Physics 8.06 Apr 1, 2008

SUPPLEMENTARY NOTES ON THE CONNECTION FORMULAE FOR THE SEMICLASSICAL APPROXIMATION

The WKB "connection formulas" allow one to continue semiclassical solutions from an allowed to a forbidden region and vice versa. However these formulas are subtle and must be used with care. The purpose of these notes is to explain how to use the them and why it is necessary to be careful. Note that we are not **deriving** the connection formulas here. The derivation is either long and dull (e.g., Griffiths or Merzbacher) or short, elegant and obscure (e.g., Landau and Lifschitz). In any case, the proper use of the connection formulas is quite independent of how they are derived. The semiclassical approximation is valid whenever the rate of change of the de Broglie wavelength is small,

$$\left|\frac{d\lambda}{dx}\right| \ll 1 \tag{1}$$

where $\lambda = \hbar/p(x)$ and $p(x) = \sqrt{2m(E - V(x))}$. Eq. (1) can be satisfied in a classically allowed region, where $E > V(x)$, and λ is real, or in a classically forbidden region where $E < V(x)$, and λ is imaginary. As derived in class the wavefunctions in the semiclassical limit are given by:

$$\psi(x) \cong c_+ \frac{1}{\sqrt{p(x)}} \exp\left[\frac{i}{\hbar}\int^x dx' p(x')\right] + c_- \frac{1}{\sqrt{p(x)}} \exp\left[-\frac{i}{\hbar}\int^x dx' p(x')\right] \tag{2a}$$

in the classically allowed region, and

$$\psi(x) \cong d_+ \frac{1}{\sqrt{\kappa(x)}} \exp\left[\frac{1}{\hbar}\int^x dx' \kappa(x')\right] + d_- \frac{1}{\sqrt{\kappa(x)}} \exp\left[-\frac{1}{\hbar}\int^x dx' \kappa(x')\right] \tag{2b}$$

in the forbidden region, where $\kappa(x) = \sqrt{2m(V(x) - E)}$. Notice that all the integrals have been written as indefinite integrals. This is because a change in the lower limit amounts to a change in the value of the constants $c_\pm$ and $d_\pm$. In specific applications the lower limits and the constants are chosen to suit the problem. To make use of the semiclassical method it is almost always necessary to continue the wavefunction from the allowed region to a forbidden region, or vice versa. The trouble is that these regions are separated by a classical turning point, x_0, where $E = V(x_0)$, so $p(x_0) = 0$ and $d\lambda/dx \to \infty$. So the semiclassical approximation breaks down at a classical turning point. The question is, then, how does one continue a solution from an allowed region through a classical turning point into a forbidden region, or vice versa? It should be possible because we are talking about the solution to a second order differential equation (the Schrödinger equation). Once one has specified two constants of integration, the solution is completely determined, so specifying the solution in one region should fix it in the forbidden region. In fact, this is not quite true, and that's the subtlety of the "Connection Formulas".

1 What are the Connection Formulas?

First, let's summarize the formulas and their domain of applicability. The formulas depend on whether the classically forbidden region lies to the left or right of the classically allowed region. To be complete we give the formulas for both cases. Figure 1 shows the situation: in (a) the forbidden region is on the right; in (b) it is on the left.

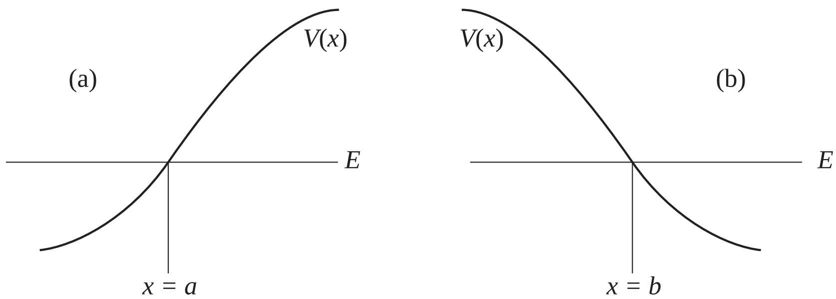

Figure 1

I. Forbidden region to the right.

   – If the wavefunction is known to be exponentially falling in the forbidden region, then it's phase and amplitude are known in the allowed region:

$$\frac{1}{\sqrt{\kappa(x)}} \exp\left[-\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right] \Rightarrow \frac{2}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' - \frac{\pi}{4}\right] \tag{3}$$

