Part I

Foundations

1

Schrödinger's Equation

Schrödinger's equation is

$$\hat{H}\psi(\mathbf{x},t) = i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t}\,. \tag{1.1}$$

Here $\psi(\mathbf{x},t)$ is a wavefunction, and $\hat{H}$ is an operator obtained from the classical Hamiltonian describing a system. The classical Hamiltonian is a function of particle coordinates $\mathbf{x}_j, \mathbf{p}_j$, where $\mathbf{x}_j$ is the 3-vector describing the position of the jth particle and $\mathbf{p}_j$ is its momentum. The Hamiltonian operator $\hat{H}$ is obtained from the classical Hamiltonian H by making the substitutions

$$\mathbf{p}_j \rightarrow \frac{\hbar}{i}\nabla_j\,, \tag{1.2}$$

where ∇_j is the gradient operator acting on the coordinates of the jth particle, $h = 6.6255 \times 10^{-27}$ erg sec is Planck's constant, $\hbar = h/2\pi = 1.054 \times 10^{-27}$ erg sec, and $i = \sqrt{-1}$.

The Schrödinger equation (1.1) can be simplified by assuming a solution of the form $\psi(\mathbf{x},t) = \Phi(\mathbf{x})e^{-iEt/\hbar}$. Then the explicit time dependence may be removed from (1.1) and the resulting time-independent equation is

$$\hat{H}\Phi(\mathbf{x}) = E\Phi(\mathbf{x})\,. \tag{1.3}$$

The real constant E is interpreted as the energy of the system. The equations (1.1) and (1.3) are called the time-dependent and time-independent Schrödinger equations.

In this work, we will be particularly interested in the description of a single particle in one dimension. The classical Hamiltonian for a single particle in a potential $V(x)$ is

$$H = \frac{p^2}{2m} + V(x) \,. \tag{1.4}$$

Therefore, the Schrödinger equations we shall study are

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \,, \tag{1.5}$$

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Phi(x) = E\Phi(x) \,. \tag{1.6}$$

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(1.4)

(1.5)

(1.6)

2

Solutions in a Constant Potential

We will deal primarily with (1.6). To gain some familiarity with the time-independent Schrödinger equation (1.6), we shall solve it in a region of space in which the potential $V(x)$ is constant, $V(x) = V$. The equation may then be rewritten

$$\frac{d^2\Phi(x)}{dx^2} = \frac{-2m}{\hbar^2}(E - V)\Phi(x)\,. \tag{2.1}$$

Three types of solution may occur, depending on whether the term $-2m(E-V)/\hbar^2$ is negative, zero, or positive. Since under any condition we have a second-order differential equation to solve, there will always be two possible particular solutions.

Case A: $\frac{-2m}{\hbar^2}\,(E - V) = -k^2 < 0\,,$

$$\Phi_1(x) = e^{+ikx}, \qquad \Phi_2(x) = e^{-ikx}\,. \tag{2.2}$$

Case B: $\frac{-2m}{\hbar^2}(E - V) = 0\,,$

$$\Phi_1(x) = 1, \qquad \Phi_2(x) = x\,. \tag{2.3}$$

Case C: $\frac{-2m}{\hbar^2}(E - V) = +\kappa^2 > 0\,,$

$$\Phi_1(x) = e^{-\kappa x}, \qquad \Phi_2(x) = e^{+\kappa x}\,. \tag{2.4}$$

The most general solution of the Schrödinger equation in each of these three cases will be a complex linear superposition of the two particular solutions,

$$\Phi(x) = A\Phi_1(x) + B\Phi_2(x)\,. \tag{2.5}$$

The relationship beteween E, V, k, and κ may be expressed in a transparent form as follows:

$$\begin{aligned} \text{Case A}: \quad & \tfrac{\hbar^2 k^2}{2m} + V = E\,, \\ \text{Case B}: \quad & V = E\,, \\ \text{Case C}: \quad & \tfrac{-\hbar^2 \kappa^2}{2m} + V = E\,. \end{aligned}$$

In case A, the classical particle moves with a kinetic energy $KE = E - V = p^2/2m = (\hbar k)^2/2m$. Therefore, $\pm\hbar k$ may be interpreted as the momentum of a particle moving in a region of constant potential $V < E$.

We can make these considerations a little more precise by the following line of reasoning. When the Hamiltonian operator $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ acts on the wavefunction $\Phi(x)$ it produces a multiple of the wavefunction (1.6). An equation of the form

$$(\text{Operator})(\text{Wavefunction}) = (\text{Number}) \times (\text{Wavefunction}) \tag{2.6}$$

is called an eigenvalue equation. (In (1.6), the number is the energy eigenvalue.) If we apply the momentum operator $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$ to the wavefunctions $\Phi_1(x) = e^{+ikx}, \Phi_2(x) = e^{-ikx}$, we should find the possible momentum states of the particle

$$\begin{aligned} \hat{p}\Phi_1(x) &= \tfrac{\hbar}{i}\tfrac{d}{dx}e^{+ikx} = (+\hbar k)e^{+ikx} = +\hbar k\Phi_1(x)\,, \\ \hat{p}\Phi_2(x) &= \tfrac{\hbar}{i}\tfrac{d}{dx}e^{-ikx} = (-\hbar k)e^{-ikx} = -\hbar k\Phi_2(x)\,. \end{aligned} \tag{2.7}$$

Therefore, $\Phi_1(x)$ represents a particle traveling in a region of constant potential $V < E$ with momentum $p = +\hbar k = +\sqrt{2m(E-V)}$ (i.e., to the right), while $\Phi_2(x)$ represents a particle traveling with momentum $p = -\hbar k = -\sqrt{2m(E-V)}$ (i.e., to the left).

A classical particle is forbidden to travel in a region in which $V > E$. This is reflected, in the quantum mechanical case, by the fact that the associated momenta are imaginary:

$$\begin{aligned} \hat{p}\Phi_1(x) &= \frac{\hbar}{i}\frac{d}{dx}e^{-\kappa x} = \frac{-\hbar\kappa}{i}e^{-\kappa x} = +i\sqrt{2m(V-E)}\Phi_1(x)\,, \\ \hat{p}\Phi_2(x) &= \frac{\hbar}{i}\frac{d}{dx}e^{+\kappa x} = \frac{+\hbar\kappa}{i}e^{+\kappa x} = -i\sqrt{2m(V-E)}\Phi_2(x)\,. \end{aligned} \tag{2.8}$$

The wavefunction $\Phi_1(x) = e^{-\kappa x}$ represents a solution of Schrödinger's equation that is exponentially decreasing toward the right, while $\Phi_2(x) = e^{+\kappa x}$ is exponentially increasing toward the right.

Case B, with $V = E$, is degenerate because the real momenta become zero in the limit $V \to E$ from below, or the imaginary momenta become zero in the limit $V \to E$ from above. Under this condition of degeneracy, mathematical theorems tell

Table 2.1 Solutions of Schrödinger's equation in a region with constant potential

Case		Two Independent Solutions	Eigenvalue of Momentum Operator	Definition of Parameters
A	$V < E$	$\Phi_1 = e^{+ikx}$ $\Phi_2 = e^{-ikx}$	$+\hbar k$ $-\hbar k$	$+\frac{\hbar^2 k^2}{2m} + V = E$
B	$V = E$	$\Phi_1 = 1$ $\Phi_2 = x$	0 Not an eigenfunction	$V = E$
C	$V > E$	$\Phi_1 = e^{-\kappa x}$ $\Phi_2 = e^{+\kappa x}$	$+i\hbar\kappa$ $-i\hbar\kappa$	$-\frac{\hbar^2 \kappa^2}{2m} + V = E$

us that at least one of the solutions must satisfy an eigenvalue equation, but the other solution need not:

$$\hat{p}\Phi_1(x) = \frac{\hbar}{i}\frac{d}{dx}1 = 0 = 0 \times \Phi_1(x)\,,$$

$$\hat{p}\Phi_2(x) = \frac{\hbar}{i}\frac{d}{dx}x = \frac{+\hbar}{i} \times 1 = \frac{+\hbar}{i} \times \Phi_1(x)\,.$$

The eigenvalue equation tells us that the corresponding momentum in case B is zero.

These results are summarized in Table 2.1.

3

Wavefunctions across a Boundary

In the previous chapter we have solved a very simple one-dimensional problem. In this chapter we shall solve a more complicated problem. We already know what a particle wavefunction looks like in a region in which the potential is constant. We now ask: What does a particle wavefunction look like if the potential has a constant value V_1 in one region of space (the line) and a different constant value V_2 in an adjacent region of space (Fig. 3.1)? We choose the break point between the two regions to be $x = a$. For the sake of concreteness, we temporarily assume the particle energy E is larger than either V_1 or V_2.

