

**Physics 221A**  
**Fall 2010**  
**Notes 7**  
**The WKB Method**

## 1. Introduction

The WKB method is important both as a practical means of approximating solutions to the Schrödinger equation, and also as a conceptual framework for understanding the classical limit of quantum mechanics. The letters WKB stand for Wentzel, Kramers and Brillouin, who first applied the method to the Schrödinger equation in the 1920's. Some people think the name of Jeffreys should be added, and refer to the WKBJ method. The WKB approximation is also called the *semiclassical* or *quasiclassical* approximation. The basic idea behind the method can be applied to any kind of wave (in optics, acoustics, etc): it is to expand the solution of the wave equation in the ratio of the wavelength to the scale length of the environment in which the wave propagates, when that ratio is small. In quantum mechanics, this is equivalent to treating  $\hbar$  formally as a small parameter. The method itself antedates quantum mechanics by many years, and was used by Liouville and Green in the early nineteenth century.

Planck's constant  $\hbar$  has dimensions of action, so its value depends on the units chosen, and it does not make sense to say that  $\hbar$  is "small." However, typical mechanical problems have quantities with dimensions of action that appear in them, for example, an angular momentum, a linear momentum times a distance, etc., and if these are large in comparison to  $\hbar$ , then we may be able to treat  $\hbar$  as small. This would normally be the case for macroscopic systems, which are well described by classical mechanics. Thus the classical limit can be thought of as one in which all actions are large in comparison to  $\hbar$ .

It is obvious that there must be some subtlety in the classical limit of quantum mechanics, since the physical interpretations of the two theories are so different. For example, quantum mechanics makes physical predictions that are fundamentally statistical, while statistics only enters into classical mechanics if there is a lack of complete information about initial conditions. Moreover there are quantum phenomena, such as interference and tunneling, that have no classical analog. We will see as we proceed how WKB theory represents these characteristic features of quantum mechanics around a framework constructed out of classical mechanics.

## 2. The WKB Ansatz

To establish the basic WKB ansatz, we work with the Schrödinger equation for an energy

eigenfunction in three dimensions,

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}), \quad (1)$$

assuming a kinetic-plus-potential Hamiltonian. In the special case that the potential is constant,  $V = V_0 = \text{const.}$ , solutions exist in the form of plane waves,

$$\psi(\mathbf{x}) = Ae^{iS(\mathbf{x})/\hbar}, \quad (2)$$

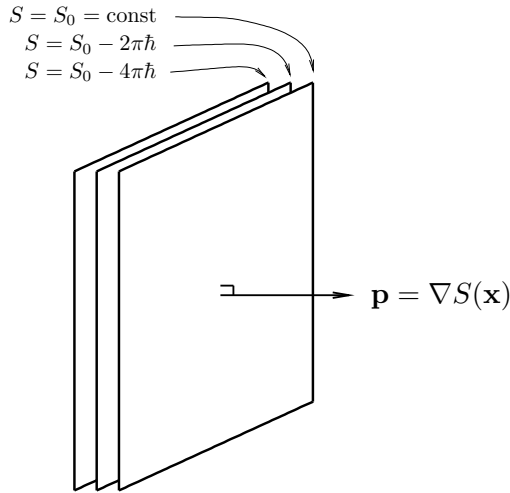
where  $A$  is the constant amplitude, and where

$$S = \mathbf{p} \cdot \mathbf{x}. \quad (3)$$

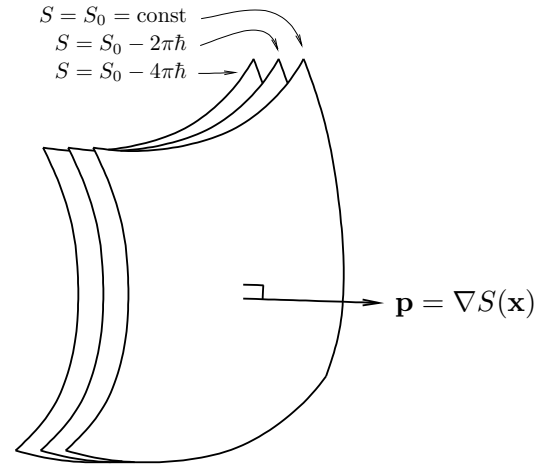
The vector  $\mathbf{p}$  is a momentum, and in fact the wave function (2) is an eigenfunction of momentum as well as energy, with eigenvalues related by

$$E = \frac{|\mathbf{p}|^2}{2m} + V_0. \quad (4)$$

We assume that  $E \geq V_0$ , so that  $\mathbf{p}$  is real.



**Fig. 1.** Plane waves are so called because the surfaces of constant phase are planes. The momentum eigenvalue is  $\mathbf{p} = \nabla S$ , where  $S/\hbar$  is the phase.



**Fig. 2.** In a slowly varying potential, the wave fronts are surfaces that curve with the same scale length as the potential. The vector  $\mathbf{p} = \nabla S$  is a “local momentum,” that is, a function of position.

The wave (2) is called a plane wave because the wave fronts, that is, the surfaces of constant phase, are planes. These are sketched in Fig. 1. The momentum  $\mathbf{p} = \nabla S$  is orthogonal to the wave fronts; it is a constant (independent of position). Two wave successive wave fronts with a phase

difference of  $2\pi$ , that is, with  $\Delta S = 2\pi\hbar$ , are separated by the wavelength  $\lambda$ , which is related to the momentum by the de Broglie formula,

$$\lambda = \frac{2\pi\hbar}{|\nabla S|} = \frac{2\pi\hbar}{|\mathbf{p}|}. \quad (5)$$

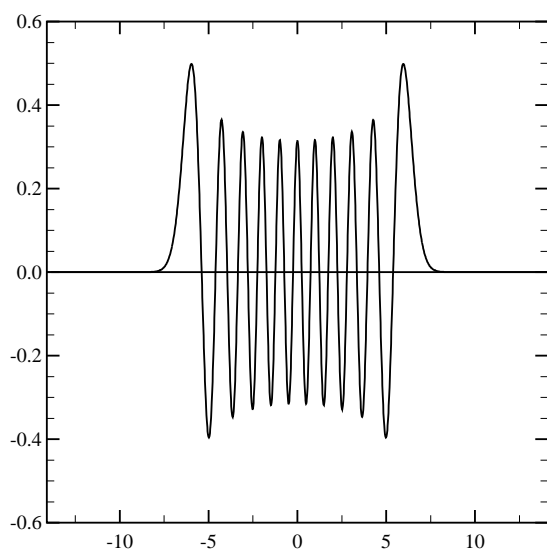
Now let us consider the case of a slowly varying potential  $V$ . Let  $L$  be some characteristic scale length of the potential. When we say that  $V$  is slowly varying, we mean that  $V$  does not change much on the scale of a wavelength, that is,

$$\lambda \ll L. \quad (6)$$

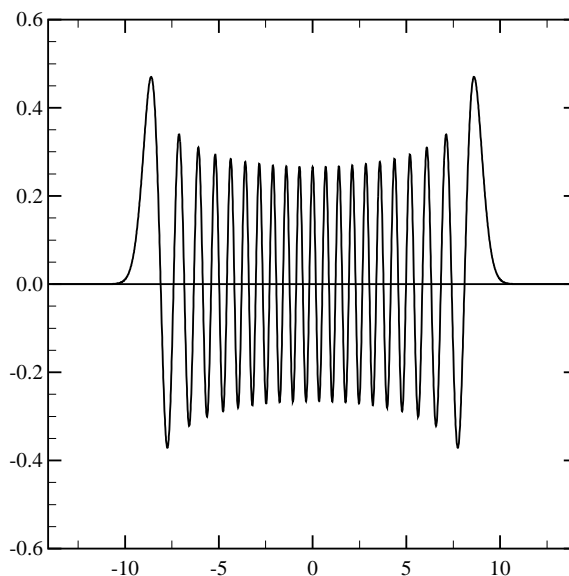
Then it is plausible that the wave fronts, that is, the surfaces of constant phase of the solution  $\psi(\mathbf{x})$  of the Schrödinger equation (1), will be curved surfaces such as illustrated in Fig. 2, and that these surfaces will deviate significantly from a plane wave on the same scale length  $L$  as the potential. For example, the radius of curvature of the wave fronts should be of the same order of magnitude as  $L$ , and the normal direction of the wave fronts should turn by an angle of order unity in a distance  $L$ . We can still write the phase of the wave as  $S(\mathbf{x})/\hbar$ , but the function  $S$  no longer has the plane wave form (3). As for the amplitude  $A$  of the wave, it is constant in a constant potential, so it is reasonable to guess that in a slowly varying potential it is also slowly varying, that is, that it has the same scale length  $L$  as the potential. We still write the wave function as

$$\psi(\mathbf{x}) = A(\mathbf{x})e^{iS(\mathbf{x})/\hbar}, \quad (7)$$

but now  $A$  and  $S$  are functions of  $\mathbf{x}$  to be determined. Notice that the phase  $S(\mathbf{x})/\hbar$  is *not* slowly varying, since it changes by  $2\pi$  (a quantity of order unity) over distance  $\lambda \ll L$ .



**Fig. 3.** Normalized harmonic oscillator eigenfunction for  $n = 20$ . Distance  $x$  is measured in units of  $(\hbar/m\omega)^{1/2}$ .



**Fig. 4.** Same as Fig. 3, except  $n = 40$ .

Some exactly solvable one-dimensional problems reinforce our confidence in the validity of Eq. (7) and the assumptions surrounding it. See, for example, the one-dimensional eigenfunctions of the harmonic oscillator illustrated in Figs. 3 and 4. The wave function is largely concentrated between the classical turning points for the given energy  $E$ , namely,  $\pm(2E/m\omega^2)^{1/2}$ . We can take  $L$  as the distance between these turning points. The wave function  $\psi(x)$  looks like a cosine wave (a sum of two terms of the form (7)) with a slowly varying amplitude.

