Lectures 9, 10 and 11: More on WKB

1 Illustration of matching in a turning point problem

Let $y(x)$ satisfy the linear homogeneous equation:

$$\epsilon^2 y''(x) - U(x)y(x) = 0 \tag{1}$$

in the interval (a_1, a_2) where $U(0) = 0$, $U'(0) > 0$, $U(x) > 0$ for $x \in (0, a_2]$ and $U(x) < 0$ for $x \in [a_1, 0)$. We seek asymptotic solution, which for $\epsilon << 1$ has the asymptotic behavior

$$y(x) \sim AU^{-1/4} \exp\left[-\frac{1}{\epsilon}\int_0^x U^{1/2}(s)ds\right][1 + o(1)] \tag{2}$$

for $x >> \epsilon^{2/3}$.

Now, consider $x = O(\epsilon^{2/3})$. We introduce rescaled variables:

$$x = \epsilon^{2/3}[U'(0)]^{-1/3} t \quad ; \quad y(x(t)) = \psi(t)$$

to obtain

$$\psi'' - t\psi = -\epsilon^{2/3}[U'(0)]^{-4/3} t^2 h(\epsilon^{2/3} t)\psi$$

where h is defined by $U(x) = \alpha x + x^2 h(x)$. As shown before, for $t \in [-M, M]$ for $M << \epsilon^{2/5}\epsilon^{-2/3}$,

$$\psi(t) \sim \psi_0(t) = C_1 Ai(t) + C_2 Bi(t) \tag{3}$$

In the regime $\epsilon^{2/3} << x << \epsilon^{2/5}$, both (2) and (3) are valid (after transforming t to x) and hence must *match*. To the leading order, note that

$$\frac{1}{\epsilon}\int_0^x U^{1/2}(s)ds \sim [U'(0)]^{1/2}\frac{2x^{3/2}}{3\epsilon} + o(1)$$

Hence, (2) in this regime reduces to

$$y(x) \sim A[U'(0)]^{-1/4} x^{-1/4} \exp\left[-\frac{2}{3}[U'(0)]^{1/2}\frac{x^{3/2}}{\epsilon}\right][1 + o(1)] \tag{4}$$

On the otherhand, from the known asymptotics for $t \to +\infty$, it follows that in the regime $1 << t << \epsilon^{-2/3}\epsilon^{2/5}$

$$Ai(t) \sim \frac{1}{2\sqrt{\pi}} t^{-1/4} e^{-\frac{2}{3}t^{3/2}}$$

$$Bi(t) \sim \frac{1}{2\sqrt{\pi}} t^{-1/4} e^{\frac{2}{3}t^{3/2}}$$

Therefore, (3) matches to (4) when

$$\frac{C_1}{2\sqrt{\pi}} = A[U'(0)]^{-1/4}\epsilon^{-1/6} \quad ; \quad C_2 = 0$$

On the otherhand, since for $t \to -\infty$, it is known that

$$Ai(t) \sim \frac{1}{\sqrt{\pi}}(-t)^{-1/4} \sin\left(\frac{2}{3}(-t)^{3/2} + \frac{\pi}{4}\right)$$

Therefore, in the regime $1 << t << \epsilon^{-2/3}\epsilon^{2/5}$

$$\psi(t) \sim \frac{C_1}{\sqrt{\pi}}(-t)^{-1/4} \sin\left(\frac{2}{3}(-t)^{3/2} + \frac{\pi}{4}\right) \tag{5}$$

On the otherhand, in the regime $x \in [a_1, 0)$ for $|x| >> \epsilon^{2/3}$, we know

$$y(x) \sim \hat{C}_3(-U(x))^{-1/4} \exp\left[-i\int_x^0 [-U(s)]^{1/2} ds\right] + \hat{C}_4(-U(x))^{-1/4} \exp\left[i\int_x^0 [-U(s)]^{1/2} ds\right]$$