In region 1 the particle wavefunction $\Phi(x)$ is in general a linear superposition of the two specific solutions:

Region 1

$$x \leq a \qquad \Phi(x) = Ae^{ik_1 x} + Be^{-ik_1 x} ,$$

$$\frac{(\hbar k_1)^2}{2m} + V_1 = E . \tag{3.1}$$

Similarly, the wavefunction in region 2 is

Region 2

$$a \leq x \qquad \Phi(x) = Ce^{ik_2 x} + De^{-ik_2 x} ,$$

$$\frac{(\hbar k_2)^2}{2m} + V_2 = E . \tag{3.2}$$

In order to find a relationship between the wavefunctions for regions 1 and 2, we try to make the total wavefunction $\Phi(x)$ "as continuous as possible" across the boundary

at $x = a$. Since Schrödinger's equation is a second-order differential equation, the solution in each region is characterized by two complex numbers [(A, B) in region 1; (C, D) in region 2]. Thus, we have two degrees of freedom to play with. That means we can choose the coefficients (A, B) and (C, D) so that the wavefunction and its first derivative are continuous at $x = a$:

$$\begin{array}{lccc} & \text{Region 1 at } x = a & & \text{Region 2 at } x = a \\ \Phi(a): & Ae^{ik_1 a} + Be^{-ik_1 a} & = & Ce^{ik_2 a} + De^{-ik_2 a} \\ \frac{d\Phi(a)}{dx}: & ik_1 Ae^{ik_1 a} - ik_1 Be^{-ik_1 a} & = & ik_2 Ce^{ik_2 a} - ik_2 De^{-ik_2 a} \end{array} . \tag{3.3}$$

This pair of simultaneous linear equations relating the coefficients (A, B) to the coefficients (C, D) can be handled in an elegant and simple way using matrix algebra:

$$\begin{bmatrix} e^{ik_1 a} & e^{-ik_1 a} \\ ik_1 e^{ik_1 a} & -ik_1 e^{-ik_1 a} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{ik_2 a} & e^{-ik_2 a} \\ ik_2 e^{ik_2 a} & -ik_2 e^{-ik_2 a} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} . \tag{3.4}$$

In fact, the treatment becomes yet simpler if we first make it slightly more complicated by writing each 2×2 matrix in (3.4) as the product of two matrices, as follows:

$$\begin{bmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{bmatrix} \begin{bmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{bmatrix} \begin{bmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} . \tag{3.5}$$

In this form, the coefficients (C, D) for the wavefunction in region 2 may be related directly and simply to the coefficients (A, B) for the wavefunction in region 1 (or vice versa). The calculation is simple because it involves multiplication by matrix inverses.

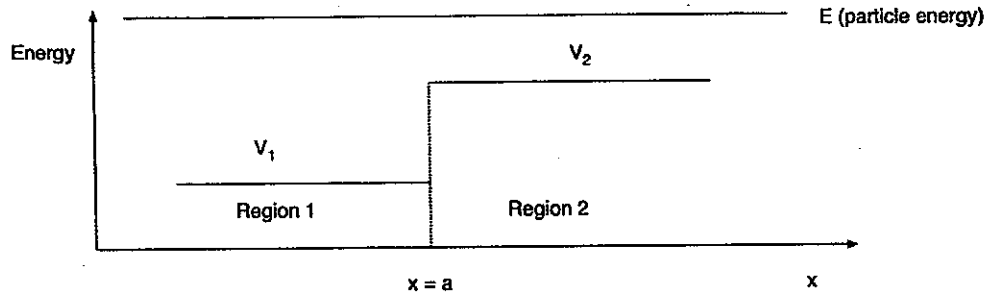

Fig. 3.1 The potential in the left-hand region is $V_1 < E$, and the potential in the right-hand region is $V_2 < E$. The wavefunction and its first derivative are matched at the boundary.

For example, to solve for (C, D) in terms of (A, B) we first multiply both sides of (3.5) by $\begin{bmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{bmatrix}^{-1}$ on the left. Then we multiply by $\begin{bmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{bmatrix}^{-1}$ on the left:

$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{bmatrix}^{-1} \times \begin{bmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{bmatrix} \begin{bmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}. \tag{3.6}$$

The coefficients (A, B) could just as easily have been solved for in terms of the coefficients (C, D) by a similar process

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{ik_1 a} & 0 \\ 0 & e^{-ik_1 a} \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{bmatrix}^{-1} \times \begin{bmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{bmatrix} \begin{bmatrix} e^{ik_2 a} & 0 \\ 0 & e^{-ik_2 a} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}. \tag{3.7}$$

Equations (3.6) and (3.7) show that the coefficients (C, D) are related by a linear transformation to the coefficients (A, B).

For reasons that will become apparent at the end of chapter 4 (Fig. 4.2), the relation (3.7) is much preferable to the relation (3.6).

In deriving the relationship between the coefficients (A, B) in region 1 and the coefficients (C, D) in region 2, we have assumed $E > V_1, E > V_2$. We now relax this assumption. To discuss the general case it is only necessary to observe that in each of the three cases $V < E, V = E, V > E$, the wavefunction $\Phi(x)$ can be expressed as a linear superposition of the two particular solutions $\Phi_1(x), \Phi_2(x)$ given in (2.2)–(2.4)

$$\begin{aligned} \Phi(x) &= A\Phi_1(x) + B\Phi_2(x), \\ \Phi'(x) &= A\Phi_1'(x) + B\Phi_2'(x). \end{aligned} \tag{3.8}$$

The matrix relation between the wavefunction and its first derivative $\Phi(x), \Phi'(x)$ and the coefficients (A, B) is

$$\begin{bmatrix} \Phi(x) \\ \frac{d\Phi(x)}{dx} \end{bmatrix} = \begin{bmatrix} \Phi_1(x) & \Phi_2(x) \\ \Phi_1'(x) & \Phi_2'(x) \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}. \tag{3.9}$$

In detail, for the three possible cases we find:

Case A: $V < E$, $\quad \frac{\hbar^2 k^2}{2m} + V = E$,

$$\begin{aligned} \Phi(x) &= Ae^{+ikx} + Be^{-ikx} \\ \frac{d\Phi(x)}{dx} &= ikAe^{+ikx} - ikBe^{-ikx} \end{aligned} \Longrightarrow$$

$$\begin{bmatrix} \Phi(x) \\ \frac{d\Phi(x)}{dx} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ +ik & -ik \end{bmatrix} \begin{bmatrix} e^{+ikx} & 0 \\ 0 & e^{-ikx} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}. \tag{3.10}$$

Case B: $V = E$,

$$\begin{array}{rcccl} \Phi(x) & = & A\times 1 & + & B\times x \\ \frac{d\Phi(x)}{dx} & = & 0 & + & B\times 1 \end{array} \Longrightarrow$$

$$\begin{bmatrix} \Phi(x) \\ \frac{d\Phi(x)}{dx} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & x \\ 0 & 1 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} . \tag{3.11}$$

Case C: $V > E$, $\quad -\frac{\hbar^2\kappa^2}{2m} + V = E$,

$$\begin{array}{rcccl} \Phi(x) & = & Ae^{-\kappa x} & + & Be^{+\kappa x} \\ \frac{d\Phi(x)}{dx} & = & -\kappa Ae^{-\kappa x} & + & \kappa Be^{+\kappa x} \end{array} \Longrightarrow$$

$$\begin{bmatrix} \Phi(x) \\ \frac{d\Phi(x)}{dx} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ -\kappa & +\kappa \end{bmatrix} \begin{bmatrix} e^{-\kappa x} & 0 \\ 0 & e^{+\kappa x} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} . \tag{3.12}$$

Each of these equations can be written in the form

$$\begin{bmatrix} \Phi(x) \\ \frac{d\Phi(x)}{dx} \end{bmatrix} = K(V)E(V;x) \begin{bmatrix} A \\ B \end{bmatrix} . \tag{3.13}$$

The 2×2 matrices K, E as well as their inverses are collected in Table 3.1.

We return now to the problem of matching the wavefunction and its first derivative across a boundary, as illustrated in Fig. 3.1. Without making any assumptions about the relative values of E, V_1, V_2, the wavefunctions in regions 1 and 2 can be written as complex linear superpositions of the particular solutions $\Phi_1(x), \Phi_2(x)$ for the appropriate cases (Table 2.1). Matching the wavefunctions and their first derivatives at the boundary $x = a$ leads via (3.13) to the matrix equation

$$K(V_1)E(V_1;a) \begin{bmatrix} A \\ B \end{bmatrix} = K(V_2)E(V_2;a) \begin{bmatrix} C \\ D \end{bmatrix} . \tag{3.14}$$

The expression for (A, B) in terms of (C, D) is then given very simply by

$$\begin{bmatrix} A \\ B \end{bmatrix} = E^{-1}(V_1;a)K^{-1}(V_1)K(V_2)E(V_2;a) \begin{bmatrix} C \\ D \end{bmatrix} . \tag{3.15}$$

We have already encountered a special case of (3.15) in the case $E > V_1, E > V_2$ in (3.7).