Returning to the three-dimensional case, it is clear from Fig. 2 that the solution  $\psi(\mathbf{x})$  looks like a plane wave if we examine it in a region of space small compared to  $L$ . Let  $\mathbf{x}_0$  be a fixed point, and let  $\mathbf{x} = \mathbf{x}_0 + \boldsymbol{\xi}$ , where  $|\boldsymbol{\xi}| \ll L$ . Then when we expand the wave function (7) about  $\mathbf{x}_0$ , we can simply evaluate the amplitude  $A$  at  $\mathbf{x}_0$ , since it does not change much on the scale of  $\boldsymbol{\xi}$ , but we must include the first correction term in the phase. Thus we have

$$\psi(\mathbf{x}_0 + \boldsymbol{\xi}) \approx A(\mathbf{x}_0)e^{iS(\mathbf{x}_0)/\hbar}e^{i\boldsymbol{\xi}\cdot\nabla S/\hbar}, \quad (8)$$

where the first two factors constitute a constant amplitude and phase, and the third shows that  $\psi$  has locally the form of a plane wave with momentum

$$\mathbf{p} = \mathbf{p}(\mathbf{x}) = \nabla S(\mathbf{x}). \quad (9)$$

Unlike the case of a plane wave,  $\mathbf{p}$  is now a function of position, so it is not constant and  $\psi(\mathbf{x})$  is no longer an eigenfunction of momentum. (The wave function  $\psi(\mathbf{x})$  is still an eigenfunction of energy, however, with energy  $E$ .) The local momentum  $\mathbf{p}(\mathbf{x})$  is orthogonal to the wave fronts, as illustrated in Fig. 2. Since displacement by the wave length  $\lambda$  in a direction orthogonal to the wave fronts must result in a phase advance of  $2\pi$ , the de Broglie relation (5) still holds, but now  $\lambda$  is also a function of position. Thus the slowly varying assumption (6) may hold in some regions of space and not others; the WKB approximation is valid where it holds. Notice that this assumption can be stated in another form,

$$\frac{|\mathbf{p}|L}{\hbar} \gg 1, \quad (10)$$

showing the dimensionless ratio of a mechanical action to  $\hbar$ . In this sense the assumption (6) is equivalent to treating  $\hbar$  as “small.”

The *momentum field* (9) gives us the beginning of a classical interpretation of the solution (7) of the Schrödinger equation. That is, we imagine that the region of space occupied by the wave (7) is also occupied by a swarm of classical particles, such that the particle at position  $\mathbf{x}$  has momentum  $\mathbf{p}(\mathbf{x}) = \nabla S(\mathbf{x})$ . This swarm defines in effect a classical ensemble out of which the probabilistic features of quantum mechanics will be represented. The momentum field  $\mathbf{p}(\mathbf{x})$  satisfies

$$\nabla \times \mathbf{p}(\mathbf{x}) = 0, \quad (11)$$

and

$$S(\mathbf{x}) = S(\mathbf{x}_0) + \int_{\mathbf{x}_0}^{\mathbf{x}} \mathbf{p}(\mathbf{x}') \cdot d\mathbf{x}', \quad (12)$$

where in the latter integral  $\mathbf{x}$  and  $\mathbf{x}_0$  are any two points and the path of integration is any path between them (we ignore topological complications in the application of Stokes' theorem). Integrals of the form (12) are well known in classical mechanics, where the function  $S$  is called *Hamilton's principal function*. It is also called simply the *action*, and it does have dimensions of action, but several different quantities in classical mechanics are called the action and one should be aware of which is meant when using this term. It was because of the interpretation of the function  $S$  as the classical action that we split off a factor of  $\hbar$  in the phase of the quantum wave function in Eqs. (2) and (7).

The result of the preceding argument is to justify the *WKB ansatz* (7), and to associate it with a picture of an ensemble of classical particles. This picture is the beginning of a classical framework for understanding the meaning of the functions  $S(\mathbf{x})$  and  $A(\mathbf{x})$ , which will get fleshed out as we proceed.

### 3. Equations for $S$ and $A$

The WKB ansatz (7) was based on some approximations, and is not by itself a systematic expansion of the wave function. But we can easily generalize it. First we bring the amplitude up into the exponent by writing

$$\psi(\mathbf{x}) = \exp\left\{\frac{i}{\hbar}[S(\mathbf{x}) - i\hbar \ln A(\mathbf{x})]\right\}, \quad (13)$$

which suggests that the WKB ansatz amounts to an expansion of  $\ln \psi$  in powers of  $\hbar$ , beginning with the power  $\hbar^{-1}$ , in which the leading term is the action  $S$  and the next term is  $-i \ln A$ . We extend this expansion to all orders, writing

$$\psi(\mathbf{x}) = \exp\left[\frac{i}{\hbar}W(\mathbf{x})\right], \quad (14)$$

where

$$W(\mathbf{x}) = W_0(\mathbf{x}) + \hbar W_1(\mathbf{x}) + \hbar^2 W_2(\mathbf{x}) + \dots, \quad (15)$$

and where

$$W_0(\mathbf{x}) = S(\mathbf{x}), \quad W_1(\mathbf{x}) = -i \ln A(\mathbf{x}). \quad (16)$$

It is now seen that the WKB ansatz, in its generalized form (14), only involves the assumptions that the logarithm of the wave function can be expanded in powers of  $\hbar$ , and that the leading term is  $O(\hbar^{-1})$ .

We now substitute Eq. (14) into the Schrödinger equation (1), and express the latter in terms of  $W$  instead of  $\psi$ . After a little algebra, we find

$$\frac{1}{2m}(\nabla W)^2 - \frac{i\hbar}{2m}\nabla^2 W + V = E. \quad (17)$$

No approximations have been made yet, and this is exactly equivalent to the Schrödinger equation (1), although the shift from  $\psi$  to its logarithm has made the Schrödinger equation nonlinear. Next

we expand  $W$  as in Eq. (15), substitute into Eq. (17), and collect terms order by order. At order  $\hbar^0$ , we find

$$\frac{1}{2m}(\nabla W_0)^2 + V(\mathbf{x}) = E, \quad (18)$$

or

$$\frac{1}{2m}(\nabla S)^2 + V(\mathbf{x}) = E. \quad (19)$$

This is the well known *Hamilton-Jacobi* equation of classical mechanics. See Eq. (B.109). At order  $\hbar^1$ , we find

$$\frac{1}{m}\nabla W_0 \cdot \nabla W_1 - \frac{i}{2m}\nabla^2 W_0 = 0, \quad (20)$$

or by Eq. (16),

$$\nabla S \cdot \nabla \ln A + \frac{1}{2}\nabla^2 S = 0. \quad (21)$$

We write this in the form,

$$2A\nabla S \cdot \nabla A + A^2\nabla^2 S = 0, \quad (22)$$

or,

$$\nabla \cdot (A^2\nabla S) = 0. \quad (23)$$

We call this equation (in its various forms) the *amplitude transport* equation.

The Hamilton-Jacobi equation (19) may be written in the form,

$$H(\mathbf{x}, \nabla S) = E, \quad (24)$$

where  $H$  is the classical Hamiltonian. Since  $\mathbf{p} = \nabla S$ , this shows that the particles that make up the classical ensemble associated with the momentum field  $\mathbf{p}(\mathbf{x})$  all have the same energy  $E$ , independent of their position. This is a generalization of Eq. (4) to the case of slowly varying potentials. Equation (24) is a form of the Hamilton-Jacobi equation that is preferable to Eq. (19), since it applies to other problems (other versions of the Schrödinger equation (1)), such as problems with magnetic fields or multiparticle problems. It requires a slight generalization in the case of time-dependent problems (see below).

In the amplitude transport equation (23) we suspect that the vector whose divergence vanishes is related to a conserved current. Reasonable definitions make this more clear. First let us define a velocity field  $\mathbf{v}(\mathbf{x})$  by

$$\mathbf{v}(\mathbf{x}) = \frac{\mathbf{p}(\mathbf{x})}{m}, \quad (25)$$

which is the classical relation between momentum and velocity for kinetic-plus-potential problems. For other problems (other versions of the Schrödinger equation) this relation is expressed by the classical Hamilton's equation,

$$\mathbf{v} = \frac{\partial H}{\partial \mathbf{p}}, \quad (26)$$

for example,

$$\mathbf{v} = \frac{1}{m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right), \quad (27)$$

in problems with a magnetic field. We associate the velocity field  $\mathbf{v}(\mathbf{x})$  with the ensemble of classical particles introduced above, imagining that the particle at position  $\mathbf{x}$  has momentum  $\mathbf{p}(\mathbf{x})$  and velocity  $\mathbf{v}(\mathbf{x})$ .

Next, we define a density  $\rho(\mathbf{x})$  by

$$\rho(\mathbf{x}) = A(\mathbf{x})^2. \quad (28)$$

This is the probability density of the quantum problem, since by the WKB ansatz (7), we have

$$\rho(\mathbf{x}) = |\psi(\mathbf{x})|^2. \quad (29)$$

This is assuming that  $A$  and  $S$  are real, which, as we shall see, is true in classically allowed regions. With these definitions of  $\rho$  and  $\mathbf{v}$ , the amplitude transport equation has the form,

$$\nabla \cdot \mathbf{J} = 0, \quad (30)$$

where

$$\mathbf{J}(\mathbf{x}) = \rho(\mathbf{x})\mathbf{v}(\mathbf{x}). \quad (31)$$

We interpret  $\rho(\mathbf{x})$  as the density of classical particles at position  $\mathbf{x}$ , whereupon  $\mathbf{J}(\mathbf{x})$  is the particle flux. It coincides with the quantum probability flux,

$$\mathbf{J} = \text{Re}[\psi^*(\mathbf{v}_{\text{op}}\psi)], \quad (32)$$

where  $\mathbf{v}_{\text{op}} = (1/m)(-i\hbar\nabla)$ , as we see by substituting the WKB ansatz (7) into Eq. (32). Then the amplitude transport equation is seen to be a version of the continuity equation for the quantum probability density and flux (without the term  $\partial\rho/\partial t$ , since the problem is time-independent). More precisely, it is an approximate version of this continuity equation, since the WKB ansatz (7) only contains the first two terms of the expansion (15).

The form (30) of the amplitude transport equation now has the following interpretation for our ensemble of classical particles. It says that if these particles move according to the classical equations of motion, then the number of particles entering some small volume in a some elapsed time is equal to the number of particles leaving that volume. That is, the particle density  $\rho(\mathbf{x})$  is constant in time, when the particles are allowed to evolve according to the classical equations of motion. Our classical ensemble is a stationary one, in the sense that the particle density and flux are time-independent, even though the particles themselves are moving along classical trajectories.

Conversely, if one can find a stationary ensemble of classical particles, such that the momentum of the particles is a function of their position,  $\mathbf{p} = \mathbf{p}(\mathbf{x})$ , and such that  $\nabla \times \mathbf{p} = 0$ , then the phase  $S$  and amplitude  $A$  of the quantum wave function can be reconstructed by Eqs. (12) and (28), respectively.

