Lecture 6

Phys 521

WKB approximation

Review geometric optics limit in 1-d

$$\psi(x,t) = A(x,t)\, e^{\frac{i}{\hbar} S(x,t)} \quad , \quad P(x,t) = A^2(x,t)$$

$$0 = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi - i\hbar\frac{\partial\psi}{\partial t}$$

$$= e^{iS/\hbar}\Bigg(A\underbrace{\left(\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V + \frac{\partial S}{\partial t}\right)}_{=0 \text{ (H-J equation)}} - \frac{\hbar^2}{2m}\frac{\partial^2 A}{\partial x^2}$$

← quantum potential

$$- i\hbar\underbrace{\left(\frac{1}{m}\frac{\partial A}{\partial x}\frac{\partial S}{\partial x} + \frac{1}{2m}A\frac{\partial^2 S}{\partial x^2} + \frac{\partial A}{\partial t}\right)}_{\frac{1}{2A}\left(\frac{\partial P}{\partial t} + \frac{1}{m}\frac{\partial}{\partial x}\left(P\frac{\partial S}{\partial x}\right)\right)}\Bigg)$$

Stationary states: $S(x,t) = W(x) - Et$, $\frac{\partial P}{\partial t} = 0$

- W real $\Leftrightarrow$ classically allowed regions
- Real and imaginary parts define two equations
- W imaginary $\Leftrightarrow$ classically forbidden regions

→ In both cases, can get an expansion in $\hbar$

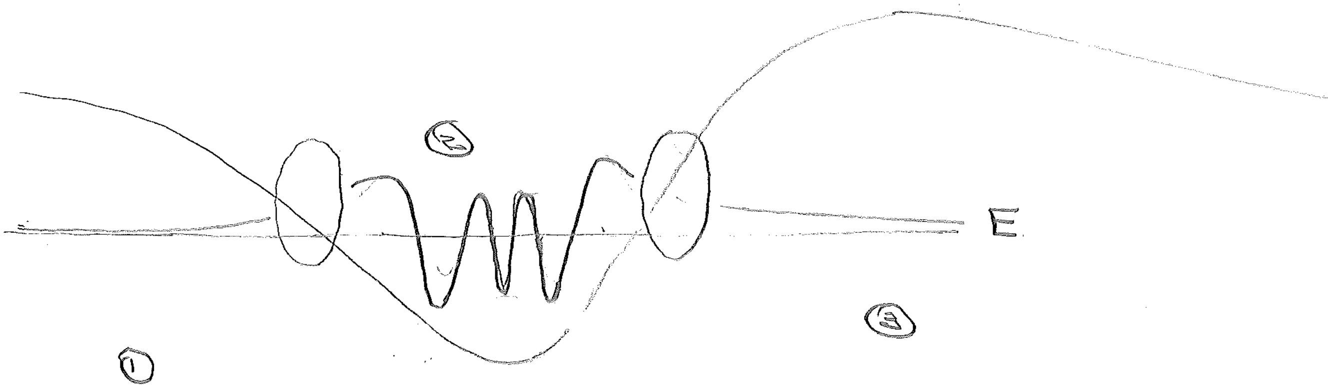
[What mean? $\lambda = h/p \ll$ (scale of variation)]

WKB approximation: $\psi(x,t) = \underbrace{\sqrt{P(x)}\, e^{\frac{i}{\hbar}W(x)}}_{\varphi(x)}\, e^{-\frac{i}{\hbar}Et}$

(1) $\left(\frac{dW}{dx}\right)^2 = 2m\left(E - V(x)\right)$

(2) $\frac{d}{dx}\left(P\frac{dW}{dx}\right) = 0 \Rightarrow P \propto \frac{1}{dW/dx}$

Validity:
$\frac{\hbar^2}{2m}\left|\frac{A''}{A}\right| \ll \frac{1}{2m}(W')^2 = \frac{\hbar^2 k^2}{2m}$
$\left|\frac{A''}{A}\right| = \left|\frac{1}{2}\frac{P''}{P} - \frac{1}{4}\frac{P'^2}{P^2}\right| \sim \left(\frac{k'}{k}\right)^2$
$\lambda\left|\frac{k'}{k}\right| \ll 1$



Region 2: $k^2(x) \equiv \frac{2m(E - V(x))}{\hbar^2}$ $\qquad \frac{1}{\hbar}W' = \pm k$
$(E > V(x))$

$$\varphi(x) = \frac{1}{\sqrt{k(x)}} \exp\left(\pm i \int^x dx'\, k(x')\right)$$

Region 1: $p^2(x) \equiv \frac{2m}{\hbar^2}\left(V(x) - E\right)$ $\qquad \frac{1}{\hbar}W' = \pm i p$
$(E < V(x))$

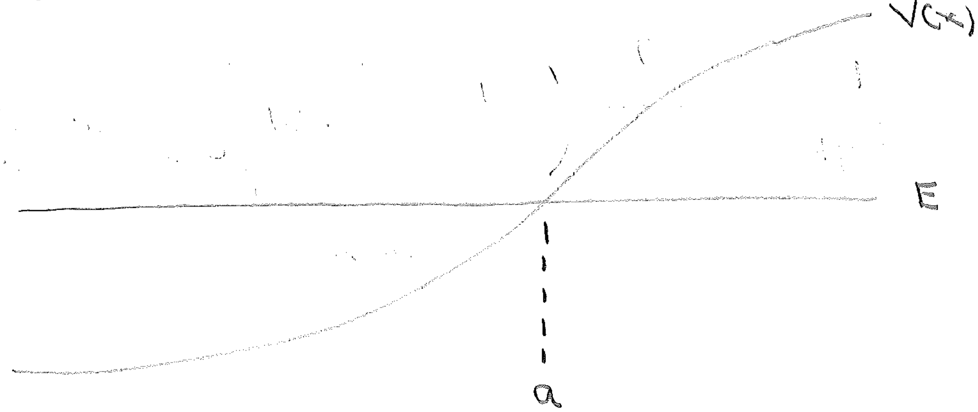
$$\varphi(x) = \frac{1}{\sqrt{p(x)}} \exp\left(\pm \int^x dx'\, p(x')\right)$$

Connection formulae:

① Come from linear approximation to potential near turning point. Not good near extrema.

② These are correspondences. Only double arrows are implications.