(3.11)

Table 3.1 The 2×2 matrices $K(V)$ and $E(V;x)$, and their inverses, for the three cases: $E > V$, $E = V$, and $E < V$

(3.12)

	$E > V$	$E = V$	$E < V$
	$k = \sqrt{2m(E-V)/\hbar^2}$		$\kappa = \sqrt{2m(V-E)/\hbar^2}$
(3.13) $K(V)$	$\begin{bmatrix} 1 & 1 \\ +ik & -ik \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 1 \\ -\kappa & +\kappa \end{bmatrix}$
$K^{-1}(V)$	$\frac{1}{2}\begin{bmatrix} 1 & +\frac{1}{ik} \\ 1 & -\frac{1}{ik} \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & -\frac{1}{\kappa} \\ 1 & +\frac{1}{\kappa} \end{bmatrix}$
$E(V;x)$	$\begin{bmatrix} e^{+ikx} & 0 \\ 0 & e^{-ikx} \end{bmatrix}$	$\begin{bmatrix} 1 & +x \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} e^{-\kappa x} & 0 \\ 0 & e^{+\kappa x} \end{bmatrix}$
(3.14) $E^{-1}(V;x)$	$\begin{bmatrix} e^{-ikx} & 0 \\ 0 & e^{+ikx} \end{bmatrix}$	$\begin{bmatrix} 1 & -x \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} e^{+\kappa x} & 0 \\ 0 & e^{-\kappa x} \end{bmatrix}$

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4

Piecewise Constant Potentials

In this chapter we solve Schrödinger's equation in one dimension with potentials more complicated than those used in the previous chapter. We consider here potentials that are constant in an interval

$$V(x) = V_j, \qquad a_{j-1} < x < a_j \; . \tag{4.1}$$

Such a potential is illustrated in Fig. 4.1. The values of the potential at the breakpoints is unimportant as long as there are only a finite number of breakpoints.

4.1 TRANSFER MATRICES

Piecewise constant potentials can be treated by a simple extension of the methods developed in chapter 3. Instead of using different pairs of letters $(A, B), (C, D)$ for the particular solutions $\Phi_1(x), \Phi_2(x)$ in each region, we denote the general solution in region j by

$$\Phi(x) = A_j \Phi_1(x) + B_j \Phi_2(x), \qquad a_{j-1} \le x \le a_j \; . \tag{4.2}$$

(Otherwise we might quickly run out of letters.) From (3.15) we know the matrix relation between the coefficients $(A, B) = (A_1, B_1)$ in region 1 and the coefficients $(C, D) = (A_2, B_2)$ in region 2 is

$$\begin{aligned} \begin{bmatrix} A_1 \\ B_1 \end{bmatrix} &= E^{-1}(V_1; a_1) K^{-1}(V_1) K(V_2) E(V_2; a_1) \begin{bmatrix} A_2 \\ B_2 \end{bmatrix} \\ &= T_{12} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix} . \end{aligned} \tag{4.3}$$

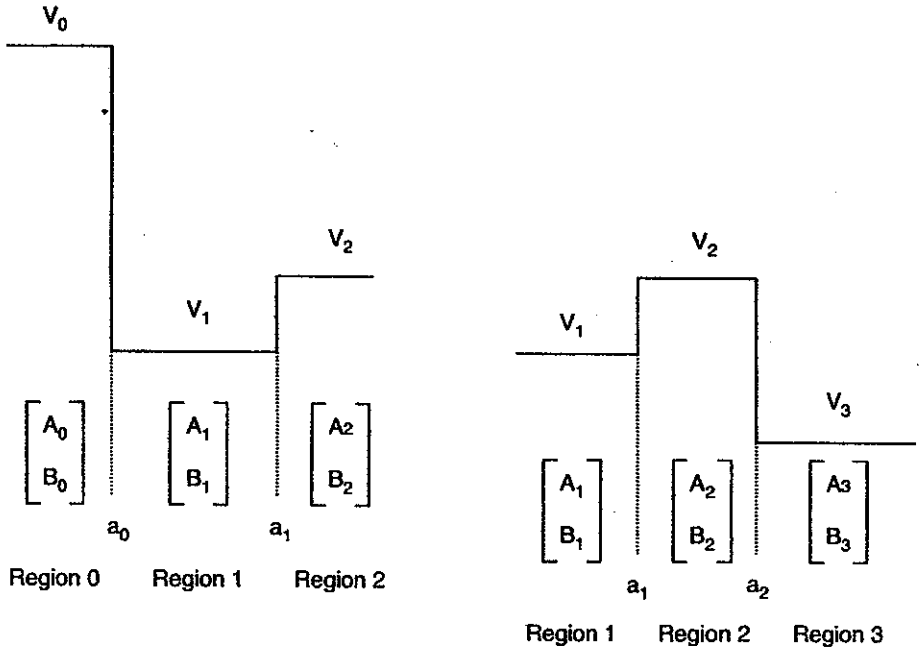

Fig. 4.1 The coefficients A_0, B_0 in the left-hand region 0 are related to the coefficients A_1, B_1 in Region 1 by a simple 2×2 transfer matrix. Similarly, the coefficients A_1, B_1 are related to A_2, B_2 by another simple transfer matrix. Thus, A_0, B_0 are related to A_2, B_2 by the product of simple 2×2 transfer matrices.

The break between regions 1 and 2 occurs at $x = a_1$. The 2×2 matrix T_{12} is called a transfer matrix because knowledge of the amplitudes A_2, B_2 can be transferred to knowledge of the amplitudes of A_1, B_1 with this matrix.

Suppose now the asymptotic region on the left (region 0) and region 1 meet at breakpoint a_0 (Fig. 4.1). The coefficients (A_0, B_0) or (A_L, B_L) and (A_1, B_1) are related by an equation of the form (3.15):

$$\begin{aligned} \begin{bmatrix} A_0 \\ B_0 \end{bmatrix} &= E^{-1}(V_L; a_0) K^{-1}(V_L) K(V_1) E(V_1; a_0) \begin{bmatrix} A_1 \\ B_1 \end{bmatrix} \\ &= T_{01} \begin{bmatrix} A_1 \\ B_1 \end{bmatrix} . \end{aligned} \tag{4.4}$$

Combining this with the matrix relation (4.3) yields an immediate linear relation between the coefficients (A_0, B_0) and (A_2, B_2)

$$\begin{bmatrix} A_0 \\ B_0 \end{bmatrix} = T_{01} T_{12} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix} . \tag{4.5}$$

Suppose now region 3 occurs to the right of region 2, the two regions meeting at breakpoint a_2 (Fig. 4.1). The coefficients (A_2, B_2) are related to (A_3, B_3) by an equation of the form (3.15):

$$\begin{bmatrix} A_2 \\ B_2 \end{bmatrix} = E^{-1}(V_2;a_2)K^{-1}(V_2)K(V_3)E(V_3;a_2)\begin{bmatrix} A_3 \\ B_3 \end{bmatrix}$$
$$= T_{23}\begin{bmatrix} A_3 \\ B_3 \end{bmatrix} . \tag{4.6}$$

Combining (4.6) with the linear relation between (A_1, B_1) and (A_2, B_2) given in (4.3) yields a linear relation between (A_1, B_1) and (A_3, B_3):

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = T_{12}T_{23}\begin{bmatrix} A_3 \\ B_3 \end{bmatrix} . \tag{4.7}$$

For a piecewise constant potential with asymptotic constant value $V_0 = V_L$ on the left and $V_{N+1} = V_R$ on the right, there are $N+1$ breakpoints $a_0, a_1, a_2, ..., a_N$, with a_j separating region j with constant potential V_j from region $(j+1)$ with constant potential $V_{j+1} (j = 1, 2, ..., N)$. The linear relationship between (A_0, B_0) and (A_{N+1}, B_{N+1}), or (A_L, B_L) and (A_R, B_R), is easily seen to be

$$\begin{bmatrix} A_0 \\ B_0 \end{bmatrix} = T_{01}T_{12}T_{23}...T_{N-1,N}T_{N,N+1}\begin{bmatrix} A_{N+1} \\ B_{N+1} \end{bmatrix}$$
$$= T_{0,N+1}\begin{bmatrix} A_{N+1} \\ B_{N+1} \end{bmatrix} . \tag{4.8}$$

The individual matrices are

$$T_{j,j+1} = E^{-1}(V_j;a_j)K^{-1}(V_j)K(V_{j+1})E(V_{j+1};a_j) . \tag{4.9}$$

Notation: We will call $T_{0,N+1}$ (or simply T) the transfer matrix for the problem of a piecewise constant potential with asymptotic constant values V_0 (or V_L) on the left and V_{N+1} (or V_R) on the right.

The transfer matrix $T_{0,N+1}$ is obtained as a product of 2×2 matrices. There are four 2×2 matrices at each breakpoint (the product at a_j is $T_{j,j+1}$, given in (4.9)), so that a problem involving N piecewise constant potentials between the asymptotic potentials V_L on the left and V_R on the right, defined by $N+1$ breakpoints, involves multiplying together $4(N+1)$ 2×2 matrices.

