The WKB Approximation

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1 Introduction

The Schroedinger equation for a particle in a potential can be solved explicitly only if the potential has a sufficiently simple form, otherwise numerical methods have to be used. In many cases it is preferable to have approximate explicit formulas, that can be further used to calculate other quantities, than to have exact numerical solutions. The WKB approximation, developed by Wentzel, Brillouin and Keller, is a semiclassical method to solve Schroedinger's equation that does not require the potential to be a perturbation of a solvable problem. Instead, it only assumes that certain classical quantities having the dimension of action (energy×time) are much larger than the Planck's constant. In this paper I will present the method in a simple but complete way, paying particular attention to the famous *connection formulas*, that are the main source of difficulty in the presentation.

To make things clear from the beginning, let me be very specific about the problems I have in mind. I want to find stationary solutions for a particle moving in a one-dimensional potential. I will consider two situations: (a) the potential has bound states, as illustrated in figure 1, or; (b) the potential has scattering states and is different from zero only in a small region around the origin, as illustrated in figure 2. In the first case I am particularly interested in computing the discrete energy levels of the system, whereas in the second case I want to compute the tunneling coefficient. In both cases the Schroedinger equation reads

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi}{\partial t}. \tag{1}$$

The wave-function also satisfies the continuity equation

$$\frac{\partial\rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \tag{2}$$

where

$$\rho(x,t) = |\psi(x,t)|^2 \tag{3}$$

is the probability density and

$$j(x,t) = \frac{\hbar}{m} Im\left(\psi^*\frac{\partial\psi}{\partial x}\right) \tag{4}$$

is the probability current. The continuity equation can be derived by multiplying eq.(1) by ψ^* and subtracting the resulting equation from its complex conjugate.

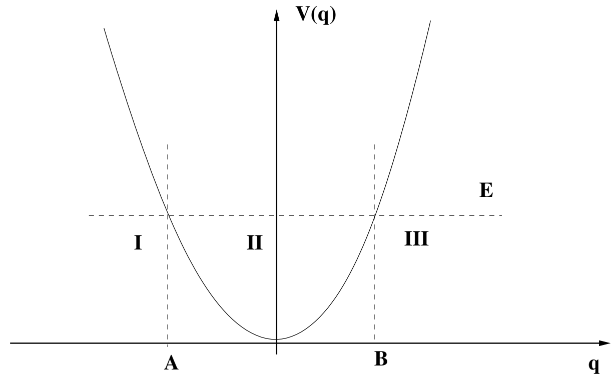

Figure 1: A particle with energy E in a bound potential. The turning points A and B, where $V = E$, separate the classically allowed region II from the forbidden regions I and III.

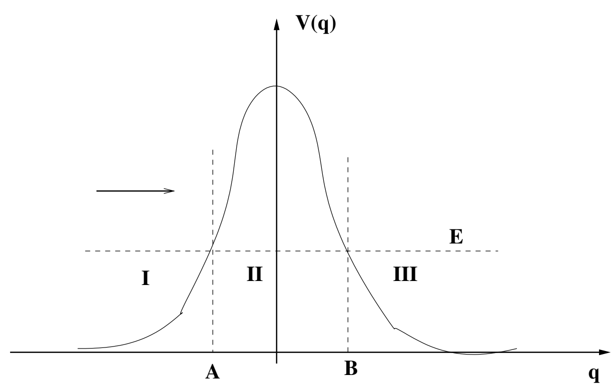

Figure 2: A particle with energy E in a scattering potential. In our calculations I will assume that the particle is incident from the left side of the barrier and that $E < V_0$.

In developing the WKB approximation it is important to write the complex wave-function ψ in terms of its modulus and phase as

$$\psi(x,t) = \sqrt{\rho(x,t)}e^{\frac{i}{\hbar}S(x,t)} \tag{5}$$

where the explicit dependence on $\hbar$ in the phase is introduced by convenience.

In terms of ρ and S the probability current becomes

$$j = \frac{\rho}{m}\frac{\partial S}{\partial x}. \tag{6}$$

The Schroedinger equation, on the other hand, reads

$$-\frac{\hbar^2}{2m}\left[\frac{1}{2\sqrt{\rho}}\frac{\partial^2 \rho}{\partial x^2} - \frac{1}{4\rho\sqrt{\rho}}\left(\frac{\partial \rho}{\partial x}\right)^2 + \frac{i}{\hbar\sqrt{\rho}}\frac{\partial \rho}{\partial x}\frac{\partial S}{\partial x} + \frac{i}{\hbar}\sqrt{\rho}\frac{\partial^2 S}{\partial x^2} - \frac{1}{\hbar^2}\sqrt{\rho}\left(\frac{\partial S}{\partial x}\right)^2\right]$$
$$+V(x)\sqrt{\rho} = i\hbar\left[\frac{1}{2\sqrt{\rho}}\frac{\partial \rho}{\partial t} + \frac{i}{\hbar}\sqrt{\rho}\frac{\partial S}{\partial t}\right] \tag{7}$$

where I have already canceled the global factor $\exp(iS/\hbar)$. In terms of explicit powers of $\hbar$ this equation has three types of factors, involving $\hbar^0$, $\hbar^1$ and $\hbar^2$. I am going to show that the factors in $\hbar^1$ vanish exactly because of the continuity equation. Indeed, the two terms of this type on the left side of the equation are