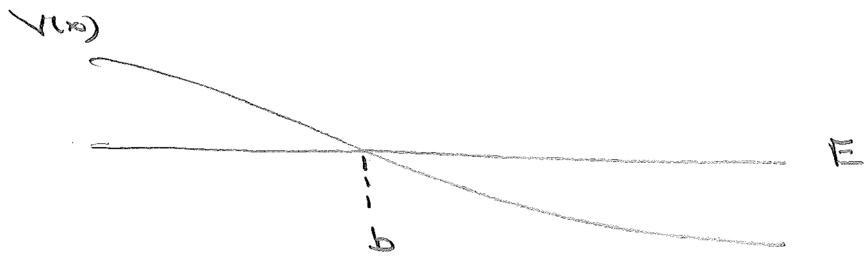
Turning point to right of classical region



$$\frac{2}{\sqrt{k}}\cos\left(\int_x^a dx'\,k(x') - \frac{\pi}{4}\right) \longleftrightarrow \frac{1}{\sqrt{p}}\exp\left(-\int_a^x dx'\,p(x')\right)$$

$$\frac{1}{\sqrt{k}}\sin\left(\int_x^a dx'\,k(x') - \frac{\pi}{4}\right) \longleftrightarrow -\frac{1}{\sqrt{p}}\exp\left(+\int_a^x dx'\,p(x')\right)$$

Turning point to left of classical region

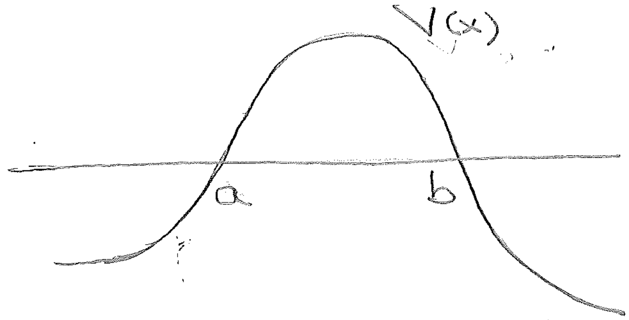


$$\frac{1}{\sqrt{p}}\exp\left(-\int_x^b dx'\,p(x')\right) \longleftrightarrow \frac{2}{\sqrt{k}}\cos\left(\int_b^x dx'\,k(x') - \frac{\pi}{4}\right)$$

$$-\frac{1}{\sqrt{p}}\exp\left(\int_x^b dx'\,p(x')\right) \longleftrightarrow \frac{1}{\sqrt{k}}\sin\left(\int_b^x dx'\,k(x') - \frac{\pi}{4}\right)$$

Transmission through a barrier

Ⓐ



$$x<a \qquad \varphi(x) = \frac{A}{\sqrt{k(x)}} \exp\left(i\int_a^x dx\, k(x)\right) + \frac{B}{\sqrt{k(x)}} \exp\left(-i\int_a^x dx\, k(x)\right)$$

$$= \frac{\overbrace{A e^{-i\pi/4}}^{A'}}{\sqrt{k}} \exp\left[-i\left(\int_x^a dx\, k - \frac{\pi}{4}\right)\right]$$

$$+ \frac{\overbrace{B e^{+i\pi/4}}^{B'}}{\sqrt{k}} \exp\left[+i\left(\int_x^a dx\, k - \frac{\pi}{4}\right)\right]$$

Note change of order of integration limits

$$= (A'+B') \frac{1}{\sqrt{k}} \cos\left(\int_x^a dx\, k - \frac{\pi}{4}\right)$$

$$- i(A'-B') \frac{1}{\sqrt{k}} \sin\left(\int_x^a dx\, k - \frac{\pi}{4}\right)$$

$$\xrightarrow[a<x<b]{} \frac{A'+B'}{2} \frac{1}{\sqrt{p}} \exp\left(-\int_a^x dx\, p\right)$$

$$+ i(A'-B') \frac{1}{\sqrt{p}} \exp\left(\int_a^x dx\, p\right)$$

use $\displaystyle\int_a^x dx\, p = \underbrace{\int_a^b dx\, p}_{\mu} - \int_x^b dx\, p$

$$\mu \equiv \int_a^b dx\, p(x)$$

$$= \frac{A'+B'}{2} e^{-\mu} \frac{1}{\sqrt{p}} \exp\left(\int_x^b dx\, p\right)$$

$$+ i(A'-B') e^{\mu} \frac{1}{\sqrt{p}} \exp\left(-\int_x^b dx\, p\right)$$

$$\frac{1}{2i}e^{i(\;)} - \frac{1}{2i}e^{-i(\;)}$$

$$\xrightarrow[x>b]{} -\frac{A'+B'}{2}\, e^{-\mu}\, \frac{1}{\sqrt{k}} \sin\left(\int_b^x dx\, k - \frac{\pi}{4}\right)$$

$$= +2i(A'-B')\, e^{\mu}\, \frac{1}{\sqrt{k}} \underbrace{\cos\left(\int_b^x dx\, k - \frac{\pi}{4}\right)}_{\frac{1}{2}e^{i(\;)} + \frac{1}{2}e^{-i(\;)}}$$

$$= \frac{1}{\sqrt{k}} \exp\left[i\left(\int_b^x dx\, k - \frac{\pi}{4}\right)\right]\left(+i(A'-B')\, e^{\mu} - \frac{A'+B'}{4i}\, e^{-\mu}\right)$$

$$+ \frac{1}{\sqrt{k}} \exp\left[-i\left(\int_b^x dx\, k - \frac{\pi}{4}\right)\right]\left(+i(A'-B')\, e^{\mu} + \frac{A'+B'}{4i}\, e^{-\mu}\right)$$

$$A'\left(+ie^{\mu} + \frac{i}{4}e^{-\mu}\right) + B'\left(-ie^{\mu} + \frac{i}{4}e^{-\mu}\right)$$

$$= +\frac{i}{2}A'\left(2e^{\mu} + \frac{1}{2}e^{-\mu}\right) - \frac{i}{2}B'\left(2e^{\mu} - \frac{1}{2}e^{-\mu}\right)$$

$$A'\left(+ie^{\mu} - \frac{i}{4}e^{-\mu}\right) + B'\left(-ie^{\mu} - \frac{i}{4}e^{-\mu}\right) = +\frac{i}{2}A'\left(2e^{\mu} - \frac{1}{2}e^{-\mu}\right)$$

$$- \frac{i}{2}B'\left(2e^{\mu} + \frac{1}{2}e^{-\mu}\right)$$

$$x>b: \quad \varphi(x) = \frac{F}{\sqrt{k}} \exp\left(i\int_b^x dx\, k\right) + \frac{G}{\sqrt{k}} \exp\left(-i\int_b^x dx\, k\right)$$

(c)

$$F = e^{-i\pi/4}\left(+\frac{i}{2}Ae^{-i\pi/4}\left(2e^{\mu}+\frac{1}{2}e^{-\mu}\right) - \frac{i}{2}Be^{+i\pi/4}\left(2e^{\mu}-\frac{1}{2}e^{-\mu}\right)\right)$$

$$= \frac{1}{2}A\left(2e^{\mu}+\frac{1}{2}e^{-\mu}\right) - \frac{i}{2}B\left(2e^{\mu}-\frac{1}{2}e^{-\mu}\right)$$

$$G = e^{i\pi/4}\left(\frac{i}{2}Ae^{-i\pi/4}\left(2e^{\mu}-\frac{1}{2}e^{-\mu}\right) - \frac{i}{2}Be^{i\pi/4}\left(2e^{\mu}+\frac{1}{2}e^{-\mu}\right)\right)$$

$$= \frac{i}{2}A\left(2e^{\mu}-\frac{1}{2}e^{-\mu}\right) + \frac{1}{2}B\left(2e^{\mu}+\frac{1}{2}e^{-\mu}\right)$$

$$\begin{pmatrix} F \\ G \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix}$$

$$M = \frac{1}{2}\begin{pmatrix} 2e^{\mu}+\frac{1}{2}e^{-\mu} & -i\left(2e^{\mu}-\frac{1}{2}e^{-\mu}\right) \\ i\left(2e^{\mu}-\frac{1}{2}e^{-\mu}\right) & 2e^{\mu}+\frac{1}{2}e^{-\mu} \end{pmatrix}$$

