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The WKB Approximation

Although this perturbation technique (due to Wentzel, Kramers, and Brillouin) has practical value essentially only for 1-D problems (or for problems separable into one-dimensionalized problems), it is of considerable interest through its connection with classical physics and the "old" (pre-1925) quantum theory. It is not only of historical theoretical importance, however. It can be very useful for problems involving quantum-mechanical tunneling.

For a one-dimensionalized Schrödinger equation, we have

$$\frac{d^2u}{dx^2} + \frac{2\mu}{\hbar^2}(E - V(x))u(x) = 0, \tag{1}$$

or

$$\frac{d^2u}{dx^2} + \frac{P^2(x)}{\hbar^2}u(x) = 0, \tag{2}$$

where $P(x)$ is the "local" (x-dependent) momentum of the particle. Thus if $V(x)$ were constant over a small range of x values, P would be the momentum of the particle in this range of x values. The WKB technique uses $\hbar$ as an expansion parameter; that is, it uses an expansion in powers of $\hbar$ that should therefore be valid in the classical limit $\hbar \to 0$. In particular, solutions are sought of the form

$$u(x) = e^{\frac{i}{\hbar}S(x)} = e^{\frac{i}{\hbar}\left(S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \cdots\right)}, \tag{3}$$

so

$$u' = \frac{i}{\hbar}(S_0' + \hbar S_1' + \hbar^2 S_2' + \cdots)e^{\frac{i}{\hbar}S(x)}, \tag{4}$$

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$$u'' = \left[-\frac{1}{\hbar^2}(S_0' + \hbar S_1' + \hbar^2 S_2' + \cdots)^2 + \frac{i}{\hbar}(S_0'' + \hbar S_1'' + \hbar^2 S_2'' + \cdots) \right] e^{\frac{i}{\hbar}S(x)}. \quad (5)$$

Substituting this relation into the Schrödinger equation, and picking off terms of order $\frac{1}{\hbar^2}$, of order $\frac{1}{\hbar}$, and of successively smaller order in powers of $\hbar$, we get (first) from the term of order $\frac{1}{\hbar^2}$:

$$-(S_0')^2 + P^2(x) = 0, \quad (6)$$

$$\frac{dS_0}{dx} = \pm P(x), \qquad S_0(x) = \pm \int_{\text{const.}}^{x} d\xi\, P(\xi). \quad (7)$$

Next, the term of order $\frac{1}{\hbar}$ leads to

$$iS_0'' - 2S_0'S_1' = 0, \qquad S_1' = \frac{i}{2}\frac{S_0''}{S_0'} = \frac{i}{2}\frac{d}{dx} ln S_0', \quad (8)$$

leading to

$$S_1(x) = \frac{i}{2} ln P(x), \qquad \text{or} \qquad e^{iS_1} = \frac{1}{\sqrt{P(x)}}. \quad (9)$$

In the next approximation, terms of order 1 in the powers of $\hbar$ development lead to

$$iS_1'' - (S_1')^2 - 2S_0'S_2' = 0, \quad (10)$$

$$S_2' = \frac{i}{2}\frac{S_1''}{S_0'} - \frac{(S_1')^2}{2S_0'} = -\frac{1}{4}\frac{S_0'''}{(S_0')^2} + \frac{3}{8}\frac{(S_0'')^2}{(S_0')^3} = -\frac{1}{4}\left(\frac{S_0''}{(S_0')^2}\right)' - \frac{1}{8}\frac{(S_0'')^2}{(S_0')^3}, \quad (11)$$

so

$$S_2 = -\frac{1}{4}\left(\frac{\left(\frac{dP}{dx}\right)}{P^2}\right) - \frac{1}{8}\int_{\text{const.}}^{x} d\xi \frac{\left(\frac{dP}{d\xi}\right)^2}{P^3(\xi)}, \quad (12)$$

or

$$S_2 = \frac{1}{4}\frac{\mu\frac{dV}{dx}}{[2\mu(E - V(x))]^{\frac{3}{2}}} - \frac{1}{8}\int_{\text{const.}}^{x} d\xi \frac{\mu^2\left(\frac{dV}{d\xi}\right)^2}{[2\mu(E - V(\xi))]^{\frac{5}{2}}}. \quad (13)$$