$$-\frac{i}{2m\sqrt{\rho}}\frac{\partial \rho}{\partial x}\frac{\partial S}{\partial x} - \frac{i}{2m}\sqrt{\rho}\frac{\partial^2 S}{\partial x^2} \tag{8}$$

which can be re-organized as

$$-\frac{i}{2\sqrt{\rho}}\frac{\partial}{\partial x}\left(\frac{\rho}{m}\frac{\partial S}{\partial x}\right) = -\frac{i}{2\sqrt{\rho}}\frac{\partial j}{\partial x} = \frac{i}{2\sqrt{\rho}}\frac{\partial \rho}{\partial t} \tag{9}$$

and exactly cancel the term in $\hbar$ on the right side.

Dividing the remaining terms in eq.(7) by $\sqrt{\rho}$ I obtain

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V_Q(x) = -\frac{\partial S}{\partial t} \tag{10}$$

where I have defined the *quantum potential*

$$\begin{aligned} V_Q(x) &= V(x) - \frac{\hbar^2}{4m\rho}\frac{\partial^2 \rho}{\partial x^2} + \frac{\hbar^2}{8m\rho^2}\left(\frac{\partial \rho}{\partial x}\right)^2 \\ &= V(x) - \frac{\hbar^2}{4m\sqrt{\rho}}\frac{\partial}{\partial x}\left(\frac{1}{\sqrt{\rho}}\frac{\partial \rho}{\partial x}\right). \end{aligned} \tag{11}$$

Equation (10) is exact and, together with the continuity equation, it is completely equivalent to Schroedinger's equation. If it were not for the terms in $\hbar^2$ in the quantum potential, eq.(10) would be the Hamilton-Jacobi equation of classical mechanics, whose solution is given by the action function (see below). The WKB approximation consists exactly in discard these terms. David Bohm proposed that we could solve these equations as they are, and find the trajectories of the particle in the quantum potential. Notice, however, that V_Q depends on the wave-function itself. Given $\psi(x, t_0)$ we would calculate V_Q and propagate the wave-function to $t_0 + dt$. This would allows us to re-calculate V_Q and proceed with the integration. The difficulty is that V_Q is singular at the nodes of the wave-function, where $\psi(x, t) = 0$.

In either case equation (10) is a partial differential equation that can be solved for $S(x, t)$ given $S(x, 0)$. However, our interest here is to calculate stationary states, whose time dependence is of the form

$$\psi(x, t) = \phi(x) e^{-\frac{iEt}{\hbar}}. \tag{12}$$

Comparing with equation (5) we see that this amounts to impose

$$\rho = \rho(x) \qquad\qquad S(x, t) = W(x) - Et \tag{13}$$

so that

$$\psi(x, t) = \sqrt{\rho(x)} e^{\frac{iW(x)}{\hbar}} e^{-\frac{iEt}{\hbar}}.$$

In terms of W and E equation (10) becomes

$$\frac{1}{2m} \left(\frac{\partial W}{\partial x} \right)^2 + V_Q(x) = E. \tag{14}$$

2 General form of the WKB wave-function

In the limit where certain classical quantities (to be more clearly specified below) become much larger than $\hbar$, it is legitimate to discard the quantum corrections to the potential V_Q and replace it by the classical potential. In this case eq.(10) reduces to the classical Hamilton-Jacobi equation

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V(x) = -\frac{\partial S}{\partial t}. \tag{15}$$

For stationary states, where

$$\rho = \rho(x) \qquad \text{and} \qquad S(x,t) = W(x) - Et$$

it reduces to

$$\frac{1}{2m}\left(\frac{\partial W}{\partial x}\right)^2 + V(x) = E. \tag{16}$$

The function $S(x,t)$ is called Hamilton's principal function, whereas $W(x)$ is Hamilton's characteristic function. Equation (16) can be solved for W as

$$W(x) = \pm \int^x \sqrt{2m(E - V(x'))}dx' \tag{17}$$

where the integrand is readily recognized as the momentum $p(x,E)$ of a particle with energy E at position x, since

$$\frac{p^2}{2m} + V(x) = E \qquad \rightarrow \qquad p(x,E) = \sqrt{2m(E - V(x))}. \tag{18}$$

Comparing the classical Hamilton-Jacobi equation (16), which is independent of $\hbar$, with its fully quantum version (14), we can see that quantum corrections to W are proportional to $\hbar^2$. The same is true for 'classical' ρ, that we compute below using the continuity equation.

Since ρ is time independent, the current must be constant, since $\partial j/\partial x = 0$ in this case. Using eqs.(6), (13) and (17) we see that

$$j = \frac{\rho}{m}p(x,E) = const.$$

and, therefore,

$$\rho(x) = \frac{const}{p(x,E)}. \tag{19}$$

Putting all this information together we obtain the general form of the time independent, stationary, wave function $\phi(x)$ as

$$\phi(x) = \frac{c}{\sqrt{p(x,E)}} e^{\pm \frac{i}{\hbar} \int^x p(x',E)dx'}. \tag{20}$$

In the next sections I will now apply these ideas to the specific problems illustrated in figures 1 and 2. In both cases, for a given total energy E the x-axis is divided into three regions by the turning points A and B. In the classically forbidden regions $V(x) > E$ and $p(x,E)$ becomes purely imaginary. In these regions it is convenient to define the real function

$$q(x,E) = \sqrt{2m(V(x)-E)} = |p(x,E)| \tag{21}$$

and re-write the general form of the wave-function as

$$\phi(x) = \frac{c}{\sqrt{q(x,E)}} e^{\pm \frac{1}{\hbar} \int^x q(x',E)dx'}. \tag{22}$$

The lower limit of integration in equations (20) and (22) will be fixed later.