Alternately, there exists constants C_3, C_4 related to $\hat{C}_3$ and $\hat{C}_4$ so that

$$y(x) \sim C_3(-U(x))^{-1/4} \sin\left[\int_x^0 [-U(s)]^{1/2} ds + \frac{\pi}{4}\right] + C_4(-U(x))^{-1/4} \cos\left[\int_x^0 [-U(s)]^{1/2} ds + \frac{\pi}{4}\right] \tag{6}$$

For $\epsilon^{2/3} << -x << \epsilon^{2/5}$, the expression above has the following asymptotic behavior for $\epsilon \to 0$:

$$y(x) \sim C_3[U'(0)]^{-1/4}(-x)^{-1/4} \sin\left[\frac{2}{3}[U'(0)]^{1/2}(-x)^{3/2} + \frac{\pi}{4}\right] + C_4[U'(0)]^{-1/4}(-x)^{-1/4} \cos\left[\frac{2}{3}[U'(0)]^{1/2}(-x)^{3/2} + \frac{\pi}{4}\right] \tag{7}$$

Taking into account expression for t in terms of x, The expressions (5) and (7) match when

$$C_3[U'(0)]^{-1/4}\epsilon^{-1/6} = \frac{C_1}{\sqrt{\pi}} \quad \text{and} \quad C_4 = 0$$

This means that constants in the two different outer regions $x >> \epsilon^{2/3}$, and $-x >> \epsilon^{2/3}$ can be connected. These relations are called *connection* relation. The constant C_3, C_4 appearing in (6) is related to constant A in (2) through (2) and (6):

$$2C_3 = A \quad \text{and} \quad C_4 = 0$$

which follows from matching solution to *inner* region solution. There is only one arbitrary constant A in this problem, as we ruled out the growing exponential solution $\exp\left[\int_0^x U^{-1/2}(s)ds\right] U^{-1/4}[1+o(1)]$ to (1)

2 Eigenvalue problem to Schroedinger Equation

As an example, we can determine the Energy levels (E) of a particle bound by a potential $V(x)$ for time-stationary Schroedinger equation in 1 dimension. This corresponds to finding eigenvalues E of the Schroedinger operator

$$\mathcal{S}y := \epsilon^2 y'' - V(x)y = Ey \quad \text{in } \mathbb{R} \tag{8}$$

where ϵ is a parameter propertional to Planck's constant and $V(x) \to +\infty$ as $x \to \pm\infty$. $V(x)$ physically means the bounding potential of the particle. We look for a *non zero* solution $y(x)$ to (1), with the property that $y \to 0$ as $x \to \pm\infty$. This corresponds to requiring zero probability of particle being outside the potential well. This is a natural requirement for infinitely deep potential well. We will assume $V \in C^\infty(-\infty, \infty)$ and that $V'(x) > 0$ for any x. If we substitute $U(x) = V(x) - E$, then the equation above transforms into (2). We will take $x = 0$ to coincide with the point where V is a minimum. We will restrict to values of E for which $E > V(0)$, since otherwise, there can be no non-zero solutions to (8) with desired property $y \to 0$ as $x \to \pm\infty$, as can be checked from WKB solutions.

Define a and b to be the two points where $U = V(x) - E = 0$. From given conditions $U(x) > 0$ for $x \in (b, \infty)$, $U < 0$ for $x \in (a, b)$ and $U > 0$ for $x \in (-\infty, a)$. There are three distinct *outer* regions, call it regions I, II and III, characterized by $x \in [b + K\epsilon^{2/3}, \infty)$, $x \in [a + K\epsilon^{2/3}, b - K\epsilon^{2/3}$ and $x \in (-\infty, a - K\epsilon^{2/3})$ for some large enough constant K.

The compliment of these regions in $\mathbb{R}$ are the *inner* regions, where formal WKB solutions are invalid.