The second approximation function, $S_2(x)$, is usually neglected. We see, from its specific form, that this may be justified, provided $V(x)$ is a mildly varying function of x, i.e., $|\frac{dV}{dx}|$ is small, and provided x is not near a classical turning point for which we would have $(E - V(x)) = 0$, hence, a zero in the denominator of the function $S_2(x)$. Assuming S_2 can be neglected, we still have to consider two different types of solutions.

1. For $(E - V(x)) > 0$, for classically allowed regions, we have oscillatory solutions

$$u(x) = \frac{C}{\sqrt{P(x)}} \cos\left(\frac{1}{\hbar}\int_{x_2}^{x} d\xi\, P(\xi) + \alpha\right), \quad (14)$$

where we have assumed $x > x_2$, x_2 is a left classical turning point (see Fig. 36.1), and C and α are integration constants.

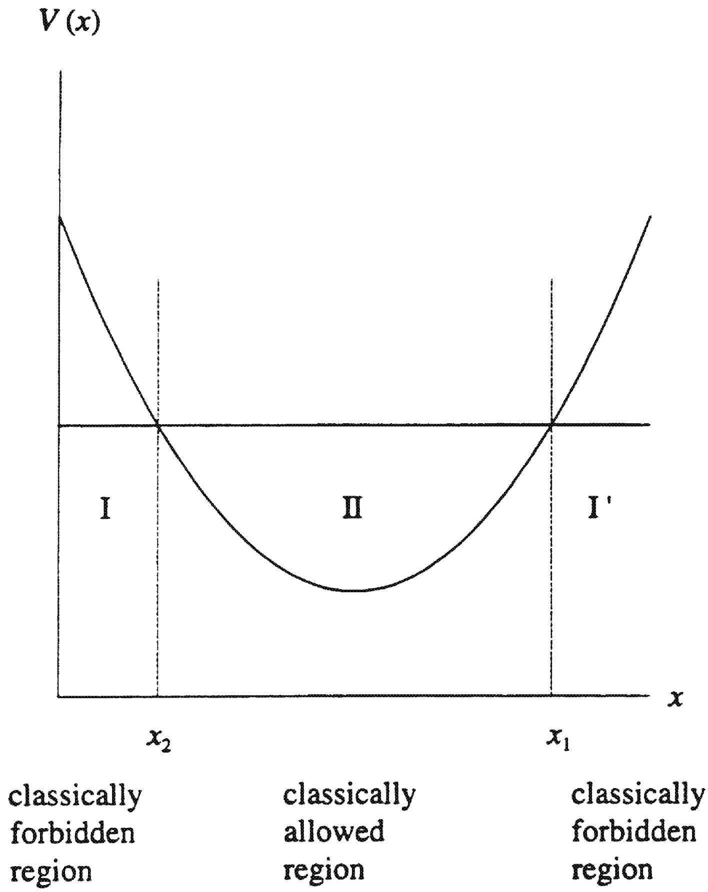

FIGURE 36.1.

