From: Quantum Mechanics by Herbert Kroemer

Chapter 5

SCATTERING BY SIMPLE BARRIERS

5.1 SCATTERING STATES AND THEIR NORMALIZATION

In this chapter, we consider solutions of the Schroedinger equations that correspond to particles coming from infinity and being scattered by a non-constant potential in their path. Because the particles have an infinite amount of space available, the single-particle energy eigenfunctions for the problem are not normalizable and hence do not correspond to physically admissible single-particle states. Nevertheless, they remain mathematically and physically meaningful for the following reasons:

(a) Mathematically, it is always possible to construct normalizable, and hence physically admissible, time-dependent wave packets from the energy eigenfunctions by linear superposition. The situation is a direct generalization of that in chapter 4, where we constructed normalizable, and hence physically admissible, wave packets from the un-normalizable plane waves. The energy

eigenfunctions extending to infinity are the generalizations of the earlier plane waves.

(b) Physically, it is inherent in the nature of scattering problems that one deals with a very large number of particles with a nonzero density. As a rule, the interaction between the particles is negligible, so that each particle behaves as if it were present alone. Furthermore, the single-particle state functions for all particles are essentially the same. Under these circumstances, it is convenient to re-normalize ψ in such a way that $|\psi|^2$ represents the *overall* density of particles,

$$\rho = |\psi|^2. \tag{5•1–1}$$

This means that $|\psi|^2\, d^3r$ is the average value $\langle dN \rangle$ of the number of particles that materialize in the volume d^3r, taken over many different measurements of this number, all on the same state ψ. With this normalization, the quantity

$$\mathbf{j} = -\frac{i\hbar}{2M}(\psi^*\nabla\psi - \psi\nabla\psi^*) \tag{5•1–2}$$

is the *overall* particle current density. As a rule, in scattering problems, it is the incident *current* density that is known and specified, rather than the spatial density. The wave function is then most conveniently used with whatever normalization leads to the desired incident current density.

5.2 MATRIX FORMALISM FOR SCATTERING BY ONE-DIMENSIONAL BARRIERS

5.2.1 Scattering Matrix and Propagation Matrix

In this section, we extend the treatment of scattering at a step, treated briefly in section 1.4, to scattering by one-dimensional barriers of finite thickness with a more complicated potential profile, such as the schematic barrier shown in **Fig. 5•2–1.** Such one-dimensional barriers are more than simple textbook exercises; they actually play an important role in modern semiconductor electronics.

We consider a potential barrier of unspecified shape, separating two regions of constant, but not necessarily equal, potential energy, as in the figure. We define two reference planes $x = x_{\mathrm{I}}$ and $x = x_{\mathrm{II}}$ somewhere within the constant-potential regions on either side of the barrier, each in a range where the kinetic energy is positive,

$$\mathcal{E} > V(x_{\mathrm{I}}),\ V(x_{\mathrm{II}}) \tag{5•2–1}$$

In those two constant-potential regions—which may be arbitrarily narrow—the wave functions are superpositions of plane waves, which may always be written in the form

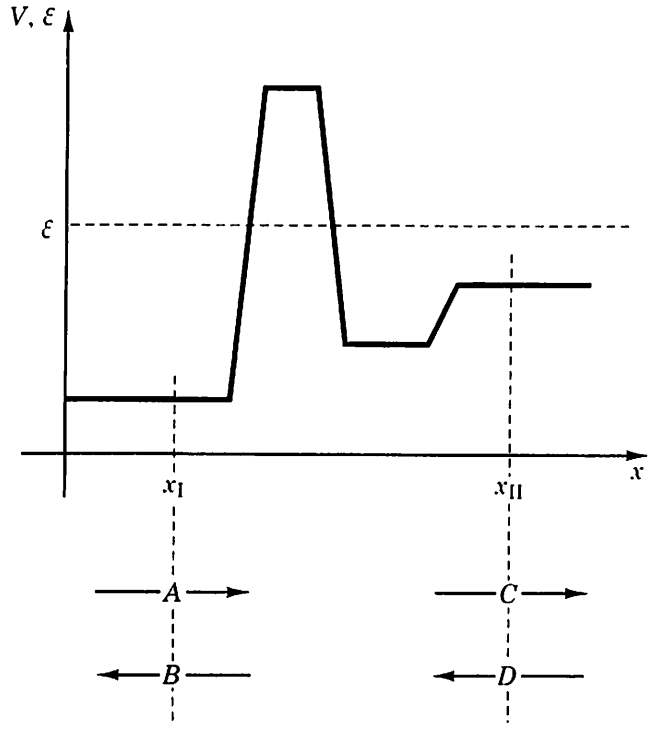

Figure 5•2–1. Scattering at an arbitrary barrier can be described by defining four complex wave amplitudes in two reference planes. We define the amplitudes in the two reference planes at x_I and x_{II} and assume that the total energy $\mathcal{E}$ exceeds the potential energy at least in the two reference planes.

$$\psi_I(x) = \frac{1}{\sqrt{K_I}}[A \cdot e^{iK_I(x-x_I)} + B \cdot e^{-iK_I(x-x_I)}], \tag{5•2–2a}$$

$$\psi_{II}(x) = \frac{1}{\sqrt{K_{II}}}[C \cdot e^{iK_{II}(x-x_{II})} + D \cdot e^{-iK_{II}(x-x_{II})}]. \tag{5•2–2b}$$

Here K_I and K_{II} are the *local* wave numbers at the two reference planes.[1] Compared to our treatment of the scattering at a simple step in section 1.4, we have split off amplitude factors of the form $1/\sqrt{K}$ from the wave amplitudes, along with phase factors that ensure that the complex amplitude coefficients contain whatever phases the waves have directly at their reference planes.

The reason for re-normalizing the amplitudes is the following. We are principally interested in the *current* densities of the four waves, and by splitting off the factors $1/\sqrt{K}$, we make these factors cancel out in the current density expressions, leading to the following simple expressions for the four partial probability current densities:

$$j_I^+ = +\frac{\hbar}{M} \cdot |A|^2, \quad j_{II}^+ = +\frac{\hbar}{M} \cdot |C|^2, \tag{5•2–3a,b}$$

$$j_I^- = -\frac{\hbar}{M} \cdot |B|^2, \quad j_{II}^- = -\frac{\hbar}{M} \cdot |D|^2. \tag{5•2–3c,d}$$

[1] Throughout this chapter, we use uppercase K to designate *local* wave numbers, reserving the use of lowercase k for the wave numbers of extended plane waves and for the so-called Bloch wave numbers for periodic potentials (defined in section 5.4).

These represent the current contributions of the four partial waves.

Of the four wave amplitudes, the amplitudes A and D of the two waves traveling *toward* the barrier may be viewed as the *physically* independent variables. The B-wave may then be considered a linear superposition of the reflected portion of the A-wave and the transmitted portion of the D-wave. This dependence may be expressed by writing

$$B = \rho_+ A + \tau_- D, \tag{5•2–4a}$$

where ρ_+ is an *amplitude* reflection coefficient for waves incident in the $+x$ direction and τ_- is an *amplitude* transmission coefficient for waves incident in the $-x$ direction. These *amplitude* coefficients should not be confused with the particle reflection and transmission coefficients introduced in section 1.5—see (1•5–11,12). Similarly,

$$C = \tau_+ A + \rho_- D, \tag{5•2–4b}$$

with obvious meanings for τ_+ and ρ_-. The four scattering coefficients are in general complex; their phase angles depend on the choice of the two reference planes.

Equations (5•2–4) may be lumped together into a single matrix equation

$$\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} \rho_+ & \tau_- \\ \tau_- & \rho_- \end{pmatrix} \begin{pmatrix} A \\ D \end{pmatrix} = \hat{S} \begin{pmatrix} A \\ D \end{pmatrix}, \tag{5•2–5}$$

where

$$\boxed{\hat{S} = \begin{pmatrix} \rho_+ & \tau_- \\ \tau_- & \rho_- \end{pmatrix}} \tag{5•2–6}$$

is the **scattering matrix**, often called the ***S*-matrix**. We have placed a caret ($\hat{}$) on top of S to indicate that $\hat{S}$ is not a numerical factor, but an operator, operating on the column matrix consisting of the amplitudes A and D.

The study of the S-matrix is a central problem in three-dimensional scattering theory. In simple *one-dimensional* problems such as ours, it is more useful to express the wave amplitudes on *one* side of the barrier in terms of the wave amplitudes on the *other* side: The central problem in one-dimensional scattering theory is the overall scattering by a *sequence* of several barriers. The wave amplitudes on the right-hand side of one barrier then also serve as the wave amplitudes on the left-hand side of the next barrier. By using a formalism that expresses the amplitudes on *one* side as functions of those on the *other*, we can work through the sequence of barriers one by one. It will turn out to be useful to work "backwards," by expressing the amplitudes in the left-hand reference plane I of Fig. 5•2–1 as linear functions of the amplitudes in the right-hand reference plane II, writing

$$A = P_{11} C + P_{12} D, \tag{5•2–7a}$$

$$B = P_{21}C + P_{22}D. \tag{5•2–7b}$$

These two equations may again be lumped together in the form of a matrix equation,

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \hat{P} \begin{pmatrix} C \\ D \end{pmatrix}, \tag{5•2–8}$$

where

$$\boxed{\hat{P} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix}} \tag{5•2-9}$$

is what we call the **propagation matrix** or, briefly, the **P-matrix**[2] of the barrier.

To appreciate this formalism, consider the combined scattering by two separate potential barriers with the propagation matrices $\hat{P}_1$ and $\hat{P}_2$, separated by a length L of field-free space (**Fig. 5•2–2**).

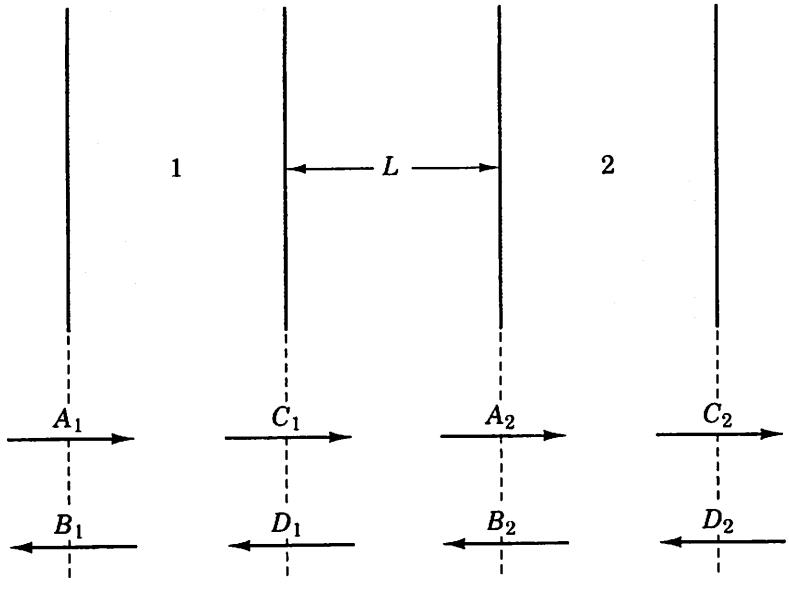

Figure 5•2–2. Combined scattering effect of a composite barrier that consists of two individual barriers separated by a distance L.

The vertical lines shown in the figure are the reference planes of the two barriers, with respect to which the wave amplitudes and the scattering coefficients are defined. The distance L is the distance between the two innermost reference planes. The problem is characterized by eight complex wave amplitudes at the four reference planes, A_1 through D_2.

[2] Various authors employ either $\hat{P}$ or its inverse $(P)^{-1}$ under various names, such as *transfer matrix*.

Our goal is to express the two leftmost wave amplitudes A_1 and B_1 as functions of the two rightmost ones, C_2 and D_2. For the amplitude relation across the two barriers, we have

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{P}_1 \begin{pmatrix} C_1 \\ D_1 \end{pmatrix} \text{ and } \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \hat{P}_2 \begin{pmatrix} C_2 \\ D_2 \end{pmatrix}. \tag{5•2–10a,b}$$

The relations between the wave amplitudes at the two ends of the field-free space section can be written as

$$\begin{pmatrix} C_1 \\ D_1 \end{pmatrix} = \hat{P}_\Delta \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \tag{5•2–11}$$

where $\hat{P}_\Delta$ is the **free-space propagation matrix**, which accounts for the phase shifts of the two waves in going from the entrance plane of barrier 2 back to the exit plane of barrier 1. It is left to the reader to show that

$$\hat{P}_\Delta = \begin{pmatrix} e^{-iK_\Delta L} & 0 \\ 0 & e^{+iK_\Delta L} \end{pmatrix}, \tag{5•2–12}$$

where K_Δ is the wave number in that space.

If we insert (5•2–10b) into the right-hand side of (5•2–11), and the resulting expression into the right-hand side of (5•2–10a), we obtain the desired expression for A_1 and B_1 in terms of C_2 and D_2, namely

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \hat{P} \begin{pmatrix} C_2 \\ D_2 \end{pmatrix}, \tag{5•2–13}$$

where

$$\hat{P} = \hat{P}_1 \hat{P}_\Delta \hat{P}_2 \tag{5•2–14}$$

is the overall propagation matrix of the combination, obtained by ordinary matrix multiplication of the individual matrices. Note that the sequence of the matrices is the same as that of the corresponding scattering sections in Fig. 5•2–2.