   – A wavefunction 90° out of phase in the allowed region continues into a growing exponential in the forbidden region as follows:

$$\frac{1}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' + \frac{\pi}{4}\right] \Rightarrow \frac{1}{\sqrt{\kappa(x)}} \exp\left[\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right] \tag{4}$$

II. Forbidden region to the left.

   – If the wavefunction is known to be exponentially falling in the forbidden region, then it's phase and amplitude are known in the allowed region:

$$\frac{1}{\sqrt{\kappa(x)}} \exp\left[-\frac{1}{\hbar}\int_x^b \kappa(x')dx'\right] \Rightarrow \frac{2}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_b^x p(x')dx' - \frac{\pi}{4}\right] \tag{5}$$

   – A wavefunction 90° out of phase in the allowed region continues into a growing exponential in the forbidden region as follows:

$$\frac{1}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_b^x p(x')dx' + \frac{\pi}{4}\right] \Rightarrow \frac{1}{\sqrt{\kappa(x)}} \exp\left[\frac{1}{\hbar}\int_x^b \kappa(x')dx'\right] \tag{6}$$

2 Are the Connection Formulas equalities?

(This section is written by Hong Liu, 2007)

Can we use the connection formulas in the directions opposite to the arrows in (3)–(6)? The answer is yes, but extra care[1] must be paid in reversing the arrows in equations (4) and (6).

[1] In contrast, the arrows in (3) and (5) can be reversed relatively straightforwardly.

To illustrate the subtleties, let us consider a specific example: Suppose the wavefunction in a forbidden region to the right is given by

$$
\begin{aligned}
\psi(x) \quad \approx \quad & \frac{d_+}{\sqrt{\kappa(x)}} \exp\left[\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right](1+O(\hbar)) \\
& + \frac{d_-}{\sqrt{\kappa(x)}} \exp\left[-\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right](1+O(\hbar)) \ . \qquad (7)
\end{aligned}
$$

Then using (4) in the direction opposite to the arrow and (3), we obtain the wave function on the left

$$
\begin{aligned}
& \frac{d_+}{\sqrt{p(x)}} \cos\left[\tfrac{1}{\hbar}\int_x^a p(x')dx' + \frac{\pi}{4}\right](1+O(\hbar)) \\
& + \frac{2d_-}{\sqrt{p(x)}} \cos\left[\tfrac{1}{\hbar}\int_x^a p(x')dx' - \frac{\pi}{4}\right](1+O(\hbar)) \ . \qquad (8)
\end{aligned}
$$

The above procedure is correct *provided in (7) we know the coefficient* d_- *before the exponentially falling term* $\exp[-\frac{1}{\hbar}\int_a^x \kappa(x')dx']$ *precisely.*

In most circumstances, however, the accuracy of the WKB approximation is not enough for us to know d_- exactly. This is due to that the second term in (7) is so small compared with the first term, that it is normally dropped completely. Note that for each term in (7), we have dropped terms of order $O(\hbar)$, as indicated in the equation. The $O(\hbar)$ contribution in the first term, which was already dropped, is much larger than the exponentially suppressed second term in the small $\hbar$ limit. Thus it is completely legitimate to drop the second term in (7). In such a situation we are simply left with

$$
\psi(x) \approx \frac{d_+}{\sqrt{\kappa(x)}} \exp\left[\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right] \qquad (9)
$$

and it is then incorrect to use equation (4) backwards to conclude that the wavefunction on the left is of the form

$$
\frac{d_+}{\sqrt{p(x)}} \cos\left[\tfrac{1}{\hbar}\int_x^a p(x')dx' + \frac{\pi}{4}\right] \ . \qquad (10)
$$

In comparing (10) with (8), we see that (10) misses the second term in (8), which is of the same order as the term in (10).

Nevertheless, one does encounter situations in which d_- in (7) is known precisely, often due to symmetry. For example, consider a situation in which

$a = 0$ and both $\psi(x)$ and $\kappa(x)$ are even functions of x. Then the symmetry requires that $d_+ = d_-$. (We will see such an example in the problem of a double well potential in pset 8). Sometimes it is also possible to use more sophisticated mathematical methods to keep track of the coefficient d_- precisely even without symmetry. In these situations one can then use the connection formulas in both directions.

