Because of this symmetry, it is clear that if $\psi(x)$ is an eigenfunction, then the function $\psi(-x)$ is also an eigenfunction. The eigenfunctions, however, have been shown to be nondegenerate. Hence, these two functions must be linearly dependent, i.e., there must exist a number C such that the expression

$$\psi(-x) = C\psi(x) \tag{5-159}$$

is an identity in x. If the transformation $x \to -x$ is made once more in Eq. (5-159), the result is

$$\psi(x) = C\psi(-x) = C^2\psi(x),$$

whence $C = \pm 1$, and

$$\psi(-x) = \pm\psi(x). \tag{5-160}$$

Every eigenfunction for a bound state in a symmetric field $[u(x) = u(-x)]$ is therefore either an even or an odd function of x. This fact, which has already been noted in connection with Eqs. (5-109) and (5-110), is expressed by the statement that $\psi(x)$ has a definite *parity*. If $\psi(-x) = \psi(x)$, the parity of ψ is *even;* if $\psi(x) = -\psi(-x)$, it is *odd*.

If the system under study is invariant to the transformation $x \to -x$, then conclusions as to the energy levels, etc., cannot be influenced by the choice of which of the two directions along x is to be positive. In other words, if no feature of the environment of the particle, as expressed in the function $V(x)$, specifies a particular direction, then the eigenfunctions of nondegenerate states have a definite parity.

That these simple considerations are not trivial is apparent from the fact that the result $\langle x^{2m+1}\rangle = 0$ can be deduced immediately from parity considerations, without reference to the explicit form of ψ. In more complex situations, the concept of parity is of fundamental importance for the classification of quantum states.

5-13 The Wentzel-Kramers-Brillouin approximation. Only a few problems in quantum mechanics can be solved exactly, and approximation methods are therefore of great practical importance. We shall conclude this chapter on one-dimensional problems with a discussion of an approximate treatment, due to Wentzel, Kramers, and Brillouin.[1] This approach, commonly known as the *WKB method*, is also called the *classical approximation*, since it deals with situations in which $\hbar$ is small compared

[1] G. Wentzel, *Z. Physik* **38**, 518 (1926); H. A. Kramers, *Z. Physik* **39**, 828 (1926); L. Brillouin, *Compt. rend.* **183**, 24 (1926) and *J. phys. et radium* **7**, 353 (1926); R. E. Langer, *Phys. Rev.* **51**, 669 (1937).

to the action. The method leads to a quantization rule which is essentially the same as that of Wilson and Sommerfeld (Section 1-12).

The one-dimensional Schrödinger equation,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0,$$

can be written in the form

$$\frac{d^2\psi}{dx^2} + \frac{p^2}{\hbar^2}\psi = 0, \tag{5-161}$$

where p is the classical momentum at the point x:

$$p = \sqrt{2m[E - V(x)]}. \tag{5-162}$$

If the energy is high enough so that the wave length $\lambda = h/p$ is very short in the classical region, compared to the extent of this region, and if the potential function changes smoothly, then the "index of refraction" for the waves varies slowly. In the discussion of geometrical optics in Section 4-2, it has been shown that, under these circumstances, the wave function can be approximated by

$$\psi(x) = \phi(x)\exp\left[\pm\frac{i}{\hbar}\int^x p(x)\,dx\right], \tag{5-163}$$

where $\phi(x)$ is a slowly varying function [Eq. (4-12)]. This is the basis for the WKB method.

By straightforward substitution of the approximate solution (5-163) into the Schrödinger equation (5-161), the differential equation for the function $\phi(x)$ is obtained:

$$\frac{\hbar}{ip}\frac{d^2\phi}{dx^2} \pm \left(2\frac{d\phi}{dx} + \frac{1}{p}\frac{dp}{dx}\phi\right) = 0. \tag{5-164}$$

It is assumed that $\hbar/p$ is small, compared to the other dimensions of the problem, and that ϕ varies slowly. Hence, we neglect the first term in Eq. (5-164) and obtain

$$\frac{2}{\phi}\frac{d\phi}{dx} + \frac{1}{p}\frac{dp}{dx} = \frac{d}{dx}\ln(\phi^2 p) = 0, \tag{5-165}$$

which yields

$$\phi = Kp^{-1/2} \qquad (K = \text{a constant}). \tag{5-166}$$

The approximate wave function is therefore

$$\psi_{\text{WKB}} = Kp^{-1/2} \exp\left(\pm \frac{i}{\hbar} \int^x p\, dx\right). \tag{5-167}$$

