Lecture #6: Linear V(x). JWKB Approximation and Quantization

JWKB: Jeffreys, Wentzel, Kramers, Brillouin.

Last time: Normalization schemes for eigenfunctions which belong to continuously variable eigenvalues.

- 1. identities
- 2. $\psi_{\delta k}, \psi_{\delta p}, \psi_{\delta E}, \psi_{box}$: different normalization schemes

3. trick using box normalization
$$(\theta \text{ is } k, p, E)$$

$$\frac{\# \text{ states}}{\delta \Theta_{\alpha L}} \left(\frac{\# \text{ particles}}{\delta x} \right)_{\alpha L} \text{ for box normalization}$$

 $\frac{dn}{dE}$ ("density of states") often needed - alternate method via JWKB next lecture 4.

1.
$$V(x) = \alpha x$$
 linear potential
solve in momentum representation, $\phi(p)$, and take F.T. to $\psi(x) \rightarrow \text{Airy functions}$

2. Semi-classical (JWKB) approx. for $\psi(x)$

*
$$p(x) = [(E - V(x))2m]^{1/2}$$
 Classical mechanical momentum function dependence on x.
* $\psi(x) = |p(x)|^{-1/2} \exp\left[\pm \frac{i}{x} \int_{x}^{x} \frac{\varphi(x')dx'}{p(x')dx'}\right]$

$$\psi(x) = |p(x)|^{-1/2} \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} \varphi(x') dx'\right]$$

envelope

- visualize $\psi(x)$ as plane wave with x-dependent wave vector *
- useful for evaluating stationary phase integrals (localization, causality) *

**** splicing across boundary between classical (
$$E > V$$
) and forbidden ($E < V$) regions Next

lecture

WKB Quantization Condition

$$\int_{x_{-}(E)}^{x_{+}(E)} p(x')dx' = \frac{h}{2}(n+1/2)n = 0,1,\dots$$

<u>Linear</u> Potential. $V(x) = \alpha x$

 $\hat{H} = \frac{\hat{p}^2}{2m} + \alpha \hat{x}$ coordinate representation momentum representation $\hat{\mathbf{x}} \rightarrow \mathbf{x}$ $\hat{p} \rightarrow p$ $\hat{p} \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x}$ $\hat{x} \to i\hbar \frac{\partial}{\partial p}$ $\begin{pmatrix} \text{note } [\hat{x}, \hat{p}] = i\hbar \text{ in both} \\ \text{representations - prove this?} \end{pmatrix}$ $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha x$ $\hat{H} = \frac{p^2}{2m} + i\hbar\alpha \frac{d}{dp}$ $0 = (H - E)\phi(p)$ $0 = \left(\frac{p^2}{2m} + i\hbar\alpha \frac{d}{dp} - E\right)\phi(p)$ 2nd order 1st order - much easier! differential equation Solve in momentum representation (a sometimes useful trick) $\frac{\mathrm{d}\phi(\mathbf{p})}{\mathrm{d}\mathbf{p}} = -\frac{\mathrm{i}}{\hbar\alpha} \left(\mathrm{E} - \mathrm{p}^2/2\mathrm{m}\right)\phi(\mathbf{p})$ Schr. Eq. Form of Solution $\phi(p) = Ne^{i}$ $\frac{d\phi}{dp}$ gives p^2 times $\phi(p)$ - when you take $\frac{d}{dp}$ $\frac{d\phi}{dp}$ gives constant times $\phi(p)$ Must solve for a and b

plug into Schr. Eq. and identify correspondences, term-by-term, to get

 $\phi(p) = Nexp$

$$a = -\frac{iE}{\hbar\alpha}$$
$$b = \frac{i}{6\hbar\alpha m}$$

$$\frac{i}{\hbar\alpha} \left(E p - p^3 / 6m \right) \right] \qquad easy? Note that, if p is real, \phi(p) is oscillatory$$

$$\phi * (p)\phi(p) = 1!$$
 \therefore N = 1

Now p is an observable, so it must be real. Thus $\phi(p)$ is defined for all (real) p and is oscillatory in p for all p. $\phi(p)$ is NEVER exponentially increasing or decreasing if p is real!

IT IS STRANGE THAT $\phi(p)$ does not distinguish between classically allowed and forbidden regions. IS THIS REALLY STRANGE? If we allow p to be imaginary in order to deal with classically forbidden regions, $\phi(p)$ becomes an increasing or decreasing exponential. When we extend the solution to the Schrödinger equation into the classically forbidden region, p is imaginary and $\phi(p)$ is exponentially increasing or decreasing.