Once the overall propagation matrix has been obtained, the quantity of dominant interest is usually the overall **transmission probability** of the composite barrier, defined as the ratio of the transmitted current density to the incident current density, in the absence of any current incident from the outgoing side. Evidently,

$$T \equiv j_{\text{II}}^{+}/j_{\text{I}}^{+} = |C/A|^2 \quad \text{while} \quad D = 0. \tag{5•2–15}$$

Setting $D = 0$ in (5•2–7a) yields

$$\boxed{T = \frac{1}{|P_{11}|^2}.} \tag{5•2–16}$$

5.2.2 Relations between Matrix Coefficients

The matrix manipulations are greatly simplified by the fact that the four coefficients of each propagation matrix are not independent of each other. We show here that, if the kinetic energy is positive at both reference planes, as specified in (5•2–1), the coefficients must obey the relations

$$P_{22} = P_{11}^* \quad \text{and} \quad P_{21} = P_{12}^* \tag{5•2–17a,b}$$

and

$$\det \hat{P} \equiv P_{11}P_{22} - P_{12}P_{21} = 1. \tag{5•2–18}$$

The first two relations, (5•2–17a,b), are a consequence of **time reversal invariance**: If $\psi(x)$ is a solution of the time-independent Schroedinger equation, then its complex conjugate $\psi^*(x)$ must also be a solution. But in this second solution, the wave propagation directions are reversed: Under the condition (5•2–1), all four waves are propagating waves, and the B^*-wave and the C^*-wave have become the incident waves, while the A^*- and D^*-waves have become the outgoing scattered waves. This means that (5•2–8) must remain valid, with unchanged matrix coefficients, if we make the substitutions

$$A \to B^*,\ B \to A^*,\ C \to D^*,\ D \to C^*. \tag{5•2–19}$$

Written out, (5•2–8) then becomes

$$\begin{pmatrix} B^* \\ A^* \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} D^* \\ C^* \end{pmatrix}. \tag{5•2–20}$$

By taking the complex conjugate and re-arranging rows and columns, this is converted to

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} P_{22}^* & P_{21}^* \\ P_{12}^* & P_{11}^* \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}. \tag{5•2–21}$$

The matrix on the right-hand side must evidently be the same as the original matrix $\hat{P}$. Comparison of the matrix coefficients then leads to (5•2–17a,b).

A second requirement is **current conservation**: The amplitudes of the incident, reflected, and transmitted waves must be such that the net probability current density in reference plane I equals that in reference plane II. Because of the current relations (5•2–3), this implies that

$$A^*A - B^*B = C^*C - D^*D. \tag{5•2–22}$$

This condition must be satisfied for any combination of incoming or outgoing waves, including specifically the case of no incoming wave from the right, that is, $D = 0$. From (5•2–7a,b), we obtain, for $D = 0$,

$$A^*A - B^*B = (P_{11}^*P_{11} - P_{21}^*P_{21})C^*C. \tag{5•2–23}$$

Comparing this with (5•2–22) for $D = 0$ yields the condition

$$P_{11}^* P_{11} - P_{21}^* P_{21} = 1, \tag{5•2-24}$$

which, because of (5•2–17a,b), is equivalent to the determinantal relation (5•2–18).

The conditions (5•2–17) and (5•2–18) are powerful conditions in the analysis of scattering properties. In applying them, it is important, however, to recall that they were derived under the assumption that the kinetic energy at *both* reference planes is positive. In the analysis of scattering by barriers, it is often necessary to break up the overall propagation matrix of a barrier into products of several factor matrices representing successive portions of the overall barrier, some of which may involve reference planes where the kinetic energy is negative. In those cases, the relations (5•2–17) and (5•2–18) will not, in general, be satisfied for the factor matrices. We will discuss such cases later.

5.3 SCATTERING BY A SQUARE BARRIER AND A SQUARE WELL

5.3.1 The Propagation Matrix

To illustrate the propagation matrix formalism, we apply it here to the scattering properties of a square barrier of height V_0 and width L (**Fig. 5•3–1**) and a square well of depth $-V_0$. In both cases, the scattering can be represented as scattering by two steps separated by a free-space section. In the case of a barrier, we assume initially that the energy of the incident particle exceeds the barrier height, $\mathcal{E} > V_0$; we will drop this assumption later.

In section 1.4, we calculated the amplitude ratios B/A and C/A for scattering at a simple upward potential step (see 1•4–20a,b) for the specific case of no returning wave ($D = 0$). However, we wrote the individual plane waves in the simple form $\psi \sim \exp(\pm ikx)$, without splitting off the re-normalizing factors of the form $\sqrt{K}$, as in (5•2–2a,b). In terms of the "old" amplitudes of section 1.4, our "new" amplitudes are

$$A = \sqrt{k}A_{\text{old}}, \quad B = \sqrt{k}B_{\text{old}}, \quad \text{and} \quad C = \sqrt{k'}C_{\text{old}}. \tag{5•3–1}$$

With the help of these conversions, we obtain, from (1•4–20a,b),

$$P_{11} = \frac{A}{C} = \sqrt{\frac{k}{k'}}\left(\frac{A}{C}\right)_{\text{old}} = \frac{k + k'}{2\sqrt{kk'}} \tag{5•3–2a}$$

and

$$P_{21} = \frac{B}{C} = \sqrt{\frac{k}{k'}}\left(\frac{B}{C}\right)_{\text{old}} = \frac{k - k'}{2\sqrt{kk'}}. \tag{5•3–2b}$$

Here, k is the wave number on the downside of the step, and k' is the wave number on the upside. The remaining two matrix coefficients follow from (5•3–2a,b) via (5•2–17a,b). If we write K and K' instead of k and k', we obtain

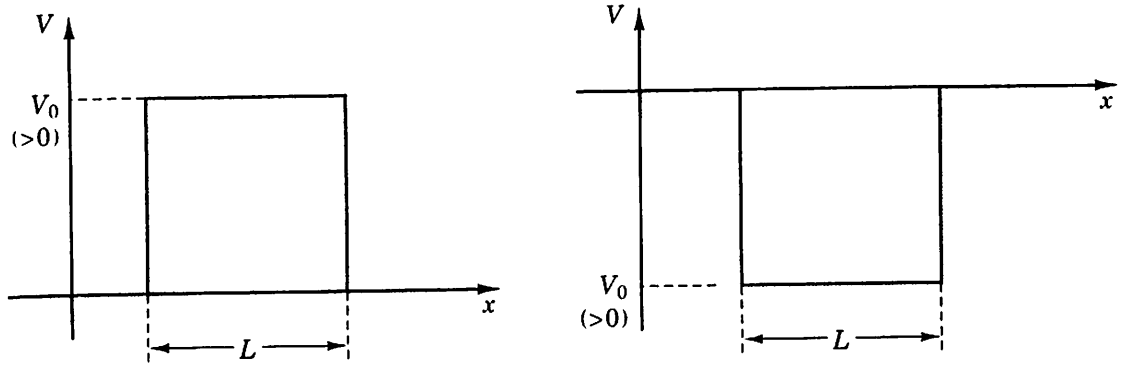

Figure 5•3–1. Square barrier ($V_0 > 0$) (left) and square well ($V_0 < 0$) (right).

the overall propagation matrix for the *upward* step:

$$\hat{P}_{\uparrow} = \frac{1}{2\sqrt{KK'}} \begin{pmatrix} K + K' & K - K' \\ K - K' & K + K' \end{pmatrix}. \tag{5•3–3a}$$

The propagation matrix for a *downward* step follows by simply interchanging K and K':

$$\hat{P}_{\downarrow} = \frac{1}{2\sqrt{KK'}} \begin{pmatrix} K' + K & K' - K \\ K' - K & K' + K \end{pmatrix}. \tag{5•3–3b}$$

If we insert (5•3–3) and the free-space matrix (5•2–12) into the matrix product (5•2–14) for the overall propagation matrix, and replace k_Δ by K', we obtain

$$\hat{P} = \frac{1}{4KK'} \begin{pmatrix} K + K' & K - K' \\ K - K' & K + K' \end{pmatrix} \begin{pmatrix} e^{-iK'L} & 0 \\ 0 & e^{+iK'L} \end{pmatrix} \begin{pmatrix} K' + K & K' - K \\ K' - K & K' + K \end{pmatrix}. \tag{5•3–4}$$

Execution of the matrix multiplications—left as an exercise to the reader—leads to

$$P_{11} = P_{22}^* = \cos K'L - i\frac{K^2 + K'^2}{2KK'} \sin K'L, \tag{5•3–5}$$

$$P_{12} = P_{21}^* = +i\frac{K^2 - K'^2}{2KK'} \sin K'L. \tag{5•3–6}$$

5.3.2 Transmission Resonances

The transmission probability for $\mathcal{E} > V_0$ follows from (5•3–5) by insertion into (5•2–16). One finds, after some manipulation, that

$$T = \frac{1}{|P_{11}|^2} = \left[1 + \left(\frac{K^2 - K'^2}{2KK'}\right)^2 \sin^2 K'L\right]^{-1}. \tag{5•3–7}$$

The two wave numbers K and K' outside and inside the barrier are related to the energy via

$$\mathcal{E} = \frac{\hbar^2 K^2}{2M} = \frac{\hbar^2 K'^2}{2M} + V_0. \tag{5•3–8}$$

If we eliminate the wave number K *outside* the barrier via (5•3–8), we can re-write (5•3–7) in a simpler form, as a function of the wave number K' inside the barrier only,

$$T = \left[1 + \frac{1}{4}\frac{\beta^2}{\beta + (K'L)^2}\frac{\sin^2 K'L}{(K'L)^2}\right]^{-1}, \tag{5•3–9}$$

where we have defined a dimensionless **barrier parameter**

$$\beta = \frac{2M}{\hbar^2} V_0 L^2, \tag{5•3–10}$$

to characterize the "strength" of the barrier or the well.

Viewed as a function of $K'L$, the transmission probability oscillates (**Fig. 5•3–2**) between full transmission, where

$$T_{\max} = 1, \tag{5•3–11}$$

and a minimum transmission curve shown as a dotted line in the figure, and given by

$$T_{\min} = \left[1 + \frac{1}{4}\frac{\beta^2}{\beta + (K'L)^2}\frac{1}{(K'L)^2}\right]^{-1} = 1 - \frac{\beta^2}{[2(K'L)^2 + \beta]^2}. \tag{5•3–12}$$

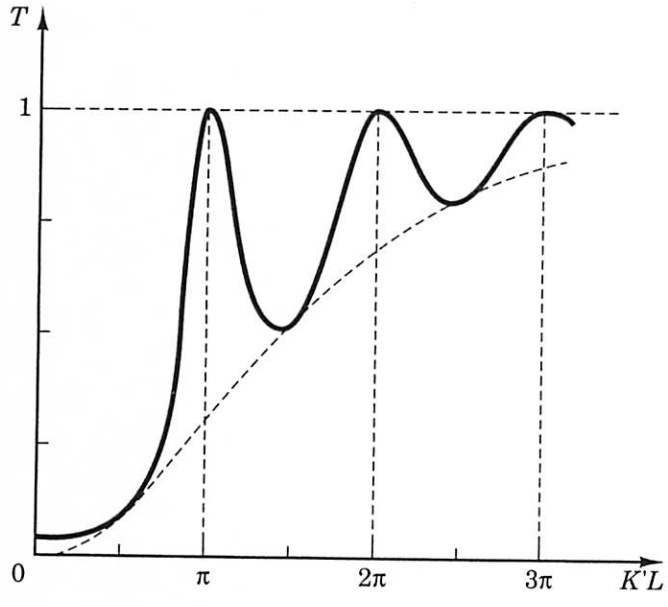

Figure 5•3–2. Transmission resonances for a rectangular barrier, for $\beta = 100$.

Written as a function of the energy $\mathcal{E}$ rather than of $K'L$, this minimum curve is simply

$$T_{\min} = 1 - \frac{V_0^2}{(2\mathcal{E} - V_0)^2}. \tag{5•3–13}$$

Full transmission ($T = 1$) is reached for those energies for which

$$K'L = n\pi, \quad \text{with} \quad n = 1, 2, 3, \ldots. \tag{5•3–14a}$$

The minimum-transmission curve $T_{\min}$ is reached for

$$K'L = n\pi, \quad \text{with} \quad n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots. \tag{5•3–14b}$$

The occurrence of the transmission resonances is the result of an interference between the wave reflected by the upward step at $x = 0$ and that reflected by the downward step at $x = L$. We saw in section 1.4 that the amplitude reflection coefficients for the two steps are equal in magnitude, but opposite in sign. This means that the two reflected waves are equally strong, but they have a relative phase shift of π, measured in their respective planes of reflection. To this is added the additional phase shift $2K'L$ that the wave reflected at $x = L$ undergoes on its round trip from $x = 0$ to $x = L$ and back. Under the resonance condition (5•3–14a), this round-trip phase shift is a multiple of 2π. The total phase shift between the two reflected waves is therefore an odd multiple of π, and because the two reflected waves are equally strong, this leads to complete mutual annihilation of the two reflected waves. By contrast, under the antiresonance condition (5•3–14b), the two reflected waves enhance each other.

Exercise: Compare the antiresonance transmission coefficient $T_{\min}$ of (5•3–12) with the value for a simple step for the same pair K, K'.

The details of the transmission resonances depend on the magnitude of the barrier parameter β defined in (5•3–10). For electrons scattered by a barrier 1 eV high and 1 nm wide, we have $\beta = 26.25$. The curve in Fig. 5•3–2 is for $\beta = 100$. The larger the value of β, the more rapid will be the oscillations and the sharper will be the resonances.

Although we stated our calculations for the case of a potential *barrier* (V_0, $\beta > 0$), they are equally valid for a square potential *well* (V_0, $\beta < 0$). The case of a well represents a simple one-dimensional model of the scattering of a particle wave by the potential well of an atom or an atomic nucleus. Note that for scattering by a well, the condition $\mathcal{E} > 0$ outside the well implies the condition

$$(K'L)^2 > -\beta > 0 \tag{5•3–15}$$

on the wave number inside the well. Very sharp transmission resonances occur when $-\beta \gg 1$ and when the leftmost inequality in (5•3–15) is satisfied only by a small excess,[3] making the quantity $\beta + (K'L)^2$ in the denominator inside the expression (5•3–9) a small number.

5.3.3 Tunneling through the Barrier for $\mathcal{E} < V_0$

Our treatment of wave propagation across a square barrier for $\mathcal{E} > V_0$ is readily extended to the case of tunneling *through* that barrier when the incident energy is less than the height of the barrier ($\mathcal{E} < V_0$). We discussed this case already briefly in section 1.4, using a brute-force fitting of five wave functions at the two steps. It is instructive to consider the problem again, this time in the framework of the propagation matrix formalism.

We may continue to treat each of the two steps as a separate barrier with a propagation matrix of its own, just as for $\mathcal{E} > V_0$, but now one of the two reference planes for each barrier is in a region of negative kinetic energy, in contrast to the assumptions we made at the beginning of the chapter. Also, the drift space separating the two barriers has a negative kinetic energy throughout.