#### 4. The Time-Dependent Case

We comment briefly on the time-dependent WKB problem. Consider the time-dependent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{x}, t)\psi = i\hbar\frac{\partial\psi}{\partial t}, \quad (33)$$

where the potential is allowed to be a function of time. Let the WKB ansatz be

$$\psi(\mathbf{x}, t) = A(\mathbf{x}, t)e^{iS(\mathbf{x}, t)/\hbar}. \quad (34)$$

Then at order  $\hbar^0$  we find

$$\frac{1}{2m}(\nabla S)^2 + V(\mathbf{x}, t) + \frac{\partial S}{\partial t} = 0, \quad (35)$$

which is also well known in classical mechanics as the time-dependent version of the Hamilton-Jacobi equation. See Eq. (B.107). It can also be written in the form,

$$H(\mathbf{x}, \nabla S, t) + \frac{\partial S}{\partial t} = 0, \quad (36)$$

where  $H(\mathbf{x}, \mathbf{p}, t)$  is the classical Hamiltonian. This form is more general than Eq. (35), because it applies to a wider class of Hamiltonians. The solution  $S(\mathbf{x}, t)$  of the time-dependent Hamilton-Jacobi equation is known as *Hamilton's principal function*, and is given in terms of a line integral (usually taken along classical orbits),

$$S(\mathbf{x}, t) = \int \mathbf{p} \cdot d\mathbf{x} - H dt = \int L dt, \quad (37)$$

where  $L$  is the classical Lagrangian. See Sec. B.23 for a discussion of Hamilton's principal function in classical mechanics. We will see it appear again when we study the Feynman path integral. At order  $\hbar^1$ , the time-dependent problem gives rise to a time-dependent version of the amplitude transport equation,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0, \quad (38)$$

which again is a version of the continuity equation for quantum probability, with an interpretation in terms of a classical ensemble. In this case, the classical ensemble, whose particles evolve according to classical mechanics, reproduce the time-dependent probability density of the quantum problem, modulo errors of order  $\hbar^2$  that result from the truncation of the series (15).

#### 5. Historical and Other Comments on the Hamilton-Jacobi Equation

A version of the Hamilton-Jacobi equation first appeared in Hamilton's researches in the 1830's into variational formulations of mechanics and their relation to optics. Hamilton discovered the form of the classical equations of motion that now bears his name, and he realized that their complete solution was equivalent to solving a certain partial differential equation, Eq. (36). These ideas were generalized by Jacobi a few years later, who developed methods for solving Eq. (24), what we



now call the time-independent Hamilton-Jacobi equation. Jacobi used these methods to solve some nontrivial problems in classical mechanics.

Renewed interest in the Hamilton-Jacobi equation arose in the period of the old quantum theory (1900-1925), after Sommerfeld's and Wilson's analysis of Bohr's quantization condition, which is expressed in terms of action integrals like (12). The old quantum theory was a collection of rules that were incomplete, logically unclear, and of limited applicability, but which gave excellent agreement with experiment in a number of important cases such as the specific heat of solids and the spectrum of hydrogen, including its fine structure. As a result, the period 1911-1925 saw a heightened interest in the formal structure of classical mechanics, in the hope that it would elucidate the difficulties of the old quantum theory. These efforts were summarized in Born's book *The Mechanics of the Atom*, published just about the time that Heisenberg's and Schrödinger's (modern) quantum theory emerged. After this, interest in classical mechanics, at least in physics circles, fell to almost zero.

In more recent times, since the advent of computers and the discovery of chaos, classical mechanics has enjoyed another revival, partly stimulated also by developments in mathematics such as the KAM (Kolmogorov-Arnold-Moser) theorem. It is now recognized that the Hamilton-Jacobi equation has no global solutions in the case of chaotic motion, and that this has an impact on the morphology and other features of the quantum wave function.

In the language of classical mechanics, the solution  $S$  of the Hamilton-Jacobi equation is the generator of the canonical transformation that trivializes the classical equations of motion. The existence of this transformation requires that the system have a sufficient number of commuting constants of motion (the classical analog of a complete set of commuting observables). The constants of motion are conveniently expressed as functions of the *actions*, themselves constants of motion that generate periodic (and commuting) flows in phase space. The variables canonically conjugate to the actions are certain angles. Such matters are discussed in advanced courses in classical mechanics.

Because of problems with chaos and other issues, the Hamilton-Jacobi equation and the other equations of WKB theory are harder to solve in the multidimensional case, so the most common applications of WKB theory are in one dimension. We now turn to that case.

## 6. One-Dimensional WKB Problems

We consider now the one-dimensional Schrödinger equation,

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x), \quad (39)$$

in which we use the one-dimensional WKB ansatz,

$$\psi(x) = A(x)e^{iS(x)/\hbar}. \quad (40)$$

The Hamilton-Jacobi equation is the one-dimensional version of Eq. (19),

$$\frac{1}{2m}\left(\frac{dS}{dx}\right)^2 + V(x) = E, \quad (41)$$

and the amplitude transport equation is the one-dimensional version of Eq. (23),

$$\frac{d}{dx} \left( A^2 \frac{dS}{dx} \right) = 0. \quad (42)$$

We solve the Hamilton-Jacobi equation (41) algebraically for  $dS/dx$ , obtaining

$$\frac{\partial S}{\partial x} = p(x) = \pm \sqrt{2m[E - V(x)]}. \quad (43)$$

The  $\pm$  sign means that there are actually two WKB solutions, with actions that differ by a sign. The general solution is a linear combination of the two solutions. Integrating Eq. (43), we have

$$S(x) = \int_{x_0}^x p(x') dx'. \quad (44)$$

Changing the lower limit of integration merely adds a constant to  $S$ , which by Eq. (40) just changes the overall phase of the wave function. We will worry about phases later, and set  $x_0$  to anything convenient.

The amplitude transport equation (42) is also easily solved. We find

$$A(x) = \frac{\text{const}}{\sqrt{p(x)}}, \quad (45)$$

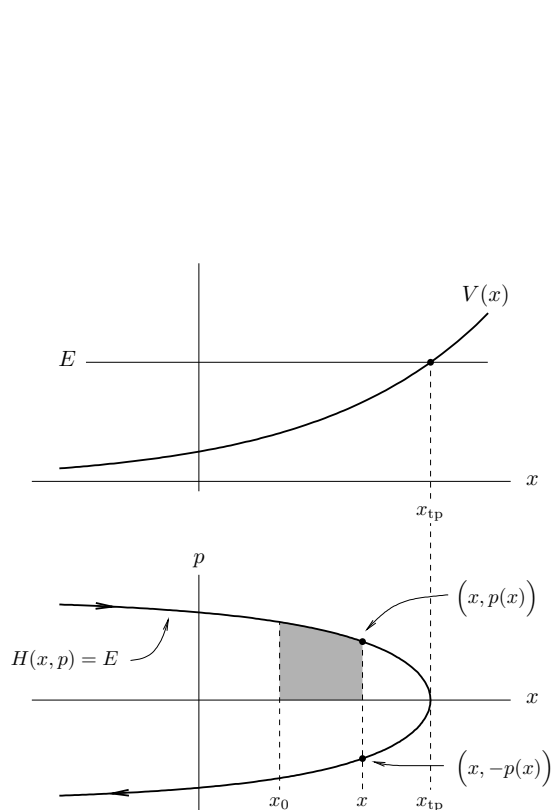
where as we see by Eq. (40) the constant of integration just establishes the normalization and phase of the wave function. For now we set this constant to anything convenient.

To proceed it is convenient to get rid of the  $\pm$  sign in Eq. (43) by committing to a definite branch of the square root function. How we do this depends on whether  $E > V(x)$  (a classically allowed region, where the kinetic energy is positive and the momentum real) or  $E < V(x)$  (a classically forbidden region, where the kinetic energy is negative and the momentum imaginary). We will adopt the following definitions,

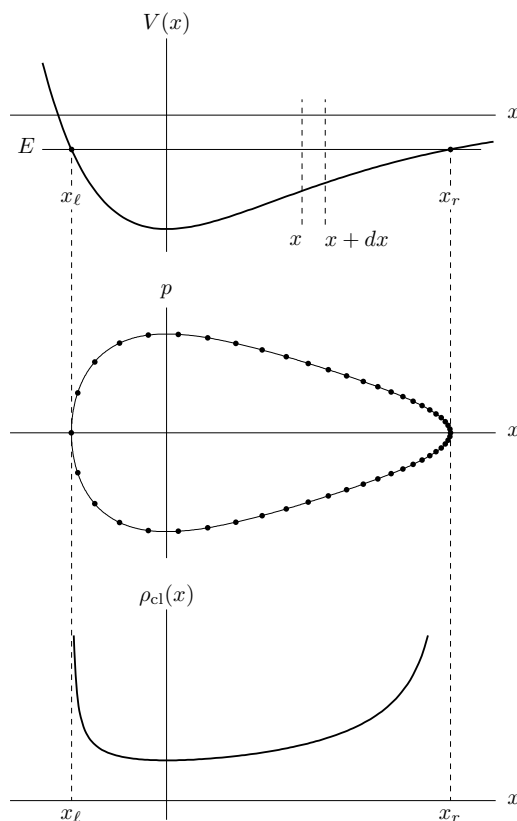
$$p(x) = \begin{cases} \sqrt{2m[E - V(x)]}, & E > V(x), \\ i\sqrt{2m[V(x) - E]}, & E < V(x). \end{cases} \quad (46)$$

Then we will define  $S(x)$  by Eq. (44), and say that the solutions of the Hamilton-Jacobi equation (41) are  $S(x)$  and  $-S(x)$ , with associated momentum functions  $p(x)$  and  $-p(x)$ . The momentum is purely imaginary in the classically forbidden region.

The classical meaning of the functions  $p(x)$  and  $A(x)$  may be seen in Fig. 5, which illustrates a portion of the  $x$ -axis in which there is a classical turning point  $x_{\text{tp}}$  (a point where  $E = V(x)$ ), with the classically allowed region to the left and the classically forbidden region to the right (upper part of figure). The energy  $E$  is the eigenvalue of the Schrödinger equation (39). The lower part of the figure is a phase space plot, showing the classical orbit of energy  $E$ . The orbit is also the contour line of the classical Hamiltonian,  $H(x, p) = E$ , because the classical motion conserves energy and therefore traces out this line. A given  $x$  value in the classically allowed region corresponds to two



**Fig. 5.** Illustration of functions  $p(x)$  and  $S(x)$  in classically allowed region.



**Fig. 6.** Meaning of classical probability density  $\rho(x)$  for a one-dimensional oscillator (the Morse oscillator).

momentum values,  $\pm p(x)$ , where the vertical line of constant  $x$  intersects the orbit, representing the particle passing  $x$  going one direction, and then passing it again going back. These are the two momentum branches corresponding to a given  $x$  value. Thus, the upper branch (the upper part of the orbit in phase space) is the graph of the function  $p = p(x)$ . By Eq. (44), the action  $S(x)$  with lower limit  $x_0$  is the area between the  $x$ -axis and the upper part of the orbit and between the limits  $x_0$  and  $x$ , as in the shaded part of the figure.