2. For $(E - V(x)) < 0$, for classically forbidden regions, we have exponential solutions. These solutions are best put in the form

$$u(x) = \frac{A}{\sqrt{|P(x)|}} e^{+\frac{1}{\hbar}\int_{x_1}^{x} d\xi |P(\xi)|} + \frac{B}{\sqrt{|P(x)|}} e^{-\frac{1}{\hbar}\int_{x_1}^{x} d\xi |P(\xi)|}, \quad \text{for } x > x_1, \tag{15}$$

or

$$u(x) = \frac{A}{\sqrt{|P(x)|}} e^{+\frac{1}{\hbar}\int_{x}^{x_2} d\xi |P(\xi)|} + \frac{B}{\sqrt{|P(x)|}} e^{-\frac{1}{\hbar}\int_{x}^{x_2} d\xi |P(\xi)|}, \quad \text{for } x < x_2. \tag{16}$$

Even to this order, the WKB solutions blow up at the classical turning points. As $x \to x_1$, or $x \to x_2$, $P(x) \to 0$, and the WKB solutions go to ∞. The exact solutions, however, have no remarkable behavior or singularities there. We need an expression that gives a continuous $u(x)$ valid for all regions. We need to relate the integration constants, C, α, from the oscillatory solutions to the A, B from the exponential solutions. In square well problems, we had a similar situation, in which we used boundary conditions at discontinuities of the potential to find C, α as functions of A, B. Unfortunately, it is precisely at the classical turning points, where u_{WKB} breaks down and becomes invalid (see Fig. 36.2). The problem was solved by Kramers through his connection formulae. In the vicinity of the classical turning points, x_1, x_2, a good approximation to an exact solution can be found and this approximation can be used to make the connection between the exponential and the oscillatory WKB approximate solutions. For this purpose, it is sufficient to consider $\frac{dV}{dx}$ to be constant over a small range of x near $x = x_1$, or near $x = x_2$, and use the exact solution for this straight-line potential of fixed slope to fit onto the oscillatory solution on one side and the exponential one on the other. The details involve Bessel functions with index $n = \pm\frac{1}{3}$. The details of the derivation will be given in an appendix.

A The Kramers Connection Formulae

At a left turning point (see Fig. 36.1), $x = x_2$, a decreasing exponential solution connects onto an oscillatory solution according to

$$\frac{1}{\sqrt{|P(x)|}} e^{-\frac{1}{\hbar}\int_x^{x_2} d\xi |P(\xi)|} \leftrightarrow \frac{2}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar}\int_{x_2}^{x} d\xi\, P(\xi) - \frac{\pi}{4}\right], \tag{17}$$

whereas an increasing exponential solution connects onto an oscillatory one according to

$$\frac{1}{\sqrt{|P(x)|}} e^{+\frac{1}{\hbar}\int_x^{x_2} d\xi |P(\xi)|} \leftrightarrow \frac{1}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar}\int_{x_2}^{x} d\xi\, P(\xi) + \frac{\pi}{4}\right]. \tag{18}$$

At a right turning point, $x = x_1$, the decreasing exponential solution connects onto an oscillatory solution according to

$$\frac{1}{\sqrt{|P(x)|}} e^{-\frac{1}{\hbar}\int_{x_1}^{x} d\xi |P(\xi)|} \leftrightarrow \frac{2}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar}\int_{x}^{x_1} d\xi\, P(\xi) - \frac{\pi}{4}\right], \tag{19}$$

whereas the increasing exponential solution connects onto an oscillatory one according to

$$\frac{1}{\sqrt{|P(x)|}} e^{+\frac{1}{\hbar}\int_{x_1}^{x} d\xi |P(\xi)|} \leftrightarrow \frac{1}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar}\int_{x}^{x_1} d\xi\, P(\xi) + \frac{\pi}{4}\right]. \tag{20}$$

B Appendix: Derivation of the Connection Formulae

In the vicinity of a classical turning point (let us choose a left turning point $x = x_2$), let us assume the potential function varies smoothly so the function V(x) can be approximated by a straight line over the region where the WKB approximation is not valid. Thus, for the left turning point, $x = x_2$, we will assume $u_{\text{WKB}}(x)$ is