The classical approximation is expected to hold in regions where the fractional change in p in one wavelength is small, that is, where

$$\left|\frac{p'\lambda}{p}\right| = \left|\frac{\hbar p'}{p^2}\right| \ll 1. \tag{5-168}$$

The WKB approximation is valid under similar conditions: ψ_{WKB} satisfies the differential equation

$$\frac{d^2\psi}{dx^2} + \left[\frac{p^2}{\hbar^2} - Q\right]\psi = 0, \tag{5-169}$$

where

$$Q = \frac{3}{4}\left(\frac{p'}{p}\right)^2 - \frac{p''}{2p}, \tag{5-170}$$

and Eq. (5–169) is an approximation to Eq. (5–161) if

$$|Q| \ll \frac{p^2}{\hbar^2},$$

or

$$\left|\frac{\hbar p'}{p^2}\right| \sqrt{\tfrac{3}{4} - \tfrac{1}{2}(pp''/p'^2)} \ll 1. \tag{5-171}$$

In nearly all practical cases, this condition is equivalent to (5–168). The condition will, in general, be fulfilled for problems where the mass is large, the energy high, and the potential smooth. However, it is clear that the WKB solutions cannot be valid near a classical turning point, where the momentum is zero.

We shall now consider the problem of finding the wave function for a particle in a given potential well. Let $V(x)$ have the form shown in Fig. 5–21. In region 1, the wave function decreases exponentially for $x \to -\infty$, and since p is imaginary $[V(x) > E]$, ψ is approximated by

$$\psi_1 = K_1|p|^{-1/2} \exp\left(\frac{1}{\hbar}\int_{x_1}^x |p|\, dx\right). \tag{5-172}$$

In region 2, ψ is oscillatory:

$$\psi_2 = K_2 p^{-1/2} \exp\left(\frac{i}{\hbar}\int^x p\, dx\right) + K_2' p^{-1/2} \exp\left(-\frac{i}{\hbar}\int^x p\, dx\right). \tag{5-173}$$

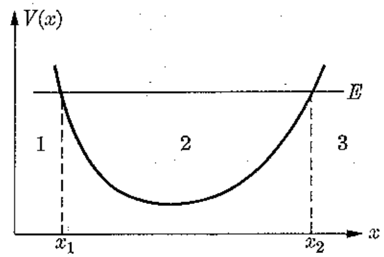

FIG. 5–21. Potential well for discussion of the WKB approximation.

In region 3, the wave function decreases exponentially for $x \to \infty$:

$$\psi_3 = K_3|p|^{-1/2} \exp\left(-\frac{1}{\hbar}\int_{x_2}^x |p|\, dx\right). \tag{5-174}$$

The regions of validity for these forms of the wave function are separated by the classical turning points, near which the approximation fails. However, since ψ_1, ψ_2, and ψ_3 are all approximations to the same function ψ, the constants K_1, K_2, K_2', and K_3 cannot all be arbitrary. In order to evaluate the constants and to connect the approximate solutions in the three regions, we assume that the potential energy function is approximately linear in the neighborhood of x_1 and x_2. Thus, at x_1, we write

$$V(x) \approx E - A(x - x_1), \tag{5-175}$$

and at x_2,

$$V(x) \approx E + B(x - x_2). \tag{5-176}$$

In the neighborhood of x_1, the Schrödinger equation (5–161) then becomes

$$\frac{d^2\psi}{dx^2} + \frac{2mA}{\hbar^2}(x - x_1)\psi = 0, \tag{5-177}$$

and near x_2,

$$\frac{d^2\psi}{dx^2} - \frac{2mB}{\hbar^2}(x - x_2)\psi = 0. \tag{5-178}$$

In Eq. (5–177), we now change the variable to

$$z = -\left(\frac{2mA}{\hbar^2}\right)^{1/3}(x - x_1), \tag{5-179}$$

and obtain

$$\frac{d^2\psi}{dz^2} - z\psi = 0. \tag{5-180}$$

Similarly, the substitution

$$z = \left(\frac{2mB}{\hbar^2}\right)^{1/3} (x - x_2) \tag{5–181}$$

reduces Eq. (5–178) to the same form (5–180).