When $\mathcal{E} < V_0$, the solution of the Schroedinger equation at the reference planes may still be written in the form (5•2–2a,b), but now the wave number K' becomes imaginary,

$$K' \rightarrow +i\kappa, \tag{5•3–16}$$

where

$$\kappa = \left[\frac{2M}{\hbar^2}(V_0 - \mathcal{E})\right]^{1/2}. \tag{5•3–17}$$

As we pointed out in section 1.4, all we have to do to adapt our earlier wave function for $\mathcal{E} > V_0$ to the case $\mathcal{E} < V_0$ is to make the substitution (5•3–16) everywhere. We recall that this converts any wave propagating to the right into a wave evanescent to the right, i.e.,

$$\exp(+iK'x) \rightarrow \exp(-\kappa x), \tag{5•3–18}$$

automatically yielding the correct boundary conditions at infinity, if the region of negative kinetic energy extends that far: The requirement that there be no wave coming in from $+\infty$ is transformed into the requirement that the wave vanish at infinity.

However, with re-normalized plane wave amplitudes as in (5•2–2a,b), making the substitution (5•3–16) introduces a nuisance factor $\sqrt{i}$ into the

[3] The text by Merzbacher, quoted in appendix G, contains an excellent discussion of scattering by a square well, including the topic of resonances in the transmission delay.

denominators. To avoid cluttering up the subsequent math, we absorb this factor into the complex amplitudes A through D and write the substituted waves in the form

$$\psi_{\mathrm{I}}(x) = \frac{1}{\sqrt{\kappa_{\mathrm{I}}}}[A \cdot e^{-\kappa_{\mathrm{I}}(x-x_{\mathrm{I}})} + B \cdot e^{+\kappa_{\mathrm{I}}(x-x_{\mathrm{I}})}], \tag{5•3–19a}$$

$$\psi_{\mathrm{II}}(x) = \frac{1}{\sqrt{\kappa_{\mathrm{II}}}}[C \cdot e^{-\kappa_{\mathrm{II}}(x-x_{\mathrm{II}})} + D \cdot e^{+\kappa_{\mathrm{II}}(x-x_{\mathrm{II}})}]. \tag{5•3–19b}$$

Consider now the propagation matrix at the upward step on the left-hand side of the barrier shown in figures 1•4–3 or 5•3–1, assuming that $0 < \mathcal{E} < V_0$. If we had not absorbed a factor $\sqrt{i}$ into the wave amplitudes C and D, we could obtain the propagation matrix by simply making the substitution (5•3–16) in the expression (5•3–3a) for the matrix for $\mathcal{E} > V_0$. If we absorb the factor $\sqrt{i}$ in the denominator of the matrix coefficients into the right-hand amplitudes, the resulting matrix becomes

$$\hat{P}_{\uparrow} = \frac{1}{2\sqrt{K\kappa}}\begin{pmatrix} K + i\kappa & K - i\kappa \\ K - i\kappa & K + i\kappa \end{pmatrix}. \tag{5•3–20a}$$

The propagation matrix for the downward step at the end of the barrier requires more care. Now, a factor $\sqrt{i}$ has been absorbed into the amplitudes A and B at the *left* reference plane. This calls for an *additional* factor $\sqrt{i}$ in the denominator of the matrix coefficients, leading to

$$\hat{P}_{\downarrow} = \frac{1}{2i\sqrt{K\kappa}}\begin{pmatrix} i\kappa + K & i\kappa - K \\ i\kappa - K & i\kappa + K \end{pmatrix}. \tag{5•3–20b}$$

Finally, the free-space propagation matrix (5•2–12) evidently becomes

$$\hat{P}_{\Delta} = \begin{pmatrix} e^{+\kappa L} & 0 \\ 0 & e^{-\kappa L} \end{pmatrix}. \tag{5•3–21}$$

When the three propagation matrices are multiplied together, the $\sqrt{i}$ corrections to $\hat{P}_{\uparrow}$ and $\hat{P}_{\downarrow}$ cancel out, and the final result is exactly the same as if we had made the substitution (5•3–16) everywhere in (5•3–4). We may therefore obtain the transmission probability T by simply making the substitution (5•3–16) in the final result (5•3–9) of the calculation for $\mathcal{E} > V_0$:

$$\begin{aligned} T &= \left[1 + \frac{1}{4}\frac{\beta^2}{\beta - (\kappa L)^2} \cdot \frac{\sinh^2 \kappa L}{(\kappa L)^2}\right]^{-1} \\ &= \left[1 + \frac{V_0^2}{4\mathcal{E} \cdot (V_0 - \mathcal{E})} \cdot \sinh^2 \kappa L\right]^{-1}. \end{aligned} \tag{5•3–22}$$

Note the replacement of the trigonometric sine by the hyperbolic sine, from whose properties it is evident that the tunneling probability exhibits no reso-

nances and that it decreases rapidly as the particle energy drops below the top of the barrier.

The result (5•3–22) becomes particularly simple when the barrier becomes relatively opaque, when $\kappa L \gg 1$. In that case,

$$T \cong \frac{16\mathcal{E} \cdot (V_0 - \mathcal{E})}{V_0^2} \cdot e^{-2\kappa L}, \tag{5•3–23}$$

the same as (1•4–32), except that there we called the barrier width w rather than L.

5.3.4 The δ-Function Limit

The propagation matrix becomes particularly simple in the limit of a δ-function well or a δ-function barrier. We go to the limits

$$L \to 0,\ V_0 \to \pm\infty,\ LV_0 = S = \text{const.} \tag{5•3–24}$$

With these,

$$K',\ \kappa \to \infty;\quad K'L,\ \kappa L \to 0, \tag{5•3–25a,b}$$

$$K'^2L,\ \kappa^2 L \to 2M|S|/\hbar^2 = 2\kappa_0, \tag{5•3–26}$$

where we have introduced the convenient abbreviation

$$\kappa_0 = MS/\hbar^2. \tag{5•3–27}$$

If the limits (5•3–25) through (5•3–26) are inserted into (5•3–5) through (5•3–7), we obtain, for the δ-function well,

$$P_{11} = 1 - i\kappa_0/K, \qquad P_{12} = -i\kappa_0/K, \tag{5•3–28a,b}$$

and for the δ-function barrier,

$$P_{11} = 1 + i\kappa_0/K, \qquad P_{12} = i\kappa_0/K. \tag{5•3–29a,b}$$

We shall use these limits in the next section.

5.3.5 Relations between Propagation Matrix Coefficients for Negative Kinetic Energies

Inspection of the propagation matrices (5•3–20a,b) and (5•3–21) for $\mathcal{E} < V_0$ shows that the coefficients of these matrices do not obey the relations (5•2–17a,b) and (5•2–18) derived earlier for the case where $\mathcal{E} > V_0$ in both reference planes. The reason for this discrepancy is that both the time reversal argument and the current continuity argument in section 5.2 take on different forms when the waves are evanescent rather than propagating at one or both of the two reference planes. Because of the general usefulness of the relations between the propagation matrix coefficients, we derive here the analogs of the

relations (5•2–17a,b) and (5•2–18) for the other possible energetic relations.

We must consider three cases:

(a) "Upward barrier," with $V(x_{\mathrm{I}}) < \mathcal{E} < V(x_{\mathrm{II}})$.
(b) "Downward barrier," with $V(x_{\mathrm{I}}) > \mathcal{E} > V(x_{\mathrm{II}})$, the inverse of case (a).
(c) $\mathcal{E} < V$ at both reference planes.

We treat only case (a) in detail; the other two cases are left to the reader, and we only state the results at the end.

Time Reversal

When taking the complex conjugate of a wave function, right-evanescent and left-evanescent waves are not interchanged, in contrast to right- and left-propagating waves. In case (a), the wave functions in the two reference planes will be of the forms (5•2–2a) to the left and (5•3–19b) to the right. The time-reversed wave function is then no longer obtained by the substitutions (5•2–19), but by

$$A \to B^*,\ B \to A^*,\ C \to C^*,\ D \to D^*. \tag{5•3–30}$$

In terms of the propagation matrix coefficients, this implies that

$$P_{22} = P_{12}^* \quad \text{and} \quad P_{21} = P_{11}^*, \tag{5•3–31a,b}$$

instead of (5•2–17a,b).

Current Continuity

For wave functions with imaginary wave numbers, the probability current density is no longer given by the forms (5•2–3). Instead,

$$j_{\mathrm{I}} = -\frac{i\hbar}{M}(A^*B - B^*A) \quad \text{or} \quad j_{\mathrm{II}} = -\frac{i\hbar}{M}(C^*D - D^*C), \tag{5•3–32}$$

where the second relation is applicable to case (a). Current continuity then demands that

$$A^*A - B^*B = -i \cdot (C^*D - CD^*). \tag{5•3–33}$$

We insert, on the left-hand side, the basic relations (5•2–7) that express A and B in terms of C and D, and we request that the resulting expression hold for all combinations of C and D. This means that both the C^*C terms and the D^*D terms on the left-hand side must vanish and that the C^*D terms on the left-hand side must add up to $-i$:

$$P_{11}^*P_{11} - P_{21}^*P_{21} = P_{12}^*P_{12} - P_{22}^*P_{22} = 0, \tag{5•3–34}$$

$$P_{11}^*P_{12} - P_{21}^*P_{22} = -i. \tag{5•3–35}$$

If we now use the earlier result (5•3–31a,b), we see that (5•3–34) is indeed satisfied and that (5•3–35) may be written as

$$\det \hat{P} = +i. \tag{5•3–36}$$

It is left to the reader to show that the following relationships hold in the remaining two cases:

CASE (b):

$$P_{22} = P_{21}^* \quad \text{and} \quad P_{12} = P_{11}^*, \tag{5•3–37a,b}$$

$$\det \hat{P} = -i. \tag{5•3–38}$$

CASE (c):

All coefficients are real, and

$$\det \hat{P} = 1. \tag{5•3–39}$$

Inspection of the individual propagation matrices for tunneling through a barrier shows that these matrices do indeed satisfy the conditions derived here.

◆ PROBLEMS TO SECTION 5.3

#5•3-1: Zero-Reflection Conditions at a Double-Step Barrier

Devise a quantum-mechanical "antireflection coating"; that is, determine the proper width L and height V_1 of an intermediate potential step to suppress the reflection of a wave of a specific incident energy at a barrier of height $V_2 < \mathcal{E}$ (**Fig. 5•3–3**).

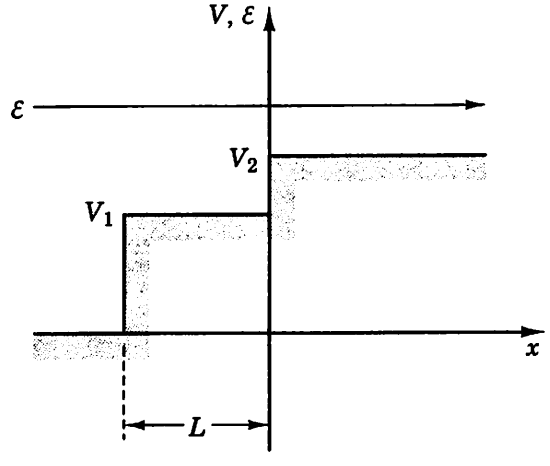

Figure 5•3–3. Zero-reflection barrier.

#5•3-2: Pair of δ-Functions

Calculate the propagation matrix for two δ-function barriers of equal strength S, separated by a distance L. Plot and discuss the transmission probability T as a function of particle energy up to 10 eV, (assuming electrons), for the specific numerical values $S = 10^{-7}$ eV · cm, $L = 2 \times 10^{-8}$ cm.

#5•3–3: Sharpness of Transmission Resonances for Deep Wells

Give a detailed discussion of the sharpness of the transmission resonances for scattering by a deep well, assuming that

$$-V_0 \gg 4\mathcal{E}. \tag{5•3–40}$$

Specifically, derive and discuss a suitable approximation for the energetic width $\Delta\mathcal{E}$ of the resonance as a function of V_0 and L under the condition (5•3–40), where $\Delta\mathcal{E}$ is defined as the width of that energy interval over which $T \geq 1/2$, the so-called full width at half-magnitude, commonly referred to by the abbreviation FWHM.

#5•3–4: Density Resonances

Investigate the probability density present in the range of a barrier, in the energetic vicinity of the transmission resonances. Express the probability density $\rho(x)$ relative to the probability density in the incident beam, $|A|^2/K$, by setting $A = \sqrt{K}$. Plot the result graphically for the lowest two transmission resonances of a barrier with $\beta = 100$.

5.4 ENERGY BANDS IN PERIODIC POTENTIALS

An important type of wave propagation is that of electrons through the periodic potential in a crystal. We apply here the propagation matrix formalism to study this problem, for the idealized case of a one-dimensional "crystal." While strictly one-dimensional crystals do not occur in nature, a solution of this simplified problem exhibits many important features of real, three-dimensional crystals. In particular, it shows the existence of allowed and forbidden energy bands.