3 The WKB wave-function for bound states

I will now consider the specific problem of bound states illustrated in figure 1. In the classically forbidden regions I and III the WKB wave-function involves real exponentials and we need to be careful not to let it diverge. In the classically allowed region II, on the other hand, both solutions (with plus or minus sign in the exponent) are well behaved and should be included. Taking this considerations into account we write

$$\phi(x) = \begin{cases} \dfrac{D_1}{2\sqrt{q}} e^{\frac{1}{\hbar}\int^x q(x',E)dx'} & x \in I \\ \\ \dfrac{C}{\sqrt{p}} \cos\left(\dfrac{1}{\hbar}\displaystyle\int^x p(x',E)dx' + \xi\right) & x \in II \\ \\ \dfrac{D_2}{2\sqrt{q}} e^{-\frac{1}{\hbar}\int^x q(x',E)dx'} & x \in III \end{cases} \tag{23}$$

where I replaced the combination of the two exponentials in region II by a cosine with a phase.

We now get to the hard part of the WKB procedure, which is to match the constants D_1, C, D_2 and ξ. These constants cannot be arbitrary, since $\phi(x)$ needs to be an approximation for the true wave-function in all space and all these constants must be related to the single undetermined constant that we could find later by normalization.

The problem is that we cannot simply match the different parts of the wave-function $\phi(x)$ because it diverges right at the matching points $x = A$ and $x = B$! At these points $p(x,E) = q(x,E) = 0$. The trick to overcome this difficulty is to go back to the original Schroedinger equation and to solve it in the neighborhood of these points by approximating the potential by a straight line. The next two sections are dedicated to that. Once we have these solutions we can compare them with our WKB forms and relate the coefficients to each other. We will find that the matching cannot be always performed and the condition for it to work is the Bohr-Sommerfeld quantization rule that discretizes the energy levels.

4 Solution near a turning point with $V' > 0$

4.1 Statement of the problem and solution

Consider a turning point x_0 with $V'(x_0) > 0$, where the prime means differentiation with respect to x. This is the case of $x = B$ for bound states (see fig.1) or $x = A$ for scattering states (see fig.2). In the vicinity of x_0 we can expand the potential as

$$V(x) \approx V(x_0) + V'(x_0)(x - x_0) = E + V'(x_0)(x - x_0). \tag{24}$$

The time-independent Schroedinger equation becomes, in operator form,

$$\frac{p^2}{2m}|\phi\rangle + [E + V'(x_0)(x - x_0)]|\phi\rangle = E|\phi\rangle \tag{25}$$

or

$$\frac{p^2}{2m}|\phi\rangle + V'(x_0)x|\phi\rangle = V'(x_0)x_0|\phi\rangle. \tag{26}$$

I am going to solve this equation step by step in this section. The final result will be written as

$$\phi(x) = c\int_0^{+\infty} \cos\left(t^3/3 - ty\right)dt \tag{27}$$

where c is a normalization constant and

$$y = \left(\frac{2mV'(x_0)}{\hbar^2}\right)^{1/3}(x_0 - x). \tag{28}$$

This is exact, but not very helpful. The variable y is zero at the turning point $x = x_0$. If we assume that the ratio $\hbar^2/mV'(x_0)$ is so small that y becomes very large as we move away from x_0, without leaving the region where the linear approximation of the potential is valid, we can derive approximate formulas for this integral that directly relate to our WKB wave-functions. In this case I will show that

$$\phi(x) \approx \begin{cases} \frac{c}{\sqrt{p(x,E)}}\cos\left(\frac{1}{\hbar}\int_{x_0}^{x} p(x',E)dx' + \pi/4\right) & x < x_0 \\ \\ \frac{c}{2\sqrt{q(x,E)}}e^{-\frac{1}{\hbar}\int_{x_0}^{x} q(x',E)dx'} & x > x_0. \end{cases} \tag{29}$$

4.2 Solving the equation

In the momentum representation $\langle p|\phi\rangle = \phi(p)$ equation (26) reads

$$\frac{p^2}{2m}\phi(p) + i\hbar V'(x_0)\frac{\partial\phi(p)}{\partial p} = V'(x_0)x_0\phi(p). \tag{30}$$

This equation has a simple solution

$$\phi(p) = A\exp\left(i\alpha p^3 - ipx_0/\hbar\right) \tag{31}$$

with

$$\alpha = \frac{1}{6m\hbar V'(x_0)} \tag{32}$$

as the reader can check by substitution. The corresponding wave-function in position representation is obtained by Fourier transforming:

$$\phi(x) = \frac{A}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{(i\alpha p^3 + ip(x-x_0)/\hbar)}dp$$

which can be easily re-arranged as

$$\phi(x) = A'\int_0^{+\infty} \cos\left(\alpha p^3 + p(x-x_0)/\hbar\right)dp.$$

Finally, changing variables to $t = p(3\alpha)^{1/3}$ and defining

$$y = \left(\frac{2mV'(x_0)}{\hbar^2}\right)^{1/3}(x_0 - x) \tag{33}$$

we obtain

$$\phi(x) = c\int_0^{+\infty} \cos\left(t^3/3 - ty\right)dt \equiv cAi(-y) \tag{34}$$

where $Ai(z)$ is the Airy function.