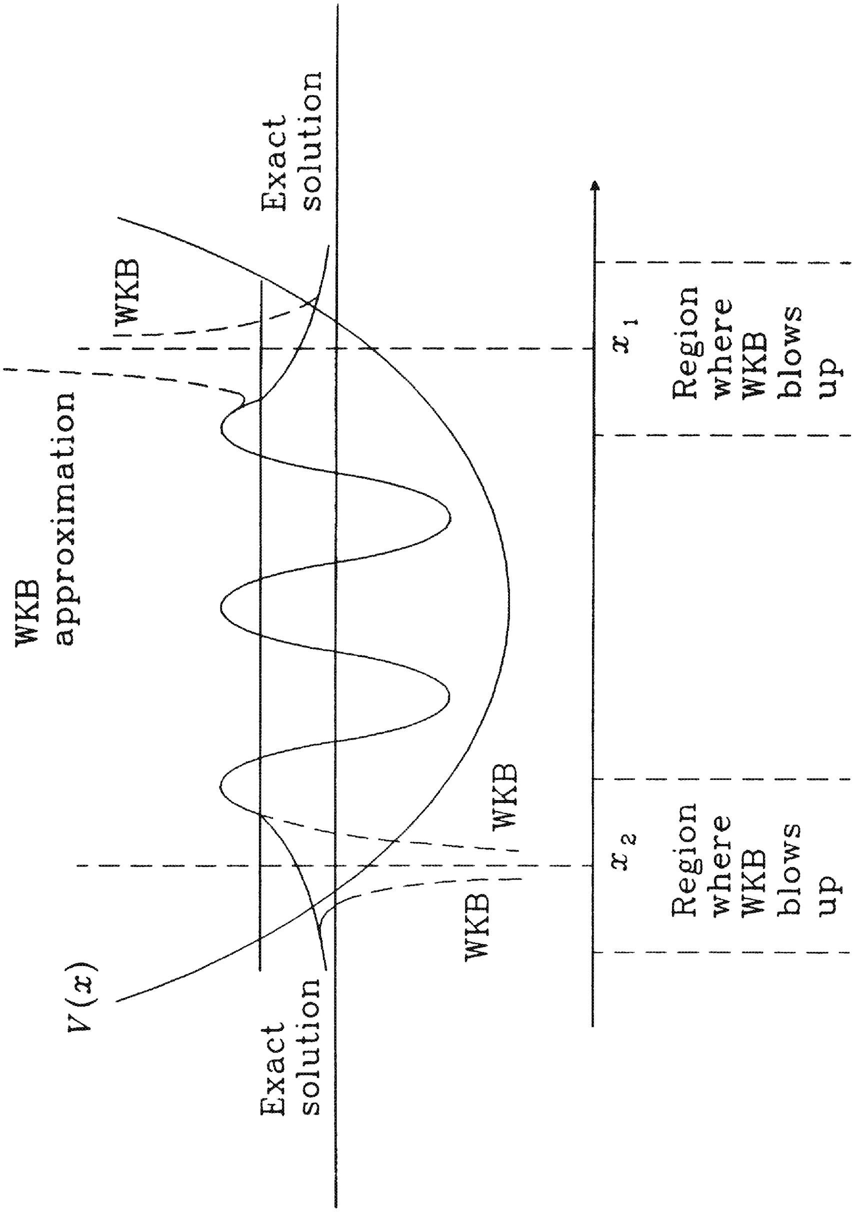

FIGURE 36.2. WKB and exact solutions for a $V(x)$ with one classically allowed region.

a good approximation for $x < x_2 - \frac{\Delta}{2}$ (in the exponential region I), and again for $x > x_2 + \frac{\Delta}{2}$ (in the oscillatory region II). We will also assume in the region, $x_2 - \frac{\Delta}{2} < x < x_2 + \frac{\Delta}{2}$, the potential $V(x)$ can be approximated by a straight line, so in this region

$$\frac{2\mu}{\hbar^2}(E - V(x)) = c^2(x - x_2), \qquad \text{where} \quad c^2 = \frac{2\mu}{\hbar^2}|\frac{dV}{dx}|_{x=x_2}. \tag{21}$$

The strategy is then the following: Find an exact solution to the equation

$$u'' + c^2(x - x_2)u(x) = 0, \tag{22}$$

valid in the region near $x = x_2$ (where the WKB solution blows up), and continue this solution into region II where it matches the oscillatory WKB solution for $x - x_2$ sufficiently large and also continue it to the left into region I where now for $x_2 - x$ sufficiently large it matches the exponential WKB solution. It will be convenient to introduce new dependent and new independent variables for eq. (22).