Transmission and reflection coefficients: Set $G=0$

$$\begin{pmatrix} F \\ 0 \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix} \Rightarrow \begin{array}{l} F = M_{11}A + M_{12}B \\ 0 = M_{21}A + M_{22}B \end{array}$$

$$\Rightarrow \frac{B}{A} = -\frac{M_{21}}{M_{22}} \Rightarrow R = \left|\frac{M_{21}}{M_{22}}\right|^2$$

$$\frac{F}{A} = \frac{\det M}{M_{22}} = \frac{1}{M_{22}} \Rightarrow T = \frac{1}{|M_{22}|^2}$$

In accord with general M-theory

$$T = \frac{1}{|M_{22}|^2} = \frac{1}{(e^{\mu} + \frac{1}{4}e^{-\mu})^2} \xrightarrow[\mu \gg 1]{} e^{-2\mu}$$

$$R = \left|\frac{M_{21}}{M_{22}}\right|^2 = \left(\frac{e^{\mu} - \frac{1}{4}e^{-\mu}}{e^{\mu} + \frac{1}{4}e^{-\mu}}\right)^2 \xrightarrow[\mu \ll 1]{} 1 - e^{-2\mu}$$

$$R + T = 1$$

E. Merzbacher, Quantum Mechanics, 2nd Edition

CHAPTER 7

The WKB Approximation

1. *The Method.* If the potential energy does not have a very simple form, the solution of the Schrödinger equation even in one dimension,

$$\frac{d^2\psi}{dx^2} + \frac{2\mu}{\hbar^2}(E - V)\psi = 0 \tag{7.1}$$

is usually a complicated problem which requires the use of approximation methods. Some of these, for instance, perturbation and variational methods, briefly described in Section 4.6, are quite general and will be discussed in detail after we have freed ourselves from the limitation to one dimension. One particular method, however, is particularly suitable for obtaining approximate solutions to ordinary differential equations, and it is appropriate that we should take it up now. This is the so-called WKB method, named after its proponents in quantum mechanics, Wentzel, Kramers, and Brillouin. The WKB method can also be applied to three-dimensional problems, if the potential is spherically symmetric and a radial differential equation can be separated.

The basic idea is simple. If $V = $ const., (7.1) has the solutions $e^{\pm ikx}$. This suggests that if V, while no longer constant, varies only slowly with x, we might try a solution of the form

$$\psi(x) = e^{iu(x)} \tag{7.2}$$

except that the function $u(x)$ now is not simply proportional to x. Substitution of (7.2) into (7.1) gives us an equation for the x-dependent "phase," $u(x)$. This equation becomes particularly simple if we use the abbreviations

$$k(x) = \left\{\frac{2\mu}{\hbar^2}[E - V(x)]\right\}^{1/2} \quad \text{if} \quad E > V(x) \tag{7.3a}$$

and

$$k(x) = -i\left\{\frac{2\mu}{\hbar^2}[V(x) - E]\right\}^{1/2} = -i\kappa(x) \quad \text{if} \quad E < V(x) \tag{7.3b}$$

We then find that $u(x)$ satisfies the equation

$$i\frac{d^2u}{dx^2} - \left(\frac{du}{dx}\right)^2 + [k(x)]^2 = 0 \tag{7.4}$$

This differential equation is entirely equivalent to (7.1), but the boundary conditions are more easily expressed in terms of $\psi(x)$ than $u(x)$. The fact that (7.4) is a nonlinear equation, whereas the Schrödinger equation is linear, would usually be regarded as a drawback, but in this chapter we shall take advantage of the nonlinearity to develop a simple approximation method for solving (7.4). Indeed, an iteration procedure is suggested by the fact that u'' is zero for the free particle. We are led to suspect that this second derivative remains relatively small if the potential does not vary too violently. When we omit this term from the equation entirely, we obtain the first crude approximation, u_0, to u:

$$u_0'^2 = [k(x)]^2 \tag{7.5}$$

or, integrating this,

$$u_0 = \pm\int^x k(x)\,dx + C \tag{7.6}$$

This is the approximation to the wave function which in Chapter 3 was employed to establish the wave equation.

A successive approximation method can now be set up, if we cast (7.4) in the form[1]

$$\left(\frac{du}{dx}\right)^2 = k^2(x) + i\frac{d^2u}{dx^2} \tag{7.7}$$

We substitute the nth approximation on the right-hand side of this equation, and obtain from (7.7) the $(n + 1)$th approximation by a mere quadrature:

$$u_{n+1}(x) = \pm\int^x \sqrt{k^2(x) + iu_n''(x)}\,dx + C_{n+1} \tag{7.8}$$

Thus, we have for $n = 0$

$$u_1(x) = \pm\int^x \sqrt{k^2(x) + iu_0''(x)}\,dx + C_1 = \pm\int^x \sqrt{k^2(x) \pm ik'(x)}\,dx + C_1 \tag{7.9}$$

Our hope that this procedure will yield a wave function which approximates

[1] If u_a and u_b are two particular solutions of (7.7) which differ not only by a constant, the general solution is

$$u(x) = u_a - i\log\left[1 + Ae^{i(u_b - u_a)}\right] + B$$

where A and B are arbitrary constants. The corresponding $\psi(x)$ is

$$\psi(x) = e^{iu(x)} = e^{iB}e^{iu_a} + Ae^{iB}e^{iu_b}$$

The two different signs in (7.6) give two particular u's, and therefore lead to the general solution of (7.1).

the correct $u(x)$ is baseless unless $u_1(x)$ is close to $u_0(x)$, i.e., unless

$$|k'(x)| \ll |k^2(x)| \tag{7.10}$$

In (7.9) both signs must be chosen the same as in the u_0 upon which u_1 is supposed to be an improvement. If condition (7.10) holds, we may expand the integrand and obtain

$$u_1(x) \simeq \int^x \left[\pm k(x) + \frac{i}{2}\frac{k'(x)}{k(x)}\right] dx + C_1 = \pm\int^x k(x)\,dx + \frac{i}{2}\log k(x) + C_1 \tag{7.11}$$

The constant of integration is of no moment, because it only affects the normalization of $\psi(x)$ which, if needed at all, is best accomplished after all the desired approximations have been made.

The approximation (7.11) to (7.4) is known as *WKB approximation.* It leads to the approximate wave function

$$\psi(x) \simeq \frac{1}{\sqrt{k(x)}} \exp\left[\pm i\int^x k(x)\,dx\right] \tag{7.12}$$

Condition (7.10) can be formulated in ways which are better suited to physical interpretation. If $k(x)$ is regarded as the effective wave number, we may for $E > V(x)$ define an effective wavelength

$$\lambda(x) = \frac{2\pi}{k(x)}$$

Condition (7.10) can then be written as

$$\lambda(x)\left|\frac{dp}{dx}\right| \ll |p(x)| \tag{7.13}$$

where $p(x) = \pm\hbar k(x)$ is the momentum which the particle would possess classically at point x. Condition (7.10) thus implies that the change of the momentum over a wavelength must be small compared to the momentum itself. This condition was already quoted in (3.12). It obviously breaks down if $k(x)$ vanishes or if $k(x)$ varies very rapidly. This certainly happens at the classical turning points for which

$$V(x) = E \tag{7.14}$$

or whenever $V(x)$ has a very steep behavior. In either case a more accurate solution must be used in the region where (7.10) breaks down. Yet the WKB method is not particularly useful unless we find ways to extend the wave function through these regions.