It is useful to carry out whatever simplifications are possible before the actual computations are performed. In the present case a great simplification is possible. Consider the product of two successive transfer matrices

$$T_{j-1,j}T_{j,j+1} = E^{-1}(V_{j-1};a_{j-1})K^{-1}(V_{j-1})$$
$$\times \underline{K(V_j)E(V_j;a_{j-1})E^{-1}(V_j;a_j)K^{-1}(V_j)} \times K(V_{j+1})E(V_{j+1};a_j) . \tag{4.10}$$

The four interior matrices, which are underlined, refer only to region j, where the potential has constant value V_j. The product of these four matrices can easily be

Table 4.1 Real 2×2 matrices $M(V;\delta)$ for the three cases $E > V$, $E = V$, $E < V$

$$M(V_j, \delta_j) = K(V_j)E(V_j; a_j)E^{-1}(V_j; a_{j-1})K^{-1}(V_j)$$

Case A	Case B	Case C
$E > V$	$E = V$	$E < V$
$k = \sqrt{2m(E-V)/\hbar^2}$		$\kappa = \sqrt{2m(V-E)/\hbar^2}$
$\begin{bmatrix} \cos k\delta & -k^{-1}\sin k\delta \\ +k\sin k\delta & \cos k\delta \end{bmatrix}$	$\begin{bmatrix} 1 & -\delta \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} \cosh \kappa\delta & -\kappa^{-1}\sinh \kappa\delta \\ -\kappa \sinh \kappa\delta & \cosh \kappa\delta \end{bmatrix}$
	$\delta = a_{j+1} - a_j$	$\cosh x = \frac{1}{2}(e^{+x} + e^{-x})$
		$\sinh x = \frac{1}{2}(e^{+x} - e^{-x})$

computed. The matrix product

$$M(V_j, \delta_j) = K(V_j)E(V_j; a_{j-1})E^{-1}(V_j; a_j)K^{-1}(V_j)\,, \tag{4.11}$$

($\delta_j = a_j - a_{j-1}$), is given in Table 4.1 for the three cases $E > V, E = V, E < V$. The matrix $M_j = M(V_j, \delta_j)$ depends only on the potential V_j in region j and the width δ_j of region j, as well as the particle energy E. Further, this matrix is always real and has determinant +1.

The computation of the transfer matrix simplifies to

$$T_{0,N+1} = E^{-1}(V_0; a_0)K^{-1}(V_0) \times M_1 M_2 \ldots M_N \times K(V_{N+1})E(V_{N+1}; a_N)\,. \tag{4.12}$$

As a result, the computation of the transfer matrix involves the product of $N+2\times 2 = N+4$ instead of $4(N+1) = 4N+4$ matrices: two matrices each for the left and right asymptotic regions, and the N real 2×2 matrices M_j for the N interior regions.

4.2 COMPUTATIONAL ALGORITHM

We show in Fig. 4.2 a very simple algorithm for constructing the transfer matrix merely by inspecting a piecewise constant potential. This algorithm would not have been as direct had we adopted the solution (3.6) instead of (3.7).

In summary, the algorithm for computing the transfer matrices that we will use is as follows. Equation (4.12) relates the amplitudes $\begin{bmatrix} A_L \\ B_L \end{bmatrix}$ in the asymptotic left-hand region with the amplitudes $\begin{bmatrix} A_R \\ B_R \end{bmatrix}$ in the asymptotic right-hand region. It is

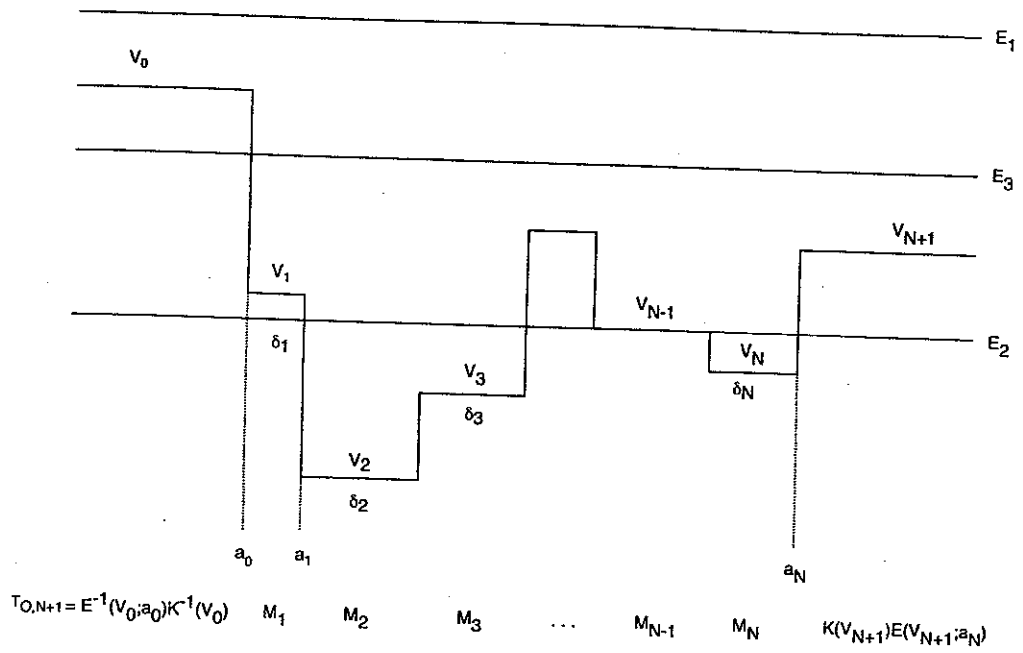

Fig. 4.2 The transfer matrix for the interior pieces of a piecewise constant potential is very simply constructed by inspection. We associate a simple 2×2 real transfer matrix with each piece of the potential and then simply multiply them in the order in which they occur.

often useful to absorb the diagonal matrix elements of $E(V_L; a_0)$ into the amplitudes $\begin{bmatrix} A_L \\ B_L \end{bmatrix}$ and the diagonal matrix elements of $E(V_R; a_N)$ into the amplitudes $\begin{bmatrix} A_R \\ B_R \end{bmatrix}$. Then

$$E(V_L; a_0) \begin{bmatrix} A_L \\ B_L \end{bmatrix} = K^{-1}(V_L) M_1 \dots M_N K(V_R) E(V_R; a_N) \begin{bmatrix} A_R \\ B_R \end{bmatrix},$$

$$\begin{bmatrix} A'_L \\ B'_L \end{bmatrix} = K^{-1}(V_L) \left\{ \prod_{j=1}^{N} M(V_j; \delta_j) \right\} K(V_R) \begin{bmatrix} A'_R \\ B'_R \end{bmatrix}. \quad (4.13)$$

The first step is the computation of the 2×2 real unimodular matrices $M(V_j; \delta_j)$ for each of the N intermediate piecewise constant potentials of energy V_j and width δ_j. These matrices can be written down by inspection for any energy E. The product of these N matrices is then computed in the order in which the potentials appear. We call the product M:

$$M = M(V_1; \delta_1) \dots M(V_N; \delta_N) = \prod_{j=1}^{N} M(V_j; \delta_j) = \begin{bmatrix} m_{11}(E) & m_{12}(E) \\ m_{21}(E) & m_{22}(E) \end{bmatrix}. \quad (4.14)$$

It remains only to premultiply M by $K^{-1}(V_L)$ and postmultiply by $K(V_R)$. We consider two cases separately.

If the asymptotic potentials V_L, V_R are both less than the energy E of the particle, the matrices K are complex:

$$T = \frac{1}{2}\begin{bmatrix} 1 & \frac{1}{ik_L} \\ 1 & \frac{1}{-ik_L} \end{bmatrix}\begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}\begin{bmatrix} 1 & 1 \\ ik_R & -ik_R \end{bmatrix} \tag{4.15}$$

$$= \frac{1}{2}\begin{bmatrix} m_{11} + \frac{k_R}{k_L}m_{22} + ik_R m_{12} + \frac{m_{21}}{ik_L} & m_{11} - \frac{k_R}{k_L}m_{22} - ik_R m_{12} + \frac{m_{21}}{ik_L} \\ m_{11} - \frac{k_R}{k_L}m_{22} + ik_R m_{12} - \frac{m_{21}}{ik_L} & m_{11} + \frac{k_R}{k_L}m_{22} - ik_R m_{12} - \frac{m_{21}}{ik_L} \end{bmatrix}. \tag{4.16}$$

This matrix with complex matrix elements can be written in the simpler-looking form

$$T(E) = \begin{bmatrix} \alpha & \beta \\ \overline{\beta} & \overline{\alpha} \end{bmatrix}, \tag{4.17}$$

where $\overline{\alpha}$ is the complex conjugate of the complex number α, and similarly for β. These two complex numbers are explicitly given by $\alpha = \alpha_R + i\alpha_I$, $\beta = \beta_R + i\beta_I$:

$$\begin{aligned} 2\alpha_R &= +m_{11} + \frac{k_R}{k_L}m_{22}, \\ 2\beta_R &= +m_{11} - \frac{k_R}{k_L}m_{22}, \\ 2\alpha_I &= +k_R m_{12} - \frac{m_{21}}{k_L}, \\ 2\beta_I &= -k_R m_{12} - \frac{m_{21}}{k_L}. \end{aligned} \tag{4.18}$$