3 An Example

A worked example will help show how the Connection Formulas are to be applied. Consider a particle trapped between the origin at $x = 0$ and a high potential V(x). Figure 2 gives an illustration. For energy E, the classical turning point is at $a = a(E)$. a is the point where $E = V(a)$. The semiclassical solution which vanishes at the origin is

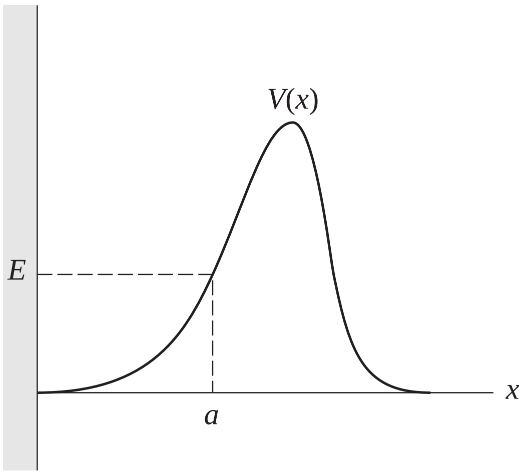

Figure 2

$$\psi(x) = \sin\left[\frac{1}{\hbar}\int_0^x p(x')dx'\right]. \tag{11}$$

This form is valid for $x < a$. What do we do as x approaches the turning point at $x = a$? We rewrite the sin[...] as the a linear combination of the two cosines for which we have connection information:

$$\begin{aligned} \psi(x) &= \sin\left[\frac{1}{\hbar}\int_0^x p(x')dx'\right] \qquad (12) \\ &= \sin\Delta\cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' - \frac{\pi}{4}\right] + \cos\Delta\cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' + \frac{\pi}{4}\right] \end{aligned}$$

where

$$\Delta = \frac{1}{\hbar} \int_0^a p(x)dx - \frac{\pi}{4}. \tag{13}$$

This much is just application of trig identities. If the coefficient of $\cos[\frac{1}{\hbar}\int_x^a p(x')dx' + \frac{\pi}{4}]$ is not zero, then the wave function continues into a growing exponential for $x > a$ according to eq. (4). The only thing we can say for certain is that $\psi(x)$ has an exponentially growing term in the forbidden region:

$$\psi(x) \sim \cos\Delta \frac{1}{\kappa(x)} \exp\left[\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right]. \tag{14}$$

$\psi(x)$ would in general also contain exponentially falling terms in the forbidden region, but we don't have the accuracy to compute them. Tiny corrections to the exponentially growing term, which we did not keep track of in our WKB approximation will be much larger than the exponentially falling term. However, if $\cos\Delta = 0$, then there is no exponentially growing term in the forbidden region. Thus, if we know that $\psi(x)$ falls exponentially in the forbidden region $\cos\Delta$ must be zero. Since a bound state wavefunction must fall exponentially in the forbidden region we learn that the WKB condition for a bound state is $\cos\Delta = 0$, or

$$\int_0^a p(x)dx = (n + \frac{3}{4})\pi\hbar \tag{15}$$

which is the Bohr-Sommerfeld Quantization condition when there is a hard wall on one side. The problem set contains other problems which require careful use of the Connection Formulas.

4 Deriving the Connection Formulae

Let us consider the case depicted in the left panel of Fig. 1, with a turning point at $x = a$ with the allowed region at $x < a$ and the classically forbidden region at $x > a$. We know that in the forbidden region

$$\psi(x) = \frac{d}{\sqrt{\kappa(x)}} \exp\left[-\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right] \quad \text{for } x \gg a \tag{16}$$

and in the allowed region

$$\psi(x) = \frac{c_+}{\sqrt{p(x)}} \exp\left[\frac{i}{\hbar}\int_x^a dx' p(x')\right] + \frac{c_-}{\sqrt{p(x)}} \exp\left[-\frac{i}{\hbar}\int_x^a dx' p(x')\right] \quad \text{for } x \ll a \,. \tag{17}$$