The solution (34) should be compared with the WKB solution derived in the previous section. However, as it is, the comparison is not immediate. In order to see that equation (34) indeed resembles the WKB forms we need to do a little more work.

I am going to assume that the ratio $\hbar^2/mV'(x_0)$ is so small that, for values of x where the linear approximation is still good, y can become much larger than 1. In this case the cosine in the Airy function oscillates very fast between $+1$ and -1 as t changes, and the integral seems to tend to zero. However, there are points along the t axis where the phase of the cosine becomes nearly constant, and in the vicinity of these points the cosine stops oscillating and contributes some finite value to the integral. All we need to do is to find these points and expand the cosine around them.

In order to do that I will re-write the Airy function as an integral from $-\infty$ to $+\infty$ as

$$Ai(-y) = \frac{1}{2}\int_{-\infty}^{+\infty} e^{i\gamma(t,y)}dt \tag{35}$$

where

$$\gamma(t, y) = t^3/3 - ty. \tag{36}$$

We need to find the points where $\partial\gamma/\partial t = 0$. This condition defines the points where γ becomes stationary. We find

$$t_\pm = \pm\sqrt{y}. \tag{37}$$

Since the important contributions to the integral come from the neighborhood of these points, we may expand γ to second order around them:

$$\begin{aligned} \gamma(t, y) &\approx \gamma(t_\pm, y) + \tfrac{1}{2}\gamma''(t_\pm, y)(t - t_\pm)^2 \\ &= \mp\tfrac{2}{3}y^{3/2} \pm \sqrt{y}(t - t_\pm)^2. \end{aligned} \tag{38}$$

(the primes now denote differentiation with respect to t and remember that $\gamma'(t_\pm, y) = 0$). This approximation takes us to Gaussian integrals around each stationary point that we know how to do:

$$Ai(-y) \approx \frac{1}{2}e^{\mp i\frac{2}{3}y^{3/2}}\int_{-\infty}^{+\infty} e^{\pm i\sqrt{y}(t-t_\pm)^2}dt \tag{39}$$

However we must be careful: $y > 0$ only if $x < x_0$. This corresponds to the classically allowed region (both in the case of bound states and scattering states). In this case $\sqrt{y}$ is real, there is no risk of divergence in the exponents and both stationary points contribute to the integral and we must sum their contributions. We get

$$\begin{aligned} Ai(-y) &\approx \tfrac{1}{2}\sqrt{\tfrac{i\pi}{\sqrt{y}}}e^{-i\frac{2}{3}y^{3/2}} + \tfrac{1}{2}\sqrt{\tfrac{-i\pi}{\sqrt{y}}}e^{i\frac{2}{3}y^{3/2}} \\ &= \sqrt{\tfrac{\pi}{\sqrt{y}}}\cos\left(\tfrac{2}{3}y^{3/2} - \pi/4\right). \end{aligned} \tag{40}$$

For $x > x_0$ we find that $y < 0$ and $\sqrt{y} = i\sqrt{-y}$. In this case only the stationary point t_+ contributes, since t_- would lead to a diverging integral. We get

$$\begin{aligned} Ai(-y) &\approx \tfrac{1}{2}e^{-\frac{2}{3}(-y)^{3/2}} \int_{-\infty}^{+\infty} e^{-\sqrt{-y}(t-t_+)^2} dt \\ &= \tfrac{1}{2}\sqrt{\tfrac{\pi}{\sqrt{-y}}} e^{-\frac{2}{3}(-y)^{3/2}}. \end{aligned} \tag{41}$$

The asymptotic analysis presented above is not rigorous, since we have not shown that the contour of integration can be deformed so as to pass through the stationary points. In any case, it gives an idea of the general procedure.

To complete the analysis we only need to relate y with $p(x, E)$. We start from

$$p(x, E) = \sqrt{2m(E - V(x))} \approx \sqrt{-2mV'(x_0)(x - x_0)} = \sqrt{2mV'(x_0)(x_0 - x)}$$

and

$$\int_{x_0}^{x} p(x', E)dx' \approx \sqrt{2mV'(x_0)} \int_{x_0}^{x} \sqrt{(x_0 - x')}dx' = -\frac{2}{3}\sqrt{2mV'(x_0)}(x_0 - x)^{3/2}.$$

Therefore,

$$\frac{2}{3}y^{3/2} = \frac{2}{3\hbar}\sqrt{2mV'(x_0)}(x_0 - x)^{3/2} = -\frac{1}{\hbar}\int_{x_0}^{x} p(x', E)dx'$$

and also

$$y^{1/2} = \frac{p(x, E)}{[2m\hbar V'(x_0)]^{1/3}}.$$

Therefore, equation (40) can be re-writen as

$$Ai(-y) \approx \frac{c}{\sqrt{p(x, E)}} \cos\left(\frac{1}{\hbar}\int_{x_0}^{x} p(x', E)dx' + \pi/4\right). \tag{42}$$

for $x < x_0$, where $c = \sqrt{\pi[2mV'(x_0)\hbar]^{1/3}}$ and we used that $\cos(-\theta) = \cos(\theta)$.