The solutions of the differential equation (5–180) are the *Airy functions.*[1] We require a function which vanishes asymptotically for large positive z ($z > 0$ corresponds to $x < x_1$ and $x > x_2$). Such a function is

$$Ai(z) = \frac{1}{\pi}\int_0^\infty \cos\left(\frac{s^3}{3} + sz\right) ds, \tag{5–182}$$

which, for large $|z|$, has the asymptotic forms

$$Ai(z) \sim \frac{1}{2\sqrt{\pi}\, z^{1/4}} \exp\left(-\tfrac{2}{3}z^{3/2}\right) \qquad (z > 0), \tag{5–183}$$

$$Ai(z) \sim \frac{1}{\sqrt{\pi}\,(-z)^{1/4}} \sin\left[\tfrac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] \qquad (z < 0). \tag{5–184}$$

[See Fig. 5–22 for a graph of $Ai(z)$].

If the energy E is large enough, the regions of validity of the linear approximations (5–175) and (5–176) contain many wavelengths. The

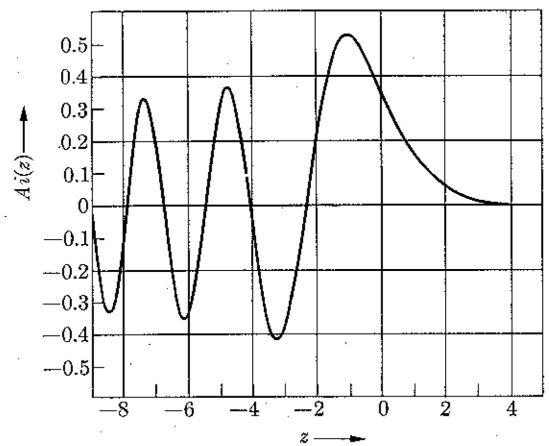

FIG. 5–22. The Airy function $Ai(z) = (1/\pi)\int_0^\infty \cos(s^3/3 + sz)\, ds$.

[1] H. and B. S. Jeffreys, *Methods of Mathematical Physics.* Cambridge: Cambridge University Press, 1956, 3rd ed., Section 17.07. J. C. P. Miller, *The Airy Integral* (British Association for the Advancement of Science, Mathematical Tables, Part-Volume B). Cambridge: Cambridge University Press, 1946.

function $Ai(z)$, which passes smoothly through the turning point, provides the required connections among the approximate forms (5–172), (5–173), and (5–174).

In the neighborhood of x_1, we have

$$p^2 \approx 2mA(x - x_1) = -(2mA\hbar)^{2/3} z,$$

and

$$\frac{1}{\hbar}\int_{x_1}^x |p|\, dx = \left(\frac{2mA}{\hbar^2}\right)^{1/3} \int_{x_1}^x \sqrt{z}\, dx = -\int_0^z \sqrt{z}\, dz = -\tfrac{2}{3}z^{3/2}. \tag{5–185}$$

Similarly,

$$\frac{1}{\hbar}\int_{x_1}^x p\, dx = \left(\frac{2mA}{\hbar^2}\right)^{1/3} \int_{x_1}^x \sqrt{-z}\, dx = -\int_0^z \sqrt{-z}\, dz = \tfrac{2}{3}(-z)^{3/2},$$

and comparison with Eqs. (5–183) and (5–184) shows that the function approximated to the left of x_1 by

$$\psi_1 \approx |p|^{-1/2} \exp\left(\frac{1}{\hbar}\int_{x_1}^x |p|\, dx\right) \qquad (x < x_1) \tag{5–186}$$

has, on the right, the approximation

$$\psi \approx 2p^{-1/2} \sin\left(\frac{1}{\hbar}\int_{x_1}^x p\, dx + \frac{\pi}{4}\right) \qquad (x > x_1). \tag{5–187}$$