Our task is to relate c_+ and c_- to d, and we expect to find the relation described by the connection formula (3). I'll take you through this derivation, and leave deriving the other three connection formulae to you. In the vicinity of the turning point a, the potential is approximately linear and we can write

$$V - E \simeq b(x-a) \quad \text{where } b \equiv \left.\frac{dV}{dx}\right|_{x=a} > 0 \,. \tag{18}$$

This linearized potential is a good description for $|x-a| < L$, where L is the "length scale over which V curves". The semiclassical forms for the wave function, (16) and (17), are not valid too close to a. For example, (16) is valid where

$$\left|\frac{d}{dx}\frac{\hbar}{\kappa(x)}\right| \gg 1 \tag{19}$$

and we must ask whether there are values of $(x-a)$ that are simultaneously large enough that (19) is valid, but not so large that (18) breaks down. If there is a range of $(x-a)$ in which both (19) and (18) are valid, then within this domain (19) becomes

$$\left|\frac{d}{dx}\frac{\hbar}{\sqrt{2mb(x-a)}}\right| = \frac{\hbar}{\sqrt{8mb}}\frac{1}{(x-a)^{3/2}} \ll 1 \,.$$

We can therefore conclude that as long as

$$L^{3/2} \gg \frac{\hbar}{\sqrt{8mb}} \,, \tag{20}$$

there is a region where (19) is valid, meaning that (16) describes the wave function, and where (18) describes the potential. The same condition (20) implies that there is a range of $a-x$, in the allowed region in which $a-x$ is big enough that (17) is a valid description of the wave function and small enough that (18) still describes the potential. The condition (20) must be satisfied by the potential near its turning points in order to ensure the validity of the analysis we are pursuing (with semiclassical wave functions far away from turning points and connection formulae prescribing how they are connected "across" the turning points.) One way of reading (20) is that it is always satisfied in the $\hbar \to 0$ limit, and indeed this is why the method is called "semiclassical". Perhaps a better way to read the condition, though, is to leave $\hbar$ fixed—it is after all a constant of nature—and view (20) as the statement of how smooth the potential must be near its turning points. Henceforth, we assume that (20) is satisfied. Within the domain of $x-a$ where both (18) and (19) hold, the wave function is given by

$$\begin{aligned} \psi(x) &= \frac{d}{[2mb(x-a)]^{1/4}} \exp\left[-\frac{1}{\hbar}\int_a^x \sqrt{2mb(x'-a)}\, dx'\right] \\ &= \frac{d}{[2mb(x-a)]^{1/4}} \exp\left[-\frac{2}{3\hbar}\sqrt{2mb}\,(x-a)^{3/2}\right] . \qquad (21) \end{aligned}$$

Now, we want to "analytically continue" this expression from $x-a>0$ to $x-a<0$. The trick is to consider $(x-a)$ a *complex variable*, which we shall write as

$$(x-a) = \rho \exp i\phi \ ,$$

and to start with $\phi = 0$ and ρ in the range such that all our approximations are valid and then to continuously change ϕ from 0 to π, all the while keeping ρ fixed. In this way, we end at a point in the allowed region (with $x-a<0$) where both (18) and (19) hold. Lets see what happens to the wave function upon performing this procedure. First, we rewrite the wave function as

$$\psi(x) = \frac{d}{(2mb\rho)^{1/4} \exp\frac{i\phi}{4}} \exp\left[-\frac{2}{3\hbar}\sqrt{2mb}\,\rho^{3/2} \exp\frac{3i\phi}{2}\right] \qquad (22)$$

which, for $\phi = 0$, is what we had before. For $\phi = \pi$, namely $x-a<0$, the wave function becomes

$$\psi(x) = \frac{d}{(2mb\rho)^{1/4} \exp\frac{i\pi}{4}} \exp\left[+i\frac{2}{3\hbar}\sqrt{2mb}\,\rho^{3/2}\right] . \qquad (23)$$

So, this is the wave function in the allowed region that we obtain by starting from the wave function in the forbidden region and analytically continuing. Note that the turning point is at $\rho = 0$, and we never went near it. By turning $x-a$ into a complex variable, we were able to start with $x-a>0$, end with $x-a<0$, and never go near $x-a=0$. We must now compare