Similarly, for $x > x_0$,

$$q(x, E) \approx \sqrt{2mV'(x_0)(x - x_0)},$$

$$\int_{x_0}^{x} q(x', E)dx' \approx \frac{2}{3}\sqrt{2mV'(x_0)}(x - x_0)^{3/2},$$

$$\frac{2}{3}(-y)^{3/2} \approx \frac{1}{\hbar}\int_{x_0}^{x} q(x', E)dx'$$

and

$$(-y)^{1/2} = \frac{q(x, E)}{[2m\hbar V'(x_0)]^{1/3}}.$$

This gives

$$Ai(-y) \approx \frac{c}{\sqrt{q(x, E)}} e^{-\frac{1}{\hbar}\int_{x_0}^{x} q(x', E)dx'}. \tag{43}$$

These results are summarized in equations (27) and (29) at the beginning of this section.

5 Solution near a turning point with $V' < 0$

This is very similar to what we did in the previous section, but with some important sign changes. The time-independent Schroedinger's equation is the same

$$\frac{p^2}{2m}|\phi\rangle + V'(x_0)x|\phi\rangle = V'(x_0)x_0|\phi\rangle \tag{44}$$

and the solution in the p representation is now written as

$$\phi(p) = A\exp\left(-i\alpha p^3 - ipx_0/\hbar\right) \tag{45}$$

with

$$\alpha = -\frac{1}{6m\hbar V'(x_0)} = \frac{1}{6m\hbar|V'(x_0)|}. \tag{46}$$

Following the same steps of the last section we can write $\phi(x)$ as

$$\phi(x) = c\int_0^{+\infty}\cos\left(t^3/3 - ty\right)dt \equiv cAi(-y) \tag{47}$$

where we defined $t = p(3\alpha)^{1/3}$ and

$$y = \left(\frac{2m|V'(x_0)|}{\hbar^2}\right)^{1/3}(x - x_0). \tag{48}$$

The asymptotic form of this expression for large y is identical to the ones we derived in section 4: for $x > x_0$, in the classically allowed region, we get

$$Ai(-y) \approx \sqrt{\frac{\pi}{\sqrt{y}}}\cos\left(\frac{2}{3}y^{3/2} - \pi/4\right). \tag{49}$$

For $x < x_0$, in the classically forbidden region, we find

$$Ai(-y) \approx \frac{1}{2}\sqrt{\frac{\pi}{\sqrt{-y}}}e^{-\frac{2}{3}(-y)^{3/2}}. \tag{50}$$

Finally we need to relate y with $p(x,E)$. We find

$$p(x,E) \approx \sqrt{2m|V'(x_0)|(x - x_0)},$$

$$\int_{x_0}^{x} p(x',E)dx' \approx \frac{2}{3}\sqrt{2m|V'(x_0)|}(x - x_0)^{3/2},$$

$$\frac{2}{3}y^{3/2} \approx \frac{1}{\hbar}\int_{x_0}^{x} p(x', E)dx'$$

and

$$y^{1/2} = \frac{p(x, E)}{[2m\hbar|V'(x_0)|]^{1/3}}.$$

Therefore, the asymptotic solutions can be re-writen as

$$\phi(x) \approx \begin{cases} \frac{c}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_{x_0}^{x} p(x', E)dx' - \pi/4\right) & x > x_0 \\ \\ \frac{c}{2\sqrt{q(x,E)}} e^{\frac{1}{\hbar}\int_{x_0}^{x} q(x',E)dx'} & x < x_0. \end{cases} \tag{51}$$

6 Semiclassical quantization

We are now in a position to match the different parts of the wave-function for bound states, as given by equation (23) that we repeat here:

$$\phi(x) = \begin{cases} \dfrac{D_1}{2\sqrt{q}} e^{\frac{1}{\hbar}\int^x q(x',E)dx'} & x \in I \\ \\ \dfrac{C}{\sqrt{p}} \cos\left(\dfrac{1}{\hbar}\displaystyle\int^x p(x',E)dx' + \xi\right) & x \in II \\ \\ \dfrac{D_2}{2\sqrt{q}} e^{-\frac{1}{\hbar}\int^x q(x',E)dx'} & x \in III \end{cases}$$

We start by connecting regions II and III, where the turning point B satisfies $V'(B) > 0$. Comparing with the approximate solutions near the turning point, equation (29), also repeated below,

$$\phi(x) \approx \begin{cases} \frac{c}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_{x_0}^x p(x',E)dx' + \pi/4\right) & x < x_0 \\ \\ \frac{c}{2\sqrt{q(x,E)}} e^{-\frac{1}{\hbar}\int_{x_0}^x q(x',E)dx'} & x > x_0. \end{cases}$$

we find that $D_2 = C$, the lower limit of the integrals should be fixed as B and $\xi = \pi/4$.

