Massachusetts Institute of Technology
Physics Department

Physics 8.322 **Spring 2007**
Quantum Theory II **March 5, 2007**

Notes on WKB Approximation for Reflection above a Barrier and The Transition Amplitude in the Adiabatic Approximation

1 Reflection above a barrier

A particularly interesting and useful application of the WKB approximation involves calculation of the exponentially small probability that a particle is reflected from a barrier that it would classically penetrate. The aim of this first section is to present a physically "intuitive" (and to my knowledge new) derivation of this probability. Two examples of such barriers are shown in Fig. 1. The first is $V_1(x) = -\frac{1}{2}\alpha x^2$ and the second is $V_2(x) = V_0 \operatorname{sech}^2(x/a)$[1].

The derivation makes use of the standard WKB result for the barrier penetration factor. When a particle encounters a barrier, $V(x)$, which exceeds its energy for $x_1 < x < x_2$, the probability of penetration is

$$F(E) = \exp\left(-\frac{2}{\hbar}\int_{x_1(E)}^{x_2(E)} dx\sqrt{2m(V(x)-E)}\right) \tag{1}$$

where the integral is over the classically forbidden region (note $V(x) > E$ throughout the integral). $x_{1,2}(E)$ are the classical turning points where $V(x) = E$.

Reflection above the barrier can be viewed as *barrier penetration in momentum space.* To see how this can be, consider for example the description of classical motion in the inverted harmonic oscillator potential, Fig. 1a. Suppose the particle is incident from the left. At large negative x it has a large positive momentum, p. As x increases toward zero, p decreases, reaching a minimum $p_0(E) = \sqrt{2mE}$, at $x = 0$. If it is transmitted, the momentum increases thereafter as it moves off to the right. Now consider this sequence of statements from the perspective of momentum space: Initially the particle has large positive momentum, which decreases to a minimum, $p_0(E)$, and then increases. In other words, the particle "reflects" from a barrier in momentum space located at p_0[2]. The situation in momentum

[1] For simplicity, in these notes I will consider only symmetric potentials, $V(x) = V(-x)$. The generalization is straightforward.

[2] For a generic potential the barrier is at $p_0 = \sqrt{2m(E - V_{\max})}$.

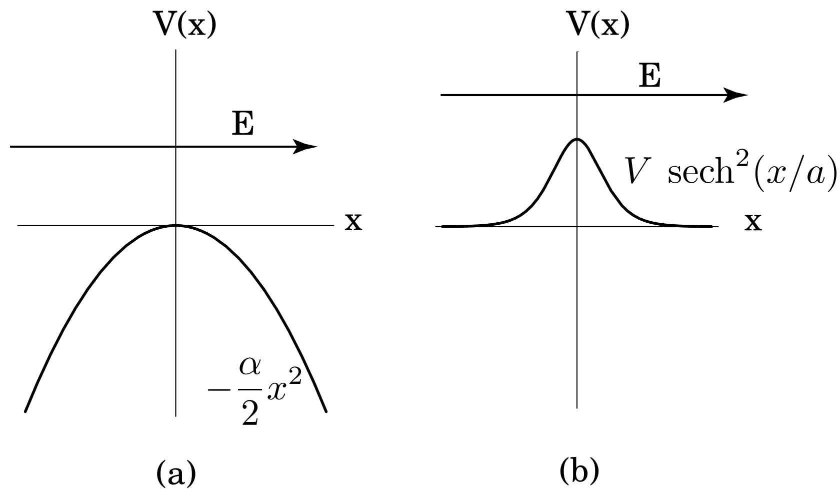

Figure 1: Parabolic (a) and Hyperbolic secant (b) barriers. The energy, E, is above the barrier.

space is illustrated in Fig. 2. If the particle were to reflect from the barrier *in coordinate space*, it must make a transition to negative momentum, $-p_0(E)$, in momentum space, and then continue to ever more negative momentum. Since values of momentum between $-p_0$ and p_0 cannot occur classically, this transition looks like *"tunneling" in momentum space.*

