

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  $\psi$  with the *incident* wave  $\psi_0$ :

$$\psi(\mathbf{r}) \cong \psi_1(\mathbf{r}) \cong \psi_0(\mathbf{r}) - \int G(\mathbf{r} - \mathbf{R})V(\mathbf{R})\psi_0(\mathbf{R}) d^3R. \quad (5\bullet6-12)$$

This is the **first-order Born approximation**. Physically, the approximation of replacing  $\psi$  by  $\psi_0$  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  $\psi_1$  into the integral, leading to a second-order wave function  $\psi_2$ . 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.

Quantum Mechanics: For Engineering,  
Materials Science & Applied Physics,  
Herbert Kroemer, ©Prentice Hall 1994

## WKB APPROXIMATION

### 6.1 WKB WAVE FUNCTIONS

#### 6.2 EXAMPLE: HARMONIC OSCILLATOR

#### 6.3 GENERAL CONNECTION RULES ACROSS A CLASSICAL TURNING POINT

#### 6.4 TUNNELING

### 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.<sup>1</sup>

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

<sup>1</sup>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.

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.,

$$\psi_{\pm}(x) = \frac{A}{\sqrt{K(x)}} \cdot \exp\left[\pm i \int^x K(y) dy\right], \quad (6\cdot1-1)$$

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

$$K(x) = \sqrt{\frac{2M}{\hbar^2} [\varepsilon - V(x)]} \quad \text{if} \quad \varepsilon > V. \quad (6\cdot1-2)$$

In the case of a constant potential, this is of course an exact solution of the Schrodinger 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

$$\frac{dj_{\pm}}{dx} = \frac{d}{dx} \left( \psi_{\pm}^* \frac{d\psi_{\pm}}{dx} - \psi_{\pm} \frac{d\psi_{\pm}^*}{dx} \right) = 0, \quad (6\cdot1-3)$$

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

$$\psi_{WKB}(x) = \frac{1}{\sqrt{K(x)}} \left\{ A \cdot \exp\left[+i \int^x K(y) dy\right] + B \cdot \exp\left[-i \int^x K(y) dy\right] \right\}, \quad (6\cdot1-4)$$

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

$$j = \frac{\hbar}{M} \cdot (|A|^2 - |B|^2). \quad (6\cdot1-5)$$

## 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

$$\psi'' = -\left[ K^2 + \frac{1}{2} \left( \frac{K''}{K} \right) - \frac{3}{4} \left( \frac{K'}{K} \right)^2 \right] \cdot \psi \quad (6\cdot1-6)$$

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

$$\varepsilon > V(x), \quad (6\cdot1-7)$$

to make sure that  $K(x)$  is real. The case  $\varepsilon < V(x)$  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 Schrodinger 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.,

$$\frac{1}{4} \left| 2 \left( \frac{K''}{K} \right) - 3 \left( \frac{K'}{K} \right)^2 \right| \ll |K|^2. \quad (6\cdot1-8)$$

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

$$\left| \frac{V''}{\varepsilon - V} + \frac{5}{4} \left( \frac{V'}{\varepsilon - V} \right)^2 \right| \cdot |\Lambda|^2 \ll 16\pi^2, \quad (6\cdot1-9)$$

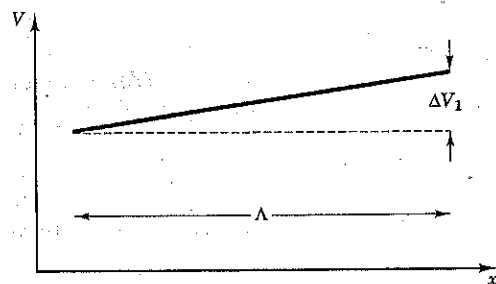
where  $\Lambda = 2\pi/K$  is the local de Broglie wavelength. Both (6•1-8) and (6•1-9) are complicated conditions. While they might in principle be satisfied by a mutual cancellation of the terms on the left-hand sides, this is of little importance in practice. We therefore impose the stronger condition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

$$\Delta V_1 \equiv |V' \cdot \Lambda| \ll \frac{8\pi}{\sqrt{5}} |\varepsilon - V| \approx 11.2 |\varepsilon - V| \quad (6\cdot1-10)$$