On the other hand, regions I and II, connected by the turning point A where $V'(A) < 0$, must match equations (51):

$$\phi(x) \approx \begin{cases} \frac{c}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_{x_0}^x p(x',E)dx' - \pi/4\right) & x > x_0 \\ \\ \frac{c}{2\sqrt{q(x,E)}} e^{\frac{1}{\hbar}\int_{x_0}^x q(x',E)dx'} & x < x_0. \end{cases}$$

In this case we find that $D_1 = C$, the lower limit of the integrals should be fixed as A and $\xi = -\pi/4$.

Putting all this information together we may write

$$\phi(x) = \begin{cases} \dfrac{C'}{2\sqrt{q}} e^{\frac{1}{\hbar}\int_A^x q(x',E)dx'} & x \in I \\ \dfrac{C'}{\sqrt{p}} \cos\left(\dfrac{1}{\hbar}\displaystyle\int_A^x p(x',E)dx' - \dfrac{\pi}{4}\right) = \dfrac{C}{\sqrt{p}} \cos\left(\dfrac{1}{\hbar}\displaystyle\int_B^x p(x',E)dx' + \dfrac{\pi}{4}\right) & x \in II \\ \dfrac{C}{2\sqrt{q}} e^{-\frac{1}{\hbar}\int_B^x q(x',E)dx'} & x \in III \end{cases}$$

The two forms in region II are written in order to connect with regions I and III respectively. But of course they must be representations of the same function and, therefore, identical. In order to assure their identity, we re-write the argument of the first cosine in terms of the argument of the second cosine:

$$\frac{1}{\hbar}\int_A^x p(x',E)dx' - \frac{\pi}{4} = \frac{1}{\hbar}\int_A^B p(x',E)dx' - \frac{\pi}{2} + \frac{1}{\hbar}\int_B^x p(x',E)dx' + \frac{\pi}{4}.$$

We now impose that

$$\frac{1}{\hbar}\int_A^B p(x',E)dx' - \frac{\pi}{2} = n\pi \tag{52}$$

so that the arguments of the two cosine become related by

$$\cos\left(\frac{1}{\hbar}\int_A^x p(x',E)dx' - \frac{\pi}{4}\right) = (-1)^n \cos\left(\frac{1}{\hbar}\int_B^x p(x',E)dx' + \frac{\pi}{4}\right).$$

This last sign, $(-1)^n$ is finally absorbed by imposing $C' = (-1)^n C$.

The final result is

$$\phi(x) = C \begin{cases} \dfrac{(-1)^n}{2\sqrt{q}} e^{\frac{1}{\hbar}\int_A^x q(x',E)dx'} & x \in I \\ \dfrac{1}{\sqrt{p}} \cos\left(\dfrac{1}{\hbar}\displaystyle\int_B^x p(x',E)dx' + \dfrac{\pi}{4}\right) & x \in II \\ \dfrac{1}{2\sqrt{q}} e^{-\frac{1}{\hbar}\int_B^x q(x',E)dx'} & x \in III \end{cases} \tag{53}$$

where C is related to the normalization of $\phi(x)$. This global matching is possible only if the quantization condition (52) is satisfied. This can be re-writen as

$$\int_A^B p(x, E)dx = \left(n + \frac{1}{2}\right)\pi\hbar \tag{54}$$

which is the well known Bohr-Sommerfeld quantization condition of the old quantum theory.

7 The WKB wave-function for scattering states

Let us now consider the problem of scattering states illustrated in figure 1, where a particle (or beam of particles) is incident from the left with E smaller than the height of the barrier. The general form of the WKB wave-function for this setting is

$$\phi(x) = \begin{cases} \dfrac{A}{\sqrt{p}} e^{\frac{i}{\hbar}\int^x p(x',E)dx'} + \dfrac{R}{\sqrt{p}} e^{-\frac{i}{\hbar}\int^x p(x',E)dx'} & x \in I \\ \dfrac{C}{\sqrt{q}} e^{\frac{1}{\hbar}\int^x q(x',E)dx'} + \dfrac{D}{\sqrt{q}} e^{-\frac{1}{\hbar}\int^x q(x',E)dx'} & x \in II \\ \dfrac{T}{\sqrt{p}} e^{\frac{i}{\hbar}\int^x p(x',E)dx'} & x \in III \end{cases} . \tag{55}$$

Notice that the forbidden region is now region II, which is finite. Therefore the exponentials with both $+$ and $-$ signs are allowed. As we shall see, this introduces a complication in the matching of the different parts of the wave-function. We will deal with that in the next section.