We spoke previously of a swarm or ensemble of classical particles that represents the WKB wave, such that the momentum of the particle at position  $\mathbf{x}$  is  $\mathbf{p}(\mathbf{x})$  (in three dimensions). From Fig. 5, we see that in the one-dimensional case there are really two swarms, one with particles going to the right and one with them going to the left. If the positions and momenta of these particles are plotted in phase space, then they lie on the line  $H = E$ , that is, they all have the same classical energy. This, in fact, is the meaning of the Hamilton-Jacobi equation (41).

The amplitude solution (45) also has a classical interpretation. As explained in Sec. 3,  $A(x)^2$  is the same as the quantum probability density  $\rho(x) = |\psi(x)|^2$  in the WKB approximation (neglecting  $O(\hbar^2)$  and higher terms in the expansion (15)), and it has an interpretation in terms of the density of the ensemble or swarm of classical particles. In the one-dimensional case, this classical density

can be understood from another standpoint, which we now discuss. The density in question is only normalizable in the case of an oscillator, so we consider that case, and refer to Fig. 6.

The top of the figure is the potential energy curve for the Morse oscillator, which is often used to model the stretching of molecular bonds. The potential rises rapidly to the left, corresponding to the strong repulsion of atoms that are brought close together, and gradually to the right, representing the attractive force between atoms as they are pulled apart, a force that dies off slowly as the distance increases. In the middle is a potential well, in which the oscillations represent molecular vibrations. We use the Morse potential here because it is a strongly nonlinear oscillator that presents features not present in the harmonic oscillator.

The classical particle oscillates between the left and right turning points  $x_\ell$  and  $x_r$  with a period  $T$ . In each period, it passes through a small interval  $[x, x + dx]$  twice, once going to the right and once to the left. We define a classical probability density  $\rho_{\text{cl}}(x)$  by requiring the probability of the particle to lie in the interval  $[x, x + dx]$  to be the fraction of the total period  $T$  that the particle spends in this interval. That is, we define

$$\rho_{\text{cl}}(x) dx = \frac{2}{T} dt, \quad (47)$$

where  $dt$  is the time it takes to pass through the interval once. Thus we have

$$\rho_{\text{cl}}(x) = \frac{2}{T} \frac{1}{v(x)} = \frac{2m}{T} \frac{1}{p(x)}. \quad (48)$$

According to Eq. (45), this probability density is equal to  $A(x)^2$ , to within a constant. The function  $\rho_{\text{cl}}(x)$  is plotted in the lower part of Fig. 6. It is smallest where the classical particle is moving most rapidly, and conversely.

The density  $\rho_{\text{cl}}(x)$  diverges at the turning points, where the velocity goes to zero. One can show that  $\rho_{\text{cl}}(x)$  goes like  $d^{-1/2}$  when  $d$ , the distance from a turning point, is small. Then, since  $A(x)$  goes like the square root of  $\rho_{\text{cl}}(x)$ , it goes like  $d^{-1/4}$  and also diverges near the turning point. Thus, the nominal prediction of WKB theory is that the wave function should diverge at turning points. The exact wave function does not actually diverge there, as can be seen from exact solutions such as those in Figs. 3 and 4, but it does become large there. In effect, the classical singularity is smoothed out by the uncertainty principle, which also causes some of the wave function to spill over into the classically forbidden region. We shall discuss the behavior of the wave function near turning points more carefully below.

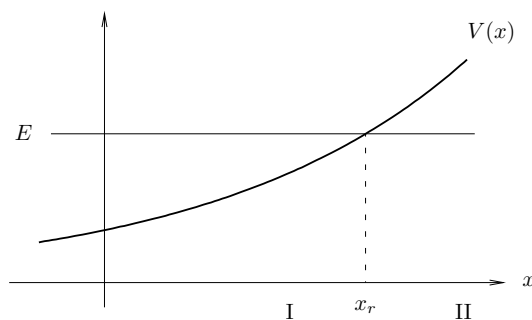
According to Eq. (47), the swarm or ensemble of particles representing the WKB wave can be thought of as a large number of particles uniformly distributed in time around the orbit. These are illustrated by the dots placed at equal time intervals along the phase space orbit in the center diagram in Fig. 6.

By its construction,  $\rho_{\text{cl}}(x)$  is normalized to unity. In the case of a scattering problem, the motion is not periodic and  $T \rightarrow \infty$ , so the density of classical particles cannot be normalized. It is still meaningful, however, to think of particles uniformly distributed along the orbit in time, in

which case we have a particle density  $\rho_{\text{cl}}(x)$  that is proportional to  $1/p(x)$ , as in the case of an oscillator. It is not surprising that  $\rho_{\text{cl}}$  cannot be normalized in this case, since the quantum wave function cannot be normalized, either.

## 7. Classically Allowed Region to the Left

Let us now examine the case in which we have a classically allowed region to the left of a turning point, with a classically forbidden region on the right, as illustrated in Fig. 7. The turning point is denoted  $x_r$  (since it is to the right of the classically allowed region). We are only sketching part of the  $x$ -axis in this diagram, and we make no assumptions about what the potential does to the left or the right of the diagram. For example, to the left it may rise again, creating a potential well, or just asymptote to zero, making a scattering problem. Or, to the right, it may go down again, creating a barrier the particle can tunnel through.



**Fig. 7.** A 1-dimensional potential  $V(x)$  rising to the right. Point  $x_r$  is a classical turning point.

First we treat region I, the classically allowed region, where  $x < x_r$  and  $E > V(x)$ . Here  $p(x)$  is real and positive as defined by Eq. (46). In this region we define  $S$  by

$$S(x) = \int_{x_r}^x p(x') dx', \quad (49)$$

which is the same as Eq. (44) except that now we are agreeing to measure the action from the turning point  $x_r$ . This is merely a matter of convenience, but it means that  $S(x)$  is real and negative in region I, and increasing to the right (since  $dS/dx = p(x) > 0$ ). Taking  $S(x)$  and  $-S(x)$  as the two solutions of the Hamilton-Jacobi equation, the WKB solution is a general linear combination of two waves,

$$\psi_{\text{I}}(x) = c_r \frac{e^{iS(x)/\hbar + i\pi/4}}{\sqrt{p(x)}} + c_\ell \frac{e^{-iS(x)/\hbar - i\pi/4}}{\sqrt{p(x)}}, \quad (50)$$

where  $c_r$  and  $c_\ell$  are two generally complex constants and where we have introduced phase shifts of  $\pm\pi/4$  in the two terms for later convenience. Properly speaking, we should have used  $-p(x)$  in the denominator of the second term, but we have absorbed the factor of  $\sqrt{-1} = i$  into the second

constant. The first term is a wave traveling to the right (since  $dS/dx > 0$ ), and the second, a wave traveling to the left; this is the meaning of the subscripts on the constants  $c_r$  and  $c_\ell$ . The general solution is a linear combination of such waves.

Next we treat region II, the classically forbidden region, where  $x > x_r$  and  $E < V(x)$ . Here  $p(x)$  is purely imaginary, as given by Eq. (46). In order to work with real quantities, we define

$$K(x) = \int_{x_r}^x |p(x')| dx' = \int_{x_r}^x \sqrt{2m[V(x') - E]} dx', \quad (51)$$

and we take  $S(x) = iK(x)$ . Again, the lower limit  $x_r$  is the classical turning point. In region II  $K(x)$  is real, positive, and increasing to the right. We also write the amplitude in the form,

$$A(x) = \frac{1}{\sqrt{|p(x)|}}, \quad (52)$$

so that  $A(x)$  is real and positive, absorbing any phases into the constants. Thus, the general WKB solution in region II is

$$\psi_{\text{II}}(x) = c_g \frac{e^{K(x)/\hbar}}{\sqrt{|p(x)|}} + c_d \frac{e^{-K(x)/\hbar}}{\sqrt{|p(x)|}}, \quad (53)$$

where  $c_g$  and  $c_d$  are a new pair of complex constants. The first term is a wave that is growing exponentially as we move to the right, while the second is damping exponentially to the right, which explains the subscripts on  $c_g$  and  $c_d$ . (It is necessary to say, “to the right,” because a wave that is growing to the right is damping to the left, and vice versa.)

We now have two solutions, Eqs. (50) and (53), in regions I and II respectively, each with two constants. The two pairs of constants cannot be independent, since the general solution to the Schrödinger equation (39) can only have two arbitrary constants overall. Therefore there must be a way of determining  $c_g$  and  $c_d$ , given  $c_r$  and  $c_\ell$ , and vice versa. The rules for doing this are called *connection rules*, and they amount to connecting the two WKB solutions through the turning point region that separates the classical allowed and classically forbidden regions.

Unfortunately, neither WKB solution (50) nor (53) is valid in the immediate neighborhood of the turning point, as shown by the divergence of the amplitude  $A(x)$ . This divergence represents a breakdown of the WKB approximation, which was based on the assumption (6), where we interpret  $\lambda$  as the local de Broglie wavelength,

$$\lambda = \frac{2\pi\hbar}{p(x)}. \quad (54)$$

But near the turning point,  $p(x) \rightarrow 0$ ,  $\lambda \rightarrow \infty$ , and the condition (6) is violated. Therefore, to find the connection between the coefficients ( $c_r, c_\ell$ ) and ( $c_g, c_d$ ) we cannot simply extend the two WKB solutions up to one another at the turning point.

Instead, we require a separate solution, or at least an approximate one, that is valid in the immediate neighborhood of the turning point. One can show that the WKB solutions (50) and (53) are valid except in a small region around the turning point, unless the slope  $V'(x_0)$  of the potential at the turning point itself should be too small.