In the outer region I,

$$y(x) = A_I \exp\left[\int_b^x \sqrt{U(s)}ds\right] U^{-1/4}(x)[1 + o(1)]$$

From what has been discussed in the last section, this particular solution has the following asymptotic behavior in outer region II,

$$y(x) = \frac{1}{2}A_I(-U(x))^{-1/4} \sin\left[\int_x^b [-U(s)]^{1/2}ds + \frac{\pi}{4}\right][1 + o(1)] \tag{9}$$

This can be written in an alternate manner, which is suitable for matching to solution in region III.

$$y(x) = -\frac{1}{2}A_I(-U(x))^{-1/4} \sin\left[\int_a^x [-U(s)]^{1/2}ds + \frac{\pi}{4} - \theta\right][1 + o(1)] \tag{10}$$

where

$$\theta = \int_a^b [-U(s)]^{1/2}ds + \frac{\pi}{2} \tag{11}$$

On the otherhand, in region III,

$$y(x) = A_{III} \exp\left[-\int_x^a [U(s)]^{1/2}ds\right][U(x)]^{-1/4}[1 + o(1)] \tag{12}$$

Corresponding to this solution, the solution in region II, that matches with a common *inner* solution in $x \in \left[a - K\epsilon^{2/3}, a + K\epsilon^{2/3}\right]$ is given by (Exercise, left to the reader)

$$y(x) = \frac{1}{2}A_{III}[-U(x)]^{-1/4} \sin\left[\int_a^x [-U(s)]^{1/2}ds + \frac{\pi}{4}\right][1 + o(1)] \tag{13}$$

In order for (13) and (10) to match, we must require either

$$A_I = -A_{III}, \theta = 2n\pi + o(1), \quad \text{or} \quad A_I = A_{III},\ \theta = (2n+1)\pi + o(1)$$

Thus, in all cases, we have the requirement

$$\theta = n\pi + o(\epsilon)$$

for some positive integer n (since θ is evidently positive). This implies

$$\int_a^b \sqrt{E - V(x)}dx = \left(n - \frac{1}{2}\right)\pi + o(\epsilon)$$

This is the quantization condition that energy E must satisfy. Note that a and b do depend on E. For example, suppose $V(x) = \alpha x^2$ (harmonic oscillator potential). Then $a = -\sqrt{\frac{E}{\alpha}}$ and $b = \sqrt{\frac{E}{\alpha}}$. Then,

$$\int_a^b \sqrt{E - V(x)}dx = \int_{-\alpha^{-1/2}\sqrt{E}}^{\alpha^{-1/2}\sqrt{E}} \sqrt{E - \alpha x^2}dx = \alpha^{-1/2}E\int_{-1}^{1} \sqrt{1 - y^2}dy = (n - \frac{1}{2})\pi + o(1)$$

Hence, using $\int_{-1}^1 \sqrt{1 - y^2}dy = \frac{\pi}{2}$, we obtain eigenvalues E in the more explicit form:

$$E = 2(n - \frac{1}{2})\alpha^{1/2} + o(1)$$

Similar expressions can be obtained for a more general $V(x)$ in the asymptotic limit $n \to \infty$, when $E >> 1$ to give us the Bohr quantization condition.

Remark 1 *The WKB result*

$$y = U^{-1/4} \exp\left[\pm\frac{1}{\epsilon}\int^x U^{1/2}(s)ds\right][1+o(1)]$$

is equally valid for independent solutions to

$$\epsilon^2 y'' - (U(x;\epsilon) + \epsilon^2 r(x;\epsilon))y(x) = 0$$

when $U(x;\epsilon)$ and $r(x;\epsilon)$ are continous in ϵ in a neighborhood of $\epsilon = 0$. The proof of this statement is very similar to what we have seen without $r(x)$.

Remark 2 *WKB type asymptotics can be applied to certain other equations of the form*

$$\epsilon^2 y'' + a(x;\epsilon)y' + V(x;\epsilon)y = 0$$

when $V(x,\epsilon) \to U(x)$ as $\epsilon \to 0$. First, we note that Liouville's transformation

$$y(x) = \exp\left[-\frac{1}{2\epsilon^2}\int^x a(s;\epsilon)ds\right] z(x)$$

Then $z(x,\epsilon)$ satisfies a second order differential equation without a z' term appearing in the equation. In this form, the analysis is similar to (1).