If we insist on working in the $\psi(x)$ picture, we must perform a Fourier Transform.

$$\psi(x) = N' \int_{-\infty}^{\infty} e^{ipx/\hbar} \phi(p) dp$$

$$\psi(x) = N' \int_{-\infty}^{\infty} exp \left[\frac{i}{\hbar \alpha} \left\{ \frac{p(\alpha x - E) + p^3 / 6m}{odd} \right\} \right] dp$$

$$e^{i\theta} = \cos \theta + i \sin \theta$$

$$\int_{-\infty}^{\infty} \sin O(p) dp = 0 \quad \text{since } \sin O(p) \text{ is odd } \text{wrt } p \rightarrow -p.$$

$$\psi(x) = N' \int_{-\infty}^{\infty} \cos \left[\frac{(\alpha x - E)p + p^3 / 6m}{\hbar \alpha} \right] dp \quad \text{Solution!}$$

$$Ai(z) = \pi^{-1/2} \int_{0}^{\infty} \cos \left(s^3/3 + sz \right) ds$$

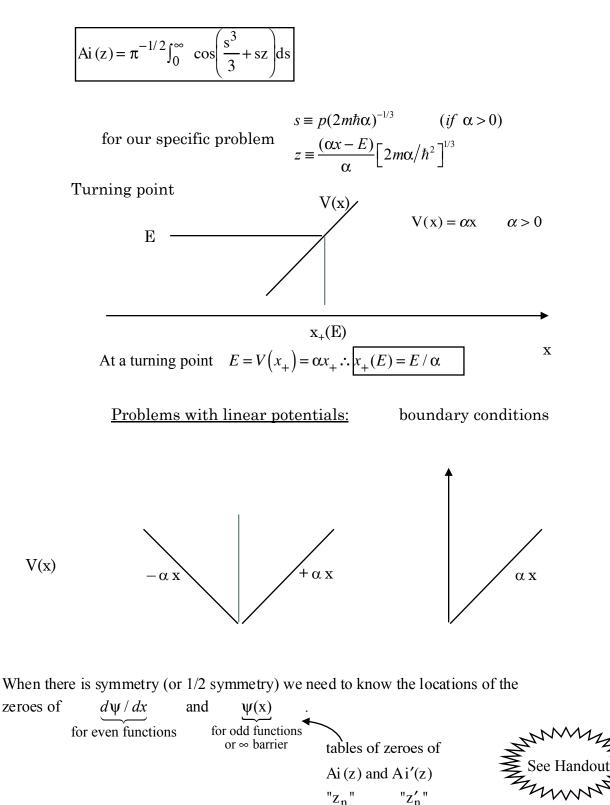
Surprise! This is a named (Airy) function and a tabulated integral

- * numerical tables for x near turning point i.e., $x \approx E/\alpha$
- * analytic "<u>asymptotic</u>" functions for x far from turning point.

useful for deriving energy levels as an explicit function of quantum numbers and for matching wave functions across boundaries.

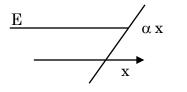
* zeroes of Airy functions $[Ai(z_i)=0]$ and of derivatives of Airy functions $[Ai'(z'_i)=0]$ are tabulated. (Useful for matching across center symmetry-point of potentials with definite even or odd symmetry.) [Two kinds of Airy functions, Ai and Bi.]

 $E = V(x) = \alpha x_{tp}$



When there is no symmetry, must match or join Ai (or, more precisely, a linear combination of Ai and Bi) and Ai' across boundaries, but we do not need to actually look at the Airy function itself near the joining point.

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This is not as bad as it seems because we are usually far from the *turning* point at an internal *joining* point and can use *analytic asymptotic expressions* for Ai(z).

2 linear potentials of different |slope|.