Let us approximate the potential in the neighborhood of the turning point by a straight line,

$$V(x) \approx V(x_r) + (x - x_r)V'(x_r), \quad (55)$$

valid when  $x - x_r$  is small. Then using  $E = V(x_r)$ , the Schrödinger equation (39) becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V'(x_r)(x - x_r)\psi = 0. \quad (56)$$

To clean this up, we introduce a shifted and scaled variable  $z$  by the substitution,

$$x = x_r + az, \quad (57)$$

where  $a$  is a positive constant chosen to absorb all the physical constants in Eq. (56). We see that the variable  $z$  is zero at the turning point, negative in the classically allowed region, and positive in the classically forbidden region. The nicest choice for  $a$  is

$$a = \left( \frac{\hbar^2}{2mV'(x_r)} \right)^{1/3}, \quad (58)$$

which causes the Schrödinger equation to become

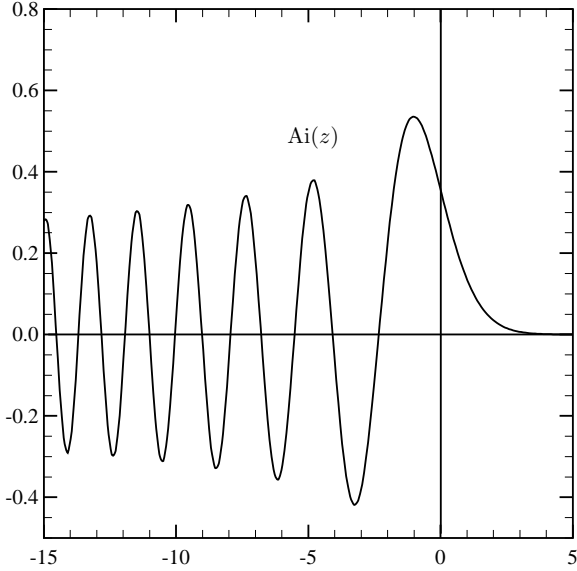
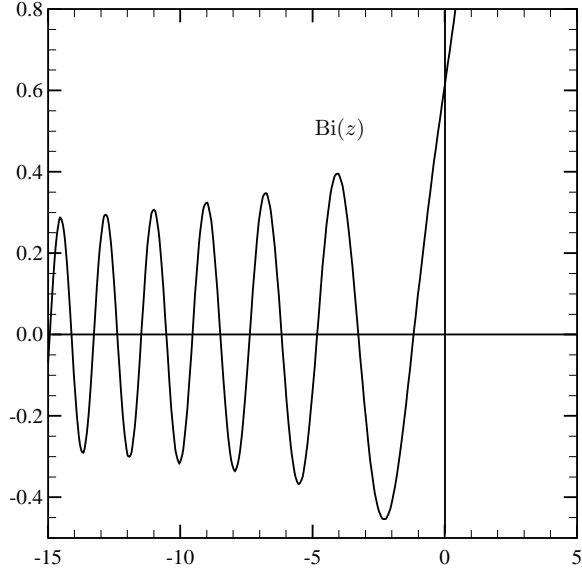
$$\frac{d^2\psi}{dz^2} - z\psi = 0. \quad (59)$$

Variable  $z$  is dimensionless, and  $a$  has dimensions of length.

Equation (59) is Airy's differential equation, whose two linearly independent solutions are the functions  $\text{Ai}(z)$  and  $\text{Bi}(z)$ . These functions are discussed in standard references on special functions of mathematical physics, such as Abramowitz and Stegun, *Handbook of Mathematical Functions* or Gradshteyn and Ryzhik *Table of Integrals, Series, and Products* by Gradshteyn and Ryzhik (these two are currently in print).

It helps to have some physical model in mind when studying the mathematical properties of the  $\text{Ai}$  and  $\text{Bi}$  functions. For this purpose, we notice that a potential  $V(x)$  that is linear in  $x$  occurs in the problem of a charged particle in a uniform electric field, where  $V(x) = qE_0x$ , or of a massive particle in a uniform gravitational field, where  $V(x) = mgx$ . Therefore, with appropriate scalings of variables as in Eq. (57), the  $\text{Ai}$  and  $\text{Bi}$  functions are the (exact) solutions of the Schrödinger equations for these two problems, as well as the approximate solutions for generic potentials near turning points.

The  $\text{Ai}$  and  $\text{Bi}$  functions are plotted in Figs. 8 and 9, respectively. The  $\text{Ai}$  function is the solution of Airy's differential equation (59) that decays exponentially as  $z \rightarrow \infty$ , and therefore represents the physically allowable solution for a particle in the uniform gravitational field (with zero total energy, since the classical turning point is at  $z = 0$ ). As seen in Fig. 8, this function is oscillatory for  $z < 0$ , with the wavelength and amplitude of the oscillations becoming smaller as  $z$  increases in the negative direction, corresponding to the increasing velocity or momentum of the particle falling in the gravitational field. The exponential damping of the function  $\text{Ai}(z)$  for  $z > 0$  corresponds to

Fig. 8. The function  $\text{Ai}(z)$ .Fig. 9. The function  $\text{Bi}(z)$ .

tunnelling into the classically forbidden region. Finally, the function  $\text{Ai}(z)$  shows the characteristic behavior of the wave function at a turning point; the wave function has a large maximum near the turning point, which is a smoothed version of the classical singularity in the probability density. As for the Bi function, it blows up exponentially in the region  $z > 0$ , and so is nonphysical for particles in gravitational fields; but we must retain this function for the general WKB problem. For  $z < 0$ , the function  $\text{Bi}(z)$  oscillates like the Ai function, but  $90^\circ$  out of phase.

Altogether, the general solution of the Schrödinger equation (39) in the neighborhood of a turning point has the form,

$$\psi_{\text{tp}}(x) = c_a \text{Ai}(z) + c_b \text{Bi}(z), \quad (60)$$

where  $c_a$  and  $c_b$  are a new pair of constants, and  $x$  and  $z$  are related by Eq. (57). We must now connect this solution with the solution  $\psi_{\text{I}}(x)$  to the left, and  $\psi_{\text{II}}(x)$  to the right.

First, working to the left, we invoke the asymptotic forms for the Ai and Bi functions for large negative  $z$ ,

$$\text{Ai}(z) = \frac{1}{\sqrt{\pi}(-z)^{1/4}} \cos \alpha(z), \quad z \ll 0, \quad (61a)$$

$$\text{Bi}(z) = \frac{1}{\sqrt{\pi}(-z)^{1/4}} \sin \alpha(z), \quad z \ll 0, \quad (61b)$$

where

$$\alpha(z) = -\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}. \quad (62)$$

Notice that  $-z$  is positive in this region. Thus, we can write the wave function at the left of the turning point region in the form,

$$\psi_{\text{tp}}(x) = \frac{1}{2\sqrt{\pi}(-z)^{1/4}} [(c_a - ic_b)e^{i\alpha(z)} + (c_a + ic_b)e^{-i\alpha(z)}]. \quad (63)$$



Compare this to the WKB solution in the classically allowed region, Eq. (50), which we write in the form,

$$\psi_{\text{I}}(x) = \frac{1}{\sqrt{p(x)}} [c_r e^{i\varphi(x)} + c_\ell e^{-i\varphi(x)}], \quad (64)$$

where

$$\varphi(x) = \frac{S(x)}{\hbar} + \frac{\pi}{4}. \quad (65)$$

Equations (63) and (64) must represent the same function. Furthermore, since the waves travelling to the left and right are linearly independent, the left and right travelling waves in the two equations must independently be equal. To show that this is true and to find the connections between the coefficients  $(c_r, c_\ell)$  and  $(c_a, c_b)$ , we first approximate the momentum function  $p(x)$  near the turning point according to Eq. (55),

$$p(x) = \sqrt{2m[E - V(x)]} = \sqrt{-2mV'(x_r)(x - x_r)} = \frac{\hbar}{a}(-z)^{1/2}, \quad (66)$$

where we use Eqs. (57) and (58). This shows that the amplitude factors in Eqs. (63) and (64) are proportional, as they should be. Next, we integrate  $p(x)$  to find the action,

$$\frac{S(x)}{\hbar} = \frac{1}{\hbar} \int_{x_0}^x p(x') dx' = \int_0^z (-z')^{1/2} dz' = -\frac{2}{3}(-z)^{3/2}, \quad (67)$$

which shows that  $\alpha(z) = \varphi(x)$ . Thus, the phases in Eqs. (63) and (64) are identical. Now we can read off the necessary relations between the coefficients, which are

$$\begin{aligned} \frac{1}{2\sqrt{\pi}}(c_a - ic_b) &= \sqrt{\frac{a}{\hbar}} c_r, \\ \frac{1}{2\sqrt{\pi}}(c_a + ic_b) &= \sqrt{\frac{a}{\hbar}} c_\ell. \end{aligned} \quad (68)$$

This completes the connection between the classically allowed region and the turning point region.

To connect to the right, that is, between the turning point region and the classically forbidden region, we invoke the asymptotic forms of the Ai and Bi functions for large positive  $z$ ,

$$\text{Ai}(z) = \frac{1}{2\sqrt{\pi} z^{1/4}} e^{-\beta(z)}, \quad z \gg 0, \quad (69a)$$

$$\text{Bi}(z) = \frac{1}{\sqrt{\pi} z^{1/4}} e^{+\beta(z)}, \quad z \gg 0, \quad (69b)$$

where

$$\beta(z) = \frac{2}{3}z^{3/2}. \quad (70)$$

Thus, the wave function to the right of the turning point region has the form,

$$\psi_{\text{tp}}(x) = \frac{1}{2\sqrt{\pi} z^{1/4}} [c_a e^{-\beta(z)} + 2c_b e^{+\beta(z)}], \quad (71)$$

whereas the WKB solution in the classically forbidden region, Eq. (53), has the form,

$$\psi_{\text{II}} = \frac{1}{\sqrt{|p(x)|}} [c_g e^{\kappa(x)} + c_d e^{-\kappa(x)}]. \quad (72)$$

where

$$\kappa(x) = \frac{1}{\hbar} K(x). \quad (73)$$

As before, Eqs. (71) and (72) must represent the same function. That the amplitudes are proportional is shown as before, for close to (but to the right of) the turning point we have

$$|p(x)| = \sqrt{2mV'(x_0)(x - x_0)} = \frac{\hbar}{a} z^{1/2}. \quad (74)$$

As for the action integral, we have

$$\kappa(x) = \frac{1}{\hbar} \int_{x_0}^x |p(x')| dx' = \int_0^z z'^{1/2} dz' = \frac{2}{3} z^{3/2} = \beta(z). \quad (75)$$

Therefore again we can read off the relations between the coefficients, which are

$$\begin{aligned} \frac{c_a}{2\sqrt{\pi}} &= \sqrt{\frac{a}{\hbar}} c_d, \\ \frac{c_b}{\sqrt{\pi}} &= \sqrt{\frac{a}{\hbar}} c_g. \end{aligned} \quad (76)$$

Finally, we can eliminate  $(c_a, c_b)$  between Eqs. (68) and (76), and find the desired connection rules between the coefficients  $(c_r, c_\ell)$  in the classically allowed region I, and the coefficients  $(c_g, c_d)$  in the classically forbidden region II.