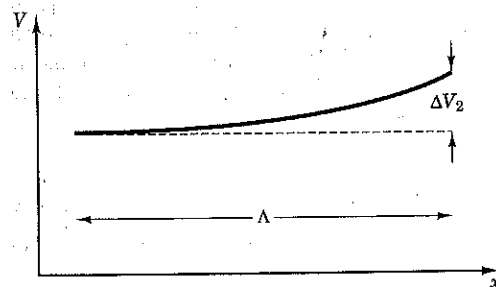
and

$$\Delta V_2 \equiv \frac{1}{2} |V'' \cdot \Lambda^2| \ll 8\pi^2 |\varepsilon - V| \approx 79.0 |\varepsilon - V|. \quad (6\cdot1-11)$$

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  $\Delta V_1$  represents the change in potential along one wavelength (**Fig. 6•1-1(a)**); similarly,  $\Delta V_2$  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



(a)



(b)

**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

$$|A(x)|^2 - |B(x)|^2 = \text{constant}. \quad (6.1-12)$$

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

$$\kappa(x) = \sqrt{\frac{2M}{\hbar^2} [V(x) - \mathcal{E}]} \text{ if } \mathcal{E} < V. \quad (6.1-13)$$

With this change, we obtain, instead of (6.1-4),

$$\psi_{\text{WKB}}(x) = \frac{1}{\sqrt{\kappa(x)}} \left\{ C \cdot \exp \left[ - \int^x \kappa(y) dy \right] + D \cdot \exp \left[ + \int^x \kappa(y) dy \right] \right\}. \quad (6.1-14)$$

The conditions (6.1-9) through (6.1-11) still hold, except that the wavelength  $\Lambda$  is replaced by

$$\Lambda' \rightarrow 2\pi/\kappa. \quad (6.1-15)$$

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

$$j = \frac{i\hbar}{M} \cdot (CD^* - C^*D), \quad (6.1-16)$$

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  $x \rightarrow +\infty$ , we must have  $D = 0$ , or else the wave function would become infinite there. Similarly, for  $x \rightarrow -\infty$ , 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.

## 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

$$V(x) = \frac{1}{2}M\omega^2x^2, \quad (6.2-1)$$

and we recall that the energy eigenvalues are then given by

$$\varepsilon_n = (n + \frac{1}{2})\hbar\omega, \quad (6.2-2)$$

where the  $n$  are the nonnegative integers. We will also need the classical turning points from (2.3-24), i.e.,

$$x_n = \sqrt{2n + 1} \cdot L, \quad (6.2-3)$$

where

$$L = \sqrt{\hbar/M\omega} \quad (6.2-4)$$

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

$$\psi(x) = \frac{2A}{\sqrt{K}} \cdot \cos \left[ \int_{-x_n}^x K dy - \alpha \right], \quad (6.2-5)$$

with a real amplitude  $A$  and a suitable phase angle  $\alpha$ . In (6.2-5), we have selected the phase angle  $\alpha$  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  $\alpha$  to the range

$$-\pi/2 < \alpha < +\pi/2. \quad (6.2-6)$$

For  $\varepsilon = \varepsilon_n$ , the local WKB wave number  $K$  in Eq. (6.1-2) in the classically allowed range  $|x| < x_n$  is given by

$$K(x) = \sqrt{\frac{2M}{\hbar^2}(\varepsilon_n - \frac{1}{2}M\omega^2x^2)} = \frac{1}{L^2} \sqrt{x_n^2 - x^2}. \quad (6.2-7)$$

For later use, we note that

$$K(0) = \frac{x_n}{L^2} = \frac{\sqrt{2n+1}}{L}. \quad (6.2-8)$$

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.<sup>2</sup> 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  $\pi$ , with the multiplier  $n/2$ :

$$\int_{-x_n}^0 K dx - \alpha = \frac{1}{L^2} \int_{-x_n}^0 \sqrt{x_n^2 - x^2} dx - \alpha = \frac{n}{2} \pi. \quad (6.2-9)$$

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

$$\begin{aligned} \int_{-x_n}^0 \sqrt{x_n^2 - x^2} dx &= \int_0^{+x_n} \sqrt{x_n^2 - x^2} dx = \frac{\pi}{4} \cdot x_n^2 \\ &= \frac{\pi}{4} \cdot (2n + 1) \cdot L^2. \end{aligned} \quad (6.2-10)$$