A similar analysis in the neighborhood of point x_2 shows that the function approximated to the right of x_2 by

$$\psi_3 = |p|^{-1/2} \exp\left(-\frac{1}{\hbar}\int_{x_2}^x |p|\, dx\right) \qquad (x > x_2), \tag{5–188}$$

is approximated in region 2 by

$$\psi \approx 2p^{-1/2} \sin\left(\frac{1}{\hbar}\int_x^{x_2} p\, dx + \frac{\pi}{4}\right) \qquad (x < x_2). \tag{5–189}$$

The functions (5–187) and (5–189) are the continuations, into the classical region, of the functions (5–186) and (5–188), respectively, which have the proper behavior at $x = \pm\infty$. Now if ψ_1 and ψ_3 are approximations to the same eigenfunction ψ, they must be the same except perhaps for a constant multiplier:

$$\sin\left(\frac{1}{\hbar}\int_{x_1}^x p\, dx + \frac{\pi}{4}\right) = C \sin\left(\frac{1}{\hbar}\int_x^{x_2} p\, dx + \frac{\pi}{4}\right). \tag{5–190}$$

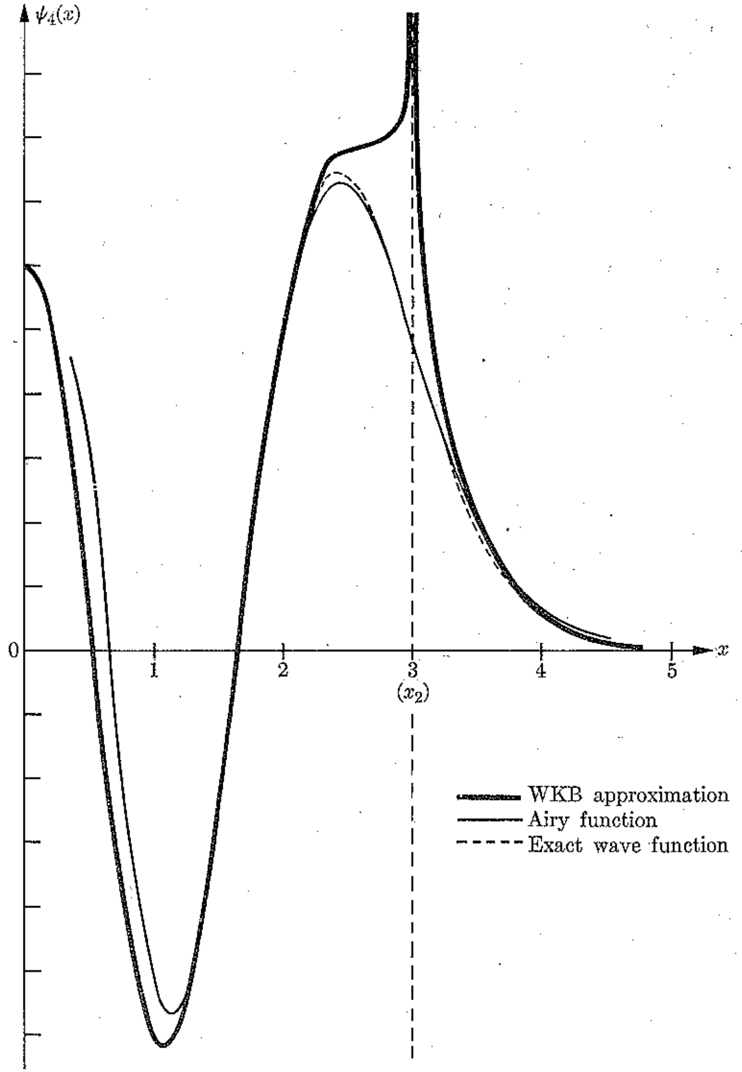

FIG. 5–23. WKB approximation to the harmonic-oscillator wave function in the state $n = 4$. To the accuracy of the graph, the WKB wave function (heavy line) coincides with the exact wave function (broken line) in the interior of the well. Near the classical turning point $x_2 = 3$, the WKB approximation breaks down. The Airy function (light line) coincides with the exact wave function at x_2 and connects the WKB approximations in the classical and non-classical regions. At small and large x, the Airy function deviates from the exact wave function.