In particular, in region I, for $x < x_2$, introduce

$$y = \frac{1}{\hbar}\int_x^{x_2} d\xi |P(\xi)| = c\int_x^{x_2} d\xi \sqrt{(x_2 - \xi)} = \frac{2}{3}c(x_2 - x)^{\frac{3}{2}}. \tag{23}$$

Similarly, in region II, for $x > x_2$, introduce

$$y = \frac{1}{\hbar}\int_{x_2}^{x} d\xi\, P(\xi) = c\int_{x_2}^{x} d\xi \sqrt{(\xi - x_2)} = \frac{2}{3}c(x - x_2)^{\frac{3}{2}}. \tag{24}$$

These relations lead to

$$\frac{du}{dx} = -c(x_2 - x)^{\frac{1}{2}}\frac{du}{dy}, \qquad \text{for region I}, \tag{25}$$

$$\frac{du}{dx} = +c(x - x_2)^{\frac{1}{2}}\frac{du}{dy}, \qquad \text{for region II}. \tag{26}$$

This process transforms the equation $u'' + c^2(x - x_2)u = 0$ into

$$\pm c^2(x_2 - x)\left(\frac{d^2u}{dy^2} + \frac{1}{3y}\frac{du}{dy} \mp u\right) = 0, \tag{27}$$

for regions I (upper signs) and II (lower signs), respectively. Now we will make the further change of dependent variable,

$$u(y) = y^{\frac{1}{3}}v(y), \tag{28}$$

in both cases, leading to the new equations

$$y^2\frac{d^2v}{dy^2} + y\frac{dv}{dy} + \left[\mp y^2 - \left(\frac{1}{3}\right)^2\right]v(y) = 0, \tag{29}$$

where upper (and lower) signs again refer to regions I (and II). This equation is the Bessel equation with index $n^2 = (\frac{1}{3})^2$ of the variable y for region II, and the variable iy for region I. Thus,

$$v_I(y) = A_+J_{+\frac{1}{3}}(iy) + A_-J_{-\frac{1}{3}}(iy) = A_+I_{+\frac{1}{3}}(y) + A_-I_{-\frac{1}{3}}(y)$$

$$v_{II}(y) = B_+ J_{+\frac{1}{3}}(y) + B_- J_{-\frac{1}{3}}(y), \tag{30}$$

or

$$u_I(y) = A_+ y^{\frac{1}{3}} I_{+\frac{1}{3}}(y) + A_- y^{\frac{1}{3}} I_{-\frac{1}{3}}(y)$$
$$u_{II}(y) = B_+ y^{\frac{1}{3}} J_{+\frac{1}{3}} + B_- y^{\frac{1}{3}} J_{-\frac{1}{3}}, \tag{31}$$

where the arbitrary constants, A_+, A_-, B_+, B_-, must still be chosen to make u and its first derivative continuous at $y = 0$, $(x = x_2)$. We therefore need the behavior of the Bessel function near $y = 0$. From

$$J_n(y) = \sum_{k=0} \frac{(-1)^k}{k!} \frac{1}{\Gamma(n+k+1)} \left(\frac{y}{2}\right)^{n+2k}, \tag{32}$$

we have near $y = 0$

$$J_{\pm\frac{1}{3}}(y) = I_{\pm\frac{1}{3}}(y) = \frac{1}{\Gamma(\pm\frac{1}{3}+1)} \left(\frac{y}{2}\right)^{\pm\frac{1}{3}} + \cdots . \tag{33}$$