2. *The Connection Formulas.* Consider the most important problem arising from the breakdown of condition (7.10): Suppose that $x = a$ is a *classical turning point*[2] for the motion with the given energy E, as shown in Figure 7.1.

[2] In Figure 7.1 the barrier is to the right of the classical turning point. Analogous considerations hold if the barrier is to the left. For a summary of results see (7.25) and (7.26).

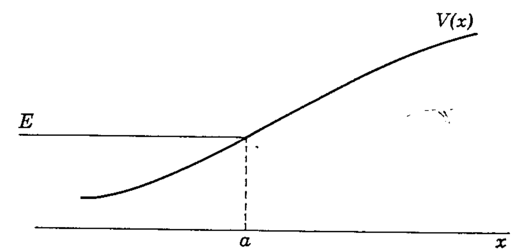


Figure 7.1. Classical turning point at $x = a$.

Assume that the WKB approximation is applicable except in the immediate neighborhood of the turning point. The discussion is considerably simplified if we change *dependent* as well as *independent* variables, introducing

$$v(x) = \sqrt{k(x)}\,\psi(x) \tag{7.15}$$

and

$$y = \int^x k(x)\,dx \tag{7.16}$$

By a little manipulation we obtain instead of the Schrödinger equation:

$$\frac{d^2v}{dy^2} + \left[\frac{1}{4k^2}\left(\frac{dk}{dy}\right)^2 - \frac{1}{2k}\frac{d^2k}{dy^2} + 1\right]v = 0 \tag{7.17}$$

From the earlier discussion it is clear that the WKB approximation is equivalent to replacing the bracket in (7.17) by unity. Indeed, if the first two terms in the bracket are neglected, we have the solutions $v(y) = e^{\pm iy}$, which by relation (7.15) give us the WKB wave functions (7.12). In the WKB region to the left of the classical turning point in Figure 7.1 y is real, and (7.17) has the approximate solution

$$v \simeq Ae^{iy} + Be^{-iy} \tag{7.18}$$

In the WKB region to the right of the turning point y is imaginary, and

$$v \simeq Ce^{|y|} + De^{-|y|} \tag{7.19}$$

We now ask the fundamental question: How are the coefficients C and D related to A and B if (7.18) and (7.19) are to represent the same state, albeit in different regions? The answer to this question can be found only if the unabridged equation (7.17) is integrated near the turning point. This requires that a somewhat special assumption be made about the behavior of the potential energy near the turning point.

We shall suppose that in the neighborhood of $x = a$ we may write

$$V(x) - E \approx \alpha(x - a) \tag{7.20}$$

where $\alpha > 0$. By (7.3*a* and *b*)

$$k(x) = \begin{cases} \left[\dfrac{2\mu\alpha}{\hbar^2}(a - x)\right]^{1/2} & \text{for } x < a \\ \exp\left(-\dfrac{i\pi}{2}\right)\left[\dfrac{2\mu\alpha}{\hbar^2}(x - a)\right]^{1/2} & \text{for } x > a \end{cases} \tag{7.21}$$

The multivaluedness of the fractional powers with which we have to deal here demands that attention must be paid to the phases. If this advice is not followed, inconsistencies arise which lead to wrong answers. All fractional powers of positive quantities are understood to be positive, and the phases have been chosen arbitrarily but definitely.

When the particular form of k given by (7.21) is substituted in (7.16), we can evaluate the integral. If the lower limit of integration is chosen to be $x = a$, i.e., such that $y(a) = 0$, y becomes a measure of the distance from the classical turning point. y is then small near the turning point because the two limits of integration are close to each other, and also because the integrand $k(x)$ is small near a. Conversely, at points far enough to the right or left of the turning point so that the WKB approximation becomes applicable, y is large in absolute value—again on both accounts. Explicitly,

$$y = \begin{cases} \dfrac{2}{3}\left(\dfrac{2\mu\alpha}{\hbar^2}\right)^{1/2}(a - x)^{3/2}e^{i\pi} & \text{for } x < a \\ \dfrac{2}{3}\left(\dfrac{2\mu\alpha}{\hbar^2}\right)^{1/2}(x - a)^{3/2}e^{-i\pi/2} & \text{for } x > a \end{cases} \tag{7.22}$$

If we express y in terms of k and then calculate the derivatives of y, (7.17) takes on a remarkably simple form:

$$\frac{d^2v}{dy^2} + \left(1 + \frac{5}{36y^2}\right)v = 0 \tag{7.23}$$

For large $|y|$ the second term in the parenthesis may be neglected. The asymptotic solutions of (7.23), $v = e^{\pm iy}$, yield again the WKB approximation. Equation (7.23) is accurate near the turning point, but the assumption is

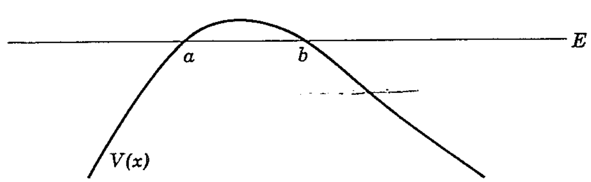
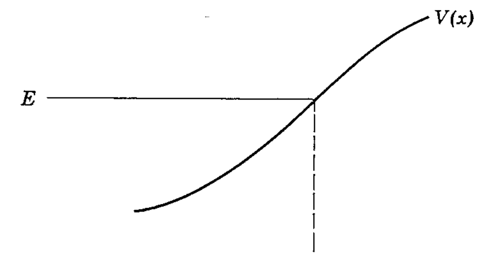


Figure 7.2. The near coincidence of two classical turning points requires special treatment in the WKB approximation.

made that it is also a good approximation to the Schrödinger equation in the intermediate region where y has moderate values.

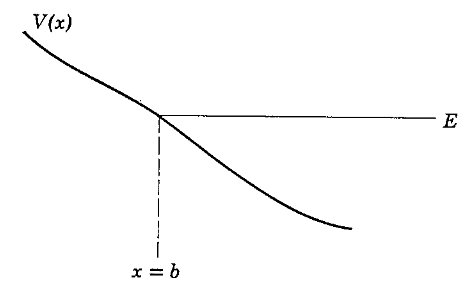
Clearly, this entire approach breaks down if, for instance, the energy is close in value to an extremum of the potential (see Figure 7.2), because, proceeding from left to right, turning point b is reached before one gets sufficiently far away from a for the WKB approximation to hold. If, on the other hand, our procedure is valid, (7.23) can be used to connect the WKB wave functions across the classical turning point. To this end the asymptotic behavior of the solutions to (7.23) must be considered in detail. The mathematical work, using integral representations of the solutions of (7.17), is found in Section 7.5. Only the results will be quoted here.



$$\frac{2}{\sqrt{k}}\cos\left(\int_x^a k\,dx - \tfrac{1}{4}\pi\right) \longleftrightarrow \frac{1}{\sqrt{\kappa}}\exp\left(-\int_a^x \kappa\,dx\right) \tag{7.25a}$$

$$\frac{1}{\sqrt{k}}\sin\left(\int_x^a k\,dx - \tfrac{1}{4}\pi\right) \longleftrightarrow -\frac{1}{\sqrt{\kappa}}\exp\left(\int_a^x \kappa\,dx\right) \tag{7.25b}$$

Figure 7.3. The turning point is to the right of the classical region.



$$\frac{1}{\sqrt{\kappa}}\exp\left(-\int_x^b \kappa\,dx\right) \longleftrightarrow \frac{2}{\sqrt{k}}\cos\left(\int_b^x k\,dx - \tfrac{1}{4}\pi\right) \tag{7.26a}$$

$$-\frac{1}{\sqrt{\kappa}}\exp\left(\int_x^b \kappa\,dx\right) \longleftrightarrow \frac{1}{\sqrt{k}}\sin\left(\int_b^x k\,dx - \tfrac{1}{4}\pi\right) \tag{7.26b}$$

Figure 7.4. The turning point is to the left of the classical region.