3 Asymptotics of solution to Inhomogeneous Equation

The WKB method can also be employed to determine asymptotics of solution to inhomogeneous equation as well. Consider solving for $y(x)$ satisfying

$$\epsilon^2 y'' - U(x)y(x) + R(x) = 0 \text{ for } x \in \mathbb{R},\ \ y(\pm\infty) = 0 \tag{14}$$

with $U(x) > 0$, with $U(x) >> x^{-2}$ as $|x| \to \infty$. Consider two independent solutions y_1, y_2 to the associated homogenous equation whose asymptotic behavior for $\epsilon << 1$ is given by

$$y_1(x;\epsilon) = [U(x)]^{-1/4} \exp\left[-\frac{1}{\epsilon}\int_0^x [U(s)]^{1/2} ds\right][1+o(1)] \tag{15}$$

$$y_2(x;\epsilon) = [U(x)]^{-1/4} \exp\left[\frac{1}{\epsilon}\int_0^x [U(s)]^{1/2} ds\right][1+o(1)] \tag{16}$$

Then, from variation of parameter formula, one particular solution has behavior

$$y(x) = y_1(x)\int_{-\infty}^x y_2(s)\frac{R(s)}{\epsilon^2 W(s)}ds - y_2(x)\int_{\infty}^x y_1(s)\frac{R(s)}{\epsilon^2 W(s)}ds \tag{17}$$

where the Wronskian $W(s) = y_1 y_2' - y_2 y_1' = \frac{2}{\epsilon}$ in our case. Using asymptotics of y_1, y_2, and defining $H(x) = \int^x [U(s)]^{1/2} ds$, we obtain

$$\begin{aligned} y(x) \sim \frac{U^{-1/4}(x)}{2\epsilon}&\int_{-\infty}^x U^{-1/4}(s)R(s)\exp\left[-\frac{1}{\epsilon}[H(x)-H(s)]\right]ds \\ &+ \frac{U^{-1/4}(x)}{2\epsilon}\int_x^\infty U^{-1/4}(s)R(s)\exp\left[-\frac{1}{\epsilon}[H(s)-H(x)]\right]ds \ \sim\ \frac{R(x)}{U(x)} + O(\epsilon) \end{aligned} \tag{18}$$

where we employed asymptotics of integrals. Now, if we require $y(x,\epsilon)$ not to have exponential growth at $x=\pm\infty$, then the solution given in (18) is the only one with that property since a nonzero linear combination $C_1y_1+C_2y_2$ grows at either $x=+\infty$ and/or $x=-\infty$ exponentially. The result in this case can be anticipated directly from (14), if it were true that $\epsilon^2 y'' << y(x)$.

4 WKB for higher order differential equations:

Application of WKB methods are not limited merely to second order differential equations. Consider for instance,

$$\epsilon^n y^{(n)} - U(x)y(x) = 0$$

As before, we may apply the *ansatz* $y(x)=e^{w(x)/\epsilon}$. Then the equation for $w(x,\epsilon)$ is formally of the form:

$$w'^n + \frac{n(n-1)}{2}\epsilon w'^{n-2}w'' + O(\epsilon^2) = U(x)$$

To the leading order, we expect $w \sim w_0$, where

$$w_0(x) = \omega_j \int^x [U(s)]^{1/n} ds \text{ where } \omega_j^n = 1, \quad \text{for } j=1,..n$$

If we substitute $w = w_0 + \epsilon\delta$,

$$\epsilon n {w_0'}^{n-1}\delta' = -\frac{1}{2}n(n-1)(w_0')^{n-2}\epsilon w_0'' + O(\epsilon^2)$$

So, formally, to the leading order

$$\delta = -\frac{n-1}{2n}\log\ U$$

This gives rise to n independent solutions:

$$y(x) \sim \exp\left[\omega_j \int^x [U(s)]^{1/n} ds\right] [U(x)]^{-(n-1)/2n}[1+o(1)]$$

for $j=1,2,..n$. This result can be rigorously using the methods similar to $n=2$.