Here, in the last equality, we have used (6.2-3). Insertion into (6.2-9) yields

$$\boxed{\alpha = \frac{\pi}{4}}, \quad (6.2-11)$$

independent of the quantum number  $n$ , harmonic oscillator. This is the **WKB phase connection rule**. Inserted into (6.2-5), (6.2-11) gives

$$\psi(x) = \frac{2A}{\sqrt{K}} \cdot \cos \left[ \int_{-x_n}^x K dy - \frac{\pi}{4} \right]. \quad (6.2-12a)$$

<sup>2</sup>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

$$\psi(x) = \frac{2A'}{\sqrt{K}} \cdot \cos \left[ \int_x^{+x_n} K dy - \frac{\pi}{4} \right], \quad (6\cdot2-12b)$$

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<sup>3</sup>

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

$$\psi_n(0) = A_0 \frac{(-1)^{n/2} \sqrt{n!}}{2^{n/2} (n/2)!}, \quad (6\cdot2-13)$$

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

$$\psi_{WKB}(0) = \frac{2A}{\sqrt{K(0)}} \cdot \cos(n\pi/2) = A \cdot \frac{2(-1)^{n/2} \sqrt{L}}{(2n+1)^{1/4}}, \quad (6\cdot2-14)$$

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:

$$A = \frac{A_0}{\sqrt{L}} \cdot \frac{(2n+1)^{1/4}}{2 \cdot 2^{n/2}} \cdot \frac{\sqrt{n!}}{(n/2)!}. \quad (6\cdot2-15)$$

<sup>3</sup>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,  $Q \rightarrow \infty$ , 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,

$$\psi_n(Q) \rightarrow A_0 \frac{2^{n/2}}{\sqrt{n!}} \cdot Q^n \exp(-Q^2/2). \quad (6\cdot2-16)$$

where

$$Q = x/L. \quad (6\cdot2-17)$$

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

$$\psi_{WKB}(x) = \frac{C}{\sqrt{\kappa}} \cdot \exp \left[ - \int_{x_n}^x \kappa dx' \right]. \quad (6\cdot2-18)$$

The integral in the exponent has the value

$$\int_{x_n}^x \kappa dx' = - \frac{x_n^2}{2L^2} \cdot \ln \left[ \frac{x + (x^2 - x_n^2)^{1/2}}{x_n} \right] + \frac{x \cdot (x^2 - x_n^2)^{1/2}}{2L^2}. \quad (6\cdot2-19)$$

In the limit of large  $x$ , this goes over into

$$\begin{aligned} - \frac{x_n^2}{2L^2} \cdot \ln \left[ \frac{2x}{x_n} \right] + \frac{x^2}{2L^2} - \frac{x_n^2}{4L^2} + \dots = \\ -m \cdot \ln \left[ Q \sqrt{\frac{2}{m}} \right] + \frac{Q^2}{2} - \frac{m}{2} + \dots, \end{aligned} \quad (6\cdot2-20)$$

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

$$\frac{x_n^2}{2L^2} = m \equiv n + \frac{1}{2}. \quad (6\cdot2-21)$$

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

$$\kappa = \frac{1}{L^2} \sqrt{x^2 - x_n^2} \xrightarrow{x \rightarrow \infty} \frac{Q}{L}, \quad (6\cdot2-22)$$

we obtain the asymptotic relation

$$\psi_{WKB}(Q) \rightarrow C \sqrt{L} \cdot \left( \frac{2e}{m} \right)^{m/2} \cdot Q^n \exp \left( - \frac{Q^2}{2} \right). \quad (6\cdot2-23)$$

Equating (6·2-16) with (6·2-23) yields

$$C = \frac{A_0}{\sqrt{L}} \cdot \frac{1}{2^{1/4}} \cdot \frac{1}{\sqrt{n!}} \cdot \left( \frac{m}{e} \right)^{m/2}. \quad (6\cdot2-24)$$

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

$$\frac{C}{A} = \frac{2^{1/2}}{e^{1/4}} \cdot \left(\frac{2n+1}{e}\right)^{n/2} \cdot \frac{(n/2)!}{n!}. \quad (6\cdot2-25)$$

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.,

$$\lim_{n \rightarrow \infty} \frac{C}{A} = 1. \quad (6\cdot2-26)$$

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.