Consider the Schrödinger equation for the momentum space wave function, $\phi(p)$,

$$\left(\frac{p^2}{2m} + V(i\hbar\frac{d}{dp})\right)\phi(p) = E\phi(p). \tag{2}$$

where I have written V as a function of the operator $x \rightarrow i\hbar\frac{d}{dp}$ which is appropriate in momentum space. Unless $V(x)$ is a sum of powers, $V(i\hbar\frac{d}{dp})$ is an integral operator. However when the WKB approximation is valid, things simplify significantly. As always, the WKB approach is to attempt to expand the logarithm of the wave function in a power series in $\hbar$,

$$\phi(p) = \exp\left(\frac{i}{\hbar}\sigma(p) + \mathcal{O}(\hbar^0)\right) \tag{3}$$

Substituting into eq. (2) and keeping the leading term in $\hbar$, we find

$$\frac{p^2}{2m} + V(-\sigma'(p)) = E \tag{4}$$

where $\sigma'(p) = \frac{d\sigma}{dp}$. This equation can be solved for $\sigma(p)$ in terms of the inverse of $V(x)$,

$$\sigma(p) = \int^p dp'\, V^{-1}(E - \frac{p'^2}{2m}) \tag{5}$$

Just to be clear about the meaning of V^{-1}, for the two examples mentioned at the very

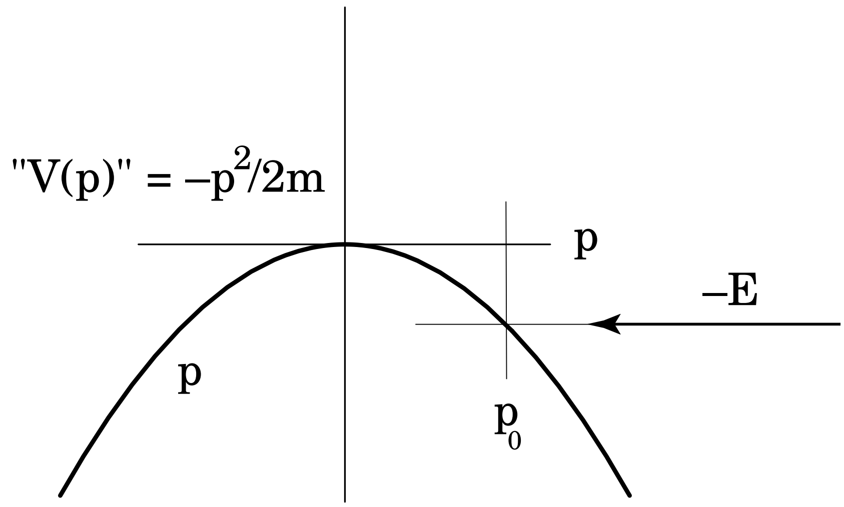

Figure 2: It is easy to show that for an inverse harmonic potential, $V(x) = -\frac{1}{2}\alpha x^2$, the problem of reflection of a particle with energy E can be transformed into the problem of tunneling of a particle with "mass" $1/\alpha$ and "energy" $-E$ through a "potential" $-\frac{p^2}{2m}$.

beginning,

$$\begin{aligned} V_1^{-1}(y) &= \pm\sqrt{\frac{-2y}{\alpha}}, \quad \text{and} \\ V_2^{-1}(y) &= \pm a\cosh^{-1}(V_0/y) = a\ln\left(\sqrt{\frac{V_0}{y}} \pm \sqrt{\frac{V_0}{y} - 1}\right) \end{aligned} \tag{6}$$

It is easy to see that $\sigma(p)$ is imaginary in the region $-p_0 < p < p_0$, where p_0 is the minimum allowed value of the classical momentum. So the transition from p_0 to $-p_0$ is damped by the factor,

$$|R(E)|^2 = \exp\left(-\frac{2}{\hbar}\int_{-p_0(E)}^{p_0(E)} dp\ \mathrm{Im}\{V^{-1}(E - \frac{p^2}{2m})\}\right) \tag{7}$$

where it is understood that any ambiguity in the sign of V^{-1} is fixed by the requirement that the imaginary part is positive, since we are interested in the solution that falls in the classically forbidden region.

1.1 Examples

The study of the two examples will make the assertions of the previous section clear.