Therefore, near $x = x_2$, after transforming back to functions of x,

$$u_I(x) = \frac{A_+ (\frac{1}{2})^{\frac{1}{3}} (\frac{2c}{3})^{\frac{2}{3}}}{\Gamma(\frac{4}{3})} (x_2 - x)^1 + \frac{A_- (\frac{1}{2})^{-\frac{1}{3}}}{\Gamma(\frac{2}{3})} + \cdots ,$$
$$u_{II}(x) = \frac{B_+ (\frac{1}{2})^{\frac{1}{3}} (\frac{2c}{3})^{\frac{2}{3}}}{\Gamma(\frac{4}{3})} (x - x_2)^1 + \frac{B_- (\frac{1}{2})^{-\frac{1}{3}}}{\Gamma(\frac{2}{3})} + \cdots . \tag{34}$$

Now, the requirement

$$u_I(x_2) = u_{II}(x_2) \qquad \text{leads to} \qquad B_- = A_-, \tag{35}$$

whereas

$$\left[\frac{du_I}{dx}\right]_{x=x_2} = \left[\frac{du_{II}}{dx}\right]_{x=x_2} \qquad \text{leads to} \qquad B_+ = -A_+. \tag{36}$$

Next, we want to continue these solutions to large values of y, far enough from the turning point, $y = 0$, so they may match the WKB solutions. For this purpose, we will attempt to use the asymptotic expansions of the Bessel functions, valid for large values of y. [Actual experience, that is, a look at the exact plots of $J_n(y)$, shows y does not have to be very large for these asymptotic expressions to be surprisingly good approximations.] For $J_n(y)$, as $y \to$ large,

$$J_n(y) \to \sqrt{\frac{2}{\pi y}} \cos(y - [n + \frac{1}{2}]\frac{\pi}{2}). \tag{37}$$

Thus,

$$J_{\pm\frac{1}{3}}(y) \to \sqrt{\frac{2}{\pi y}} \cos(y - \frac{\pi}{4} \mp \frac{\pi}{6}), \tag{38}$$

whereas

$$I_{\pm\frac{1}{3}}(y) \to \frac{1}{\sqrt{2\pi y}}\left(e^{y} + e^{-y}e^{-(\frac{1}{2}\pm\frac{1}{3})i\pi}\right), \tag{39}$$

but for large values of y, e^{-y} is completely negligible compared with e^{+y}. The e^{-y} term comes into play only for the difference $(I_{+\frac{1}{3}} - I_{-\frac{1}{3}})$ for which the e^{y} terms cancel. For this difference, as $y \to$ large,

$$(I_{+\frac{1}{3}} - I_{-\frac{1}{3}}) \to \frac{1}{\sqrt{2\pi y}}e^{-y}\left(e^{-\frac{5i\pi}{6}} - e^{-\frac{i\pi}{6}}\right) = -\sqrt{\frac{2}{\pi y}}e^{-y}\cos\frac{\pi}{6}. \tag{40}$$

Otherwise,

$$I_{\pm\frac{1}{3}} \to \frac{1}{\sqrt{2\pi y}}e^{+y}. \tag{41}$$

Now, with the $B_{\pm}$ determined from the boundary conditions at $x = x_2$, we have

$$\text{In region I:} \quad u_I(y) = y^{\frac{1}{3}}(A_+ I_{+\frac{1}{3}}(y) + A_- I_{-\frac{1}{3}}(y)). \tag{42}$$

$$\text{In region II:} \quad u_{II}(y) = y^{\frac{1}{3}}(-A_+ J_{+\frac{1}{3}}(y) + A_- J_{-\frac{1}{3}}(y)). \tag{43}$$