We consider the case of a one-dimensional periodic potential $V(x)$, with period a (**Fig. 5•4–1**). We treat each cell as a potential barrier that is characterized by the propagation matrix

$$\hat{P} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix}. \tag{5•4–1}$$

As reference planes with respect to which the various wave amplitudes and matrix coefficients are defined, we use the boundaries of the cell. We single out one particular cell and denote the complex wave amplitudes at its left boundary with A and B and those at its right boundary with C and D, as in (5•2–8):

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \hat{P} \begin{pmatrix} C \\ D \end{pmatrix}. \tag{5•4–2}$$

However, we are not dealing, with a *single* cell, but with a periodic arrangement of an infinite number of cells. Because of the translational periodicity of the potential, all bulk-like physical properties of the crystal must be periodic, too. In particular, the probability density and the probability current density

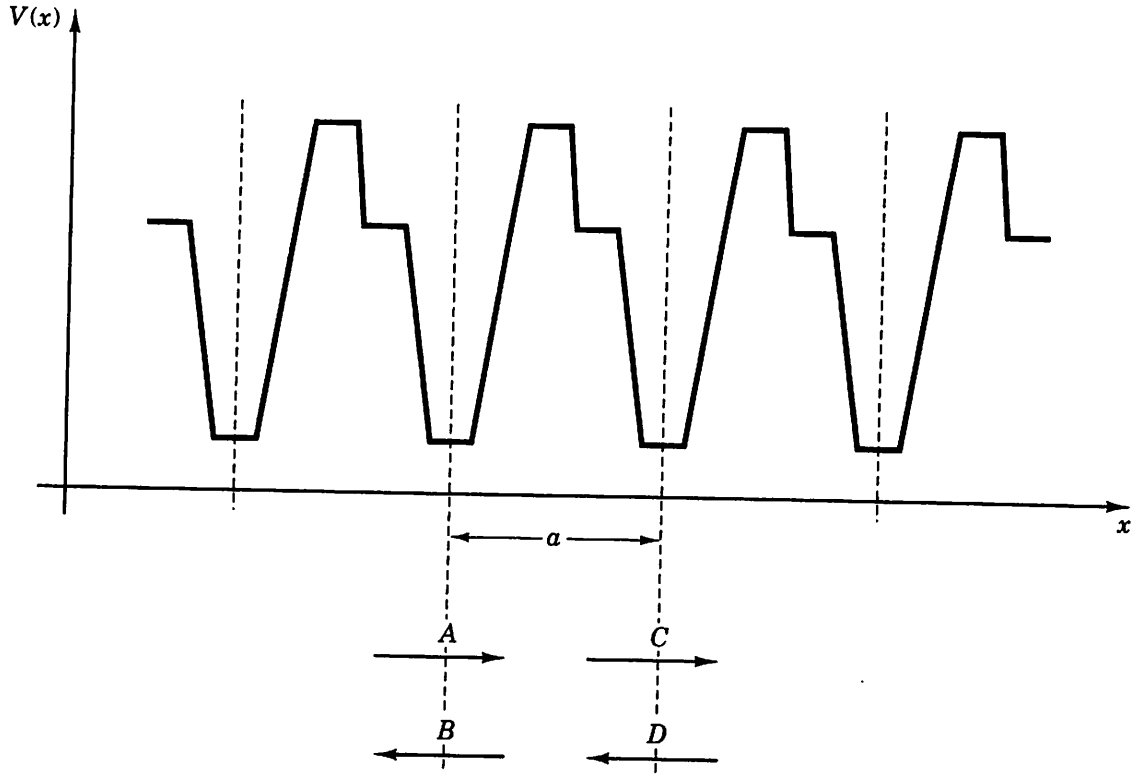

Figure 5•4–1. One-dimensional periodic potential. Each cell is represented by a potential barrier with a propagation matrix $\hat{P}$; the cell boundaries serve as reference planes.

must be periodic:

$$\psi^*(x)\,\psi(x) = \text{periodic with period } a, \tag{5•4–3a}$$

$$\text{Im}\left(\psi^* \frac{d\psi}{dx}\right) = \text{periodic with period } a. \tag{5•4–3b}$$

From (5•4–3a), it follows that $\psi(x)$ must be of the form

$$\psi(x) = u(x)\exp[i\alpha(x)], \tag{5•4–4}$$

where $u(x)$ is periodic and $\alpha(x)$ is a real function that can always be chosen in such a way that it is *not* periodic, because any periodic part could be lumped into $u(x)$. When (5•4–4) is inserted into (5•4–3b), we conclude that

$$\text{Im}\left(u^2 + i|u|^2 \frac{d\alpha}{dx}\right) = \text{periodic with period } a. \tag{5•4–5}$$

Because $u(x)$ is periodic, the first term in the parentheses is certainly periodic, and (5•4–5) reduces to

$$\frac{d\alpha}{dx} = \text{periodic with period } a. \tag{5•4–6}$$

But the only way a non-periodic function $\alpha(x)$ can have a "periodic" derivative is if the derivative is simply a constant, which we call k. This means that

$$\alpha(x) = kx. \tag{5•4–7}$$

We have neglected any integration constant C, because a term e^{iC} can always be incorporated into $u(x)$. Thus, we conclude that $\psi(x)$ must be of the form

$$\boxed{\psi(x) = u(x) \cdot e^{ikx}.} \tag{5•4–8}$$

From this, it follows that

$$\boxed{\psi(x + a) = \psi(x) \cdot e^{ika}.} \tag{5•4–9}$$

Conversely, any function $\psi(x)$ that satisfies (5•4–9) for all x can always be written in the form (5•4–8). The two equivalent forms (5•4–8) and (5•4–9) constitute the one-dimensional form of **Bloch's theorem**, the most fundamental theorem of the electron dynamics in crystals. The quantity k is called the **Bloch wave number**. We shall extend Bloch's theorem to three dimensions in chapter 17.

Applied to the wave amplitudes A through D, Bloch's theorem implies that

$$C = Ae^{ika}, D = Be^{ika}, \tag{5•4–10}$$

or

$$\begin{pmatrix} A \\ B \end{pmatrix} = e^{-ika} \begin{pmatrix} C \\ D \end{pmatrix}. \tag{5•4–11}$$

If this is inserted into (5•4–2), we obtain the condition

$$\hat{P} \begin{pmatrix} C \\ D \end{pmatrix} = e^{-ika} \begin{pmatrix} C \\ D \end{pmatrix}, \tag{5•4–12}$$

which may be re-written in the form

$$\begin{pmatrix} P_{11} - e^{-ika} & P_{12} \\ P_{21} & P_{22} - e^{-ika} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = 0. \tag{5•4–13}$$

This is a set of two linear homogeneous equations for the two unknowns C and D. Such a set has a non-trivial solution only if its determinant vanishes:

$$\begin{vmatrix} P_{11} - e^{-ika} & P_{12} \\ P_{21} & P_{22} - e^{-ika} \end{vmatrix} = (P_{11} - e^{-ika})(P_{22} - e^{-ika}) - P_{12}P_{21} = 0. \tag{5•4–14}$$

With the help of the relations (5•2–17) and (5•2–18) between the propagation matrix coefficients, this may be re-arranged to read

$$e^{-2ika} - 2Re(P_{11})e^{-ika} = -1. \tag{5•4–15}$$

If we take the real and imaginary parts of this and simplify the results using elementary trigonometric identities, we obtain the two relations

$$2\cos ka \cdot [\cos ka - \mathrm{Re}(P_{11})] = 0 \tag{5•4–16a}$$

and

$$2\sin ka \cdot [\cos ka - \mathrm{Re}(P_{11})] = 0, \tag{5•4–16b}$$

both of which must be satisfied. Evidently, this requires that

$$\cos ka = \mathrm{Re}(P_{11}). \tag{5•4–17}$$

However, this condition has a solution with a real value of k only if

$$\boxed{|\mathrm{Re}(P_{11})| \leq 1.} \tag{5•4–18}$$

If one now plots $\mathrm{Re}(P_{11})$ as a function of energy, one invariably finds that there are energy bands of finite width, alternating between **allowed bands**, where (5•4–18) is satisfied, and **forbidden bands**, where it is not.

In every energy range where (5•4–18) is satisfied, there exist two solutions of the Schroedinger equation of the required Bloch wave form (5•4–8), with two real values of k differing from each other only in sign.

In energy ranges where (5•4–18) is not satisfied, k is imaginary. The solutions of the Schroedinger equation then do not satisfy Bloch's theorem, and therefore, they cannot correspond to legitimate bulk states actually occurring inside a crystal.[4]

We illustrate this formation of energy bands here for the simplest of all periodic potentials, a periodic array of positive δ-functions with the spacing a (**Fig. 5•4–2**), introduced by Kronig and Penney in the early days of quantum mechanics to demonstrate some of the quantum-mechanical consequences of a periodic potential.

We showed in (5•3–29b) that the coefficient P_{11} of a δ-function is of the form

$$P_{11} = 1 + i\kappa_0/K, \tag{5•4–19}$$

where κ_0 is given by (5•3–27). However, the coefficient P_{11} calculated in section 5.3 corresponded to a set of reference planes that coincided with each other and with the δ-function itself. For our purposes, we must use reference planes

[4] Under certain circumstances, such solutions may correspond to so-called **surface states** or to other effects associated with an imperfect crystal periodicity.

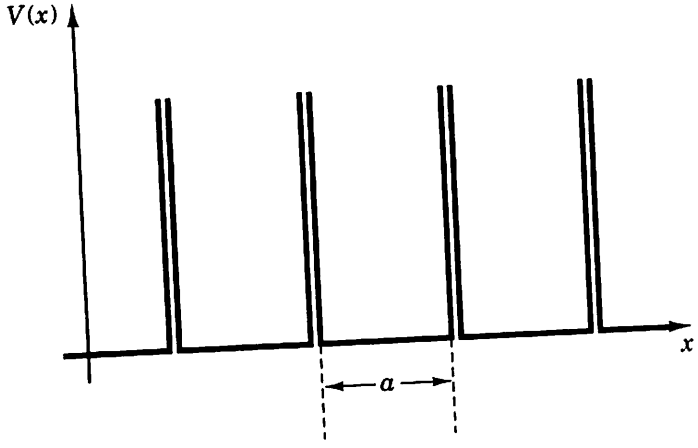

Figure 5•4–2. The Kronig-Penney potential: A periodic potential built up from a periodic array of δ-function barriers.

separated by the distance a. This adds a phase factor e^{-iKa} to the coefficient P_{11}, and we obtain

$$P_{11} = (1 + i\kappa_0/K)e^{-iKa}. \tag{5•4–20}$$

The real part of this may be written

$$\mathrm{Re}(P_{11}) = \cos Ka + P \cdot \frac{\sin Ka}{Ka}, \tag{5•4–21}$$

where we have introduced the parameter

$$P = \kappa_0 a \tag{5•4–22}$$

as a dimensionless measure of the strength of the periodic potential.

With (5•4–21), the condition (5•4–18) may be written

$$-1 \leq \cos Ka + P \cdot \frac{\sin Ka}{Ka} \leq +1. \tag{5•4–23}$$

This condition is illustrated in **Fig. 5•4–3,** where we have plotted the right-hand side of (5•4–21) as a function of Ka for $P = 5$. Only the positive-K branch is shown; the negative-K branch is its mirror image.

It is evident that the curve alternates between Ka-regions where (5•4–23) is satisfied and regions where it is not. One readily sees that the upper edges of the allowed bands (and the lower edges of the forbidden ones) occur at the values $Ka = n\pi$, where n is an integer. At those points, the cosine terms in (5•4–21) and (5•4–23) equal ± 1, with zero slope, while the sine term equals zero, with a sign of the slope equal to the sign of the cosine term. Thus, for Ka-values just below the multiples of π, the condition (5•4–23) is satisfied, while for values just above them, it is not. It is also readily seen that the widths of the forbidden bands decrease with increasing Ka, due to the decrease in the sine term, which is the term that is responsible for the formation of the forbidden bands.

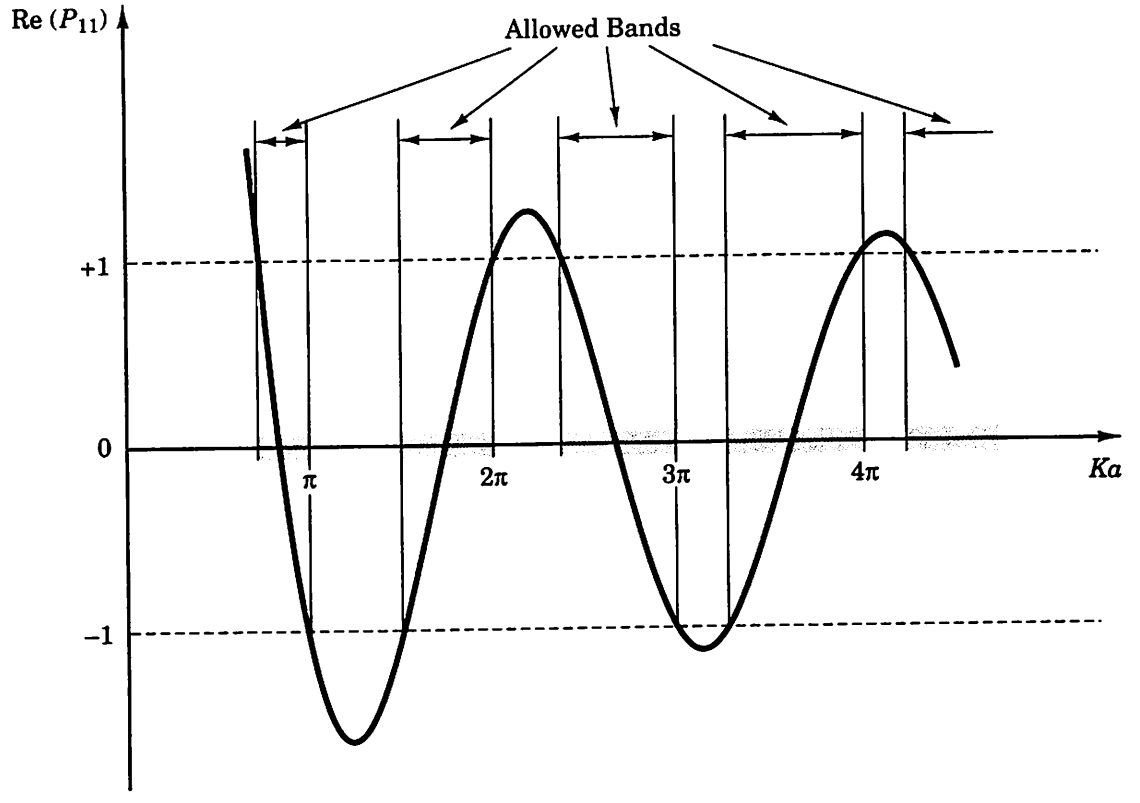

Figure 5•4–3. The condition $|\mathrm{Re}(P_{11})| \leq 1$ for a δ-function potential with a dimensionless barrier strength parameter $P = 5$.

5.5 BOUND STATES AS A SCATTERING PROBLEM

5.5.1 The Propagation Matrix for a Bound State

Although we developed the propagation matrix formalism for the purpose of treating the scattering of waves coming in from infinity, the formalism remains applicable—and surprisingly useful—for the determination of the energies of *bound* states of one-dimensional potential wells. From the propagation matrix point of view, the wave functions of bound states are simply waves whose wave numbers happen to be purely imaginary at any pair of reference planes placed sufficiently far toward $\pm\infty$ and for which two of the amplitudes in those reference planes vanish, namely, A and D. The evanescent plane "wave" to the left of the leftmost reference plane then has a representation of the form

$$\begin{pmatrix} 0 \\ B \end{pmatrix}, \tag{5•5–1a}$$

whereas the evanescent plane "wave" to the right of the rightmost reference plane has a representation of the form

$$\begin{pmatrix} C \\ 0 \end{pmatrix}. \tag{5•5–1b}$$

In order for such a pair of waves to be connected by a propagation matrix $\hat{P}$,

$$\begin{pmatrix} 0 \\ B \end{pmatrix} = \hat{P} \begin{pmatrix} C \\ 0 \end{pmatrix}, \tag{5•5–2}$$

this propagation matrix must have vanishing diagonal matrix coefficients, especially

$$\boxed{P_{11} = 0.} \tag{5•5–3}$$

Inasmuch as P_{11} is a function of the energy, (5•5–3) is an equation for the energy, the roots of which are the energies of the bound states of that well whose propagation matrix is $\hat{P}$.