The formulas connecting the wave functions to the left and right of the turning point in Figure 7.1 are

$$\frac{\cos(-y - \frac{1}{4}\pi)}{\sqrt{k}} \longleftrightarrow \frac{1}{2}\frac{e^{-|y|}}{\sqrt{\kappa}} \tag{7.24a}$$

$$\frac{\sin(-y - \frac{1}{4}\pi)}{\sqrt{k}} \longleftrightarrow -\frac{e^{|y|}}{\sqrt{\kappa}} \tag{7.24b}$$

We recognize these wave functions as the appropriate WKB solutions to the Schrödinger equation. Caution must be exercised in the use of the formulas. Suppose that we know the wave function is adequately represented far to the right of the turning point (Figure 7.3) by the increasing exponential in (7.24*b*). It is then in general not legitimate to infer that to the far left of the turning point the wave function is given by $\sin(-y - \frac{1}{4}\pi)/\sqrt{k}$. After all, an admixture of decreasing exponential would be considered negligible to the far right of the turning point although it might, according to (7.24*a*), contribute an appreciable amount of $\cos(-y - \frac{1}{4}\pi)/\sqrt{k}$ to the wave function on the left. Conversely, a minute admixture of $\sin(-y - \frac{1}{4}\pi)/\sqrt{k}$ to $\cos(-y - \frac{1}{4}\pi)/\sqrt{k}$ on the left (Figure 7.4) might be negligible there but might lead to a very appreciable exponentially increasing portion on the right, if the solutions are used for sufficiently large $|y|$. Thus we see that unless we have assured ourselves properly of the absence of the other linearly independent component in the wave function, the *connection formulas*, summarized for both kinds of classical turning points in equations (7.25*a*, *b*) and (7.26*a*, *b*), should be used only in the directions indicated by the double arrow if considerable error is to be avoided.[3]

Exercise 7.1. Show that the WKB approximation is consistent with conservation of probability, even across classical turning points.

3. ***Application to Bound States.*** The WKB approximation can be applied to derive an equation for the energies of bound states. The basic idea emerges if we choose a simple well-shaped potential with two classical turning points as shown in Figure 7.5. The WKB approximation will be used in regions 1, 2, and 3 away from the turning points, and the connection formulas will serve near $x = a$ and $x = b$. The usual requirement that ψ must be finite dictates that the solutions which increase exponentially as one moves outward from the turning points must vanish rigorously. Thus, in region 1 the unnormalized wave function is

[3] For a detailed exposition, see N. Fröman and P. O. Fröman, *JWKB Approximation*, North-Holland Publishing Co., Amsterdam 1965.

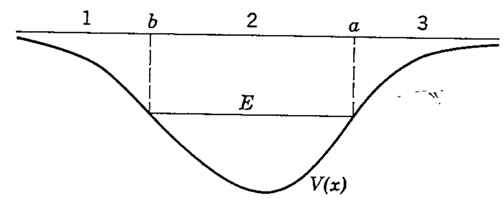


Figure 7.5. Simple potential well. Classically, a particle of energy E is confined to the region between a and b.

$$\psi_1 \simeq \frac{1}{\sqrt{\kappa}} \exp\left(-\int_x^b \kappa\, dx\right) \qquad \text{for } x < b$$

Hence, by equation (7.26*a*),

$$\psi_2 \simeq \frac{2}{\sqrt{k}} \cos\left(\int_b^x k\, dx - \tfrac{1}{4}\pi\right) \qquad \text{for } b < x < a$$

This may also be written as

$$\begin{aligned}\psi_2 &\simeq \frac{2}{\sqrt{k}} \cos\left(\int_b^a k\, dx - \int_x^a k\, dx - \tfrac{1}{4}\pi\right)\\ &= -\frac{2}{\sqrt{k}} \cos\left(\int_b^a k\, dx\right) \sin\left(\int_x^a k\, dx - \tfrac{1}{4}\pi\right)\\ &\quad + \frac{2}{\sqrt{k}} \sin\left(\int_b^a k\, dx\right) \cos\left(\int_x^a k\, dx - \tfrac{1}{4}\pi\right)\end{aligned}$$

By (7.25) only the second of these two terms gives rise to a decreasing exponential satisfying the boundary conditions at infinity. Hence, the first term must vanish. We obtain the condition

$$\int_b^a k\, dx = (n + \tfrac{1}{2})\pi \tag{7.27}$$

where $n = 0, 1, 2, \ldots$. This equation determines the possible discrete values of E. E appears in the integrand as well as in the limits of integration, since the turning points a and b are determined such that $V(a) = V(b) = E$.

If we introduce the classical momentum $p(x) = \pm\hbar k(x)$ and plot $p(x)$ versus x in phase space, the bounded motion in a potential well can be pictured by a closed curve (Figure 7.6). It is then evident that condition (7.27) may be written as

$$J \equiv \oint p(x)\, dx = (n + \tfrac{1}{2})h \tag{7.28}$$

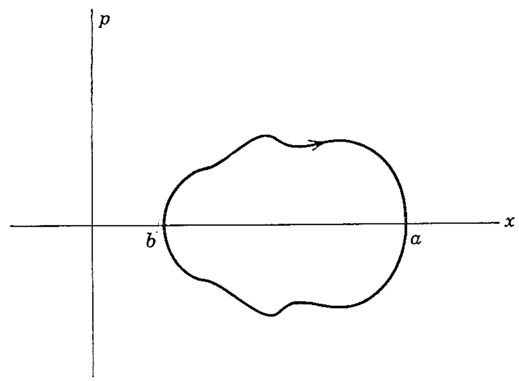


Figure 7.6. Phase space representation of the periodic motion of a particle confined between the classical turning points at $x = a$ and $x = b$.

This equation is very similar to the quantum condition (1.2) in the old quantum theory which occupied a position intermediate between classical and quantum mechanics.

The left-hand side of (7.28), which equals the area enclosed by the curve representing the motion in phase space, is called the *phase integral* J in classical terminology. It also measures the phase change which the oscillatory wave function ψ_2 undergoes between the turning points, for if the WKB approximation is used all the way from b to a,

$$\int_b^a k(x)\,dx = (n + \tfrac{1}{2})\pi$$

is the phase change across the well. Dividing this by 2π, we see that according to the WKB approximation $\frac{1}{2}n + \frac{1}{4}$ quasi wavelengths fit between b and a. Hence, n represents the number of nodes in the wave function, a fact which helps to visualize the elusive ψ.