A. $\mathbf{V_1(x) = -\frac{1}{2}\alpha x^2}$

The relevant function is

$$V_1^{-1}(E - \frac{p^2}{2m}) = \sqrt{\frac{p^2}{\alpha m} - 2\frac{E}{\alpha}} = \frac{i}{\sqrt{\alpha}}\sqrt{2E - p^2/m} \tag{8}$$

which is imaginary when $p^2 < 2mE$ as expected. So the semiclassical wavefunction in momentum space falls exponentially when $p^2 < 2mE$ as a glance at Fig. 2 shows it must. Note that if the particle's energy is *below the barrier in coordinate space* then it is *above the barrier in momentum space*. For the inverted harmonic oscillator, $V_{\max} = 0$, so for $E < 0$ the transition from p to $-p$ is classically allowed. Then reflection from the barrier is classically allowed and tunnelling is exponentially small.

Returning to $E > 0$ where reflection in coordinate space is exponentially small, combining eqs. (1) and (8) we obtain a reflection probability of

$$|R_1(E)|^2 = \exp\left(-\frac{2}{\hbar}\int_{-\sqrt{2mE}}^{\sqrt{2mE}} dp\sqrt{\frac{2}{\alpha}(E - \frac{p^2}{2m})}\right) \tag{9}$$

The integral can be evaluated with the result:

$$|R_1(E)|^2 = e^{-\frac{2\pi E}{\hbar\omega}}$$

where $\omega \equiv \sqrt{\alpha/m}$ in an analogy with the frequency of a normal oscillator. This result can be checked against the exact result,

$$|R_1(E)|^2_{\text{exact}} = \frac{e^{-\frac{2\pi E}{\hbar\omega}}}{1 + e^{-\frac{2\pi E}{\hbar\omega}}}$$

with which it agrees to exponential accuracy.

B. $\mathbf{V_2(x) = V_0 sech^2(x/a)}$

Looking back at eq. (6), we see that $V_2^{-1}(y)$ can be imaginary if $V_0 < y$, since there is no real number whose cosh is less than unity. Since the argument of V_2^{-1} is $E - p^2/2m$ the reflection coefficient is exponentially small when $p^2/2m < E - V_0$, as expected. In this case

$$V_2^{-1}(E - \frac{p^2}{2m}) = \pm a\cosh^{-1}\sqrt{\frac{V_0}{E - \frac{p^2}{2m}}} = \pm ia\cos^{-1}\sqrt{\frac{V_0}{E - \frac{p^2}{2m}}}$$

The reflection coefficient is given by

$$|R_2(E)|^2 = \exp\left(-\frac{2a}{\hbar}\int_{-p_0}^{p_0} dp\cos^{-1}\sqrt{\frac{V_0}{E - \frac{p^2}{2m}}}\right) \tag{10}$$

where $p_0 = \sqrt{2m(E - V_0)}$. With a little work this integral can be performed with the result,

$$|R_2(E)|^2 = \exp\left(-\frac{2\pi a}{\hbar}\sqrt{2mV_0}\left(\frac{E}{V_0} - 1\right)\right)$$

1.2 Relation to the "standard" result of Landau and Lifschitz

Landau and Lifschitz analyse the problem in the complex x-plane, but their analysis is difficult to follow. Without loss of generality assume that the potential, $V(x)$ is symmetric in x and takes on its maximum at $x = 0$. Here is their "recipé": When the energy is above the barrier, the classical momentum, $p(x) = \sqrt{2m(E - V(x))}$ does not vanish for any real x. Instead it typically vanishes for an *imaginary* value of x. Let $x_0 = iy_0$ be the zero of $p(x)$. Only positive values of y_0 are to be considered. Then the result quoted by Landau and Lifschitz is,

$$|R(E)|^2 = \exp -\frac{4}{\hbar}\,\mathrm{Im} \int_0^{x_0} dx \sqrt{2m(E - V(x))} = \exp -\frac{4}{\hbar} \int_0^{y_0} dy \sqrt{2m(E - V(iy))} \quad (11)$$

It is easy to show that this result is identical to ours. Consider the argument of the exponential in eq. (11) and integrate by parts on y,

$$\int_0^{y_0} dy\, p(iy) = yp(iy)|_0^{y_0} + \int_0^{p_0} dp\, y(p) \quad (12)$$

$p(iy)$ vanishes at $y = y_0$ so the surface term vanishes. The limit in the p-integral, p_0 is the value of the classical momentum at $y = 0$, the top of the barrier. The function $y(p)$ is the solution to the equation, $p = \sqrt{2m(E - V(iy))}$, which is $-iV^{-1}(E - p^2/2m)$, just what appears in eq. (7). So, in essence, the connection between the two approaches is summarized by $\int pdx = -\int xdp$.