Note that this approach does not require an actual determination of the energy eigenfunctions, which is often a more difficult task than assembling the propagation matrix numerically. The method lends itself well to complicated potentials. A convenient approach consists of calculating and multiplying together the individual propagation matrices for a given energy and then repeating this process for suitably spaced energy values in the range of interest. A simple plot of P_{11} reveals the roots, which may then be refined by more precise numerical calculations.

By comparing the condition (5•5–3) for a bound state with the condition (5•4–18) for an allowed energy band in a potential composed of a periodic array of quantum wells, we see that the allowed bands may be viewed as the result of broadening each bound state of a single well into a band.

Rather than plotting P_{11}, it is often more instructive and more convenient to plot the quantity $T = 1/|P_{11}|^2$. As we saw in (5•2–16), this quantity plays the role of a transmission probability for propagating states, and a plot of T for energies corresponding to propagating states is usually of interest anyway. If such a plot is extended to bound-state energies, the bound states show up dramatically as poles in the plot. Note, however, that the quantity T can no longer be interpreted as a transmission probability when the incident and transmitted "waves" are evanescent rather than propagating waves. Having T go to infinity simply means that there is a right-evanescent wave present on the right-hand side, without any right-evanescent wave on the left-hand side.

5.5.2 Example: Bound States of a Square Well of Finite Depth

We apply the preceding formalism here to the bound states of a single well of depth $|V_0|$, as shown in Fig. 5•3–1b. The propagation matrix coefficient P_{11} for the case of a particle going over a barrier, with $0 < V_0 < \mathcal{E}$, was given in (5•3–5). The only difference for the case of bound states inside a well is that the wave number K *outside* the well is now imaginary. From (5•3–8), which

remains valid for negative kinetic energies inside the barrier,

$$K = i\sqrt{2M|V_0|/\hbar^2 - K'^2} = i\kappa, \tag{5•5–4}$$

or, by re-introducing the barrier parameter β from (5•3–10),

$$KL = i\sqrt{|\beta| - (K'L)^2} = i\kappa L. \tag{5•5–5}$$

Substituting $K \to +i\kappa$ in (5•3–5) yields

$$P_{11} = \cos K'L + \frac{|\beta| - 2(K'L)^2}{2K'L\sqrt{|\beta| - (K'L)^2}} \sin K'L. \tag{5•5–6}$$

Exercise: Construct the overall propagation matrix as a product of the matrices in (5•3–20b), (5•2–12), and (5•3–20a), in that order, with $K_\Delta = K'$. Show that the resulting product is the same as that obtained by making the substitution $K \to +i\kappa$ in the original product in (5•3–4).

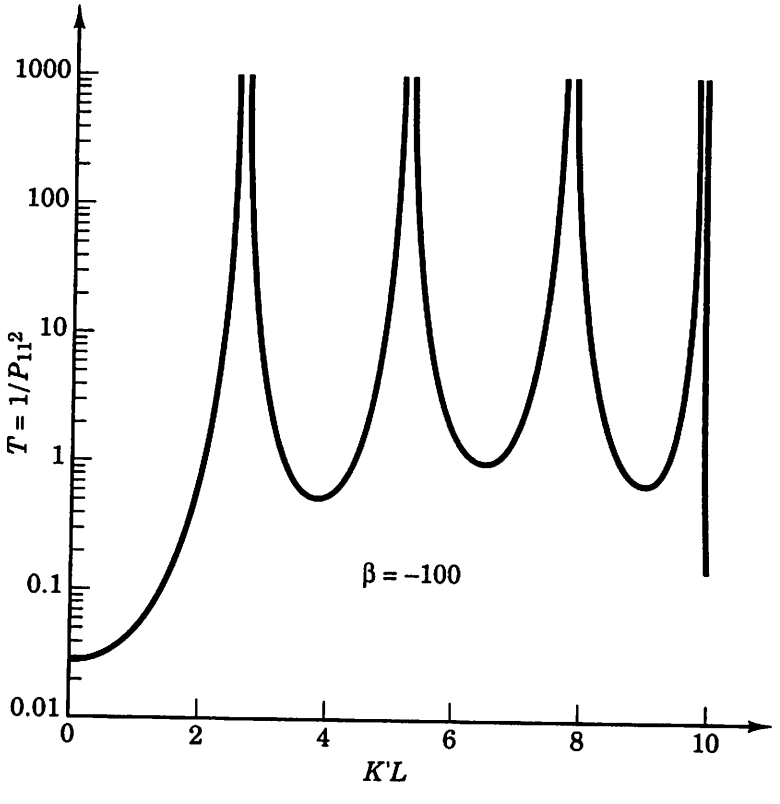

Figure 5•5–1. Semilogarithmic plot of $T = 1/|P_{11}|^2$, as a function of the wave phase $K'L$ inside the well, for a square well with the barrier parameter $\beta = -100$, up to $K'L = \sqrt{100} = 10$, corresponding to energies up to the top of the well. The plot clearly shows four poles, representing bound states; an accurate numerical calculation yields the values $K'L = 2.613$, 5.191, 7.675, and 9.813.

An example of a typical plot of T vs. $K'L$ is shown in **Fig. 5.5–1**.

◆ PROBLEM TO SECTION 5.5

#5•5-1: Transmission Properties of a Composite Barrier

Consider a composite barrier of the general type shown in **Fig. 5•5–2**, containing N discontinuities separating by $N + 1$ flat-potential sections.

The propagation matrix of such a structure has the form

$$\hat{P} = \hat{D}^{(1)} \cdot \hat{F}^{(1)} \cdot \hat{D}^{(2)} \cdot \ldots \cdot \hat{F}^{(N-1)} \cdot \hat{D}^{(N)}, \qquad (5•5–7)$$

where the $\hat{D}$'s are the propagation matrices associated with the discontinuities and the $\hat{F}$'s are associated with the flat-potential sections.

(a) Write a computer program that determines the current transmission probability T as a function of the incident energy $\mathcal{E}$, for a potential that contains an arbitrary number of discontinuities with arbitrary lengths L_n and arbitrary potential energies V_n.

(b) Execute the program for the following four-step potential

n:	0	1	2	3	4
L_n[nm]:	0	1	2	3	0
V_n[eV]:	0	+1	−2	0	−1

Calculate and plot T for this potential, in the incident energy range $0 \leq \mathcal{E} \leq 2$ eV, in steps no coarser than 0.1 eV. *Note:* The choice of the length L_N of the exit side of the potential is irrelevant, but specifying a zero length is a convenient way to signal the end of the composite barrier to the program, without having to specify the number of potential steps beforehand.

(c) Re-run the program in the energy range appropriate for bound states of the structure. Plot T vs. $\mathcal{E}$ in that range, and determine the energy of any bound states that might be present, to better than ±0.05 eV. Also, explore the existence of quasi-bound states showing up as resonances in T, with $T < \infty$ in the energy range $0 > \mathcal{E} > V_4$.

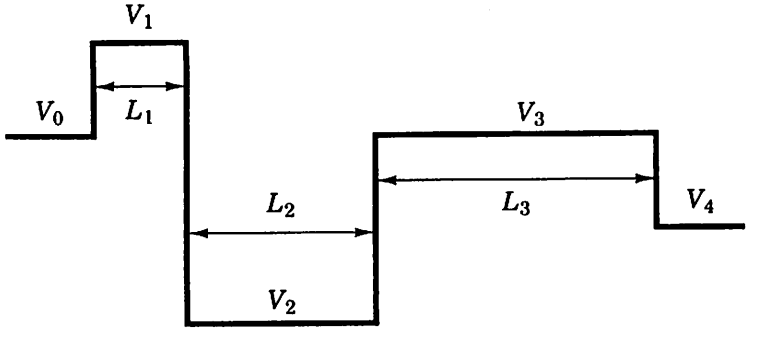

Figure 5•5–2. Barrier containing several flat-potential regions of varying lengths and heights.

5.6 THREE-DIMENSIONAL SCATTERING PROBLEMS: THE BORN APPROXIMATION

5.6.1 The Schroedinger Equation as an Integral Equation

The propagation matrix method developed in sections 5.2 through 5.5, while ideally suited for the treatment of one-dimensional scattering problems, is unsuited for scattering in three dimensions. With a few exceptions—for example, the Coulomb potential—such problems require approximation methods. We present here, in outline, the most important of these methods, the **Born approximation**.

To derive this approximation, we first re-write the Schroedinger equation as

$$\nabla^2\psi(\mathbf{r}) + \frac{2M\mathcal{E}}{\hbar^2}\psi(\mathbf{r}) = -\int s(\mathbf{R})\delta(\mathbf{R} - \mathbf{r})\, d^3R, \tag{5•6–1}$$

where

$$s(\mathbf{R}) = -\frac{2M}{\hbar^2}V(\mathbf{R})\psi(\mathbf{R}), \tag{5•6–2}$$

and $\delta(\mathbf{R} - \mathbf{r})$ is a three-dimensional Dirac δ-function located at $\mathbf{R} = \mathbf{r}$.

In the absence of the integral on the right-hand side, (5•6–1) would simply be the Schroedinger equation for plane waves whose wave vector $\mathbf{k}$ satisfies

$$k^2 = 2M\mathcal{E}/\hbar^2, \tag{5•6–3}$$

and we could simplify (5•6–1) further by writing it as

$$\nabla^2\psi_0(\mathbf{r}) + k^2\psi_0(\mathbf{r}) = 0. \tag{5•6–4}$$

The integral term in (5•6–1) acts as a perturbation, in the form of a sum over an infinite number of δ-function scattering sources, each with a strength $s \cdot d^3\mathbf{R}$. The source strength depends both on the local potential $V(\mathbf{R})$ and on the *actual* wave function $\psi(\mathbf{r})$ at each point. It is therefore an unknown quantity itself.

As a preliminary, consider first the solution of a simpler problem, a single δ-function source of unit strength, located at $\mathbf{r} = 0$. That is, we look for solutions of the equation

$$\nabla^2 G(\mathbf{r}) + k^2 G(\mathbf{r}) = -\delta(\mathbf{r}). \tag{5•6–5}$$

The function $G(\mathbf{r})$ is called **Green's function** for the scattering problem. Solutions of (5•6–5) are easily found. The simplest is

$$G(\mathbf{r}) = \frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{4\pi r}. \tag{5•6–6}$$

Exercise: Show that (5•6–6) satisfies (5•6–5). For $r > 0$, this is easily done by insertion. For $r \to 0$, (5•6–5) implies that

$$\lim_{\Omega \to 0} \int_{\Omega} \nabla^2 G d^3r = -1, \tag{5•6–7}$$

where the integral goes over any volume Ω that includes $\mathbf{r} = 0$. By Gauss' integral theorem, the integral can be converted to a surface integral:

$$\int_{\Omega} \nabla^2 G d^3r = \oint_S (\nabla G) \cdot d\mathbf{S}. \tag{5•6–8}$$

By choosing as the surface a sphere of vanishing radius, show that (5•6–5) is satisfied.

Consider next the function

$$\psi(\mathbf{r}) = -\int G(\mathbf{r} - \mathbf{R}) \cdot s(\mathbf{R})\, d^3R, \tag{5•6–9}$$

where $G(\mathbf{r})$ satisfies (5•6–5). By inserting $\psi(\mathbf{r})$ on the left-hand side of (5•6–1) and using (5•6–5), one confirms easily that $\psi(\mathbf{r})$ is a solution of (5•6–1). It is not the most general solution, however: We may add to it any arbitrary solution $\psi_0(\mathbf{r})$ of the *homogeneous* equation (5•6–4), such as

$$\psi_0(\mathbf{r}) = A \cdot \exp(i\mathbf{k} \cdot \mathbf{r}). \tag{5•6–10}$$

If we add ψ_0, and insert $s(\mathbf{R})$ from (5•6–2), we obtain the integral equation

$$\boxed{\psi(\mathbf{r}) = \psi_0(\mathbf{r}) - \int G(\mathbf{r} - \mathbf{R}) V(\mathbf{R}) \psi(\mathbf{R})\, d^3R.} \tag{5•6–11}$$

Note that this equation is not based on choosing, for ψ_0 and G, the specific examples given; all that is required is that ψ_0 and G satisfy (5•6–4) and (5•6–5).

The integral equation (5•6–11) is mathematically equivalent to the time-independent Schroedinger equation, but it is much better adapted to the treatment of scattering problems. This is because the two functions ψ_0 and G may be chosen in such a way that the ψ_0-term represents an incident wave and the integral the scattered wave. To achieve this separation, we choose ψ_0 to be a plane wave, as in (5•6–10), and G to be a wave going outward from each scattering point $\mathbf{r} = \mathbf{R}$, as in (5•6–6).

Note that (5•6–11) is a re-formulation of the scattering problem, not its solution: The unknown wave function is still contained inside the integral. This simply reflects the physical fact that the scattered intensity depends on the magnitude of the actual wave function at each scattering point, rather than on

the magnitude of the incident wave alone. Multiple scattering effects are therefore automatically included in (5•6–11).

5.6.2 The Born Approximation

So far, (5•6–11) is exact. Suppose now that the scattering potential is so weak that the scattered-wave contribution of the integral in (5•6–11) is everywhere small compared to the incident plane wave. The contribution of the integral may then be approximated by replacing the *actual* wave function ψ with the *incident* wave ψ_0:

$$\boxed{\psi(\mathbf{r}) \cong \psi_1(\mathbf{r}) \equiv \psi_0(\mathbf{r}) - \int G(\mathbf{r} - \mathbf{R})V(\mathbf{R})\psi_0(\mathbf{R})\, d^3R.} \qquad (5\text{•}6\text{–}12)$$

This is the **first-order Born approximation**. Physically, the approximation of replacing ψ by ψ_0 inside the scattering integral implies neglecting all multiple-scattering effects.