It is a simple matter to verify that

$$|\alpha|^2 - |\beta|^2 = \frac{k_R}{k_L} \tag{4.19}$$

If the asymptotic potentials V_L, V_R are both greater than the energy E of the particle, then the matrices K are real and

$$\begin{aligned} T &= \frac{1}{2}\begin{bmatrix} 1 & \frac{-1}{\kappa_L} \\ 1 & \frac{1}{\kappa_L} \end{bmatrix}\begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}\begin{bmatrix} 1 & 1 \\ -\kappa_R & \kappa_R \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} m_{11} + \frac{\kappa_R}{\kappa_L}m_{22} - \kappa_R m_{12} - \frac{m_{21}}{\kappa_L} & m_{11} - \frac{\kappa_R}{\kappa_L}m_{22} + \kappa_R m_{12} - \frac{m_{21}}{\kappa_L} \\ m_{11} - \frac{\kappa_R}{\kappa_L}m_{22} - \kappa_R m_{12} + \frac{m_{21}}{\kappa_L} & m_{11} + \frac{\kappa_R}{\kappa_L}m_{22} + \kappa_R m_{12} + \frac{m_{21}}{\kappa_L} \end{bmatrix} \\ &= \begin{bmatrix} \alpha_1 + \alpha_2 & \beta_1 + \beta_2 \\ \beta_1 - \beta_2 & \alpha_1 - \alpha_2 \end{bmatrix}, \end{aligned} \tag{4.20}$$

where the real numbers $\alpha_1, \alpha_2, \beta_1, \beta_1$ are given by

$$\begin{aligned} 2\alpha_1 &= +m_{11} + \frac{\kappa_R}{\kappa_L} m_{22} , \\ 2\beta_1 &= +m_{11} - \frac{\kappa_R}{\kappa_L} m_{22} , \\ 2\alpha_2 &= -\kappa_R m_{12} - \frac{m_{21}}{\kappa_L} , \\ 2\beta_2 &= +\kappa_R m_{12} - \frac{m_{21}}{\kappa_L} . \end{aligned} \tag{4.21}$$

It is a simple matter to verify that

$$\begin{aligned} \det T &= (\alpha_1^2 - \alpha_2^2) - (\beta_1^2 - \beta_2^2) \\ &= (\alpha_1^2 + \beta_2^2) - (\alpha_2^2 + \beta_1^2) \\ &= \frac{\kappa_R}{\kappa_L} . \end{aligned} \tag{4.22}$$

The transfer matrices (4.16) and (4.20) are related by

$$\begin{array}{ccc} (4.16) & \leftrightarrow & (4.20) \\ +ik & \leftrightarrow & -\kappa \end{array} \tag{4.23}$$

It happens frequently that the determinant of the transfer matrix must be computed. This is a relatively simple task, as the determinant of a product of matrices is the product of the determinants of the individual matrices, and for a nonsingular matrix M, $\det M^{-1} = 1/(\det M)$. To compute $\det T_{0,N+1}$ from (4.8) we observe that the determinants of all matrices $E(V;a)$ are 1 (i.e., Table 2.1). In addition, for every matrix $K(V_j)$ there is a matrix $K^{-1}(V_j)$, except on the far left and the far right, where $K^{-1}(V_L)$ and $K(V_R)$ are unmatched. Therefore,

$$\det T_{0,N+1} = \frac{\det K(V_R)}{\det K(V_L)} . \tag{4.24}$$

This result can be seen even more easily from (4.12) or (4.13), since $\det M_j = 1$ (see Table 4.1).

4.3 SCATTERING MATRICES

The complex numbers A_L, B_L are probability amplitudes for particles moving toward and away from the scattering potential on the left; B_R and A_R are probability amplitudes for a particle moving toward and away from the scattering potential on the right. These four numbers are not independent: there are two linear relations among them. These are provided by the transfer matrix T, which relates the pair $\begin{bmatrix} A_L \\ B_L \end{bmatrix}$ on the left with the pair $\begin{bmatrix} A_R \\ B_R \end{bmatrix}$ on the right.

There is another useful relation among these four amplitudes. This relates the amplitudes $\begin{bmatrix} A_L \\ B_R \end{bmatrix}$ for particles moving toward the scattering potential to the amplitudes $\begin{bmatrix} A_R \\ B_L \end{bmatrix}$ for particles leaving the scattering region. This linear relation defines the scattering matrix, or S-matrix $S(E)$:

$$\begin{bmatrix} A_R \\ B_L \end{bmatrix} = S \begin{bmatrix} A_L \\ B_R \end{bmatrix} = \begin{bmatrix} S_{11}(E) & S_{12}(E) \\ S_{21}(E) & S_{22}(E) \end{bmatrix} \begin{bmatrix} A_L \\ B_R \end{bmatrix} . \tag{4.25}$$

The T- and S-matrices have dual interpretations. The transfer matrix relates amplitudes in space—on the left and on the right of the scattering region. The scattering matrix relates amplitudes before the interaction with those after the interaction. This duality is illustrated in Fig. 4.3.

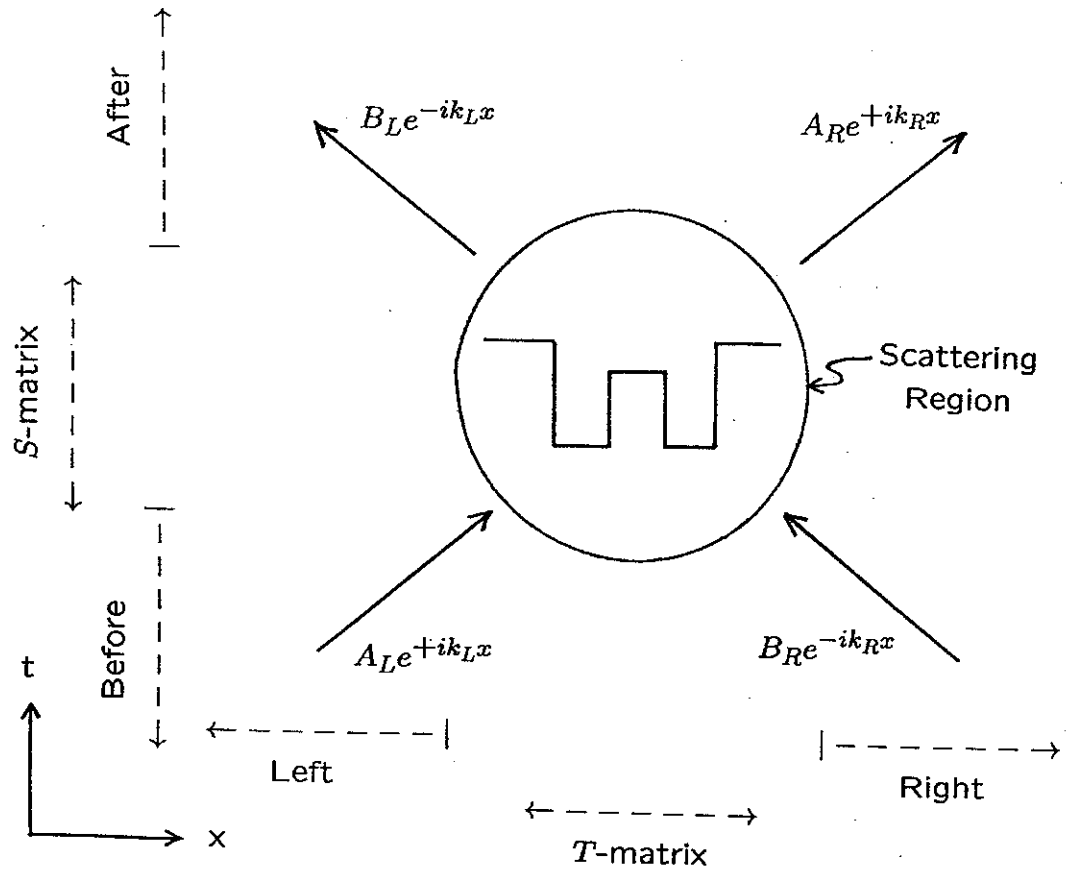

Fig. 4.3 The transfer matrix relates amplitudes on the left of the scattering region with those on the right. The scattering matrix relates incoming amplitudes ("before") with outgoing amplitudes ("after").

It is a simple matter to construct the matrix elements of the S-matrix from those of the T-matrix. We first write out the two equations summarized by the T-matrix:

$$\begin{array}{rcl} A_L &=& t_{11}A_R + t_{12}B_R\,, \\ B_L &=& t_{21}A_R + t_{22}B_R\,. \end{array} \tag{4.26}$$

Then we regroup the complex amplitudes, placing the amplitudes $\begin{bmatrix} A_R \\ B_L \end{bmatrix}$ for outgoing waves on the left and the incoming amplitudes $\begin{bmatrix} A_L \\ B_R \end{bmatrix}$ on the right:

$$\begin{array}{rcl} -t_{11}A_R &=& -A_L + t_{12}B_R \\ -t_{21}A_R + B_L &=& t_{22}B_R\,, \end{array} \tag{4.27}$$

$$\begin{bmatrix} -t_{11} & 0 \\ -t_{21} & 1 \end{bmatrix} \begin{bmatrix} A_R \\ B_L \end{bmatrix} = \begin{bmatrix} -1 & t_{12} \\ 0 & t_{22} \end{bmatrix} \begin{bmatrix} A_L \\ B_R \end{bmatrix}. \tag{4.28}$$

The linear relation we desire is obtained by multiplying by the inverse of the matrix on the left:

$$\begin{bmatrix} A_R \\ B_L \end{bmatrix} = \begin{bmatrix} -t_{11} & 0 \\ -t_{21} & 1 \end{bmatrix}^{-1} \begin{bmatrix} -1 & t_{12} \\ 0 & t_{22} \end{bmatrix} \begin{bmatrix} A_L \\ B_R \end{bmatrix}. \tag{4.29}$$