## 8. The Connection Rules

We now summarize the connection rules, first for the case of the classically allowed region to the left of the turning point. This is the case analyzed in Sec. 7. The potential is sketched in Fig. 7, with turning point  $x_r$ .

In region I, the classically allowed region where  $x < x_r$  and  $E > V(x)$ ,  $p(x)$  is real and positive and is given by Eq. (46). The action  $S$  is given by Eq. (49), which we now write with a slight change of notation,

$$S(x, x_r) = \int_{x_r}^x p(x') dx', \quad (77)$$

indicating both limits of the integral. The action  $S(x, x_r)$  is real, negative, and increasing to the right in region I. The wave function (50) is now written as

$$\psi_{\text{I}}(x) = \frac{1}{\sqrt{p(x)}} \left( c_r e^{i[S(x, x_r)/\hbar + \pi/4]} + c_\ell e^{-i[S(x, x_r)/\hbar + \pi/4]} \right), \quad (78)$$

In region II, the classically forbidden region where  $x > x_r$  and  $E < V(x)$ ,  $p(x)$  is purely imaginary and is given by Eq. (46). Note that

$$p(x) = i|p(x)| \quad (79)$$

in this region. The tunneling action is defined by

$$K(x, x_r) = \int_{x_r}^x |p(x')| dx', \quad (80)$$

which differs from Eq. (51) in that we now specify explicitly the lower limit of integration. In region II  $K(x, x_r)$  is real, positive, and increasing to the right. The wave function in this region is now written as

$$\psi_{\text{II}}(x) = \frac{1}{\sqrt{|p(x)|}} \left( c_g e^{K(x, x_r)/\hbar} + c_d e^{-K(x, x_r)/\hbar} \right). \quad (81)$$

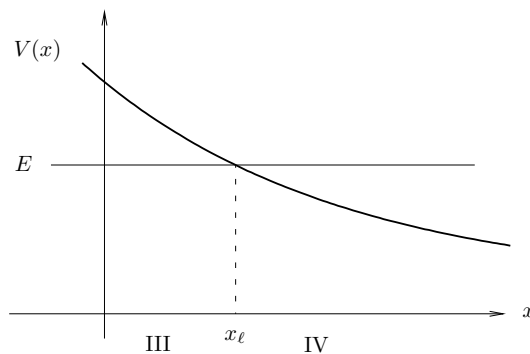
The connections between the coefficients in regions I and II are given by

$$\begin{pmatrix} c_g \\ c_d \end{pmatrix} = \begin{pmatrix} i & -i \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} c_r \\ c_\ell \end{pmatrix}, \quad (82)$$

or

$$\begin{pmatrix} c_r \\ c_\ell \end{pmatrix} = \begin{pmatrix} -\frac{i}{2} & 1 \\ +\frac{i}{2} & 1 \end{pmatrix} \begin{pmatrix} c_g \\ c_d \end{pmatrix}. \quad (83)$$

Next we consider the case of a turning point separating a classically forbidden region (III) to the left, and a classically allowed region (IV) to the right, as illustrated in Fig. 10. The turning point is  $x_\ell$ , which is not to be confused with the turning point  $x_r$  in Fig. 7. The analysis of this case is similar to what we did in Sec. 7, so we shall skip all details and simply quote the results.



**Fig. 10.** A 1-dimensional potential  $V(x)$  falling to the right. Point  $x_\ell$  is a classical turning point.

In classically forbidden region III, we have  $x < x_\ell$  and  $E < V(x)$ , function  $p(x)$  is given by Eq. (46) and is pure imaginary, and we define

$$K(x, x_\ell) = \int_{x_\ell}^x |p(x')| dx', \quad (84)$$

which is real, negative, and increasing to the right. The WKB wave in this region is

$$\psi_{\text{III}}(x) = \frac{1}{\sqrt{|p(x)|}} \left( c_g e^{K(x, x_\ell)/\hbar} + c_d e^{-K(x, x_\ell)/\hbar} \right), \quad (85)$$

where  $c_g$  and  $c_d$  are the coefficients of the waves growing and damping to the right, respectively.

In classically allowed region IV, we have  $x > x_\ell$  and  $E > V(x)$ , function  $p(x)$  is given by Eq. (46) and is real and positive, and we define

$$S(x, x_\ell) = \int_{x_\ell}^x p(x') dx', \quad (86)$$

which is real, positive, and increasing to the right. As above, we have explicitly indicated the lower limit of integration  $x_\ell$  (different from that in Eq. (77)). The WKB wave function in this region is

$$\psi_{\text{IV}}(x) = \frac{1}{\sqrt{p(x)}} \left( c_r e^{i[S(x, x_\ell) - \pi/4]} + c_\ell e^{-i[S(x, x_\ell) - \pi/4]} \right), \quad (87)$$

where  $c_r$  and  $c_\ell$  are the coefficients of waves travelling to the right and left, respectively. Notice that the phases  $e^{\pm i\pi/4}$  have been introduced with the opposite sign in comparison to Eq. (78); this is more convenient for matching the asymptotic forms of the Airy functions in the turning point regions.

The connections between the coefficients in regions III and IV is given by

$$\begin{pmatrix} c_g \\ c_d \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -i & +i \end{pmatrix} \begin{pmatrix} c_r \\ c_\ell \end{pmatrix}, \quad (88)$$

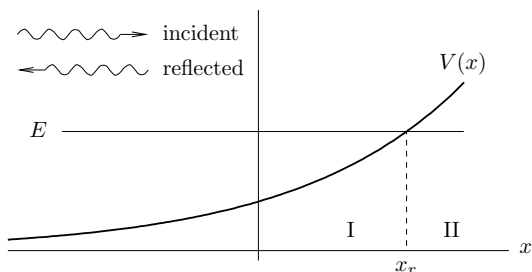
or

$$\begin{pmatrix} c_r \\ c_\ell \end{pmatrix} = \begin{pmatrix} 1 & +\frac{i}{2} \\ 1 & -\frac{i}{2} \end{pmatrix} \begin{pmatrix} c_g \\ c_d \end{pmatrix}. \quad (89)$$

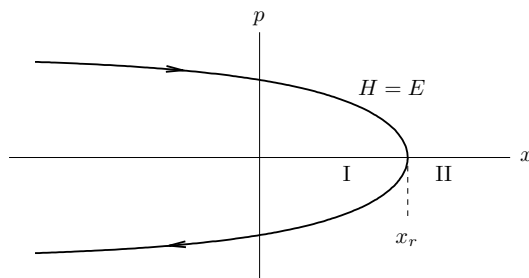
The principal limitation of these formulas is that they cannot be used when two turning points are too close together, for example, when the energy is too close to the top of a potential barrier. The latter case is important in practice, and can be handled by extensions of the WKB method that are beyond the scope of this course.

## 9. A Scattering Problem

As a first example of the connection rules, let us consider a one-dimensional scattering problem in which a particle of energy  $E$  comes in from the left, encounters an impenetrable potential barrier, and reflects back to the left. As sketched in Fig. 11, the potential  $V(x)$  approaches zero as  $x \rightarrow -\infty$  and goes to  $\infty$  as  $x \rightarrow +\infty$ . The particle cannot penetrate the barrier, so all particles launched from the left reflect and go back to the left. The orbit in phase space is illustrated in Fig. 12.



**Fig. 11.** Particle scattering from an impenetrable barrier. Point  $x_r$  is the turning point at energy  $E$ . Regions I and II are the classically allowed and forbidden regions, respectively.



**Fig. 12.** Phase space plot for potential in Fig. 11. Arrows show direction of motion on orbit  $H = E$ .

To solve the Schrödinger equation by WKB theory, we observe that the boundary conditions require that the wave function go to zero Region II, so the coefficient of the growing term  $c_g$  in this region must be zero. Let us set  $c_d = 1$  for the coefficient of the damping term in this region, which amounts to a normalization of the wave function overall. Then applying the connection rule (83), we find the coefficients of the right- and left-travelling waves in the classically allowed Region I,

$$\begin{pmatrix} c_r \\ c_\ell \end{pmatrix} = \begin{pmatrix} -\frac{i}{2} & 1 \\ +\frac{i}{2} & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \quad (90)$$

Then Eq. (78) gives the wave function in Region I,

$$\psi_I(x) = \frac{1}{\sqrt{p(x)}} \left( e^{i[S(x, x_r)/\hbar + \pi/4]} + e^{-i[S(x, x_r)/\hbar + \pi/4]} \right) = \frac{2}{\sqrt{p(x)}} \cos \left[ \frac{S(x, x_r)}{\hbar} + \frac{\pi}{4} \right]. \quad (91)$$

The wave function is an energy eigenfunction of positive energy, in the continuous part of the spectrum. It is nondegenerate, as expected from the fact that  $\psi \rightarrow 0$  as  $x \rightarrow +\infty$ . See Sec. 6.2. It is also real, as expected on the basis of time-reversal invariance. (More precisely, time-reversal invariance requires that the wave function be proportional to a real wave function; in this case, the proportionality factor is real. See Sec. 6.3.)

Another way to write the solution is

$$\psi_I(x) = \frac{e^{i\pi/4}}{\sqrt{p(x)}} \left( e^{iS(x, x_r)/\hbar} + r e^{-iS(x, x_r)/\hbar} \right), \quad (92)$$

where we define  $r$  as the *reflection amplitude*. For this problem the reflection amplitude is a phase factor,

$$r = e^{-i\pi/2} = -i. \quad (93)$$

A useful way to visualize the reflection amplitude  $r$  is to imagine that as the classical particles move along their orbits, they accumulate an action given by

$$S(t) = \int_0^t p(t') \frac{dx(t')}{dt'} dt'. \quad (94)$$

If we let the initial time  $t = 0$  be the time when the particle reaches the turning point  $x = x_r$ , then  $S(t) = S(x)$  on the upper branch of the orbit, when  $t < 0$ , and  $S(t) = -S(x)$  on the lower branch of the orbit, where  $t > 0$ . The function  $S(t)$  is a monotonically increasing function for all  $t$ , since when  $p > 0$ ,  $dx/dt > 0$ , and when  $p < 0$ ,  $dx/dt < 0$ . The upper branch is also the incident wave, while the lower branch is the reflected wave.

Then  $S(t)/\hbar$  is the phase of the incident wave in Eq. (92) up to the turning point region, whereupon the phase actually loses meaning since the wave there is no longer of WKB form. After the particle emerges from the turning point region, however, the WKB form becomes valid again, but now the phase is  $S(t)/\hbar - \pi/2$ . That is, it is as if the particle has suffered a phase shift of  $-\pi/2$  on passing through the turning point. This phase shift is also the reflection amplitude, as we have defined it. This is an example of a general rule, that a WKB wave suffers a phase shift of  $-\pi/2$  on passing through a turning point.