Setting $\int_{x_1}^{x} = \int_{x_1}^{x_2} - \int_{x}^{x_2}$, we require that the expression

$$\sin\left(\frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx - \frac{1}{\hbar}\int_{x}^{x_2} p\,dx + \frac{\pi}{4}\right) = C\sin\left(\frac{1}{\hbar}\int_{x}^{x_2} p\,dx + \frac{\pi}{4}\right),$$

be an identity in x. This condition is satisfied only if

$$\frac{1}{\hbar}\int_{x_1}^{x_2} p\,dx = (n + \tfrac{1}{2})\pi \qquad (n \text{ an integer}); \tag{5–191}$$

the constant C is then equal to $(-1)^n$.

The (unnormalized) WKB approximation to the bound-state wave function is therefore

$$\psi_{\text{WKB}} = \begin{cases} (-)^n|p|^{-1/2}\exp\left(-\frac{1}{\hbar}\int_{x}^{x_1}|p|\,dx\right) & (x < x_1), \\ (-)^n 2p^{-1/2}\sin\left(\frac{1}{\hbar}\int_{x_1}^{x} p\,dx + \frac{\pi}{4}\right) & (x_1 < x < x_2), \\ |p|^{-1/2}\exp\left(-\frac{1}{\hbar}\int_{x_2}^{x}|p|\,dx\right) & (x_2 < x). \end{cases} \tag{5–192}$$

(Note that the approximate wave function for the nth bound state has $n + 1$ zeros.)

The WKB approximation to the state ψ for the harmonic oscillator is compared to the correct wave function in Fig. 5–23.

The condition (5–191) can be written

$$\oint p\,dx = (n + \tfrac{1}{2})h. \tag{5–193}$$

The symbol $\oint$ denotes the integral taken over a complete cycle of the classical motion, i.e., the area included by the path of the representative point in the p–x plane. This is the Wilson-Sommerfeld condition [Eq. (1–43)], except that n is replaced by $n + 1/2$. Since the classical approximation is reliable only when n is large, this modification is not of great significance.

5–14 Penetration of a potential barrier; WKB approximation. The penetration of a square potential barrier has been discussed in Section 5–2. For a barrier of more complicated shape, the Schrödinger equation cannot usually be solved exactly, and the WKB approximation is often suited for the problem. The wave function is oscillatory outside the barrier and has exponential character in the nonclassical region. In the approximate wave functions (5–192), the exponentially increasing solution in the nonclassical region was discarded because it violates the boundary conditions for ψ at $\pm\infty$. In the present case, however, the nonclassical region is of finite width, and both exponential solutions must be included. We require therefore a second connection formula.

We use the second solution of the differential equation (5–180), which is the Airy function

$$Bi(z) = \frac{1}{\pi}\int_0^\infty \left[e^{-sz-(1/3)s^3} + \sin\left(\frac{s^3}{3} + sz\right)\right] ds, \qquad (5\text{–}194)$$

with the asymptotic forms

$$Bi(z) \sim \frac{1}{\sqrt{\pi}\, z^{1/4}} \exp\left(\tfrac{2}{3}z^{3/2}\right) \qquad (z > 0), \qquad (5\text{–}195)$$

$$Bi(z) \sim \frac{1}{\sqrt{\pi}\,(-z)^{1/4}} \cos\left[\tfrac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] \qquad (z < 0). \qquad (5\text{–}196)$$

An argument which follows the same lines as that of the preceding section leads to the connection formula linking an increasing exponential solution in region 1 to an oscillatory solution in region 2 (Fig. 5–24):

$$\psi_{\text{WKB}} = \begin{cases} |p|^{-1/2} \exp\left(\dfrac{1}{\hbar}\displaystyle\int_x^{x_1} |p|\, dx\right) & (x < x_1), \\ p^{-1/2} \cos\left(\dfrac{1}{\hbar}\displaystyle\int_{x_1}^{x} p\, dx + \dfrac{\pi}{4}\right) & (x > x_1). \end{cases} \qquad (5\text{–}197)$$

A potential barrier of arbitrary shape is indicated in Fig. 5–25. We assume that a beam of particles is incident from the left. In region 3, the wave function for the transmitted particles is of the form

$$\psi_3 = Ap^{-1/2} \exp i\left(\frac{1}{\hbar}\int_{x_2}^{x} p\, dx + \frac{\pi}{4}\right) \qquad (x > x_2), \qquad (5\text{–}198)$$

where the phase factor $e^{i\pi/4}$ has been included to facilitate the application of Eq. (5–197). In terms of trigonometric functions, ψ_3 can be written

$$\psi_3 = Ap^{-1/2}\left[\cos\left(\frac{1}{\hbar}\int_{x_2}^{x} p\, dx + \frac{\pi}{4}\right) + i \sin\left(\frac{1}{\hbar}\int_{x_2}^{x} p\, dx + \frac{\pi}{4}\right)\right]. \qquad (5\text{–}199)$$