The result is

$$S = \begin{bmatrix} \dfrac{1}{t_{11}} & -\dfrac{t_{12}}{t_{11}} \\[2ex] \dfrac{t_{21}}{t_{11}} & \dfrac{\det(T)}{t_{11}} \end{bmatrix} = \begin{bmatrix} s_{11}(E) & s_{12}(E) \\[2ex] s_{21}(E) & s_{22}(E) \end{bmatrix}. \tag{4.30}$$

Conservation of momentum provides the following quantities conserved by the T- and S-matrices:

$$\begin{array}{lrcl} T & k_L|A_L|^2 - k_L|B_L|^2 &=& k_R|A_R|^2 - k_R|B_R|^2\,, \\ S & k_L|A_L|^2 + k_R|B_R|^2 &=& k_R|A_R|^2 + k_L|B_L|^2\,. \end{array} \tag{4.31}$$

When the asymptotic potentials on the left and right are equal, $V_L = V_R$, these conservation laws simplify to

$$\begin{array}{lrcl} T & |A_L|^2 - |B_L|^2 &=& |A_R|^2 - |B_R|^2 \\ S & |A_L|^2 + |B_R|^2 &=& |A_R|^2 + |B_L|^2 = 1\,. \end{array} \tag{4.32}$$

One additional linear relation among two pairs of amplitudes is possible. This relates the amplitudes for right-going waves with the amplitudes for left-going waves:

$$\begin{bmatrix} A_L \\ A_R \end{bmatrix} = U \begin{bmatrix} B_R \\ B_L \end{bmatrix}. \tag{4.33}$$

This last relation is almost never used.

In this work we will deal entirely with transfer matrices. However, there are many one-dimensional quantum mechanical problems that are not elementary and that can only be treated with S-matrices.

5

Momentum Conservation

We have seen in chapter 2 that the wavefunction $\Phi_1(x) = e^{+ikx}$ represents a particle traveling to the right in a region of constant potential $V < E$ with a momentum $p = +\hbar k, k = \sqrt{2m(E-V)/\hbar^2}$. Similarly, $\Phi_2(x) = e^{-ikx}$ represents a particle traveling to the left, with a momentum $p = -\hbar k$.

The most general wavefunction in such a region is a complex linear superposition of the two particular solutions,

$$\Phi(x) = Ae^{+ikx} + Be^{-ikx} \,. \tag{5.1}$$

The complex number A is the probability amplitude for finding the particle moving to the right with momentum $\hbar k$. Its absolute square, $|A|^2 = \overline{A}A = A^*A$, is the probability for finding the particle with momentum $+\hbar k$. Similarly, B is the probability amplitude for finding the particle with momentum $-\hbar k$, and $|B|^2 = \overline{B}B = B^*B$ is the probability for finding the particle with momentum $-\hbar k$.

Since a measurement of particle momentum will yield only one of the two results $p = +\hbar k$ or $p = -\hbar k$, the probability of finding the particle of energy $E = (\hbar k)^2/2m + V$ with momentum either $+\hbar k$ or $-\hbar k$ is one. Therefore

$$|A|^2 + |B|^2 = 1 \,. \tag{5.2}$$

The average particle momentum in the region of constant potential V is the momentum $\hbar k$ multiplied by the probability that the particle has momentum $\hbar k$, plus the momentum $-\hbar k$ multiplied by the probability that the particle has momentum $-\hbar k$:

$$p_{av} = <\hat{p}> = (+\hbar k)\mathrm{Pr}(\hbar k) + (-\hbar k)\mathrm{Pr}(-\hbar k) = \hbar k(|A|^2 - |B|^2) \,. \tag{5.3}$$

We will now describe the quantum mechanical version of the law of momentum conservation. We start with a simple problem (Fig. 5.1). In the left-hand region with constant potential $V_1 < E$ the wavefunction and average momentum are

$$\begin{aligned} \Phi(x) &= Ae^{+ik_1x} + Be^{-ik_1x}\,, \\ <\hat{p}> &= \hbar k_1(|A|^2 - |B|^2)\,. \end{aligned} \tag{5.4}$$

In the right-hand region with constant potential $V_2 < E$ we have

$$\begin{aligned} \Phi(x) &= Ce^{+ik_2x} + De^{-ik_2x}\,, \\ <\hat{p}> &= \hbar k_2(|C|^2 - |D|^2)\,. \end{aligned} \tag{5.5}$$

We want to show that the average momentum in the left-hand region is equal to the average momentum in the right-hand region:

$$\hbar k_1(|A|^2 - |B|^2) = \hbar k_2(|C|^2 - |D|^2)\,. \tag{5.6}$$

The verification of (5.6) is easily carried out using transfer matrix methods. The complex amplitudes (A, B) and (C, D) are related by

$$\begin{bmatrix} A \\ B \end{bmatrix} = T_{12}\begin{bmatrix} C \\ D \end{bmatrix} = E^{-1}(V_1;a)K^{-1}(V_1)K(V_2)E(V_2;a)\begin{bmatrix} C \\ D \end{bmatrix}\,. \tag{5.7}$$

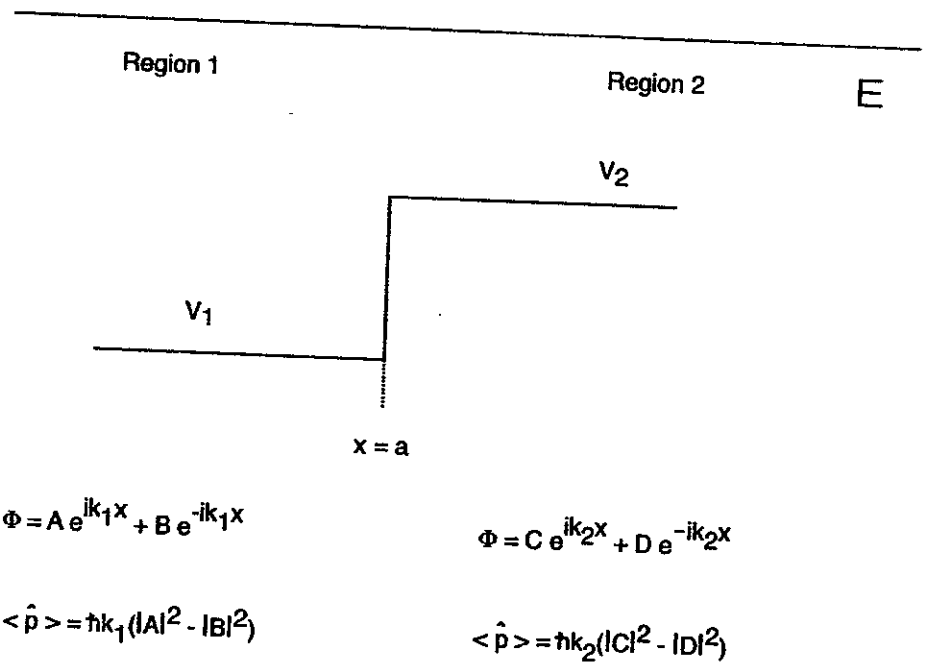

Fig. 5.1 The mean value of the particle momentum in region 1 is the same as the mean value of the momentum in region 2.

We could simplify this calculation by choosing the break point a to be at the origin of coordinates. However, it will be useful to allow a to be nonzero. Then the complex phase factors in the E matrices can be absorbed into the amplitudes (A, B) and (C, D) as follows:

$$\begin{aligned}\begin{bmatrix} A' \\ B' \end{bmatrix} &= E(V_1; a)\begin{bmatrix} A \\ B \end{bmatrix} = \begin{pmatrix} e^{+ik_1 a}A \\ e^{-ik_1 a}B \end{pmatrix}, \\ \begin{bmatrix} C' \\ D' \end{bmatrix} &= E(V_2; a)\begin{bmatrix} C \\ D \end{bmatrix} = \begin{pmatrix} e^{+ik_2 a}C \\ e^{-ik_2 a}D \end{pmatrix}. \end{aligned} \tag{5.8}$$

These phase factors will be unimportant in the final analysis since (5.6) involves only the absolute squares of the complex amplitudes.

The result (5.7) then reduces to

$$\begin{aligned}\begin{bmatrix} A' \\ B' \end{bmatrix} &= \frac{1}{2}\begin{pmatrix} 1 & \frac{1}{ik_1} \\ 1 & \frac{1}{-ik_1} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix}\begin{bmatrix} C' \\ D' \end{bmatrix} \\ &= \begin{bmatrix} \frac{k_1+k_2}{2k_1} & \frac{k_1-k_2}{2k_1} \\ \frac{k_1-k_2}{2k_1} & \frac{k_1+k_2}{2k_1} \end{bmatrix}\begin{bmatrix} C' \\ D' \end{bmatrix}. \end{aligned} \tag{5.9}$$

Now we compute $|A'|^2, |B'|^2$, and take their difference

$$\begin{aligned} |A'|^2 &= \left(\frac{k_1+k_2}{2k_1}\right)^2 |C'|^2 + \left(\frac{k_1-k_2}{2k_1}\right)^2 |D'|^2 + \frac{k_1^2-k_2^2}{(2k_1)^2}(\overline{C'}D' + C'\overline{D'}) \\ |B'|^2 &= \left(\frac{k_1-k_2}{2k_1}\right)^2 |C'|^2 + \left(\frac{k_1+k_2}{2k_1}\right)^2 |D'|^2 + \frac{k_1^2-k_2^2}{(2k_1)^2}(\overline{C'}D' + C'\overline{D'}) \\ |A'|^2 - |B'|^2 &= \frac{k_2}{k_1}(|C'|^2 - |D'|^2). \end{aligned} \tag{5.10}$$

This last equation is what we have set out to prove when we recognize that $|A'|^2 = |A|^2$, and so on.