A turning point is an example of a *caustic*, which is a generalization of the concept of a *focus*. When light passes through a focus of a lens, it also suffers a phase shift, but it is  $-\pi$  instead of  $-\pi/2$ , since the focus involves a two dimensional family of rays.

The one-dimensional version of the probability flux is

$$J = \text{Re} \left[ \psi^* \left( -\frac{i}{\hbar} \frac{d}{dx} \right) \psi \right]. \quad (95)$$

If  $\psi$  is a solution of the time-dependent Schrödinger equation, then the one-dimensional version of the continuity equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0. \quad (96)$$

But if  $\psi$  is an energy eigenfunction, then  $\partial \rho / \partial t = 0$ , so  $J$  is independent of  $x$ .

The incident and reflected waves are the two terms in the WKB solution (92). Each of these is separately a solution of the Schrödinger equation in the WKB approximation, up to the turning point region where the WKB form breaks down and the waves become strongly coupled with one another. Therefore we can compute the flux for both the incident and reflected waves up to the turning point region, and the values must be independent of  $x$ . The easiest place to do the computation is in the asymptotic region  $x \rightarrow -\infty$ , where the particles are free and the local momentum  $p(x) = dS(x)/dx$  is the constant  $\sqrt{2mE}$ . We find

$$J_{\text{inc}} = \frac{1}{m}, \quad J_{\text{refl}} = -|r|^2 \frac{1}{m}. \quad (97)$$

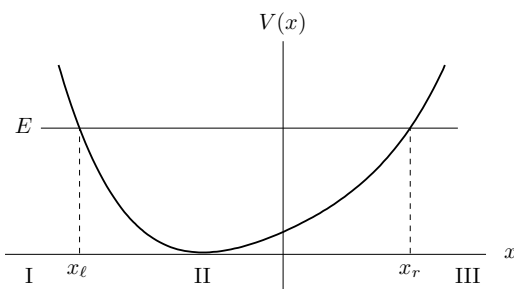
Now defining the *reflection probability*  $R$  as the absolute value of the ratio of the reflected flux to the incident flux, we have

$$R = \left| \frac{J_{\text{refl}}}{J_{\text{inc}}} \right| = |r|^2 = 1. \quad (98)$$

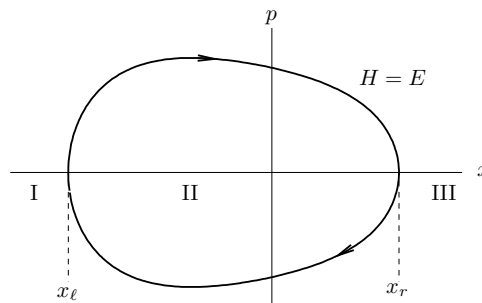
This is obviously what we expect, since all particles launched from the left must bounce back to the left.

## 10. An Oscillator

We now apply WKB theory to a one-dimensional bound-state problem. Consider a particle moving in the potential well illustrated in Fig. 13. At the energy  $E$ , the left turning point is  $x_\ell$  and the right one is  $x_r$ . We assume the potential rises to infinity to the left of  $x_\ell$  and to the right of  $x_r$ , so no tunnelling out of the well is possible. Region I,  $x < x_\ell$ , and Region III,  $x > x_r$ , are the classically forbidden regions, while Region II,  $x_\ell < x < x_r$ , is the classically allowed region. Figure 14 shows the orbit  $H = E$  in phase space, with arrows indicating the direction of motion.



**Fig. 13.** A potential well. There are two turning points at energy  $E$ .



**Fig. 14.** Orbit  $H = E$  in phase space for the potential in Fig. 13.

Let us begin with a somewhat intuitive approach. The particles accumulate a phase  $(1/\hbar) \int p dx$  as they move around the orbit, but lose a phase  $\pi/2$  when passing through a turning point, so on going completely around the orbit and passing through two turning points the total phase is

$$\frac{1}{\hbar} \oint p dx - \pi. \quad (99)$$

Notice that  $\oint p dx$  is the area in phase space of the orbit. But if the wave function is single-valued, then the phase (99) must be  $2n\pi$ , for an integer  $n$ . Thus we find

$$\oint p dx = (n + \frac{1}{2})2\pi\hbar. \quad (100)$$

Since the area is positive, we have  $n = 0, 1, 2, \dots$ . This is the *Bohr-Sommerfeld quantization rule* for a one-dimensional oscillator. The discrete set of classical orbits that satisfy this condition are regarded as *quantized* orbits.

A region of phase space with area  $2\pi\hbar$  is sometimes called a *Planck cell*. The Bohr-Sommerfeld rule says that the  $n$ -th quantized orbit encloses  $n + \frac{1}{2}$  Planck cells. In particular, the ground state encloses one half of a Planck cell.

In classical mechanics, the quantity

$$I = \frac{1}{2\pi} \oint p dx \quad (101)$$

is called the *action* of the orbit. (Do not confuse this with other quantities called the “action.”) It depends on the orbit, that is,  $I$  is a function of the energy of the orbit,  $I = I(E)$ . This function

can be inverted to give the energy as a function of the action,  $E = E(I)$ . It can be shown (see Prob. 1(a)) that

$$\omega = \frac{dE}{dI}. \quad (102)$$

The Bohr-Sommerfeld quantization rule can be stated by saying that the action is quantized,

$$I_n = (n + \frac{1}{2})\hbar. \quad (103)$$

The quantized values of the action are universal (they apply to all oscillators). The corresponding quantized energies are obtained through the classical action-energy relationship,

$$E_n = E(I_n). \quad (104)$$

These are the energy eigenvalues of a one-dimensional oscillator in the WKB approximation. They are not exact, in general, but they are often good approximations to the true eigenvalues.

To analyze this problem more carefully, and to get the wave functions, we begin by writing down the wave functions in the three regions in terms of a set of unknown coefficients. We have

$$\psi_{\text{I}}(x) = \frac{1}{\sqrt{|p(x)|}} [a_g e^{K(x, x_\ell)/\hbar} + a_d e^{-K(x, x_\ell)/\hbar}], \quad (105a)$$

$$\begin{aligned} \psi_{\text{II}}(x) &= \frac{1}{\sqrt{p(x)}} [b_\ell e^{iS(x, x_\ell)/\hbar - i\pi/4} + b_r e^{-iS(x, x_\ell)/\hbar + i\pi/4}] \\ &= \frac{1}{\sqrt{p(x)}} [b'_\ell e^{iS(x, x_r)/\hbar + i\pi/4} + b'_r e^{-iS(x, x_r)/\hbar - i\pi/4}], \end{aligned} \quad (105b)$$

$$\psi_{\text{III}}(x) = \frac{1}{\sqrt{|p(x)|}} [c_g e^{K(x, x_r)/\hbar} + c_d e^{-K(x, x_r)/\hbar}], \quad (105c)$$

where  $(a_g, a_d)$  and  $(c_g, c_d)$  are the coefficients of the growing and damping waves in Regions I and III, respectively, and where  $(b_\ell, b_r)$  and  $(b'_\ell, b'_r)$  are the coefficients of the waves moving to the left and right in Region II. The wave in this region is written in two different ways, by referring the action either to the left or the right turning point. Equation (105a) is patterned on Eq. (85), the unprimed and primed versions of Eq. (105b) are patterned on Eqs. (87) and (78), respectively, and Eq. (105c) is patterned on Eq. (81).

To find all the coefficients, we work from the left. In Region I, boundary conditions require  $a_d = 0$ , since  $e^{-K/\hbar}$  blows up as  $x \rightarrow -\infty$ . Take  $a_g = 1$  as a provisional normalization. Then by Eq. (89) we have

$$\begin{pmatrix} b_r \\ b_\ell \end{pmatrix} = \begin{pmatrix} 1 & +\frac{i}{2} \\ 1 & -\frac{i}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \quad (106)$$

Next we note that the two expressions for the wave in Region II must be equal, and that

$$S(x, x_\ell) = \int_{x_\ell}^x p dx = \int_{x_\ell}^{x_r} p dx + \int_{x_r}^x p dx = \pi I + S(x, x_r), \quad (107)$$



where we use the fact that

$$\text{Area} = 2\pi I = \oint p dx = 2 \int_{x_\ell}^{x_r} p(x) dx. \quad (108)$$

Thus, in Region II we have

$$\begin{aligned} b_\ell e^{i[\pi I + S(x, x_r)]/\hbar - i\pi/4} + b_r e^{i[-\pi I - S(x, x_r)]/\hbar + i\pi/4} \\ = b'_\ell e^{iS(x, x_r)/\hbar + i\pi/4} + b'_r e^{-iS(x, x_r)/\hbar - i\pi/4}. \end{aligned} \quad (109)$$

But the right- and left-travelling waves are linearly independent, so this equation can only be satisfied if

$$\begin{aligned} b_\ell e^{i\pi I/\hbar - i\pi/4} &= b'_\ell e^{i\pi/4}, \\ b_r e^{-i\pi I/\hbar + i\pi/4} &= b'_r e^{-i\pi/4}, \end{aligned} \quad (110)$$

or, with Eq. (106),

$$\begin{pmatrix} b'_r \\ b'_\ell \end{pmatrix} = \begin{pmatrix} e^{-i\pi I/\hbar + i\pi/2} \\ e^{i\pi I/\hbar - i\pi/2} \end{pmatrix}. \quad (111)$$

Finally, Eq. (82) gives

$$\begin{pmatrix} c_g \\ c_d \end{pmatrix} = \begin{pmatrix} i & -i \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} b'_r \\ b'_\ell \end{pmatrix} = \begin{pmatrix} -2 \cos\left(\frac{\pi I}{\hbar}\right) \\ \cos\left(\frac{\pi I}{\hbar} - \frac{\pi}{2}\right) \end{pmatrix}. \quad (112)$$

But boundary conditions on the right require  $c_g = 0$ , so

$$\frac{\pi I}{\hbar} - \frac{\pi}{2} = n\pi, \quad (113)$$

which is equivalent to the Bohr-Sommerfeld rule (100) or (103). Also, we find the coefficient  $c_d$ ,

$$c_d = \cos n\pi = (-1)^n. \quad (114)$$

The wave function in the classically allowed region is conveniently written,

$$\psi_{\text{II}}(x) = \frac{2}{\sqrt{p(x)}} \cos\left[\frac{S(x, x_\ell)}{\hbar} - \frac{\pi}{4}\right]. \quad (115)$$

We will leave the normalization of this wave function as an exercise.