The connecting wave function of exponential type in region 2 is obtained by comparison with Eqs. (5–197) and (5–192):

$$\psi_2 = A|p|^{-1/2}\left[\exp\left(\frac{1}{\hbar}\int_x^{x_2} |p|\, dx\right) + \frac{i}{2}\exp\left(-\frac{1}{\hbar}\int_x^{x_2} |p|\, dx\right)\right]. \qquad (5\text{–}200)$$

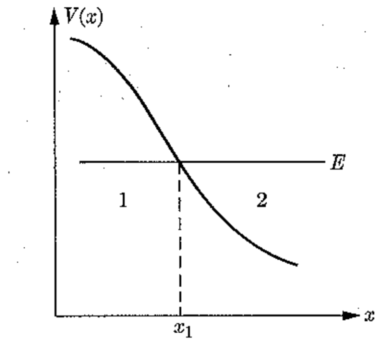

FIG. 5–24. Potential near the classical turning point x_1 at the edge of a barrier.

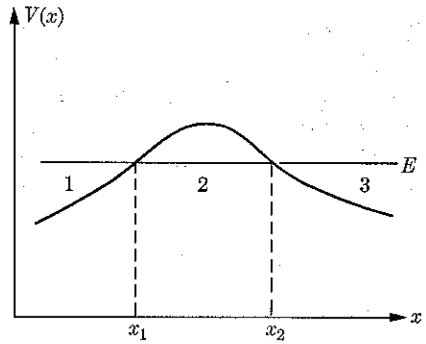

FIG. 5–25. Potential barrier.

In order to find the appropriate wave function in region 1, we rewrite the integrals in the last expression, using (see Fig. 5–25)

$$\int_x^{x_2} |p|\, dx = \int_{x_1}^{x_2} |p|\, dx - \int_{x_1}^{x} |p|\, dx,$$

and introducing the definition

$$T = \exp\left(-\frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V - E)}\, dx\right), \qquad (5\text{–}201)$$

so that Eq. (5–200) becomes

$$\psi_2 = A|p|^{-1/2}\left[T^{-1} \exp\left(-\frac{1}{\hbar}\int_{x_1}^{x} |p|\, dx\right) + \frac{i}{2}\, T \exp\left(\frac{1}{\hbar}\int_{x_1}^{x} |p|\, dx\right)\right]. \qquad (5\text{–}202)$$

By comparison with Eqs. (5–192) and (5–197), the connecting oscillatory wave function in region 1 is now seen to be

$$\psi_1 = Ap^{-1/2}\left[2T^{-1} \sin\left(\frac{1}{\hbar}\int_x^{x_1} p\, dx + \frac{\pi}{4}\right) + \frac{i}{2}\, T \cos\left(\frac{1}{\hbar}\int_x^{x_1} p\, dx + \frac{\pi}{4}\right)\right]. \qquad (5\text{–}203)$$

It is convenient to rewrite this expression in terms of exponentials:

$$\psi_1 = \frac{A}{ip^{1/2}}\left\{(T^{-1} - \tfrac{1}{4}T) \exp\left[i\left(\frac{1}{\hbar}\int_x^{x_1} p\, dx + \frac{\pi}{4}\right)\right] - (T^{-1} + \tfrac{1}{4}T) \exp\left[-i\left(\frac{1}{\hbar}\int_x^{x_1} p\, dx + \frac{\pi}{4}\right)\right]\right\}. \qquad (5\text{–}204)$$

The first term in the braces is recognized as a wave moving to the left, and hence represents the reflected wave, while the second term represents the incoming wave, which moves to the right.