The WKB treatment of reflection above the barrier has an important application to the study of the adiabatic approximation.

2 The transition amplitude in the adiabatic approximation

When a Hamiltonian changes slowly enough in time, a system initially prepared in an energy eigenstate will not make a transition to a different energy eigenstate provided the two states remain well separated in energy. If the Hamiltonian changes slowly and smoothly, then the WKB approximation can be used to estimate the transition probability.

For simplicity I consider two states and a Hamiltonian

$$H(t) = \begin{pmatrix} f(t) & \epsilon \\ \epsilon & -f(t) \end{pmatrix} \quad (13)$$

where $f(t)$ is a function that increases monotonically with t and is scaled by a parameter T, the "transition time", that determines the adabaticity. The simplest case, $f(t) = t/T$, will serve as a concrete example when needed. At any time the eigenvalues of $H(t)$ are

$$E_\pm(t) = \pm\sqrt{f(t)^2 + \epsilon^2} \equiv \pm E(t)$$

and the eigenvectors are

$$\begin{aligned} \phi_+(t) &= \begin{pmatrix} \sin\theta/2 \\ \cos\theta/2 \end{pmatrix} \\ \phi_-(t) &= \begin{pmatrix} \cos\theta/2 \\ -\sin\theta/2 \end{pmatrix} \end{aligned} \quad (14)$$

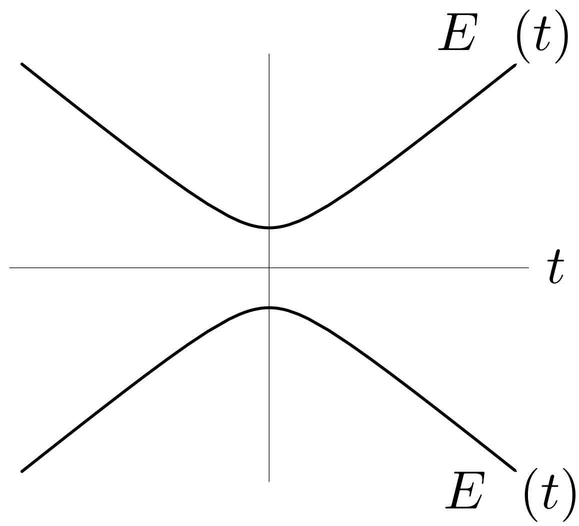

Figure 3: Eigenvalues of the time dependent Hamiltonian, $E_{\pm}(t) = \pm\sqrt{\epsilon^2 + \alpha^2 t^2}$.

where

$$\tan\theta = -\frac{\epsilon}{f(t)}.$$

A generic example of the energy level diagram is shown in Fig. 3.

2.1 Adiabatic solutions

First let's write down the solutions in the adiabatic limit[3]. The lower (upper) energy state, $\Psi^{(\pm)}(t)$, follows $\phi_{\pm}(t)$,

$$\Psi^{(\pm)}_{\text{adiabatic}}(t) = \phi_{\pm}(t) e^{\mp \frac{i}{\hbar}\int^t dt' E(t')} \text{ corresponding to } E = \pm E(t) \tag{15}$$

2.2 WKB analysis

Suppose the function $f(t)$ varies very slowly with t. Then we can show that the WKB approximation applies to this problem, under conditions analogous to the ones required for WKB propagation in one dimension.

First we write the full, time dependent Schrödinger equation for this problem without approximation. Let $\psi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$. Then $i\hbar\dot{\psi} = H\psi$ implies

$$\begin{aligned} i\hbar\dot{a} &= fa + \epsilon b \\ i\hbar\dot{b} &= \epsilon a - fb. \end{aligned} \tag{16}$$

[3] We do not need to allow for an adiabatic phase here because we are not considering a *closed* path in the space of states, and therefore the phase can be transformed away.