It is sometimes possible to improve the approximation by re-inserting the first-order wave function ψ_1 into the integral, leading to a second-order wave function ψ_2. The process can be repeated ad infinitum. Because only straightforward integrations over known functions are involved, this kind of iterative improvement of the wave function is well adapted to computer calculations.

Unfortunately, higher-order Born approximations are no panacea. Mathematically, the iteration represents a disguised power series expansion of the wave function, in terms of the powers of the overall strength of the perturbing potential. Each order adds a new power to the series. Like other power series expansions, the Born approximation may diverge. Indeed, it is usually only semi-convergent: The higher-order corrections tend to stop decreasing past a certain optimum order and then oscillate with increasing amplitude, leading to an alternating divergent series. For weak scattering potentials without singularities, this ultimate divergence is usually of no practical consequence, because the overshoot oscillations do not set in until long after one has cut off the series. They are, however, a problem with scattering potentials that are very strong or that contain singularities, such as the Coulomb potential $V(\mathbf{r}) \propto 1/r$. In the case of the Coulomb potential, a very peculiar phenomenon occurs: The first-order Born approximation happens to coincide with the known *exact* solution of the scattering problem, but the second-order integral diverges. Truncating the expansion after the first order then leads to the correct answer. Unfortunately, one cannot count on such lucky accidents. Alternative methods have been developed for such cases, but their discussion lies outside the scope of this text.

Chapter 6

WKB APPROXIMATION

6.1 WKB WAVE FUNCTIONS

6.1.1 Plane Waves with Variable Wavelength and Amplitude

Except for the Born approximation in the preceding chapter, we have so far always been concerned with *exact* solutions of the Schroedinger equation. We now turn to another approximation method, the so-called **WKB approximation**, which is an excellent approximation for slowly varying one-dimensional potentials and hence bridges the gap between classical and quantum mechanics. It is named after Wentzel, Kramers, and Brillouin, who, around 1926, were the first to employ this approximation in quantum mechanics, even though as a basic mathematical technique, it is much older.[1]

We take as our point of departure the remark in section 1.3 that in the presence of a force, both the *local* wave number K and the probability density

[1] For complete references, and an in-depth treatment, see N. Fröman and P. O. Fröman, "JWKB Approximation" Amsterdam: North-Holland, 1965. Another excellent discussion, centered around numerous examples, is found in Flügge, cited in appendix G.

ρ of an object wave *must* be functions of position. Consider, therefore, a time-independent wave function of a form similar to the terms in (5•2–2a), i.e.,

$$\psi_{\pm}(x) = \frac{A}{\sqrt{K(x)}} \cdot \exp\left[\pm i \int^{x} K(y)\, dy\right], \tag{6•1–1}$$

with a wave number $K(x)$ that depends on position according to

$$K(x) = \sqrt{\frac{2M}{\hbar^2}[\mathcal{E} - V(x)]} \qquad \text{if} \qquad \mathcal{E} > V. \tag{6•1–2}$$

In the case of a constant potential, this is of course an exact solution of the Schroedinger equation, with the amplitude A being a constant.

We might expect that in the case of a sufficiently slowly varying potential, a wave function of the form (6•1–1), with $K(x)$ given by (6•1–2), might remain at least a good approximation. We note first that the position-denominator in (6•1–1) leads to a probability density inversely proportional to K and, hence, to the local velocity $v = \hbar K/M$, as is needed in order to have a divergence-free probability current density, an essential requirement for any approximation.

Exercise: Show that

$$\frac{dj_{\pm}}{dx} = \frac{d}{dx}\left(\psi_{\pm}^{*}\frac{d\psi_{\pm}}{dx} - \psi_{\pm}\frac{d\psi_{\pm}^{*}}{dx}\right) = 0, \tag{6•1–3}$$

which means that current conservation is obeyed exactly. Show further that this result depends, not on the choice (6•1–2) for $K(x)$, but only on $K(x)$ being real and nonzero.

The most general wave function involving terms of the form (6•1–1) is a linear superposition of the two terms with different signs in the exponent, such as

$$\psi_{WKB}(x) = \frac{1}{\sqrt{K(x)}}\left\{A \cdot \exp\left[+i \int^{x} K(y)\, dy\right] + B \cdot \exp\left[-i \int^{x} K(y)\, dy\right]\right\}, \tag{6•1–4}$$

where both A and B are constants. The (unstated) lower integration limits in (6•1–4) depend on the choice of the phase of the two amplitudes A and B. In effect, those limits establish reference planes for the waves.

It is left to the reader to show that the probability current density associated with (6•1–4)—for positive K—is

$$j = \frac{\hbar}{M} \cdot (|A|^2 - |B|^2). \tag{6•1–5}$$

6.1.2 Validity Conditions

In order to determine how good an approximation the WKB wave function is, we look at its second derivative. The reader may confirm that

$$\psi'' = -\left[K^2 + \frac{1}{2}\left(\frac{K''}{K}\right) - \frac{3}{4}\left(\frac{K'}{K}\right)^2\right] \cdot \psi \tag{6•1–6}$$

for both ψ_+ and ψ_-. The WKB approximation is obtained if we specifically select $K(x)$ according to (6•1–2), assuming that

$$\mathcal{E} > V(x), \tag{6•1–7}$$

to make sure that $K(x)$ is real. The case $\mathcal{E} < V(x)$ will be discussed later.

If we choose the form (6•1–2) for $K(x)$, the $K^2\psi$-term in (6•1–6) represents the Schroedinger equation by itself. The other terms are extra terms; their magnitude is a measure of the degree of deviation of the approximation (6•1–1) from an exact solution. In order for (6•1–1) to be a good approximation, these extra terms must remain small compared to the $K^2\psi$-term, i.e.,

$$\frac{1}{4}\left|2\left(\frac{K''}{K}\right) - 3\left(\frac{K'}{K}\right)^2\right| \ll |K|^2. \tag{6•1–8}$$

To understand the meaning of this condition better, we convert it to the form

$$\left|\frac{V''}{\mathcal{E} - V} + \frac{5}{4}\left(\frac{V'}{\mathcal{E} - V}\right)^2\right| \cdot |\Lambda|^2 \ll 16\pi^2, \tag{6•1–9}$$

where $\Lambda = 2\pi/K$ is the *local* de Broglie wavelength. Both (6•1–8) and (6•1–9) are complicated conditions. While they might in principle be satisfied by a mutual cancellation of the terms on the left-hand sides, this is of little importance in practice. We therefore impose the stronger condition that both of the terms on the left-hand side of (6•1–8) be *separately* small. This leads to two conditions that may be written

$$\Delta V_1 \equiv |V' \cdot \Lambda| \ll \frac{8\pi}{\sqrt{5}}|\mathcal{E} - V| \approx 11.2|\mathcal{E} - V| \tag{6•1–10}$$

and

$$\Delta V_2 \equiv \tfrac{1}{2}|V'' \cdot \Lambda^2| \ll 8\pi^2|\mathcal{E} - V| \approx 79.0|\mathcal{E} - V|. \tag{6•1–11}$$

We refer to these as the **first and second WKB conditions.** Both have a simple meaning, which we can bring out as follows. If the potential V varies slowly enough with position, the quantity ΔV_1 represents the change in potential along one wavelength (**Fig. 6•1–1(a)**); similarly, ΔV_2 represents that change in potential that would build up due to the *curvature* of the potential along one wavelength, starting with $V' = 0$ (**Fig. 6•1–1(b)**). The relations (6•1–9) and (6•1–10) then state that the changes in potential, *both* due to a finite

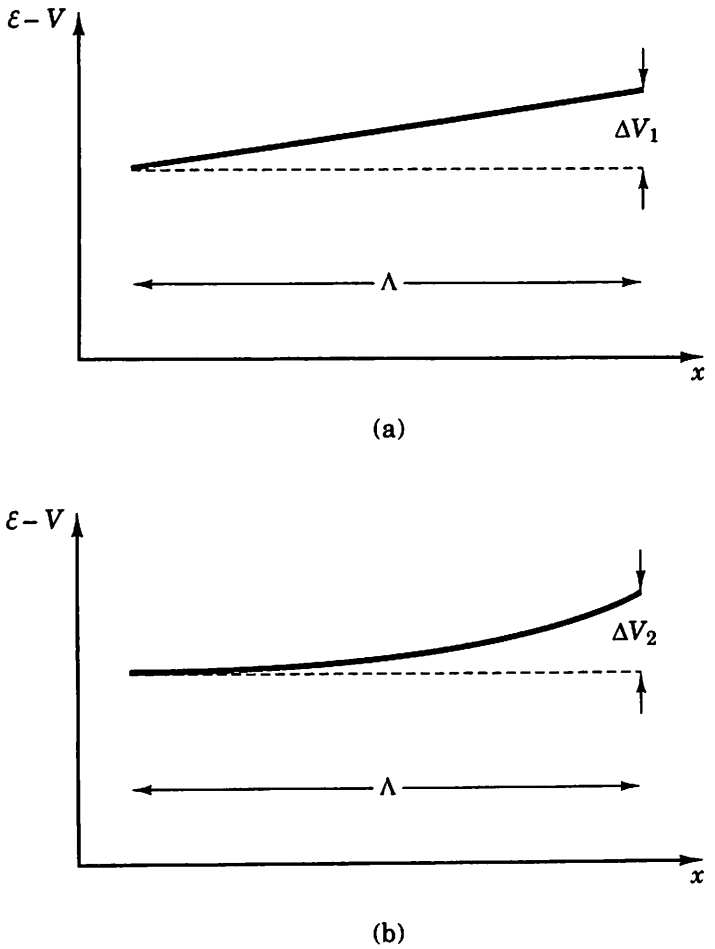

Figure 6•1–1. **(a)** The first WKB condition is that the potential change along a wavelength is sufficiently small compared to the minimal kinetic energy along the path of that wavelength. **(b)** The second WKB condition demands that the curvature of the potential be small.

slope and due to a finite curvature, taken per wavelength, must stay small compared to the stated large multiples of the kinetic energy of the particle.

Both conditions are easily met, and whenever they are satisfied, the WKB wave function (6•1–4) *with constant amplitudes A and B* is a good approximate solution of the Schroedinger equation.

If the correction terms in (6•1–6) cannot be neglected, the true wave function can still be written in the form (6•1–4), but then the amplitudes A and B no longer can be treated as constants, but become themselves position dependent. It is left to the reader to show that in this case the continuity equation (6•1–3) requires that

$$|A(x)|^2 - |B(x)|^2 = \text{constant}. \qquad (6\text{•}1\text{–}12)$$

Position-dependent amplitudes mean that scattering is taking place between the forward- and backward-propagating waves; *the WKB approximation itself is a zero-scattering approximation.*

It is in principle possible to extend the WKB approximation to higher orders, but they are hardly ever used. A much more practical approach to the calculation of any reflected waves is simply inserting the first-order WKB wave function into the Born approximation.

6.1.3 Exponentially Growing and Decaying Approximations for Negative Kinetic Energy; the Connection Problem

The preceding discussion assumed that the total energy $\mathcal{E}$ of the particle exceeds the potential energy, i.e., $\mathcal{E} > V(x)$. However, the relation (6•1–6) holds regardless of this assumption, as do the validity conditions (6•1–8) through (6•1–11) that follow from (6•1–6). This means that wave functions of the form (6•1–1) with imaginary K remain good approximations even for $\mathcal{E} < V(x)$, under the same conditions (6•1–8) through (6•1–11). In fact, this applicability to both positive and negative kinetic energies forms the basis for one of the most important applications of the WKB approximation: tunneling through barriers.

The only change we make in the negative-energy case is again a replacement of K by $i\kappa$, where

$$\kappa(x) = \sqrt{\frac{2M}{\hbar^2}[V(x) - \mathcal{E}]} \text{ if } \mathcal{E} < V. \tag{6•1–13}$$

With this change, we obtain, instead of (6•1–4),

$$\psi_{WKB}(x) = \frac{1}{\sqrt{\kappa(x)}}\left\{C \cdot \exp\left[-\int^x \kappa(y)\,dy\right] + D \cdot \exp\left[+\int^x \kappa(y)\,dy\right]\right\}. \tag{6•1–14}$$

The conditions (6•1–9) through (6•1–11) still hold, except that the wavelength Λ is replaced by

$$\Lambda' \to 2\pi/\kappa. \tag{6•1–15}$$

What *does* assume a significantly different form is the expression for the probability current density. It is again left to the reader to show that, instead of (6•1–5), we now have

$$j = \frac{i\hbar}{M} \cdot (CD^* - C^*D), \tag{6•1–16}$$

Note that a current can flow only if both a right-evanescent (C) and a left-evanescent (D) wave are present and the ratio of the two amplitudes is a complex number.

In bound-state problems, the range for which $V(x) > \mathcal{E}$ extends to infinity. In those cases, one of the two coefficients in (6•1–14) must be zero. For $x \to +\infty$, we must have $D = 0$, or else the wave function would become infinite there. Similarly, for $x \to -\infty$, we must have $C = 0$, for the same reason. In either case, there is, of course, no current.

In order for the Schroedinger equation to have any physically meaningful solutions at all, we must have $V(x) < \mathcal{E}$ over at least *some* range of x, and this means that there must be at least one *classical turning point* $x = a$ where $V(x) - \mathcal{E}$ changes its sign. In realistic problems, $V(x) - \mathcal{E}$ will go through zero

as a continuous function, rather than as a step. In the immediate vicinity of the classical turning point, neither the first nor the second WKB condition can be satisfied, and both the oscillating form (6•1–4) and the evanescent form (6•1–14) of the WKB approximation diverge, signaling the collapse of the approximation.

Suppose, however, that sufficiently far from $x = a$, the WKB approximation is applicable on both sides of a, on one side in the form (6•1–4) and on the other in the form (6•1–14), with neither form remaining a valid approximation if it is extended right up to a. This raises the question: what is the relationship between the coefficients A and B on one side to C and D on the other? This is the *connection problem* of the WKB approximation, to be treated in the sections that follow.

6.2 EXAMPLE: HARMONIC OSCILLATOR

6.2.1 Phase Connection Rule

It is useful to discuss the WKB wave functions and their connection rules for a case for which we know already the exact wave functions: the energy eigenstates of the harmonic oscillator.