The constant A can be adjusted for unit incoming current, so that the absolute magnitude of the amplitude of the incoming wave is $v^{-1/2}$. Then

$$A = \frac{\sqrt{m}}{T^{-1} + \frac{1}{4}T}. \tag{5–205}$$

With this value for A, the amplitude of the reflected wave has the magnitude

$$v^{-1/2}\,\frac{1 - T^2/4}{1 + T^2/4}. \tag{5–206}$$

The transmitted wave [Eq. (5–198)] has the amplitude

$$Ap^{-1/2} = v^{-1/2}\,\frac{T}{1 + T^2/4}. \tag{5–207}$$

The reflection coefficient R is defined as the ratio of reflected to incident wave amplitudes:

$$|R| = \frac{1 - T^2/4}{1 + T^2/4}. \tag{5–208}$$

The square of the reflection coefficient is equal to the fraction of the incident current that is reflected.

The transmission coefficient is the ratio of transmitted to incident wave amplitudes:

$$|\text{Trans. coeff.}| = \frac{T}{1 + T^2/4}. \tag{5–209}$$

It is consistent with the error of the WKB approximation to neglect powers of T higher than the first, so that

$$|\text{Trans. coeff.}| \approx T = \exp\left\{-\frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m[V(x) - E]}\,dx\right\} \qquad (T \ll 1). \tag{5–210}$$

To the same approximation,

$$|R|^2 \approx 1 - T^2. \tag{5–211}$$

As an example of the application of Eq. (5–210) for the transmission coefficient, let us consider the cold emission of electrons from a metal. In the absence of an external electric field, the electrons are bound by a po-

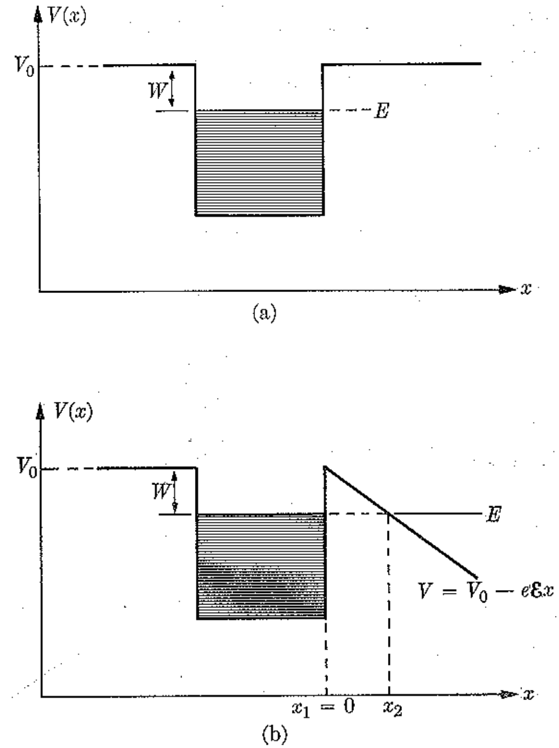

FIG. 5–26. Potential for electrons in a metal. (a) No external field. (b) With external field $\mathcal{E}$.

tential, as shown in Fig. 5–26(a). The lower levels in the well are filled, according to the Pauli exclusion principle (Chapter 12). The work function W is the energy required to remove an electron from the highest occupied state.

When an external electric field $\mathcal{E}$ is applied to the metal, the potential at the surface takes the form indicated in Fig. 5–26(b). Now the potential barrier has a finite width, and electrons are able to escape. The variation of cold emission with work function and applied field is easily obtained from Eq. (5–210). We set $x_1 = 0$, and find x_2 as follows [cf. Fig. 5–26(b)]:

$$V_0 - e\mathcal{E}x_2 = V_0 - W$$

$$x_2 = \frac{W}{e\mathcal{E}}.$$

Also,

$$V - E = V_0 - e\mathcal{E}x - E = W - e\mathcal{E}x.$$

The transmission probability therefore is

$$T^2 = \exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V-E)}\, dx\right)$$

$$= \exp\left(-\frac{2}{\hbar}\int_{0}^{W/e\mathcal{E}} \sqrt{2m(W-e\,\mathcal{E}x)}\, dx\right)$$

$$= \exp\left(-\frac{4}{3}\,\frac{\sqrt{2m}}{\hbar}\,\frac{W^{3/2}}{e\mathcal{E}}\right). \tag{5-212}$$

This expression is in qualitative agreement with experiment.