We now prove momentum conservation in the general case where $E > V_L$, $E > V_R$, shown in Fig. 5.2. The potential may be approximated by a piecewise constant potential by choosing the breakpoints close enough ($a_{j+1} - a_j \sim \epsilon, \epsilon$ very small) and allowing N to be large enough. The transfer matrix $T_{0,N+1}$ can be expressed in the form (4.12). The phase factors in the exponentials that occur at the ends of $T_{0,N+1}$ may be absorbed into the amplitudes, as in (5.8). The product of the matrices M_j that occur in the interior of (4.12) need not be computed explicitly. We have only to observe that each M_j is real and has determinant $+1$. The product of real matrices with determinant $+1$ is itself a real matrix with determinant $+1$. Thus, no matter what the potential,

$$M_1 M_2 \ldots M_N = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad ad - bc = 1, \quad a, b, c, d \quad \text{real}. \tag{5.11}$$

The relation between (A_0, B_0) and (A_{N+1}, B_{N+1}) or (A_L, B_L) and (A_R, B_R) is therefore

$$\begin{aligned}\begin{bmatrix} A'_L \\ B'_L \end{bmatrix} &= \frac{1}{2}\begin{pmatrix} 1 & \frac{1}{ik_L} \\ 1 & \frac{1}{-ik_L} \end{pmatrix}\begin{bmatrix} a & b \\ c & d \end{bmatrix}\begin{bmatrix} 1 & 1 \\ ik_R & -ik_R \end{bmatrix}\begin{bmatrix} A'_R \\ B'_R \end{bmatrix} \\ &= \begin{bmatrix} \alpha & \beta \\ \overline{\beta} & \overline{\alpha} \end{bmatrix}\begin{bmatrix} A'_R \\ B'_R \end{bmatrix}, \end{aligned} \tag{5.12}$$

$$\begin{aligned} 2\alpha &= \left(a + d\frac{k_R}{k_L}\right) + i\left(+bk_R - \frac{c}{k_L}\right), \\ 2\beta &= \left(a - d\frac{k_R}{k_L}\right) + i\left(-bk_R - \frac{c}{k_L}\right). \end{aligned} \tag{5.13}$$

Again we compute $|A'_L|^2, |B'_L|^2$ and take their difference

$$\begin{aligned} |A'_L|^2 &= |\alpha|^2|A'_R|^2 + |\beta|^2|B'_R|^2 + \overline{\alpha}\beta\,\overline{A'_R}B'_R + \alpha\overline{\beta}A'_R\overline{B'_R}, \\ |B'_L|^2 &= |\beta|^2|A'_R|^2 + |\alpha|^2|B'_R|^2 + \overline{\alpha}\beta\overline{A'_R}B'_R + \alpha\overline{\beta}A'_R\overline{B'_R}, \\ |A'_L|^2 - |B'_L|^2 &= (|\alpha|^2 - |\beta|^2)(|A'_R|^2 - |B'_R|^2) \\ &\overset{\text{by (5.12)}}{=} (ad - bc)\frac{k_R}{k_L}(|A'_R|^2 - |B'_R|^2) \\ &\overset{\text{by (5.11)}}{=} \frac{k_R}{k_L}(|A'_R|^2 - |B'_R|^2). \end{aligned} \tag{5.14}$$

Since $|A'_L|^2 = |A_L|^2$ and so on, we have the desired result that (average) momentum is conserved on transmission through a barrier of arbitrary shape

$$\hbar k_L(|A_L|^2 - |B_L|^2) = \hbar k_R(|A_R|^2 - |B_R|^2). \tag{5.15}$$

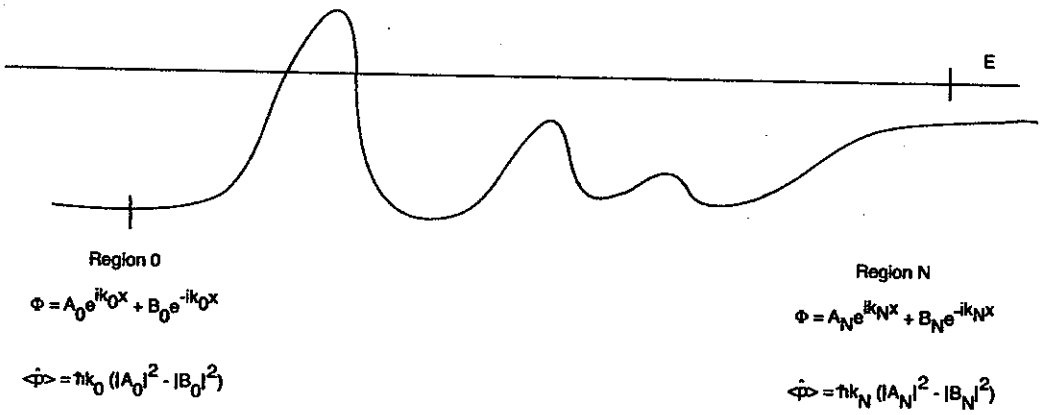

Fig. 5.2 In the general scattering case, the average momentum of the particle in the asymptotic left-hand region is the same as the average momentum in the asymptotic right-hand region, no matter what the shape of the potential.

6

Preview of Boundary Conditions

We will solve the time-independent Schrödinger equation in one dimension with piecewise constant potentials subject to three distinct boundary conditions:

Part II	Scattering
Part III	Bound States
Part IV	Periodic Potentials

Each boundary condition imposes a different condition on the transfer matrix.

6.1 BOUNDARY CONDITION FOR SCATTERING

In the case of scattering (Fig. 6.1) the wavefunctions in the asymptotic left-hand and right-hand regions are

$$\Phi_L(x) = A_L e^{+ik_L x} + B_L e^{-ik_L x}\,, \qquad \Phi_R(x) = A_R e^{+ik_R x} + B_R e^{-ik_R x}\,. \quad (6.1)$$

The amplitudes for the wavefunction on the left- and right-hand side of the potential are related by the transfer matrix

$$\begin{bmatrix} A_L \\ B_L \end{bmatrix} = T \begin{bmatrix} A_R \\ B_R \end{bmatrix} = \begin{bmatrix} t_{11}(E) & t_{12}(E) \\ t_{21}(E) & t_{22}(E) \end{bmatrix} \begin{bmatrix} A_R \\ B_R \end{bmatrix}. \quad (6.2)$$

We assume that the constant potentials on the left and right of the scattering potential are equal. We also assume that a particle is incident from the left with nonzero

probability amplitude ($A_L \neq 0$), but not from the right ($B_R = 0$). There is some probability amplitude (A_R) that the particle is transmitted through the barrier, and some amplitude (B_L) that it is reflected. This provides a simple relation between the amplitudes

$$\begin{bmatrix} A_L \\ B_L \end{bmatrix} = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \begin{bmatrix} A_R \\ 0 \end{bmatrix} \Longrightarrow \begin{array}{rcl} A_L &=& t_{11}(E)A_R \\ B_L &=& t_{21}(E)A_R \end{array} . \tag{6.3}$$

The squares of A_R, B_L describe the transmission probability $T(E)$ and reflection probability $R(E)$ for the particle incident on the scattering potential

$$\begin{array}{rcccl} T(E) &=& |A_R/A_L|^2 &=& 1/|t_{11}(E)|^2 \\ R(E) &=& |B_L/A_L|^2 &=& |t_{21}(E)|^2/|t_{11}(E)|^2 . \end{array} \tag{6.4}$$

We remark that these results can be determined from the S-matrix (4.25) with (4.30).

6.2 BOUNDARY CONDITION FOR BOUND STATES

In the case of bound states (Fig. 6.2) the wavefunctions in the asymptotic left- and right-hand regions, forbidden to a classical particle, are

$$\Phi_L(x) = A_L e^{-\kappa_L x} + B_L e^{+\kappa_L x} , \quad \Phi_R(x) = A_R e^{-\kappa_R x} + B_R e^{+\kappa_R x} . \tag{6.5}$$

In order to have a wavefunction that is bounded by the classically forbidden right-hand region, $B_R = 0$. Then

$$\begin{bmatrix} A_L \\ B_L \end{bmatrix} = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \begin{bmatrix} A_R \\ 0 \end{bmatrix} \Longrightarrow \begin{array}{rcl} A_L &=& t_{11}(E)A_R \\ B_L &=& t_{21}(E)A_R \end{array} . \tag{6.6}$$

In order to have a wavefunction that is bounded by the classically forbidden left-hand region, $A_L = 0$. Since $A_R \neq 0$ (otherwise the wavefunction would vanish everywhere), $t_{11}(E)$ must be zero. Thus, the zeros of $t_{11}(E)$ define the energies at which the potential supports bound states. This result can also be determined from the S-matrix (4.25) with (4.30).