According to (7.28), the area of phase space between one bound state and the next is equal to h. From this observation we infer the statement, often heard in statistical mechanics, that each quantum state occupies a volume h in phase space. This rule is useful in the domain where classical mechanics is actually applicable but some concession is to be made to the quantum structure of matter.

That the term *classical approximation* for the WKB method may not be amiss can be seen by noting that for high energies ψ_2 has a very short wavelength. It is a rapidly oscillating function of position but its amplitude is modulated slowly by a factor $1/\sqrt{k(x)}$. The probability, $|\psi_2|^2\,dx$, of finding the particle in an interval dx at x is proportional to the reciprocal of the

classical velocity, $1/v(x)$. This is also classically the relative probability of finding the particle in the interval dx if a random determination of its position is made as the particle shuttles back and forth between the turning points. We see thus that the probability concepts used in quantum and classical mechanics, although basically different, are nevertheless related to each other in the limit in which the rapid phase fluctuations of quantum mechanics can be legitimately averaged to give the approximate classical motion.

Exercise 7.2. Show that the WKB approximation gives the energy levels of the linear harmonic oscillator correctly. Sketch the WKB approximation to the eigenfunctions for $n = 0$ and 1.

4. *Transmission through a Barrier.* The WKB method will now be applied to calculate the transmission coefficient for a barrier upon which particles are incident from the left with insufficient energy to pass to the other side classically. This problem is very similar to that of the rectangular potential barrier, Section 6.5, but no special assumption will be made here concerning the shape of the barrier.

If the WKB approximation is assumed to hold in the three regions indicated in Figure 7.7, the solution of the Schrödinger equation may be written as

$$\psi(x) = \begin{cases} \dfrac{A}{\sqrt{k(x)}} \exp\left(i\displaystyle\int_a^x k\,dx\right) + \dfrac{B}{\sqrt{k(x)}} \exp\left(-i\displaystyle\int_a^x k\,dx\right) & (x < a) \\ \dfrac{C}{\sqrt{\kappa(x)}} \exp\left(-\displaystyle\int_a^x \kappa\,dx\right) + \dfrac{D}{\sqrt{\kappa(x)}} \exp\left(\displaystyle\int_a^x \kappa\,dx\right) & (a < x < b) \\ \dfrac{F}{\sqrt{k(x)}} \exp\left(i\displaystyle\int_b^x k\,dx\right) + \dfrac{G}{\sqrt{k(x)}} \exp\left(-i\displaystyle\int_b^x k\,dx\right) & (b < x) \end{cases} \tag{7.29}$$

The connection formulas (7.25) and (7.26) can now be used to establish linear relations between the coefficients in (7.29) in much the same way as

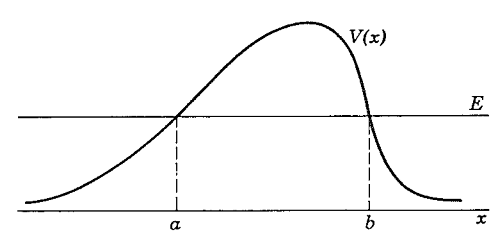


Figure 7.7. Potential barrier.

was done in Chapter 6 for the rectangular barrier. However, it must be observed that the connection formulas are applicable only if the ratios

$$\left|\frac{F+iG}{F-iG}\right| \quad \text{and} \quad \left|\frac{B-iA}{B+iA}\right|$$

are not too close to zero. The result of the calculation is remarkably simple and again best expressed in terms of a matrix M which connects F and G with A and B:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2\theta + \dfrac{1}{2\theta} & i\left(2\theta - \dfrac{1}{2\theta}\right) \\ -i\left(2\theta - \dfrac{1}{2\theta}\right) & 2\theta + \dfrac{1}{2\theta} \end{pmatrix}\begin{pmatrix} F \\ G \end{pmatrix} \tag{7.30}$$

where the parameter

$$\theta = \exp\left(\int_a^b \kappa(x)\,dx\right) \tag{7.31}$$

measures the height and thickness of the barrier as a function of energy.

Exercise 7.3. Verify (7.30).

The *transmission coefficient* is defined as

$$T = \frac{|\psi_{\text{trans}}|^2 v_{\text{trans}}}{|\psi_{\text{inc}}|^2 v_{\text{inc}}} = \frac{|\psi_{\text{trans}}\sqrt{k_{\text{trans}}}|^2}{|\psi_{\text{inc}}\sqrt{k_{\text{inc}}}|^2} = \frac{|F|^2}{|A|^2}$$

assuming that there is no wave incident from the right, $G = 0$. From (7.30) we obtain

$$T = \frac{1}{|M_{11}|^2} = \frac{4}{\left(2\theta + \dfrac{1}{2\theta}\right)^2} \tag{7.32}$$

For a high and broad barrier $\theta \gg 1$, and

$$T \approx \frac{1}{\theta^2} = \exp\left(-2\int_a^b \kappa\,dx\right) \tag{7.33}$$

Hence, θ is a measure of the opacity of the barrier.

As an example we calculate θ for a one-dimensional model of a Coulomb repulsion barrier (Figure 7.8) such as a proton (charge Z_1e) has to penetrate to reach a nucleus (charge Z_2e). The essence of this calculation survives the

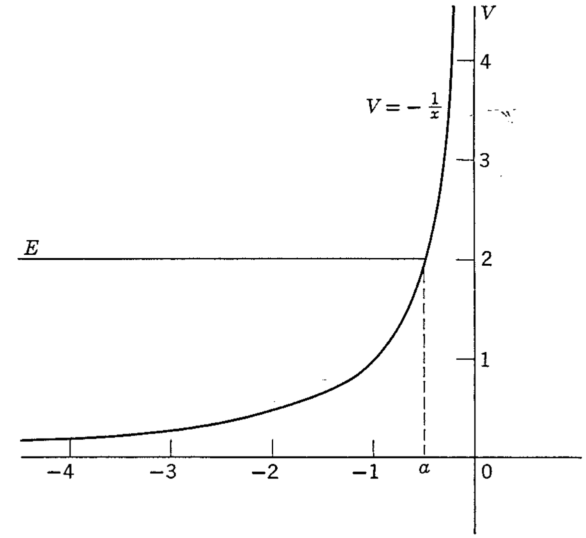


Figure 7.8. One-dimensional analog of a Coulomb barrier which repels particles incident from the left.

generalization to three dimensions (Section 11.8). Thus, let V be defined for $x < 0$ as

$$V = -\frac{Z_1 Z_2 e^2}{x} \tag{7.34}$$

The turning point a is determined by

$$E = -\frac{Z_1 Z_2 e^2}{a}$$

and we take $b = 0$. Evidently

$$\int_a^0 \kappa\,dx = \frac{\sqrt{2\mu E}}{\hbar}\int_a^0 \sqrt{\frac{a}{x} - 1}\,dx = \sqrt{\frac{2\mu}{E}}\,\frac{Z_1 Z_2 e^2}{\hbar}\int_0^1 \sqrt{\frac{1}{u} - 1}\,du = \frac{Z_1 Z_2 e^2}{\hbar v}\,\pi$$

Hence,

$$\frac{1}{\theta^2} = \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar v}\right) \tag{7.35}$$

This transmission coefficient, which inhibits the approach of a positive charged particle to the nucleus, is called the *Gamow factor*. This quantity is also decisive in the description of nuclear alpha decay, since the alpha particle, once it is formed inside the nucleus, cannot escape unless it penetrates the surrounding Coulomb barrier.[4]

As a final application of the WKB method let us consider the passage of a particle through a potential well which is bounded by barriers as shown in Figure 7.9. It will be assumed that $V(x)$ is symmetric about the origin, which is located in the center of the well, and that $V = 0$ outside the interval between $-c$ and c.