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Problems

5-1. Discuss the function ψ_2 [Eq. (5-15)] for the case $E > V_0$.

5-2. Calculate the probability current for the wave function (5-27) and show that it is continuous at each boundary of the potential barrier. Construct a solution of this problem which is an even function of $(x - a/2)$ and draw a graph of $|\psi|^2$ for $E = (1/2)V_0$. What is the amplitude of ψ at $x = a/2$? Study the dependence of $|\psi(a/2)|^2/|\psi(\infty)|^2$ on E.

5-3. Derive relations analogous to (5-31) and (5-33) for the quantity $|R|^2$ as a function of E, and prove that $|R|^2 + |T|^2 = 1$.

5-4. Consider a step potential barrier, as shown in Fig. 5-27. Calculate the transmission coefficient $|T|^2$ and the reflection coefficient $|R|^2$ as functions of the parameter d. What values of d give maximum and minimum transmission?

5-5. Carry out the details of the calculation of ψ for a particle of positive total energy in the potential well (5-34) and draw a graph of the transmission coefficient as a function of E.

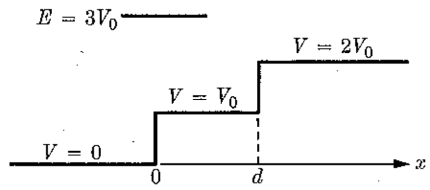

FIG. 5-27. The step potential of Problem 5-4.

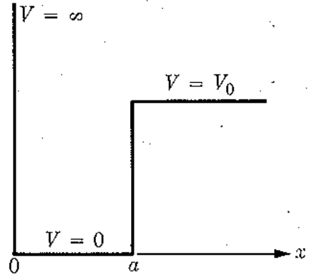

FIG. 5-28. The potential well of Problem 5-6.

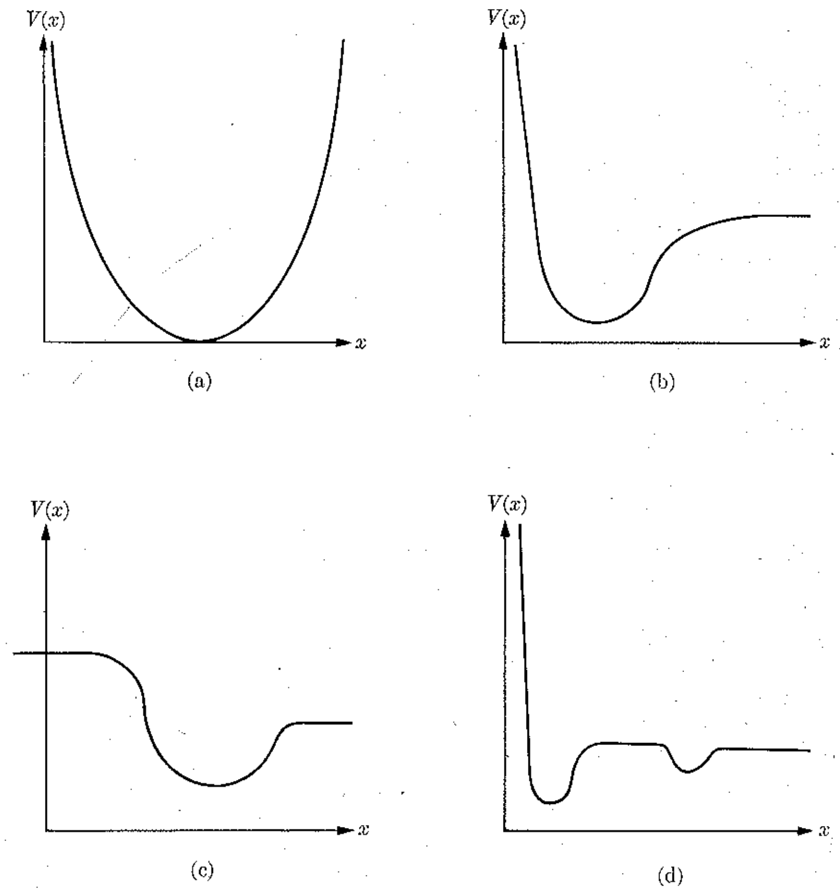

FIG. 5-29. Potential energy curves for Problem 5-10.