Or, equivalently,

$$\begin{aligned} -\hbar^2\ddot{a} - (f^2+\epsilon^2)a - i\hbar\dot{f}a &= 0 \\ b &= \frac{1}{\epsilon}(i\hbar\dot{a} - fa). \end{aligned} \tag{17}$$

The first of these equations is the one-dimensional Schrödinger equation with a classical potential $-(f^2+\epsilon^2)$ and a "quantum potential", $i\hbar\dot{f}$. In the usual WKB manner, we attempt a solution of the form,

$$a(t) = \exp(\frac{i}{\hbar}\sigma_0(t) + \sigma_1(t) + \mathcal{O}(\hbar))$$

with result,

$$\begin{aligned} \mathcal{O}(\hbar^0): &\qquad \dot{\sigma}_0^2 = \epsilon^2 + f^2 \\ \mathcal{O}(\hbar^1): &\qquad 2\dot{\sigma}_0\dot{\sigma}_1 + \ddot{\sigma}_0 + \dot{f} = 0 \end{aligned} \tag{18}$$

The first of these is of standard WKB form with $x \leftrightarrow t$ and $\epsilon^2 + f^2(t)$ playing the role of $2m(E - V(x))$. The solution is

$$\dot{\sigma}_0 \to \dot{\sigma}_0^{\pm}(t) = \pm\sqrt{e^2 + f^2(t)} = \pm E(t) \tag{19}$$

The second equation can also be solved analytically, with the result

$$\sigma_1^{\pm}(t) = -\frac{1}{4}\ln E^2(t) \mp \frac{1}{2}\ln(f(t) + E(t)) \tag{20}$$

The exponential time dependence of $a_{\pm}(t)$ determined by $\sigma_0^{\pm}(t)$ matches the adiabatic result, and the prefactor determined by $\sigma_1^{\pm}(t)$, after some algebra, reproduces the factors of $\sin\theta/2$ or $\cos\theta/2$ found in the upper component of $\phi_{\pm}$. When $b_{\pm}$ is constructed from the lower of eqs. (17) we find up to a multiplicative constant,

$$\Psi^{(\pm)}_{\mathrm{WKB}}(t) = \Psi^{(\pm)}_{\mathrm{adiabatic}}(t) \tag{21}$$

While this may seem obvious, it is comforting that the time evolution governed by WKB is unitary. The prefactor determined by $\sigma_1^{\pm}$ was crucial in this result.

2.3 Transition rate in the adiabatic approximation

Now we have the machinery easily to calculate the amplitude that a system prepared initially in (say) $\Psi^{(+)}$ as $t \to -\infty$, has made a transition to $\Psi^{(-)}$ as $t \to +\infty$.

The result follows simply from the form of eq. (19) and the analogy to reflection above the barrier in ordinary 1-dimensional WKB. We are interested in the following conditions,

$$\begin{aligned} \lim_{t\to-\infty}\Psi(t) &= \Psi^{(+)}(t) \\ \lim_{t\to+\infty}\Psi(t) &= T\Psi^{(+)}(t) + R\Psi^{(-)}(t) \end{aligned} \tag{22}$$

T is the amplitude that the system is "transmitted" through the approximate level crossing without making a transition. R is the amplitude that the system is reflected into the other state. The calculation of R amounts to calculation of the reflection coefficient for one-dimensional scattering of a system with energy zero in a potential

$$\text{``}V\text{''}(t) = -(f^2(t) + \epsilon^2)$$

as can be seen from the first of eqs (17) (It is clear from the discussion following eq. (18) that the $i\hbar\dot{f}$ plays no role in the calculation of the reflection factor. It serves to enforce probability conservation.). Thus $T = 1$ and R is exponentially small, given by eq. (7) with

$$\begin{aligned} V(x) &\rightarrow -(f^2(t) + \epsilon^2) \\ E &\rightarrow 0 \qquad (23) \\ 2m &\rightarrow 1 \qquad (24) \end{aligned}$$

So the transition probability in the WKB treatment of the adiabatic approximation is

$$|R|^2 = \exp\left(-\frac{2}{\hbar}\int_{-\epsilon}^{\epsilon} dp \ \mathrm{Im}\{f^{-1}(\sqrt{p^2 - \epsilon^2})\}\right)$$

which is our final result.

2.4 Example

Here is a concrete example:

$$f(t) = t/T \quad \rightarrow \quad f^{-1}(y) = Ty$$

which gives

$$|R|^2 = \exp\left(-\frac{4T}{\hbar}\int_{-\epsilon}^{\epsilon} dp \ \sqrt{\epsilon^2 - p^2}\right) = \exp\left(-\frac{\pi T\epsilon^2}{\hbar}\right)$$

which decreases exponentially with both the transition time and the square of the minimum separation of the energy levels.