6.3 BOUNDARY CONDITION FOR PERIODIC POTENTIALS

Many solids are adequately approximated by a long sequence of identical potentials (Fig. 6.3). If the transfer matrix for each unit cell in this potential is $T(E)$, then the transfer matrix for N identical cells "in series" is $[T(E)]^N$.

For reasons that will be justified later, it is useful to assume periodic boundary conditions. That is, we identify the wavefunction at one end of the potential with that at the other, so that $\begin{bmatrix} A \\ B \end{bmatrix}_0 = \begin{bmatrix} A \\ B \end{bmatrix}_N$:

$$\begin{bmatrix} A \\ B \end{bmatrix}_0 = [T(E)]^N \begin{bmatrix} A \\ B \end{bmatrix}_N . \tag{6.7}$$

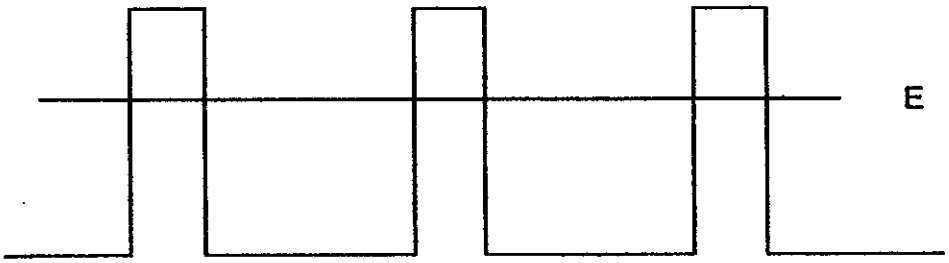

Fig. 6.1 Typical boundary conditions for scattering

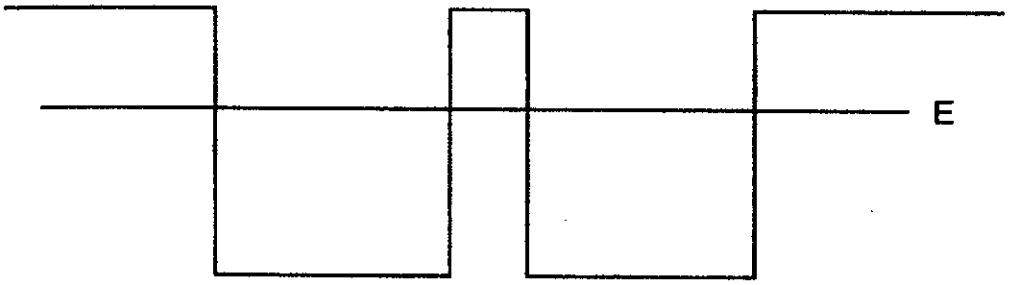

Fig. 6.2 A typical arrangement for bound states

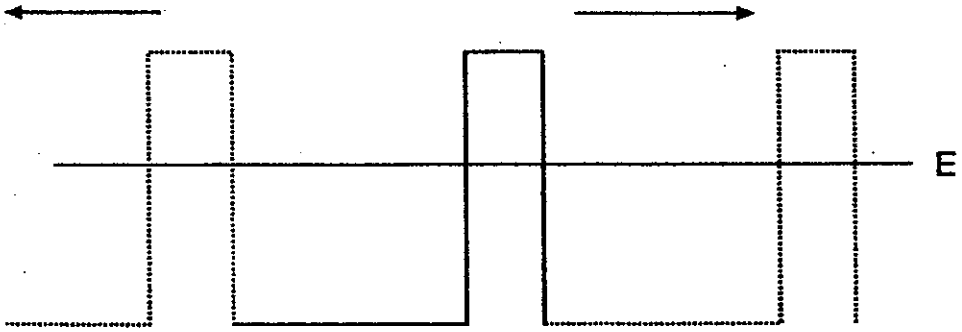

Fig. 6.3 A typical periodic potential geometry

This identification requires $[T(E)]^N = I_2$, the unit 2×2 matrix. Therefore, the problem of identifying the allowed states and energies for a periodic potential reduces to the problem of determining the values of E for which $[T(E)]^N = I_2$.

To approach this problem, we search for a similarity transformation S that diagonalizes $T(E)$:

$$\begin{aligned} S\,[T(E)]^N\,S^{-1} &= SI_2S^{-1}\,, \\ \left[ST(E)S^{-1}\right]^N &= I_2\,, \\ \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}^N &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \end{aligned} \tag{6.8}$$

Therefore, the condition simplifies to $\lambda_j^N = 1$ $(j = 1, 2)$. Since the transfer matrix $T(E)$ is unimodular, the product of the two eigenvalues is $+1$, so that $\lambda_1 = \lambda = \lambda_2^{-1}$. The eigenvalues of the unit cell transfer matrix $T(E)$ are determined from

$$\begin{aligned} \det \left| \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right| &= \lambda^2 - (t_{11} + t_{22})\lambda + (t_{11}t_{22} - t_{12}t_{21}) \\ &= \lambda^2 - \lambda\,\mathrm{tr}(T) + \det(T)\,. \end{aligned} \tag{6.9}$$

Since $\det(T) = 1$,

$$\begin{aligned} \lambda &= \tfrac{1}{2}\mathrm{tr}(T) \pm \sqrt{\left(\tfrac{1}{2}\mathrm{tr}(T)\right)^2 - 1} \\ &= \tfrac{1}{2}\mathrm{tr}(T) \pm i\sqrt{1 - \left(\tfrac{1}{2}\mathrm{tr}(T)\right)^2}\,. \end{aligned} \tag{6.10}$$

If we define an angle ϕ by

$$\begin{aligned} \cos\phi &= \tfrac{1}{2}\mathrm{tr}(T)\,, \\ \sin\phi &= \sqrt{1 - \left(\tfrac{1}{2}\mathrm{tr}(T)\right)^2}\,, \\ \lambda^{\pm 1} &= \cos\phi \pm i\sin\phi = e^{\pm i\phi}\,. \end{aligned} \tag{6.11}$$

It is easily seen that the periodic boundary condition $\lambda^N = 1$ is satisfied if $N\phi = 2\pi k$, where k is an integer. The result is

$$\mathrm{tr}(T) = t_{11} + t_{22} = 2\cos\left(2\pi\frac{k}{N}\right)\,. \tag{6.12}$$

Allowed states exist for values of the energy, E, for which the transfer matrix of the unit cell, $T(E)$, satisfies the condition (6.12).

In the following parts of this book we will explore the implications of these three types of boundary conditions.

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7

Units

Most of the calculations that will be carried out in Parts II, III, and IV of this work will be numerical computations based on equations (6.4), (6.6), and (6.12). In order to compute the transfer matrices, and in particular the real 2×2 matrices $M(V;\delta)$ for each region of a piecewise constant potential, we must provide information about the energy and width of each piece of the potential. This means we must adopt a system of units for measuring energy and length.

For an electron with mass $m = 0.911 \times 10^{-27}$ gm and charge $q = -1.602 \times 10^{-19}$ Coul, a useful unit in which to measure energy is the electron-volt (eV). This is the energy gained (or lost) by an electron when it moves through a potential difference of one volt:

$$\begin{aligned} \Delta E &= |qV| \\ &= |(-1.602 \times 10^{-19}\ \text{Coul}) \times (1\ \text{volt})| \\ &= 1.602 \times 10^{-19}\ \text{J}\ (= \text{kg m}^2/\text{sec}^2) \\ &= 1.602 \times 10^{-12}\ \text{erg}\ (= \text{gm cm}^2/\text{sec}^2)\ . \end{aligned} \tag{7.1}$$

Electron-volts are convenient units because it is very easy to change the energy of a charged particle by changing the imposed potential difference (voltage) across the region through which the charge moves.

To determine a useful length scale, we search for a length a for which the dimensionless product ka is approximately 1 for an electron moving with an energy of 1 eV:

$$\begin{aligned}
\frac{\hbar^2 k^2}{2m} &= E = 1\,\text{eV}\,, \\
k^2 &= \frac{2mE}{\hbar^2} \\
&= \frac{2(0.911\times 10^{-27}\,\text{gm})(1.602\times 10^{-12}\,\text{erg})}{(1.054\times 10^{-27}\,\text{erg sec})^2} \qquad (7.2)\\
&= 2.626\times 10^{+15}\,\text{cm}^{-2}\,, \\
k &= 0.512\times 10^{+8}\,\text{cm}^{-1}\,.
\end{aligned}$$

Therefore a useful length scale is 10^{-8} cm = 1 Å (angstrom). To give some perspective to these units, the "diameter" of a hydrogen atom in its ground state is about 1 Å and the electron is bound to the proton in this state with an energy of about 13.6 eV.

All energies will be measured in electron-volts, and all lengths will be measured in angstroms throughout the remainder of this work. In these units the relation between k and E is

$$k = \sqrt{\frac{2m}{\hbar^2}E} = \sqrt{\frac{2m}{\hbar^2}\,q\,\frac{E}{q}}\,. \qquad (7.3)$$

In this expression, E/q is measured in terms of electron-volts. Using the physical values given above,

$$k = 0.5125\sqrt{E}\,, \qquad (7.4)$$

with E measured in electron-volts.