L^+(x)$ and $\Psi_R^-(x)$ are scattered by the sample, characterized by the potential $V(x)$. Outgoing waves $\Psi_L^-(x)$ and $\Psi_R^+(x)$ consist of waves transmitted through the sample as well as waves reflected from the sample. Outside 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

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

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

$$E = E(q). \tag{1.5}$$

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,

$$E = \frac{\hbar^2 k^2}{2m}. \tag{1.6}$$

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

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

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

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

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

on the left boundary of the sample, and

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

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

$$\begin{pmatrix} \Psi_{\mathrm{L}}^-(x=0) \\ \Psi_{\mathrm{R}}^+(x=\ell) \end{pmatrix} = \mathbf{S} \begin{pmatrix} \Psi_{\mathrm{L}}^+(x=0) \\ \Psi_{\mathrm{R}}^-(x=\ell) \end{pmatrix}, \tag{1.10}$$

where the matrix $\mathbf{S}$,

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

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

$$\begin{pmatrix} \Psi_{\mathrm{R}}^+(x=\ell) \\ \Psi_{\mathrm{R}}^-(x=\ell) \end{pmatrix} = \mathbf{M} \begin{pmatrix} \Psi_{\mathrm{L}}^+(x=0) \\ \Psi_{\mathrm{L}}^-(x=0) \end{pmatrix}. \tag{1.12}$$

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 **S** matrix.

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

$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} S_{21} - \dfrac{S_{22}S_{11}}{S_{12}} & \dfrac{S_{22}}{S_{12}} \\ \dfrac{-S_{11}}{S_{12}} & \dfrac{1}{S_{12}} \end{pmatrix}. \tag{1.13}$$

Equivalently, we can express the elements of the scattering matrix **S** in terms of the elements of the transfer matrix:

$$\mathbf{S} = \begin{pmatrix} -\dfrac{M_{21}}{M_{22}} & \dfrac{1}{M_{22}} \\ M_{11} - \dfrac{M_{12}M_{21}}{M_{22}} & \dfrac{M_{12}}{M_{22}} \end{pmatrix}. \tag{1.14}$$

The scattering matrix **S** contains four complex parameters. In general, the matrix **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,

$$\int_0^\ell \Psi^*\Psi \, dx, \tag{1.15}$$

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:

$$j(x=0) = j(x=\ell). \tag{1.16}$$

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

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

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

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

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

$$|\Psi_L^-|^2 + |\Psi_R^+|^2 = |\Psi_L^+|^2 + |\Psi_R^-|^2, \tag{1.19}$$

or, in vector notation

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

where Ψ^* is the complex conjugate of Ψ.

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

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

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

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

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

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

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

$$\mathbf{S}^\dagger\mathbf{S} = \mathbf{1}, \tag{1.24}$$

which means that the scattering matrix is *unitary*.

The explicit form of equation (1.24) is given by

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

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

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

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

$$|\det \mathbf{S}| = 1. \tag{1.27}$$