Once the matching of the coefficients has been completed, we will calculate the transmission and reflection coefficients, given by

$$t = \frac{|T|^2}{|A|^2}$$

and

$$r = \frac{|R|^2}{|A|^2}.$$

8 The other Airy function

8.1 The Airy equation

Let us return to the Schroedinger equation in the vicinity of a turning point x_0, but this time in the x representation. Starting from

$$\frac{p^2}{2m}|\phi\rangle + V'(x_0)x|\phi\rangle = V'(x_0)x_0|\phi\rangle. \tag{56}$$

we find

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + V'(x_0)(x - x_0)\phi(x) = 0. \tag{57}$$

In terms of

$$y = \left(\frac{2mV'(x_0)}{\hbar^2}\right)^{1/3}(x_0 - x) \tag{58}$$

we obtain

$$\frac{\partial^2\phi}{\partial y^2} + y\phi = 0 \tag{59}$$

which is the Airy equation. Let us check that

$$\phi(x) = \int_0^{+\infty} \cos{(t^3/3 - ty)}dt = Ai(-y) \tag{60}$$

is indeed a solution. We differentiate twice with respect to y and manipulate the result as follows:

$$\begin{aligned}
\phi'' &= -\int_0^{+\infty} t^2 \cos{(t^3/3 - ty)}dt \\
&= -\int_0^{+\infty} \left\{\frac{\partial}{\partial t}[\sin{(t^3/3 - ty)}] - y\cos{(t^3/3 - ty)}\right\} dt \\
&= \sin{(t^3/3 - ty)}|_0^{\infty} - y\phi = -y\phi.
\end{aligned} \tag{61}$$

The boundary term is a bit delicate: at $t = 0$ it is clearly zero, but at $t = \infty$ it is not well defined. The argument is that it oscillates so fast for large t that any average of this term will be zero, and therefore we set it to zero.

8.2 The function Bi

The Airy equation is a second order equation and must have two independent solutions. Looking at $Ai(-y)$ we may guess that the other solution has the same form with the cosine replaced by a sine. That, however, does not work. The other solution is given by

$$\phi(x) = \int_0^{+\infty} \left[e^{-t^3/3-yt} + \sin\left(t^3/3 - ty\right) \right] dt \equiv Bi(-y). \tag{62}$$

The need of the extra exponential becomes evident when we calculate the second derivative of Bi with respect to y:

$$\begin{aligned} \phi'' &= \int_0^{+\infty} \left[t^2 e^{-t^3/3-yt} - t^2 \sin\left(t^3/3 - ty\right) \right] dt \\ &= \int_0^{+\infty} \left\{ -\frac{\partial}{\partial t}[e^{-t^3/3-yt}] + \frac{\partial}{\partial t}[\cos\left(t^3/3 - ty\right)] - y e^{-t^3/3-yt} - y \sin\left(t^3/3 - ty\right) \right\} dt \\ &= -e^{-t^3/3-yt}|_0^\infty + \cos\left(t^3/3 - ty\right)|_0^\infty - y\phi = -y\phi. \end{aligned} \tag{63}$$

If it were not for the extra exponential term, the boundary term resulting from the cosine at $t = 0$ would leave a factor 1, which is canceled by a similar factor coming from that exponential.

8.3 Asymptotic form of Bi

Far from the turning point x_0 we can derive simplified expressions for the Bi functions just as we did with Ai. I will not do that here and will only present the results. We find that, for $V'(x_0) > 0$,

$$\phi(x) \approx \begin{cases} \frac{c}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_{x_0}^x p(x', E)dx' - \pi/4\right) & x < x_0 \\ \frac{c}{\sqrt{q(x,E)}} e^{\frac{1}{\hbar}\int_{x_0}^x q(x',E)dx'} & x > x_0 \end{cases} \tag{64}$$

and, for $V'(x_0) < 0$,

$$\phi(x) \approx \begin{cases} \frac{c}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_{x_0}^x p(x', E)dx' + \pi/4\right) & x > x_0 \\ \frac{c}{\sqrt{q(x,E)}} e^{-\frac{1}{\hbar}\int_{x_0}^x q(x',E)dx'} & x < x_0. \end{cases} \tag{65}$$

Notice that both forms diverge as $x \to \pm\infty$ in the forbidden regions. This is why the function Bi does not appear in the calculation of bound states, where the forbidden regions extend to infinity. However, in scattering problems, the forbidden region is finite, no divergence occurs and Bi has to be included.

9 Semiclassical tunneling

Using the results from sections 5 and 8 we can match the different parts of the wave-function for scattering states, as given by equation (55) that we repeat here:

$$\phi(x) = \begin{cases} \frac{A}{\sqrt{p}} e^{\frac{i}{\hbar}\int^x p(x',E)dx'} + \frac{R}{\sqrt{p}} e^{-\frac{i}{\hbar}\int^x p(x',E)dx'} & x \in I \\ \frac{C}{\sqrt{q}} e^{\frac{1}{\hbar}\int^x q(x',E)dx'} + \frac{D}{\sqrt{q}} e^{-\frac{1}{\hbar}\int^x q(x',E)dx'} & x \in II \\ \frac{T}{\sqrt{p}} e^{\frac{i}{\hbar}\int^x p(x',E)dx'} & x \in III \end{cases}$$

We start with region III, where the solution represents a particle moving to the right only. Near the turning point B, where $V'(B) < 0$ we can write the solution as a combination of Ai and Bi as

$$\phi(x) \approx FAi(-y) + GBi(-y).$$

In the allowed region III these functions have asymptotic forms given by equations (51) and (65):

$$\begin{aligned} \phi(x) &\approx \frac{F}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_B^x p(x',E)dx' - \pi/4\right) + \frac{G}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_B^x p(x',E)dx' + \pi/4\right) \\ &= \frac{1}{\sqrt{p(x,E)}} \left[F \cos\left(\frac{1}{\hbar}\int_B^x p(x',E)dx' - \pi/4\right) + G \sin\left(\frac{1}{\hbar}\int_B^x p(x',E)dx' - \pi/4\right)\right] \end{aligned}$$

The desired form for region III can be recovered with the choice $G = iF$. We get

$$\phi(x) \approx \frac{F}{\sqrt{p(x,E)}} \exp\left(\frac{i}{\hbar}\int_{x_0}^x p(x',E)dx' - \pi/4\right)$$

which gives our first coefficient $T = Fe^{-i\pi/4}$.