We write the potential energy in the form

$$V(x) = \tfrac{1}{2}M\omega^2 x^2, \tag{6•2–1}$$

and we recall that the energy eigenvalues are then given by

$$\mathcal{E}_n = (n + \tfrac{1}{2})\hbar\omega, \tag{6•2–2}$$

where the n are the nonnegative integers. We will also need the classical turning points from (2•3–24), i.e.,

$$x_n = \sqrt{2n + 1} \cdot L, \tag{6•2–3}$$

where

$$L = \sqrt{\hbar/M\omega} \tag{6•2–4}$$

is the natural unit of length for the oscillator (see (2•3–7)).

Because for a one-dimensional stationary bound state there can be no net current flow, the WKB wave function (6•1–4) must be a pure standing wave. In this case, the two propagating waves in that function may be lumped together into a real cosine wave, which may be written in the form

$$\psi(x) = \frac{2A}{\sqrt{K}} \cdot \cos\left[\int_{-x_n}^{x} K\,dy - \alpha\right], \tag{6•2–5}$$

with a real amplitude A and a suitable phase angle α. In (6•2–5), we have selected the phase angle α in such a way that the left classical turning point serves as one of the integration limits and, hence, as a reference plane for the

phase of the wave, even though at that point (6•2–5) is no longer a good approximation. Without loss of generality, we may restrict α to the range

$$-\pi/2 < \alpha < +\pi/2. \tag{6•2–6}$$

For $\mathcal{E} = \mathcal{E}_n$, the local WKB wave number K in Eq. (6•1–2) in the classically allowed range $|x| < x_n$ is given by

$$K(x) = \sqrt{\frac{2M}{\hbar^2}(\mathcal{E}_n - \tfrac{1}{2}M\omega^2 x^2)} = \frac{1}{L^2}\sqrt{x_n^2 - x^2}. \tag{6•2–7}$$

For later use, we note that

$$K(0) = \frac{x_n}{L^2} = \frac{\sqrt{2n+1}}{L}. \tag{6•2–8}$$

We insert (6•2–7) into (6•2–5), evaluate the result at $x = 0$, and compare it with the known exact wave function at that point. To be specific, we assume that n is an even number.[2] In this case, the exact wave function is symmetric about the point $x = 0$, and it has $n/2$ nulls on each side of the plane $x = 0$. In order for the WKB wave function to be itself an even function of x, with the same number of nulls, it is necessary that the argument of the cosine function in Eq. (6•2–5), evaluated at $x = 0$, be an integer multiple of π, with the multiplier $n/2$:

$$\int_{-x_n}^{0} K\,dx - \alpha = \frac{1}{L^2}\int_{-x_n}^{0} \sqrt{x_n^2 - x^2}\,dx - \alpha = \frac{n}{2}\pi. \tag{6•2–9}$$

The integral is simply the area of a quarter-circle of radius x_n:

$$\begin{aligned}\int_{-x_n}^{0} \sqrt{x_n^2 - x^2}\,dx &= \int_{0}^{+x_n} \sqrt{x_n^2 - x^2}\,dx = \frac{\pi}{4}\cdot x_n^2 \\ &= \frac{\pi}{4}\cdot(2n+1)\cdot L^2.\end{aligned} \tag{6•2–10}$$

Here, in the last equality, we have used (6•2–3). Insertion into (6•2–9) yields

$$\boxed{\alpha = \frac{\pi}{4},} \tag{6•2–11}$$

independent of the quantum number n harmonic oscillator. This is the **WKB phase connection rule.** Inserted into (6•2–5), (6•2–11) gives

$$\psi(x) = \frac{2A}{\sqrt{K}}\cdot\cos\left[\int_{-x_n}^{x} K\,dy - \frac{\pi}{4}\right]. \tag{6•2–12a}$$

[2] The reader is invited to carry through the argument for odd values of n. While the details are different, the final results are the same.

Although we have derived this result here for the harmonic oscillator, we shall see that it holds generally, provided that the potential energy varies sufficiently smoothly across the classical turning point, that it may be approximated by a harmonic oscillator parabola until well into the ranges on both sides where the WKB wave functions are good approximations.

Switch of Reference Plane

In the preceding treatment, we arbitrarily used the left-hand classical turning point as reference plane. We could just as well have used the right-hand classical turning point. It is left to the reader to show that in this case, the WKB wave function between the two turning points may be written as

$$\psi(x) = \frac{2A'}{\sqrt{K}} \cdot \cos\left[\int_x^{+x_n} K\,dy - \frac{\pi}{4}\right]. \tag{6•2–12b}$$

where $A' = (-1)^n A$. Note that in this formulation, the variable x appears as the lower rather than the upper integration limit, and that the integral remains positive. The phase shift remains $\pi/4$.

6.2.2 The WKB Amplitudes and Their Connection Rule[3]

To determine the WKB amplitudes A and C, and especially their ratio C/A, we match the WKB wave functions to the true harmonic oscillator wave functions at $x = 0$ and for large values of x.

From the second term in the recursion relations (2•3–30) for the harmonic oscillator wave functions, we find, for even order n, that

$$\psi_n(0) = A_0 \frac{(-1)^{n/2}\sqrt{n!}}{2^{n/2}\,(n/2)!}, \tag{6•2–13}$$

where A_0 is the normalization coefficient of the ground-state wave function, from (2•3–10) or (2•3–15), depending on the normalization employed. On the other hand, the WKB wave function (6•2–5), taken at $x = 0$, is

$$\psi_{WKB}(0) = \frac{2A}{\sqrt{K(0)}} \cdot \cos(n\pi/2) = A \cdot \frac{2(-1)^{n/2}\sqrt{L}}{(2n+1)^{1/4}}, \tag{6•2–14}$$

where, in the second equality, we have drawn on (6•2–8) and (6•2–9). Equating the WKB value to the exact value yields the WKB amplitude A inside the classically allowed range:

$$A = \frac{A_0}{\sqrt{L}} \cdot \frac{(2n+1)^{1/4}}{2 \cdot 2^{n/2}} \cdot \frac{\sqrt{n!}}{(n/2)!}. \tag{6•2–15}$$

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[3] The derivation of the amplitude connection rule, contained in this sub-section, is fairly tedious. The reader may safely skip the details and move directly to the final result, Eq. (6•2–26).

In the opposite limit, $Q \to \infty$, the exact wave function is dominated by the highest power term in the Hermite polynomial part of the wave function. The asymptotic limit is obtained easily from the leading term in the recursion relation (2•3–30), namely,

$$\psi_n(Q) \to A_0 \frac{2^{n/2}}{\sqrt{n!}} \cdot Q^n \exp(-Q^2/2). \tag{6•2–16}$$

where

$$Q = x/L. \tag{6•2–17}$$

In the classically forbidden ranges, the WKB wave function must be purely evanescent. In the right-hand range, $x > +x_n$, we may write it as

$$\psi_{WKB}(x) = \frac{C}{\sqrt{\kappa}} \cdot \exp\left[-\int_{x_n}^{x} \kappa dx'\right]. \tag{6•2–18}$$

The integral in the exponent has the value

$$\int_{x_n}^{x} \kappa dx' = -\frac{x_n^2}{2L^2} \cdot \ln\left[\frac{x + (x^2 - x_n^2)^{1/2}}{x_n}\right] + \frac{x \cdot (x^2 - x_n^2)^{1/2}}{2L^2}. \tag{6•2–19}$$

In the limit of large x, this goes over into

$$\begin{aligned} &-\frac{x_n^2}{2L^2} \cdot \ln\left[\frac{2x}{x_n}\right] + \frac{x^2}{2L^2} - \frac{x_n^2}{4L^2} + \cdots = \\ &-m \cdot \ln\left[Q\sqrt{\frac{2}{m}}\right] + \frac{Q^2}{2} - \frac{m}{2} + \cdots, \end{aligned} \tag{6•2–20}$$

where, in the second equality, we have substituted $x = QL$ and

$$\frac{x_n^2}{2L^2} = m \equiv n + \tfrac{1}{2}. \tag{6•2–21}$$

All omitted terms decrease with increasing x and Q.

If we insert (6•2–22) and (6•2–20) into (6•2–18) and simplify the pre-factor according to

$$\kappa = \frac{1}{L^2}\sqrt{x^2 - x_n^2} \xrightarrow[x \to \infty]{} \frac{Q}{L}, \tag{6•2–22}$$

we obtain the asymptotic relation

$$\psi_{WKB}(Q) \to C\sqrt{L} \cdot \left(\frac{2e}{m}\right)^{m/2} Q^n \exp\left(-\frac{Q^2}{2}\right). \tag{6•2–23}$$

Equating (6•2–16) with (6•2–23) yields

$$C = \frac{A_0}{\sqrt{L}} \frac{1}{2^{1/4}} \frac{1}{\sqrt{n!}} \cdot \left(\frac{m}{e}\right)^{m/2}. \tag{6•2–24}$$

We are principally interested in the ratio C/A of the two amplitudes:

$$\frac{C}{A} = \frac{2^{1/2}}{e^{1/4}} \cdot \left(\frac{2n+1}{e}\right)^{n/2} \cdot \frac{(n/2)!}{n!}. \tag{6•2–25}$$

This rather elaborate-looking expression is simpler than it appears: For $n = 2$, 4, 6, one obtains the numerical values 1.013, 1.006, 1.004, rapidly converging toward the (exact) limit 1.0, i.e.,

$$\boxed{\lim_{n\to\infty} \frac{C}{A} = 1.} \tag{6•2–26}$$

This is the WKB amplitude connection rule for the harmonic oscillator. Like the phase connection rule, it holds more generally, as we shall see presently.

6.3 GENERAL CONNECTION RULES ACROSS A CLASSICAL TURNING POINT

6.3.1 The Problem

We now show that the phase and amplitude connection rules (6•2–11) and (6•2–26) for the harmonic oscillator remain applicable to the connection across the classical turning points of many other "well-behaved" potentials.

Consider a particle of energy $\mathcal{E}$, moving in a potential $V(x)$, with a classical turning point at $x = c$ (**Fig. 6•3–1**). Suppose that

$$V(x) > \mathcal{E} \text{ for all } x > c, \tag{6•3–1}$$

and that the second derivative of the potential at the classical turning point is positive.

If the potential varies sufficiently smoothly with position, there will be a wide interval (x_I, x_{II}) straddling the classical turning point, inside which the

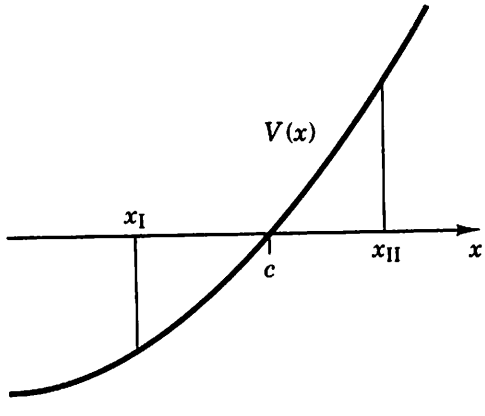

Figure 6•3–1. Connection across a classical turning point. The WKB wave function, forming a valid approximation *outside* the interval (x_I, x_{II}) is connected across this interval using a piece of the solution of an exactly solvable potential, such as the harmonic oscillator potential.

potential may be approximated by a section of a harmonic oscillator parabola of the form

$$V_0(x) = V_{00} + \tfrac{1}{2}M\omega^2(x - x_0)^2. \tag{6•3–2a}$$

We also assume that the energy $\mathcal{E}$ happens to coincide with one of the harmonic oscillator eigenvalues:

$$\mathcal{E} = V_{00} + \hbar\omega \cdot \left(n + \frac{1}{2}\right). \tag{6•3–2b}$$

Exercise: Given specific values of $\mathcal{E}$, a, $V'(a)$, and $V''(a)$, determine the associated fitting parameters V_{00}, ω, x_0, and n.

Suppose now that the fitting interval (x_I, x_{II}) is sufficiently wide and the potential sufficiently smooth that the WKB approximation is a good approximation at both ends of the interval *and beyond*.

Under the assumption (6•3–1), there can again be no net current flow, and the WKB wave function in the classically allowed range must once more be a pure standing wave of the form (6•2–5), with $K = K(x)$ given by (6•1–2). Most important, the phase angle α must then again be given by (6•2–11), i.e., $\alpha = -\pi/4$. This is readily seen by the following argument. If the WKB approximation is indeed applicable in the range $x > x_{II}$, then the WKB wave function must be a pure right-evanescent wave of the form (6•2–18). Because the WKB approximation is a zero-scattering approximation, a purely right-evanescent WKB wave function must connect to a purely right-evanescent harmonic oscillator wave function. But the latter is just the function (6•2–5) with $\alpha = -\pi/4$.

Similarly, one also confirms that under the stated assumptions, the amplitude connection rule also carries over. If the curvature of the potential is small, we are in the high-n limit (6•2–26), and we have

$$C = A. \tag{6•3–3}$$

6.3.2 Example: An Electron in a Uniform Electric Field

We illustrate the use of the WKB *phase* connection rule by determining the energy levels of an electron that is driven against an infinitely high abrupt potential wall by an electric field E (**Fig. 6•3–2**).

The potential energy is

$$V(x) = \begin{Bmatrix} \infty \\ eEx \end{Bmatrix} \text{ for } \begin{Bmatrix} x < 0 \\ x > 0 \end{Bmatrix}. \tag{6•3–4}$$

The quantum-mechanical problem corresponding to this potential can be solved rigorously in closed form, in terms of the so-called **Airy function**, a

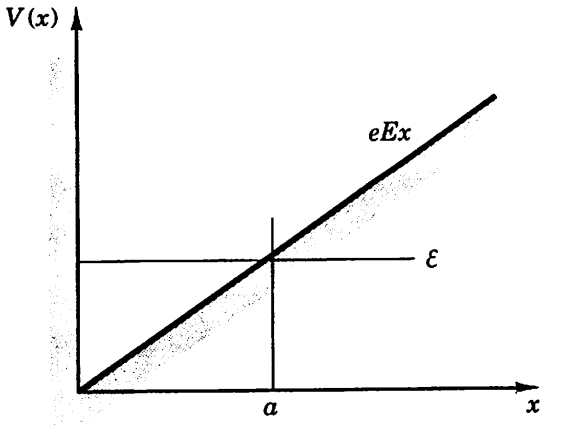

Figure 6•3–2. Potential energy for an electron in a uniform electric field at a potential wall.

linear superposition of Bessel functions of the order $\pm 1/3$. The exact values of the energy eigenvalues are

$$\mathcal{E}_n = A_n \mathcal{E}_0, \qquad n = 1, 2, 3, \ldots \tag{6•3–5}$$

where A_n is the nth root of the Airy function[4] and $\mathcal{E}_0$ is the quantity

$$\mathcal{E}_0 = \left[\frac{\hbar^2 (eE)^2}{2m_e}\right]^{1/3}, \tag{6•3–6}$$

which we may view as the **natural unit of energy** of the problem, defined in terms of the coefficients $\hbar^2/2m_e$ and eE occurring in the Schroedinger equation.