Let us now for a first choice pick $A_+ = -A_-$. Then,

$$u_I(y) = -y^{\frac{1}{3}}A_-(I_{+\frac{1}{3}}(y) - I_{-\frac{1}{3}}(y)) \to \frac{A_-}{y^{\frac{1}{6}}}\sqrt{\frac{2}{\pi}}e^{-y}\cos\frac{\pi}{6}. \tag{44}$$

Similarly, with this choice of constants,

$$\begin{aligned} u_{II}(y) &\to \frac{A_-}{y^{\frac{1}{6}}}\sqrt{\frac{2}{\pi}}\left(\cos(y - \frac{\pi}{4} - \frac{\pi}{6}) + \cos(y - \frac{\pi}{4} + \frac{\pi}{6})\right) \\ &= \frac{A_-}{y^{\frac{1}{6}}}\sqrt{\frac{2}{\pi}}\left[\cos(y - \frac{\pi}{4})\right]2\cos\frac{\pi}{6}. \end{aligned} \tag{45}$$

Thus, with this choice of constants, viz. $A_+ = -A_-$, we get

$$\text{in I} \quad \frac{e^{-y}}{y^{\frac{1}{6}}} \quad \leftarrow \quad u(y) \quad \to \quad \frac{2}{y^{\frac{1}{6}}}\cos(y - \frac{\pi}{4}) \quad \text{in II}. \tag{46}$$

Now, substituting the values for y for regions I and II, through eqs. (23) and (24), with (21), we can translate this equation into the connection formula

$$\frac{1}{\sqrt{|P(x)|}}e^{-\frac{1}{\hbar}\int_x^{x_2} d\xi |P(\xi)|} \to \frac{2}{\sqrt{P(x)}}\cos\left[\frac{1}{\hbar}\int_{x_2}^{x} d\xi\, P(\xi) - \frac{\pi}{4}\right]. \tag{47}$$

This relation gives us one of the connection formulae for a left turning point.

To get the second connection formula, choose $A_+ = A_-$. Then, we have

$$u_I(y) = A_+ y^{\frac{1}{3}}(I_{+\frac{1}{3}} + I_{-\frac{1}{3}}) \to \frac{A_+}{\sqrt{2\pi}}\frac{1}{y^{\frac{1}{6}}}2e^{y}, \tag{48}$$

and

$$
\begin{aligned}
u_{II}(y) &= A_+ y^{\frac{1}{3}}(-J_{+\frac{1}{3}} + J_{-\frac{1}{3}}) \\
&\to A_+ \frac{1}{y^{\frac{1}{6}}}\sqrt{\frac{2}{\pi}}\Big(-\cos(y - \frac{\pi}{4} - \frac{\pi}{6}) + \cos(y - \frac{\pi}{4} + \frac{\pi}{6})\Big) \\
&= \frac{A_+}{y^{\frac{1}{6}}}\sqrt{\frac{2}{\pi}}\cos(y + \frac{\pi}{4}).
\end{aligned} \tag{49}
$$

Thus, with this choice of constants, we are led to

$$
\text{in I} \quad \frac{A_+}{y^{\frac{1}{6}}}\sqrt{\frac{2}{\pi}}e^{+y} \quad \leftarrow \quad u(y) \quad \rightarrow \quad \frac{A_+}{y^{\frac{1}{6}}}\sqrt{\frac{2}{\pi}}\cos(y + \frac{\pi}{4}) \quad \text{in II.} \tag{50}
$$

Substituting for the values of y in regions I and II, this relation translates into the second connection formula at the left turning point, x_2,

$$
\frac{1}{\sqrt{|P(x)|}}e^{+\frac{1}{\hbar}\int_x^{x_2} d\xi |P(\xi)|} \leftrightarrow \frac{1}{\sqrt{P(x)}}\cos\left[\frac{1}{\hbar}\int_{x_2}^{x} d\xi\, P(\xi) + \frac{\pi}{4}\right]. \tag{51}
$$

Derivations for the connection formulae at a right turning point, x_1, go in precisely parallel fashion.