(23) to the form of the wave function we were expecting to get in the allowed region, namely (17). Using (18)—and, note that we are in the region where this is valid—we can rewrite the wave function in the allowed region (17) as follows:

$$
\begin{aligned}
\psi(x) &= \frac{c_+}{[2mb(a-x)]^{1/4}} \exp\left[\frac{i}{\hbar}\int_x^a dx'\sqrt{2mb(a-x')}\right] \\
&\qquad + \frac{c_-}{[2mb(a-x)]^{1/4}} \exp\left[-\frac{i}{\hbar}\int_x^a dx'\sqrt{2mb(a-x')}\right] \\
&= \frac{c_+}{[2mb(a-x)]^{1/4}} \exp\left[+i\frac{2}{3\hbar}\sqrt{2mb}\,(a-x)^{3/2}\right] \\
&\qquad + \frac{c_-}{[2mb(a-x)]^{1/4}} \exp\left[-i\frac{2}{3\hbar}\sqrt{2mb}\,(a-x)^{3/2}\right] \\
&= \frac{c_+}{[2mb\rho]^{1/4}} \exp\left[+i\frac{2}{3\hbar}\sqrt{2mb}\,\rho^{3/2}\right] \\
&\qquad + \frac{c_-}{[2mb\rho]^{1/4}} \exp\left[-i\frac{2}{3\hbar}\sqrt{2mb}\,\rho^{3/2}\right] \ . \qquad (24)
\end{aligned}
$$

We now see that if we choose

$$
c_+ = \frac{d}{\exp\frac{i\pi}{4}} \qquad (25)
$$

then the wave function (23) that we obtained by analytically continuing the forbidden-region wave function to the allowed region is the same as the "c_+ term" in (24)! This looks good, but what has happened to the c_- term??? Let's try to figure out why we found the c_+ term, but not the c_- term. To do this, we start with (24), including both the c_+ and c_- terms, and try to analytically continue it in the opposite direction to what we did before, back to the forbidden region. We do the analytical continuation by changing ϕ from π to 0. Note that the imaginary part of $(x-a)$ is *positive* during the continuation. You can easily check that if you start with (24) and perform this procedure, as you begin the continuation into the complex plane (i.e. as you start reducing ϕ from π) the magnitude of the c_- term becomes exponentially small compared to the magnitude of the c_+ term. As we discussed in lecture, the semiclassical approximation entails dropping such exponentially small terms. So, if we start with (24) and "continue backward", we lose the c_- term and the c_+ term turns into the correct wave function in the forbidden region once ϕ is back to 0. Analogously, when we started with the forbidden-region wave function and "continued forward", we only obtained the c_+ term. Now that we understand why we lost the c_- term, how can we find it?? Simple. Start with the forbidden-region wave function (22) again. This time, change ϕ from 0 to $-\pi$. As before, we start in the forbidden region and end in the allowed region. This time, though, the imaginary part of $x-a$ is negative during the continuation. This means that near $\phi = -\pi$, the magnitude of the c_+ term is exponentially smaller than that of the c_- term, so we expect this time to "lose" the c_+ term. And, lo and behold, the wave function in the allowed region that we obtain by starting from the forbidden region and continuing ϕ from 0 to $-\pi$ is

$$\psi(x) = \frac{d}{(2mb\rho)^{1/4}\exp\left(-\frac{i\pi}{4}\right)} \exp\left[-i\frac{2}{3\hbar}\sqrt{2mb}\,\rho^{3/2}\right] , \tag{26}$$

which is *not* the same as (23). Instead, it is precisely the c_- term in (24), as long as we choose

$$c_- = \frac{d}{\exp\left(-\frac{i\pi}{4}\right)} . \tag{27}$$

By doing the analytic continuation from $\phi = 0$ to $\phi = -\pi$, we have lost the c_+ term and obtained the c_- term! By performing these two different analytic continuations, we are able to start from the wave function in the forbidden region and determine the complete wave function in the allowed region. What we find is that in the allowed region, the wave function is given by (24) or, equivalently, (17) with c_+ and c_- specified by (25) and (27). That is, in the allowed region

$$\psi(x) = \frac{2d}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' - \frac{\pi}{4}\right] \tag{28}$$

which is the connection formula (3) we set out to prove. Elegant, n'est-ce pas?