This same solution, with $G = iF$, must work in region II, where

$$\begin{aligned} \phi(x) &\approx F[Ai(-y) + iBi(-y)] \\ &\approx F\left[\frac{1}{2\sqrt{q(x,E)}} e^{\frac{1}{\hbar}\int_B^x q(x',E)dx'} + \frac{i}{\sqrt{q(x,E)}} e^{-\frac{1}{\hbar}\int_B^x q(x',E)dx'}\right]. \end{aligned}$$

Therefore, fixing the lower limit of integration in region II as $x_0 = B$, the coefficients must be $C = F/2 = T/2e^{i\pi/4}$ and $D = iTe^{i\pi/4}$.

We now repeat the matching between regions I and II, where $x_0 = A$ and $V'(A) > 0$. In the vicinity of $x = A$ we write

$$\phi(x) \approx fAi(-y) + gBi(-y).$$

In region II this becomes

$$\begin{aligned}\phi(x) &\approx \frac{f}{2\sqrt{q(x,E)}} e^{-\frac{1}{\hbar}\int_A^x q(x',E)dx'} + \frac{g}{\sqrt{q(x,E)}} e^{\frac{1}{\hbar}\int_A^x q(x',E)dx'} \\ &= \frac{1}{\sqrt{q(x,E)}} \left[\frac{fe^{-\Delta/\hbar}}{2} e^{-\frac{1}{\hbar}\int_B^x q(x',E)dx'} + ge^{\Delta/\hbar} e^{\frac{1}{\hbar}\int_B^x q(x',E)dx'} \right]\end{aligned}$$

where we have defined

$$\Delta = \int_A^B q(x,E)dx.$$

Comparing with the form in region II we see that

$$\begin{aligned} C &= \frac{fe^{-\Delta/\hbar}}{2} \equiv \frac{T}{2} e^{i\pi/4} \\ D &= ge^{\Delta/\hbar} \equiv iTe^{i\pi/4} \end{aligned}$$

or

$$\begin{aligned} f &= Te^{\Delta/\hbar + i\frac{\pi}{4}} \\ g &= iTe^{-\Delta/\hbar + i\frac{\pi}{4}} \end{aligned}$$

Finally, we look at region I to determine A and R as a function of T. In this region we have

$$\begin{aligned}\phi(x) &\approx fAi(-y) + gBi(-y) \\ &\approx \frac{f}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_A^x p(x',E)dx' + \pi/4\right) + \frac{g}{\sqrt{p(x,E)}} \cos\left(\frac{1}{\hbar}\int_A^x p(x',E)dx' - \pi/4\right).\end{aligned}$$

Writing the cosines as exponentials and comparing with the general form in region I we see that

$$\begin{aligned} A &= \tfrac{fe^{i\pi/4}+ge^{-i\pi/4}}{2} \\ &= \tfrac{Te^{i\pi/2+\Delta/\hbar}+iTe^{-\Delta/\hbar}}{2} \\ &= iT\cosh\left(\Delta/\hbar\right) \end{aligned}$$

and

$$\begin{aligned} R &= \tfrac{fe^{-i\pi/4}+ge^{i\pi/4}}{2} \\ &= \tfrac{Te^{\Delta/\hbar}+iTe^{-\Delta/\hbar+i\pi/2}}{2} \\ &= T\sinh\left(\Delta/\hbar\right). \end{aligned}$$

The final result is

$$\phi(x) = T\begin{cases} \dfrac{i\cosh\left(\Delta/\hbar\right)}{\sqrt{p}} e^{\frac{i}{\hbar}\int_A^x p(x',E)dx'} + \dfrac{\sinh\left(\Delta/\hbar\right)}{\sqrt{p}} e^{-\frac{i}{\hbar}\int_A^x p(x',E)dx'} & x \in I \\ \dfrac{i^{1/2}}{2\sqrt{q}} e^{\frac{1}{\hbar}\int_B^x q(x',E)dx'} + \dfrac{i^{3/2}}{\sqrt{q}} e^{-\frac{1}{\hbar}\int_B^x q(x',E)dx'} & x \in II \\ \dfrac{1}{\sqrt{p}} e^{\frac{i}{\hbar}\int_B^x p(x',E)dx'} & x \in III \end{cases} . \tag{66}$$

The transmission and reflection coefficients are

$$t = \frac{1}{\cosh^2\left(\Delta/\hbar\right)} \approx 4e^{-2\Delta/\hbar} \tag{67}$$

and

$$r = \tanh^2\left(\Delta/\hbar\right) \approx 1 - 4e^{-2\Delta/\hbar}. \tag{68}$$