Along with the energy $\mathcal{E}_0$, a natural unit L of length may be associated with the problem, defined by the requirement

$$\mathcal{E}_0 = eEL = \frac{\hbar^2}{2m_e L^2}, \tag{6•3–7}$$

which leads to

$$L = \left[\frac{\hbar^2}{2m_e eE}\right]^{1/3}. \tag{6•3–8}$$

Numerically, for an electric field of, say, 10^6 V/cm,

$$\mathcal{E}_0 = 72.5 \text{ meV}; \qquad L = 0.725 \text{ nm}. \tag{6•3–9a,b}$$

We will use here the WKB approximation to obtain an approximate value for the various energy levels, to be compared with the exact value.

Because of the infinitely high potential wall at $x = 0$, the wave function must vanish there. This means that the argument of the cosine function in

[4] See, for example, problem 40 in the book by Flügge, cited earlier. For the Airy function itself and its roots, see M. Abramowitz and A. Segun, *Handbook of Mathematical Functions* (New York: Dover, 1965), chapter 10.

(6•2–12b), evaluated at $x = 0$, must be an odd multiple of $\pi/2$:

$$\int_0^a K(x)\,dx - \frac{\pi}{4} = (2n - 1)\cdot\frac{\pi}{2}. \tag{6•3–10}$$

Here we have written a instead of x_n for the as-yet unknown classical turning point,

$$a = \frac{\mathcal{E}}{eE} = L\cdot\frac{\mathcal{E}}{\mathcal{E}_0}, \tag{6•3–11}$$

and the different values of n belong to the different energy eigenvalues, starting with $n = 1$.

With the help of (6•3–7), the WKB wave number may be written

$$K(x) = \sqrt{\frac{2m_e}{\hbar^2}(\mathcal{E} - eEx)} = \frac{1}{L^{3/2}}\sqrt{a - x}, \tag{6•3–12}$$

and the integral in (6•3–10) is easily found to be

$$\int_0^a K(x)\,dx = \frac{1}{L^{3/2}}\int_0^a \sqrt{a - x}\,dx = \frac{2}{3}\left(\frac{a}{L}\right)^{3/2} = \frac{2}{3}\left(\frac{\mathcal{E}}{\mathcal{E}_0}\right)^{3/2}. \tag{6•3–13}$$

If this is inserted into (6•3–10), we obtain an expression in the form (6•3–5) for the approximate energy levels, with

$$A_n = \left[\frac{3\pi}{8}(4n - 1)\right]^{2/3}. \tag{6•3–14}$$

The three lowest values are

$$A_1 = 2.321, \qquad A_2 = 4.082, \qquad A_3 = 5.517, \tag{6•3–15a,b,c}$$

remarkably close to the first three roots of the Airy function,

$$A_1 = 2.338, \qquad A_2 = 4.088, \qquad A_3 = 5.521. \tag{6•3–16a,b,c}$$

Even the lowest level differs from the exact value by less than 1%.

6.3.3 Amplitude Connection Rules

We combine the phase connection rule (6•2–11) with the amplitude connection rule (6•3–3) to write the connection between the standing wave (6•2–5) and the right-evanescent wave (6•2–18) in the form

$$\boxed{\frac{2}{\sqrt{K}}\cdot\cos\left[\int_x^c K\,dx' - \frac{\pi}{4}\right] \leftarrow \frac{1}{\sqrt{\kappa}}\cdot\exp\left[-\int_c^x \kappa dx'\right],} \tag{6•3–17a}$$

where c indicates the classical turning point.

In the form (6•3–17a), the connection rule applies to the case where the evanescent wave decays into a barrier to the *right* of the classical turning point. In the case of an evanescent wave decaying into a barrier to the *left* of the classical turning point, we have

$$\boxed{\frac{2}{\sqrt{K}} \cdot \cos\left[\int_x^c K dx' - \frac{\pi}{4}\right] \leftarrow \frac{1}{\sqrt{\kappa}} \cdot \exp\left[-\int_c^x \kappa dx'\right].} \qquad (6\text{•}3\text{–}17b)$$

Note that we have indicated the connection between the two wave functions with unidirectional arrows. What is meant by this is the following. If we start from a purely decaying wave function on the classically *forbidden* side of the turning point, the wave function on the *allowed* side will, to a good approximation, be given by the cosine-type wave function with the indicated amplitude and phase. However, if a wave function on the allowed side of the barrier is of the cosine type, as in (6•3–17a) or (6•3–17b), the continuation of this wave function as a purely evanescent wave deep into a barrier is *not necessarily* a good approximation! It would be valid only if the WKB approximation and the connection rules were exact, for arbitrary barriers. But they are only approximations, which means that an *exact* continuation of the cosine-type wave function into the interior of the barrier would very likely contain a small contribution from the exponentially growing wave function. Near the classical turning point this contribution is likely to be negligible, but unless it is *exactly* zero, it will ultimately dominate if we continue the wave function sufficiently deep into the barrier. Hence, we write the unidirectional arrow.

6.4 TUNNELING

6.4.1 The WKB Wave Function inside a Barrier

As long as we are dealing with infinitely thick classically forbidden bariers, the connection rules (6•3–17a) and (6•3–17b) are all we ever need. The situation changes, however, when we consider tunneling *through* a barrier of finite width, as in **Fig. 6•4–1**. Inside a tunneling barrier, both left-evanescent and right-evanescent waves will in general be present simultaneously, and the overall wave function will be a superposition of the form (6•1–14). Furthermore, a current will in general be flowing through the barrier, related to the two amplitudes C and D in (6•1–14) via the relation (6•1–16). Evidently, C and D cannot both be real, and the wave function becomes complex, as is appropriate for wave functions representing a current-carrying state.

The case of main interest is that of a purely outgoing wave on the exit side of the barrier, which we may write in the form

$$\psi(x) = \frac{F}{\sqrt{K(x)}} \cdot \exp\left\{i\left[\int_b^x K(y)\, dy - \frac{\pi}{4}\right]\right\}, \qquad (6\text{•}4\text{–}1)$$

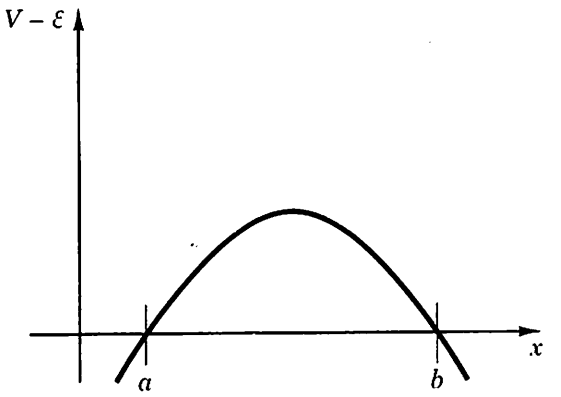

Figure 6•4–1. Smooth barrier potential.

Without loss in generality, we may assume that all phases are chosen such that F is real, in which case the probability current density to the right of the classical turning point is simply

$$j = \frac{\hbar}{M} \cdot F^2. \tag{6•4–2}$$

This current density must be equal to the current density (6•1–16) inside the barrier, which leads to the condition

$$i(CD^* - C^*D) = F^2. \tag{6•4–3}$$

With the wave function on each side of the classical turning point being complex, we need connection rules for both the real and the imaginary parts. The relation (6•3–17b) is evidently the connection rule for the real part. This implies that

$$D = F/2 \tag{6•4–4}$$

and that C is imaginary. Insertion of $D = F/2$ into (6•4–3) yields

$$C = -iF. \tag{6•4–5}$$

Hence, we obtain the overall complex connection rule across the classical turning point at $x = b$, the exit of a barrier:

$$\begin{aligned} &\frac{1}{\sqrt{\kappa(x)}}\left[\frac{1}{2}\exp\left(+\int_x^b \kappa dy\right) - i \cdot \exp\left(-\int_x^b \kappa dy\right)\right] \\ &\qquad \leftrightarrow \frac{1}{\sqrt{K(x)}} \cdot \exp\left\{i\left[\int_b^x K dy - \frac{\pi}{4}\right]\right\}. \end{aligned} \tag{6•4–6}$$

The imaginary part alone may be written

$$\frac{1}{\sqrt{\kappa(x)}}\exp\left(-\int_x^b \kappa dy\right) \leftrightarrow -\frac{1}{\sqrt{K(x)}} \cdot \sin\left[\int_b^x K dy - \frac{\pi}{4}\right]. \tag{6•4–7}$$

Note the absence of the factor 2, compared to (6•3–17b).

While (6•3–17b) is the connection rule between a standing wave and an evanescent wave that decays going into a barrier to the left, (6•4–7) is the

connection rule for a wave that *grows* going into a barrier to the left. If the barrier is to the right of a classical turning point at $x = a$, we obtain

$$\frac{1}{\sqrt{K(x)}} \cdot \sin\left[\int_x^a K dy - \frac{\pi}{4}\right] \leftrightarrow -\frac{1}{\sqrt{\kappa(x)}} \exp\left(+\int_a^x \kappa dy\right). \qquad (6\cdot4\text{–}8)$$

6.4.2 The Tunneling Probability

We are now ready to calculate the probability of a particle incident on the barrier from the left actually penetrating through the barrier. We work our way from the exit side of the barrier to the entry side. We assume that an outgoing wave of the form (6•4–1) is present to the right of the barrier, with an as-yet unknown real amplitude F. As we saw, this outgoing wave is connected to the complex superposition of left- and right-evanescent waves (6•4–6). We re-write this superposition by shifting the integration limits, which serve as reference planes, to the left classical turning point, $x = a$. This leads to the form

$$\psi = \frac{F}{\sqrt{\kappa(x)}}\left[\frac{\gamma}{2}\exp\left(+\int_a^x \kappa dy\right) - \frac{i}{\gamma} \cdot \exp\left(-\int_a^x \kappa dy\right)\right], \qquad (6\cdot4\text{–}9)$$

where

$$\gamma \equiv \exp\left(-\int_a^b \kappa dy\right) \qquad (6\cdot4\text{–}10)$$

is the attenuation factor of the amplitude of each of the evanescent waves inside the barrier, in the direction of evanescence.

The case of principal interest to us is that of a relatively opaque barrier, characterized by the condition

$$\gamma \ll 1. \qquad (6\cdot4\text{–}11)$$

In this limit, the right-evanescent term in (6•4–9) will dominate near the left turning point, and we may, to the first order, neglect the left-evanescent term. But according to (6•3–17a), this right-evanescent term is connected across the left classical turning point to a standing wave of the form (6•2–5), with an amplitude

$$A = -\frac{i}{\gamma} \cdot F. \qquad (6\cdot4\text{–}12)$$

If we write the cosine function in (6•2–5) as a superposition of an incident and a reflected plane wave, we see that the incident plane wave has the amplitude A specified by (6•4–12), corresponding to an incident probability current density

$$j^+ = \frac{\hbar}{M} \cdot |A|^2 = \frac{\hbar}{M} \cdot \frac{|F|^2}{\gamma^2}. \qquad (6\cdot4\text{–}13)$$

But the ratio of the transmitted current density (6•4–2) to the incident current density is, of course, the tunneling probability T:

$$T \equiv \frac{j_T}{j_I^+} = \frac{|F|^2}{|A|^2} = \gamma^2 = \exp\left(-2\int_a^b \kappa dy\right). \tag{6•4–14}$$

In our treatment, we assumed specifically that the potential changed smoothly through both classical turning points, so that the WKB connection rules had to be used at both ends of the tunnel. In several cases of practical interest this is not the case. It then becomes necessary to treat the discontinuous end(s) of the tunnel by the propagation matrix method developed in chapter 5. Problem 6.4–1, next, is an example.

◆ PROBLEM TO SECTION 6.4

#6•4-1: Tunneling through a Barrier with an Applied Voltage

In solid-state physics, one encounters the problem of the tunneling of electrons through a thin oxide layer between two metals, as a function of the voltage ΔV applied between the metals. A simple model of this problem is the tunneling through the trapezoidal barrier shown in **Fig. 6.4–2.**

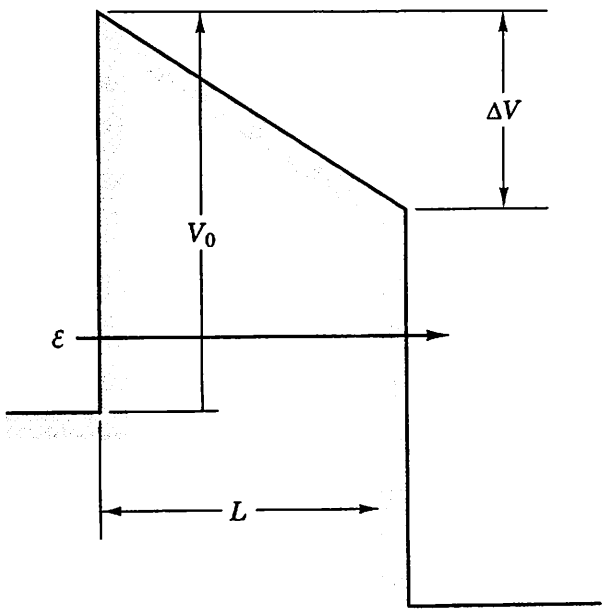

Figure 6•4–2. Trapezoidal barrier model for the tunneling of electrons through an oxide barrier between two metals.

Determine the tunneling probability as a function of ΔV, provided that ΔV remains less than $V_0 - \mathcal{E}$. For simplification, assume that L and V_0 are large enough that the total tunneling probability remains very small compared to unity.