In this section the effect of barrier penetration will be studied for a particle with an energy E below the peak of the barriers. We are particularly interested in the form of the free particle wave functions in regions 1 and 7:

$$\begin{aligned} \psi_1 &= \frac{A_1}{\sqrt{k}} \exp(ikx) + \frac{B_1}{\sqrt{k}} \exp(-ikx) \\ \psi_7 &= \frac{A_7}{\sqrt{k}} \exp(ikx) + \frac{B_7}{\sqrt{k}} \exp(-ikx) \end{aligned} \tag{7.36}$$

When the WKB method is applied to connect the wave function in regions 1 and 7, the relation between the coefficients is again most advantageously

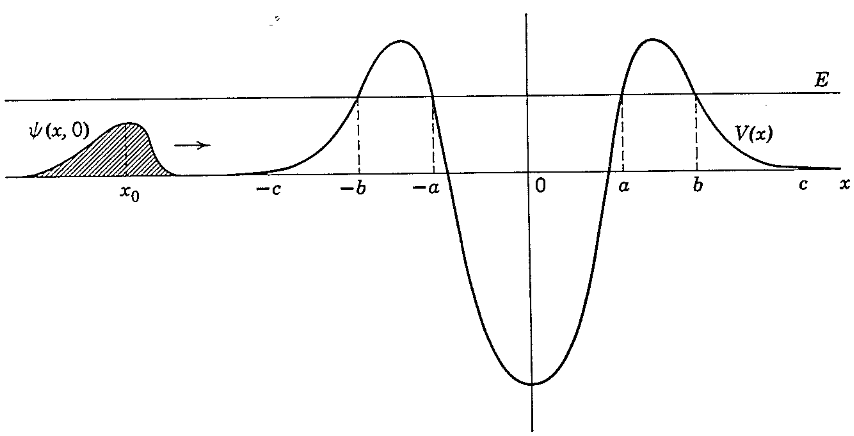


Figure 7.9. Potential barriers surrounding a well are favorable for the occurrence of narrow transmission resonances. We define as region 1: $x < -c$; region 2: $-c < x < -b$; region 3: $-b < x < -a$; region 4: $-a < x < a$; region 5: $a < x < b$; region 6: $b < x < c$; region 7: $c < x$. A wave packet is seen to be incident from the left.

[4] See J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics*, John Wiley and Sons, New York, 1952. Alpha decay is treated in Chapter 11.

recorded in matrix notation:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} e^{-2i\rho}\left[\left(4\theta^2 + \frac{1}{4\theta^2}\right)\cos L - 2i\sin L\right] & i\left(4\theta^2 - \frac{1}{4\theta^2}\right)\cos L \\ -i\left(4\theta^2 - \frac{1}{4\theta^2}\right)\cos L & e^{2i\rho}\left[\left(4\theta^2 + \frac{1}{4\theta^2}\right)\cos L + 2i\sin L\right] \end{pmatrix} \times \begin{pmatrix} A_7 \\ B_7 \end{pmatrix} \tag{7.37}$$

In writing these equations, the following abbreviations have been used:[5]

$$L = \frac{J}{2\hbar} = \int_{-a}^{a} k(x)\,dx, \qquad \rho = \int_{b}^{c} k(x)\,dx - kc \tag{7.38}$$

It follows from the definition of L and from inspection of Figure 7.9 that

$$\frac{\partial L}{\partial E} > 0 \tag{7.39}$$

The final matrix relation (7.37) has the form (6.46) subject to the conditions (6.47) and (6.48). This result is expected since, as was pointed out in Section 6.6, the matrix which links the asymptotic parts of a Schrödinger eigenfunction has the same general form for all potentials which are symmetric about the origin.

According to (6.63) the transmission coefficient is

$$T = \frac{1}{|M_{11}|^2} = \frac{4}{\left(4\theta^2 + \frac{1}{4\theta^2}\right)^2 \cos^2 L + 4\sin^2 L} \tag{7.40}$$

This quantity reaches its maximum value, unity, whenever $\cos L = 0$, or

$$L = (2n+1)\frac{\pi}{2}, \qquad J = (n + \tfrac{1}{2})h \tag{7.41}$$

The condition determining the location of the transmission peaks is seen to be the same as the quantum condition (7.28) for bound states. If $\theta \gg 1$, so

[5] For a thorough discussion of barrier penetration in the WKB approximation, see D. Bohm, *Quantum Theory*, Prentice-Hall, New York, 1951. Our notation is adapted from Bohm's.

that penetration through the barriers is strongly inhibited, T has sharp, narrow *resonance* peaks at these energies. A graph of T in the resonance region will be similar to Figure 6.10.

Exercise 7.4. Show that the distance D between neighboring resonances (in terms of energy) is approximately

$$D \approx \frac{\pi}{\partial L/\partial E} \tag{7.42}$$

It is instructive to consider the motion of a simple broad wave packet incident from the left (see Figure 7.9). A wave packet, which at $t = 0$ is localized entirely in region 1 near the coordinate x_0 far to the left of the barrier and moving toward positive x, may be represented as

$$\psi(x, 0) = \int_0^\infty f(E)e^{ik(x-x_0)}\, dE \tag{7.43}$$

where $\hbar k = \sqrt{2\mu E}$. The amplitude $f(E)$ is a smoothly varying real function of energy with a fairly sharp peak and a width ΔE. If $\psi(x, 0)$ is normalized to unity, $f(E)$ satisfies the normalization condition

$$\int_0^\infty |f(E)|^2\, v\, dE = \frac{1}{2\pi\hbar} \tag{7.44}$$

It can be shown that (7.43) may be replaced by an expansion in terms of eigenfunctions of the form (7.36). The first step in the proof is the observation that in region 1

$$\psi(x, 0) = \int_0^\infty f(E)e^{-ikx_0}\left(e^{ikx} + \frac{B_1}{A_1}\, e^{-ikx}\right) dE \qquad (x < -c) \tag{7.45}$$

the coefficients A_1 and B_1 being the same as those which appear in (7.36). Equation (7.45) holds because the integral

$$\int_0^\infty f(E)\, \frac{B_1}{A_1}\, e^{-ik(x+x_0)}\, dE \tag{7.46}$$

differs from zero only for values of x near $x = -x_0$. Hence, it vanishes in region 1.