## GENERAL CONNECTION RULES ACROSS A CLASSICAL TURNING POINT

### 6.3.1 The Problem

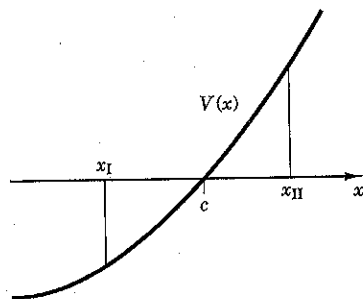
We now show that the phase and amplitude connection rules (6·2-11) and (6·2-26) for the harmonic oscillator remain applicable to the connection across the classical turning points of many other "well-behaved" potentials.

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

$$V(x) > \mathcal{E} \text{ for all } x > c, \quad (6\cdot3-1)$$

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

$$V_0(x) = V_{00} + \frac{1}{2}M\omega^2(x - x_0)^2. \quad (6\cdot3-2a)$$

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

$$\mathcal{E} = V_{00} + \hbar\omega \cdot \left(n + \frac{1}{2}\right). \quad (6\cdot3-2b)$$

---

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

$$C = A. \quad (6\cdot3-3)$$

### 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

$$V(x) = \begin{cases} \infty & \text{for } \{x < 0\} \\ eEx & \text{for } \{x > 0\} \end{cases}. \quad (6\cdot3-4)$$

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



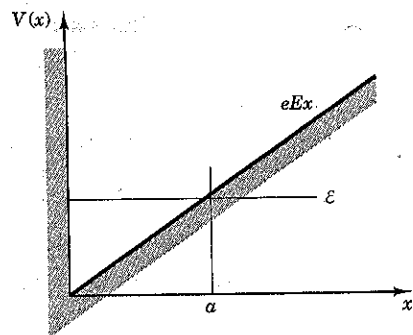


Figure 6-3-2. Potential energy for an electron in a uniform electric field at a potential wall.

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

$$\varepsilon_n = A_n \varepsilon_0, \quad n = 1, 2, 3, \dots \quad (6\cdot3-5)$$

where  $A_n$  is the  $n$ th root of the Airy function<sup>4</sup> and  $\varepsilon_0$  is the quantity

$$\varepsilon_0 = \left[ \frac{\hbar^2 (eE)^2}{2m_e} \right]^{1/3}, \quad (6\cdot3-6)$$

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 Schrodinger equation.

Along with the energy  $\varepsilon_0$ , a natural unit  $L$  of length may be associated with the problem, defined by the requirement

$$\varepsilon_0 = eEL = \frac{\hbar^2}{2m_e L^2}, \quad (6\cdot3-7)$$

which leads to

$$L = \left[ \frac{\hbar^2}{2m_e eE} \right]^{1/3}. \quad (6\cdot3-8)$$

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

$$\varepsilon_0 = 72.5 \text{ meV}; \quad L = 0.725 \text{ nm}. \quad (6\cdot3-9a,b)$$

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

<sup>4</sup>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  $\pi/2$ :

$$\int_0^a K(x) dx - \frac{\pi}{4} = (2n - 1) \cdot \frac{\pi}{2}. \quad (6\cdot3-10)$$

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

$$a = \frac{\varepsilon}{eE} = L \cdot \frac{\varepsilon}{\varepsilon_0}, \quad (6\cdot3-11)$$

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

$$K(x) = \sqrt{\frac{2m_e}{\hbar^2} (\varepsilon - eEx)} = \frac{1}{L^{3/2}} \sqrt{a - x}, \quad (6\cdot3-12)$$

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

$$\int_0^a K(x) dx = \frac{1}{L^{3/2}} \int_0^a \sqrt{a - x} dx = \frac{2}{3} \left( \frac{a}{L} \right)^{3/2} = \frac{2}{3} \left( \frac{\varepsilon}{\varepsilon_0} \right)^{3/2}. \quad (6\cdot3-13)$$