## 11. Example: The Harmonic Oscillator

The harmonic oscillator has the Hamiltonian,

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad (116)$$

so the orbits in phase space are ellipses. The  $x$ -intercept of an orbit of energy  $E$  is obtained by setting  $p = 0$  and solving for  $x$ ,

$$x_0 = \sqrt{\frac{2E}{m\omega^2}}, \quad (117)$$

and the  $p$ -intercept by setting  $x = 0$  and solving for  $p$ ,

$$p_0 = \sqrt{2mE}. \quad (118)$$

The area is

$$\pi \sqrt{\frac{2E}{m\omega^2}} \sqrt{2mE} = \frac{2\pi E}{\omega} = (n + \frac{1}{2})2\pi\hbar, \quad (119)$$

which we have assigned to the Bohr-Sommerfeld quantized value. Solving for  $E$ , we find

$$E_n = (n + \frac{1}{2})\hbar\omega. \quad (120)$$

The WKB approximation to the energy levels of the harmonic oscillator is exact. The WKB wave function, however, is only approximate.

### Problems

1. In this problem we work with one-dimensional, kinetic-plus-potential Hamiltonians,

$$H = \frac{p^2}{2m} + V(x). \quad (121)$$

(a) Prove Eq. (102) when the motion is governed by the Hamiltonian (121).

(b) A classical charged particle in periodic motion radiates at the frequency  $\omega$  of the motion as well as all higher harmonics  $k\omega$ ,  $k = 2, 3, \dots$ . In many cases the power radiated at higher harmonics is small, but the general principle holds. This follows from standard methods of classical electromagnetic theory, applied to a particle in periodic motion.

In quantum mechanics, the frequency of the radiation emitted by a particle is  $\Delta E/\hbar$ , where  $\Delta E$  is the energy difference between an initial and final state. This follows from the Einstein relation  $E = \hbar\omega$  for the energy of a photon and the Bohr notion that mechanical systems (atoms etc) have discrete energy levels. This part of the argument was understood in the days of the old quantum theory, well before modern quantum mechanics had been developed.

Consider a one-dimensional oscillator in quantum state  $n$  with energy  $E_n$  where  $n$  is large, and suppose it makes a transition to lower energy level  $n - \Delta n$ , where  $\Delta n$  is small. Using the Bohr-Sommerfeld quantization rule, show that the frequency of the emitted radiation is approximately a harmonic of the classical frequency  $\omega$  at classical energy  $E_n$ .

Notice that if the power radiated in higher harmonics of the classical problem is small, it means that the most probable quantum transition is one with  $\Delta n = 1$ .

2. Consider the Bohr-Sommerfeld quantization of a 1-dimensional oscillator in a potential  $V(x)$ .

(a) Integrate the square of the WKB wave function  $\psi$  between the two turning points to obtain the normalization constant. The wave function blows up at the turning points, but you can do the

integral anyway. Write out the normalized wave function. (The damped waves in the classically forbidden regions can be ignored.) Replace  $\cos^2$  by the average value  $1/2$  in the integrand before doing the integral. Express the normalization constant both in terms of the classical period  $T$  and the quantity  $\partial E_n/\partial n$ , where  $n$  is treated as a continuous quantity.

(b) Now assume the potential well is symmetric,  $V(-x) = V(x)$ , with  $V(0) = 0$ . Show that

$$|\psi(0)|^2 = \frac{1}{\pi\hbar} \sqrt{\frac{2m}{E}} \frac{\partial E_n}{\partial n} \cos^2\left(\frac{n\pi}{2}\right), \quad (122)$$

and

$$|\psi'(0)|^2 = \frac{\sqrt{8m^3 E}}{\pi\hbar^3} \frac{\partial E_n}{\partial n} \sin^2\left(\frac{n\pi}{2}\right). \quad (123)$$

Carry your calculations only out to leading order in  $\hbar$ .

3. Consider the potential energy illustrated in Fig. 15.

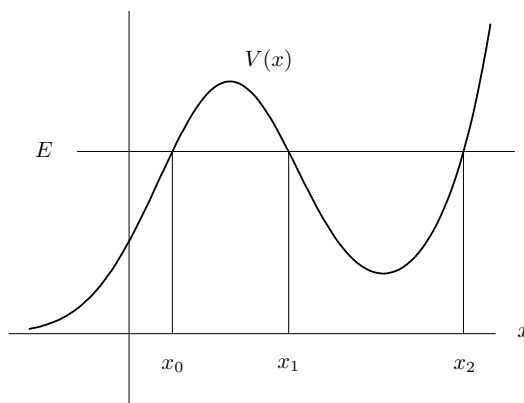


Fig. 15. Potential for problem 3.

For the energy shown, there are three turning points. In the region to the left of  $x_0$  let  $\psi$  have the form,

$$\psi(x) = \frac{1}{p(x)^{1/2}} \left( e^{iS(x,x_0)/\hbar} + r e^{-iS(x,x_0)/\hbar} \right), \quad (124)$$

where  $r$  is the reflection amplitude. Find  $r$  as a function of the energy  $E$ . Please use the following notation:

$$\Phi = \frac{2}{\hbar} S(x_2, x_1), \quad (125)$$

and

$$\kappa = \frac{1}{\hbar} K(x_1, x_0). \quad (126)$$

Hint: work from right to left.

Show that  $|r|^2 = 1$ , which means that all particles sent in from the left come back (ingoing and outgoing fluxes are equal). Show that when the energy is not close to a nominal Bohr-Sommerfeld

energy level of the well, then  $r \approx -i$  (the value  $r$  would have if there were no well to the right of  $x_0$ ), but that when  $E$  increases through such an energy level, then the phase of  $r$  rapidly increases by  $2\pi$ . This is a resonance. Estimate the range  $\Delta E$  over which this change takes place. Assume that the energy is not too close to the top of the well, i.e., the quantity  $e^{-\kappa}$  is small.

Estimate the ratio  $\psi_{\text{in}}/\psi_{\text{out}}$  of the wave function inside and outside the well, in the case where  $E$  is far from a Bohr-Sommerfeld energy level of the well, and in the case where  $E$  is equal to one of these energy levels.

4. As you know, the radial wave equation in 3-dimensional problems with central force potentials looks like a 1-dimensional Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2 f}{dr^2} + U(r)f(r) = Ef(r), \quad (127)$$

except that  $r$  ranges from 0 to  $\infty$ , and the potential  $U(r)$  is the sum of the centrifugal potential and the true potential  $V(r)$ ,

$$U(r) = \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r). \quad (128)$$

Therefore one-dimensional WKB theory can be applied to the radial wave equation. It can be shown that more accurate results are obtained in the WKB treatment if the quantity  $\ell(\ell+1)$  in the centrifugal potential is replaced by  $(\ell + \frac{1}{2})^2$ . This is called the *Langer modification*. Just accept this fact for the purposes of this problem; the justification has to do with the singularity of the centrifugal potential as  $r \rightarrow 0$ .

(a) Take the case of a free particle,  $V(r) = 0$ . Find the WKB solution in the classically allowed region. For boundary conditions in the classically forbidden region near  $r = 0$ , just assume that there is only a growing wave (as  $r$  increases). Evaluate all functions explicitly; use the abbreviation  $k = \sqrt{2mE}/\hbar$ . Take the limit  $r \rightarrow \infty$ , and reconcile the result with the asymptotic forms of the spherical Bessel function  $j_\ell(\rho)$ , quoted by Sakurai in his Eq. (A.5.15). (Sakurai's  $\rho = kr$ .)

(b) Consider a potential  $V(r)$  which is not zero, but which approaches 0 as  $r \rightarrow \infty$ . Since the particle approaches a free particle as  $r \rightarrow \infty$ , we might expect the solution at large  $r$  to look like a free particle solution, but with a phase shift. Explicitly, if the free particle solution has the form  $f(r) = \cos(kr + \alpha_f)$  as  $r \rightarrow \infty$ , where  $\alpha_f$  is the phase shift for the free particle, and the solution in the presence of the potential has the form  $f(r) = \cos(kr + \alpha_p)$  as  $r \rightarrow \infty$ , where  $\alpha_p$  is the phase shift in the presence of the potential, then we define  $\delta = \alpha_p - \alpha_f$  as the phase shift in the potential scattering, measured relative to the phase shift of a free particle. Use WKB theory to write down an expression for  $\delta$ , which will involve the limit of a certain quantity as  $r \rightarrow \infty$ .

(c) Does this limit exist? It can be shown that it does if  $V(r)$  falls off more rapidly as  $r \rightarrow \infty$  than the centrifugal potential, i.e., more rapidly than  $1/r^2$ ; the limit also exists when the true potential falls off exactly as fast as the centrifugal potential, i.e., as  $1/r^2$ . Therefore consider the case that

$V(r)$  approaches 0 as  $1/r^\alpha$ , where  $0 < \alpha < 2$ . Show that the phase shift exists only if  $1 < \alpha < 2$ . In particular, in the important case of the Coulomb potential ( $\alpha = 1$ ), the phase shift does not exist (the asymptotic form of the radial wave function  $f$  is more complicated than a phase-shifted free particle solution).

**5.** Consider a quantum particle bouncing off the floor. The vertical coordinate is  $x$ , and  $V(x) = mgx$ . The floor at  $x = 0$  acts like a hard wall.

(a) Write down the Schrödinger equation and solve it in terms of Airy functions. Let  $z_n$  be the  $n$ -th root of the Airy function, that is,  $\text{Ai}(z_n) = 0$ , where the roots satisfy

$$\dots < z_2 < z_1 < z_0 < 0. \quad (129)$$

Express the energy eigenvalues as a dimensionless multiple of the reference energy,

$$K = \left( \frac{mg^2 \hbar^2}{2} \right)^{1/3}. \quad (130)$$

(b) For the classical bouncing ball, sketch the orbits in phase space. Let  $h = E/mg$  be the height to which the ball bounces (but don't confuse  $h$  with  $\hbar$ ). Find the Bohr-Sommerfeld approximations to the energy eigenvalues  $E_n$ ,  $n = 0, 1, \dots$ . Recall that the wave suffers a phase shift of  $-\pi/2$  on passing through a turning point at a soft wall, but  $-\pi$  when reflecting off a hard wall. Express your answer as a dimensionless multiple of  $K$ . The first three zeroes of the Airy function are  $-2.33811$ ,  $-4.08795$  and  $-5.52056$ . Compare the Bohr-Sommerfeld approximation to the exact eigenvalues for the first three eigenstates.