If thus (7.45) represents the incident wave packet in region 1, it is necessary to check if the corresponding expansion in the other regions also gives the correct answer, $\psi(x, 0) = 0$, since the initial wave function is entirely confined in region 1. In particular, in region 7 we require

$$\int_0^\infty f(E)e^{-ikx_0}\left(\frac{A_7}{A_1}\, e^{ikx} + \frac{B_7}{A_1}\, e^{-ikx}\right) dE = 0 \qquad (x > c) \tag{7.47}$$

The first of these two integrals vanishes in region 7 for the same reason that (7.46) vanishes in region 1. However, the second integral in (7.47) leads to an unwanted contribution to $\psi(x, 0)$ in region 7, unless $B_7 = 0$ is chosen, eliminating any wave incident from the right.

From equation (7.37), for $B_7 = 0$,

$$\frac{A_7}{A_1} = \frac{1}{M_{11}} = \sqrt{T}\, e^{-i\varphi} = \frac{e^{2i\rho}}{\frac{1}{2}\left(4\theta^2 + \frac{1}{4\theta^2}\right)\cos L - i \sin L} \tag{7.48}$$

Hence, the initial wave function in region 7 may be expressed as

$$\psi(x, 0) = \int_0^\infty f(E)\sqrt{T}\, e^{-i\varphi}e^{ik(x-x_0)}\, dE \qquad (x > c) \tag{7.49}$$

By a somewhat more delicate argument it can also be shown that setting $B_7 = 0$ suffices to insure that the appropriate superposition of WKB wave functions gives no contribution to $\psi(x, 0)$ in the remaining internal regions.

Once the initial wave function has been written as a superposition of (approximate) eigenfunctions of the Schrödinger equation for the barrier and well, the wave function at arbitrary times is obtained simply by inserting the appropriate oscillatory phase. To the right of the barrier we obtain

$$\psi(x, t) = \int_0^\infty f(E)\sqrt{T} \exp(-i\varphi) \exp\left[ik(x - x_0) - \frac{i}{\hbar}Et\right] dE \qquad (x > c) \tag{7.50}$$

In order to study the behavior of the transmitted wave packet near a *resonance* we assume that the incident wave packet has a mean energy E_0 corresponding to a resonance and that the width ΔE of the packet considerably exceeds the width of the resonance (but is much smaller than the interval between neighboring resonances).

Under the conditions favorable for the occurrence of pronounced resonances ($\theta \gg 1$) it may usually be assumed that in the vicinity of the resonance to a reasonable approximation

$$\cos L \simeq \mp\left(\frac{\partial L}{\partial E}\right)_{E=E_0}(E - E_0), \qquad \sin L \simeq \pm 1$$

Using these approximations and evaluating the slowly varying quantity θ at $E = E_0$, we get

$$\sqrt{T}\, e^{-i\varphi} \simeq \mp \frac{\Gamma/2}{E - E_0 + i(\Gamma/2)}\, e^{2i\rho} \tag{7.51}$$

where by definition

$$\Gamma = \frac{1}{\theta^2(\partial L/\partial E)_{E=E_0}} \tag{7.52}$$

Exercise 7.5. Apply the resonance approximation to the transmission coefficient T, and show that near E_0 it has the characteristic resonance shape, Γ being its width at half-maximum.

Except for uncommonly long-range potential barriers, the phase ρ may be assumed constant, and equal to ρ_0, over the width of the resonance. With all these approximations, the wave function in region 7 at any time t becomes

$$\psi(x, t) \simeq \mp f(E_0) \exp\left[i\frac{k_0}{z}(x - x_0) + 2i\rho_0 \right] \times \frac{\Gamma}{2} \int_{-\infty}^{\infty} \frac{\exp\left[\frac{i}{\hbar}E\left(\frac{x - x_0}{v_0} - t\right)\right]}{E - E_0 + i(\Gamma/2)} dE \quad (7.53)$$

In arriving at this form the approximation

$$k = k_0 + (k - k_0) = k_0 + \frac{k^2 - k_0^2}{k + k_0} \approx k_0 + \frac{k^2 - k_0^2}{2k_0} = \frac{k_0}{2} + \frac{E}{\hbar v_0}$$

has been used and the integration has been extended to $-\infty$ without appreciable error, assuming that t is not too large.

The integral in (7.53) is a well-known Fourier integral which can be evaluated by integration in the complex E-plane. The result is that in the region $x > c$

$$\psi(x, t) \simeq \begin{cases} \pm \pi i \Gamma f(E_0) e^{2i\rho_0} \exp\left[\frac{1}{\hbar}\left(iE_0 + \frac{\Gamma}{2}\right)\left(\frac{x - x_0}{v_0} - t\right)\right] & \text{if } t > \frac{x - x_0}{v_0} \\ 0 & \text{if } t < \frac{x - x_0}{v_0} \end{cases} \quad (7.54)$$

This wave function describes a wave packet with a discontinuous front edge at $x = x_0 + v_0 t$ and an exponentially decreasing tail to the left. After the pulse arrives at a point x the probability density decays according to the formula

$$|\psi(x, t)|^2 = \pi^2\Gamma^2 |f(E_0)|^2 \exp\left[\frac{\Gamma}{\hbar}\left(\frac{x - x_0}{v_0} - t\right)\right]$$

We may calculate the probability that at time t the particle has been transmitted and is found in region 7. For a wave packet whose energy spread covers a single resonance such that

$$D \gg \Delta E \gg \Gamma \quad (7.55)$$

this probability is

$$\int_0^{x_0 + v_0 t} |\psi(x, t)|^2 \, dx = \pi^2 \hbar \Gamma v_0 |f(E_0)|^2 \left\{1 - \exp\left[-\frac{\Gamma}{\hbar}\left(t + \frac{x_0}{v_0}\right)\right]\right\} \qquad \left(t > -\frac{x_0}{v_0}\right)$$

From (7.44) we obtain as a crude estimate

$$2\pi\hbar v_0 |f(E_0)|^2 \simeq \frac{1}{\Delta E}$$

Hence, an order of magnitude estimate for the probability that transmission has occurred is

$$\frac{\Gamma}{\Delta E}\left\{1 - \exp\left[-\frac{\Gamma}{\hbar}\left(t + \frac{x_0}{v_0}\right)\right]\right\} \quad (7.56)$$

The total transmission probability for the incident wave packet (7.43) is found by letting $t \to \infty$ and is thus approximately equal to $\Gamma/\Delta E$. Equation (7.56) leads to the following simple interpretation: The wave packet reaches the well at time $-x_0/v_0$. A fraction $\Gamma/\Delta E$ of the packet is transmitted according to an exponential time law with a mean lifetime

$$\tau = \frac{\hbar}{\Gamma} \quad (7.57)$$

and the remaining portion of the wave packet is reflected promptly. The study of resonance transmission has thus afforded us an example of the familiar *exponential decay law*, and the well with surrounding barriers can actually serve as a one-dimensional model of nuclear alpha decay. Decay processes will be encountered again in Chapters 11 and 18, but it is well to point out here that the exponential decay law can be derived only as an approximate, and not a rigorous, result of quantum mechanics and that it holds only if the decay process is essentially independent of the manner in which the decaying state was formed and of the particular details of the incident wave packet.

Exercise 7.6. Show that condition (7.55) implies that the time it takes the incident wave packet to enter the well must be long compared with the classical period of motion and short compared with the lifetime of the decaying state.

Exercise 7.7. Resonances in the double well may be also defined as quasi-bound states by requiring $A_1 = B_7 = 0$ (no incident wave), or $M_{11} = 0$