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

$$A_n = \left[ \frac{3\pi}{8} (4n - 1) \right]^{2/3}. \quad (6\cdot3-14)$$

The three lowest values are

$$A_1 = 2.321, \quad A_2 = 4.082, \quad A_3 = 5.517, \quad (6\cdot3-15a,b,c)$$

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

$$A_1 = 2.338, \quad A_2 = 4.088, \quad A_3 = 5.521. \quad (6\cdot3-16a,b,c)$$

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

$$\frac{2}{\sqrt{K}} \cdot \cos \left[ \int_x^c K dx' - \frac{\pi}{4} \right] \leftarrow \frac{1}{\sqrt{\kappa}} \cdot \exp \left[ - \int_c^x \kappa dx' \right], \quad (6\cdot3-17a)$$

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

$$\frac{2}{\sqrt{K}} \cdot \cos \left[ \int_x^c K dx' - \frac{\pi}{4} \right] \leftarrow \frac{1}{\sqrt{\kappa}} \cdot \exp \left[ - \int_c^x \kappa dx' \right]. \quad (6\cdot3-17b)$$

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.

## TUNNELING

### 6.4.1 The WKB Wave Function inside a Barrier

As long as we are dealing with infinitely thick classically forbidden barriers, 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

$$\psi(x) = \frac{F}{\sqrt{K(x)}} \cdot \exp \left\{ i \left[ \int_b^x K(y) dy - \frac{\pi}{4} \right] \right\}, \quad (6\cdot4-1)$$

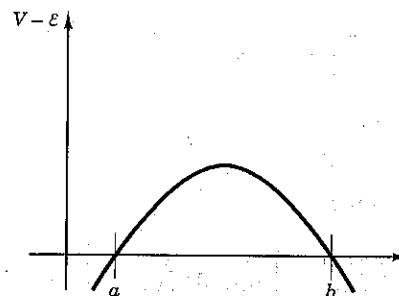


Figure 6·4-1. Smooth barrier potential.

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

$$j = \frac{\hbar}{M} \cdot F^2. \quad (6\cdot4-2)$$

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

$$i(CD^* - C^*D) = F^2. \quad (6\cdot4-3)$$

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

$$D = F/2 \quad (6\cdot4-4)$$

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

$$C = -iF. \quad (6\cdot4-5)$$

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

$$\frac{1}{\sqrt{\kappa(x)}} \left[ \frac{1}{2} \exp \left( + \int_x^b \kappa dy \right) - i \cdot \exp \left( - \int_x^b \kappa dy \right) \right] \leftrightarrow \frac{1}{\sqrt{K(x)}} \cdot \exp \left\{ i \left[ \int_b^x K dy - \frac{\pi}{4} \right] \right\}. \quad (6\cdot4-6)$$

The imaginary part alone may be written

$$\frac{1}{\sqrt{\kappa(x)}} \exp \left( - \int_x^b \kappa dy \right) \leftrightarrow \frac{1}{\sqrt{K(x)}} \cdot \sin \left[ \int_b^x K dy - \frac{\pi}{4} \right]. \quad (6\cdot4-7)$$

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

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

## 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 rewrite 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

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

where

$$\gamma \equiv \exp \left( - \int_a^b \kappa dy \right) \quad (6\cdot4-10)$$

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

$$\gamma \ll 1. \quad (6\cdot4-11)$$

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

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

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

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

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

$$T \equiv \frac{j_T}{j^+} = \frac{|F|^2}{|A|^2} = \gamma^2 = \exp \left( -2 \int_a^b \kappa dy \right). \quad (6\cdot4-14)$$

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  $\Delta V$  applied between the metals. A simple model of this problem is the tunneling through the trapezoidal barrier shown in Fig. 6·4-2.

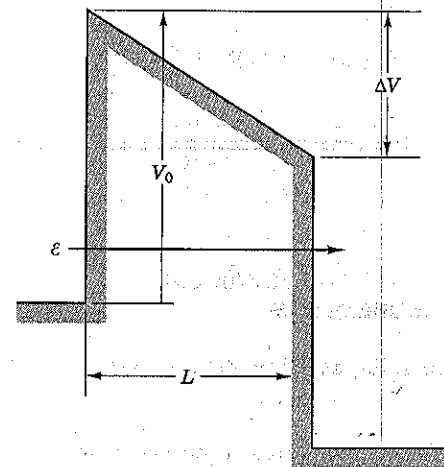


Figure 6·4-2. Trapezoidal barrier model for the tunneling of electrons through an oxide barrier between two metals.

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