For $\alpha > 0$ there are 2 cases (classical and non-classical regions)

(i) $z \ll 0, E > V(x)$ classically allowed region

Ai(z)
$$\rightarrow \pi^{-1/2} (\underbrace{-z}_{positive})^{-1/4} \sin \left[\frac{2}{3} (\underbrace{-z}_{x \text{ is in here}})^{3/2} + \underbrace{\pi/4}_{\text{phase}} \right]$$

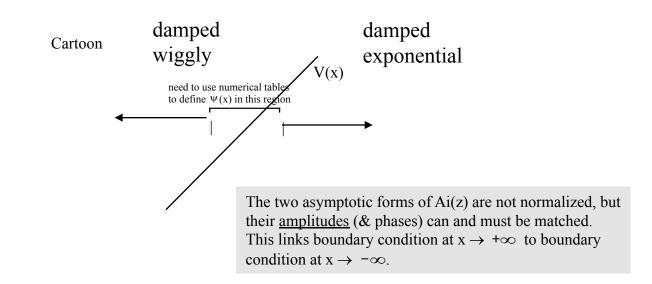
asymptotic form for $z \ll 0$.

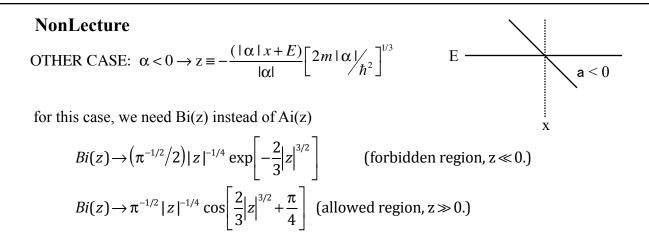
* oscillatory, but wave vector, k, varies with x

* Ai vanishes as $x \rightarrow -\infty$ because of $(-z)^{-1/4}$ factor

* Bi is needed for case where Airy function must vanish as $x \to +\infty$ in classical region

(ii)
well
$$\begin{cases} z >> 0 \ , \ E < V(x) \ forbidden \ region \\ Ai(z) \rightarrow (\pi^{-1/2}/2) \underbrace{z^{-1/4}}_{\text{positive}} \underbrace{e^{-(2/3)z^{-3/2}}}_{\frac{decreasing}{exponential}} \\ * \ not \ oscillatory, \ monotonic \\ * \ Ai \ vanishes \ as x \ \rightarrow \ +\infty \\ * \ Bi \ vanishes \ as x \ \rightarrow \ -\infty \ in \ forbidden \ region \end{cases}$$
 asymptotic form for $z \gg 0$.





What is so great about $V(x) = \alpha x$? $\Psi(x)$ seems ugly — need lookup tables, complicated solutions!

But Ai(z) turns out to be key to generalization of quantization of *all* (well behaved) V(x)!

These are semi-classical JWKB $\Psi(x)$ functions — They blow up near turning points (i.e. on both sides). The Ai(z)'s permit matching of JWKB $\Psi(x)$ s across the large gap where Ψ_{JWKB} is invalid, ill-defined.

(JEFFREYS) WENTZEL

KRAMERS

BRILLOUIN

JWKB provides a way to get $\Psi_n(x)$ and E_n without solving differential equations or performing a Fourier Transform.

But actually, the differential equations are easy to solve numerically. The reason we care about JWKB is that it provides a basis for:

- * physical interpretation (semi-classical)
- * RKR inversion from $E_{vJ} \rightarrow V_J(R)$. [Rydberg, Klein, Rees]
- * semi-classical quantization.
- * the link to classical mechanics is essential for wavepacket pictures.

(generalize on e^{ikx} for free particle by letting $k = p(x)/\hbar$ depend explicitly on x (why does this not violate $[x,p]=i\hbar$?)

$$\Psi_{JWKB} = \underbrace{\left[p(x)\right]^{-1/2}}_{\text{classical envelope}} \exp\left[\pm\frac{i}{\hbar}\int_{c}^{x}p(x')dx'\right]$$
No violation because k(x) and p(x) are classical mechanical functions of x, not QM operators.
$$p(x) = \left[2m(E - V(x))\right]^{1/2}$$
phase factor: choose c to satisfy boundary conditions

p(x) is pure real (classically allowed) or pure imaginary (classically forbidden). p(x) is not the Q.M. momentum. It is a classically motivated function of x, which has the form of the classical mechanical momentum and has the property that the $\lambda = \frac{h}{p}$ varies with x in a reasonable way.

 $|p(x)|^{-1/2}$ is probability amplitude envelope because probability $\propto \frac{1}{v}$ so amplitude $\propto \sqrt{\frac{1}{v}}$ (v is velocity)

*
$$\exp\left[\frac{i}{\hbar}\int_{c}^{x}p(x')dx'\right]$$
 is the generalization of $e^{ipx/\hbar}$ to non-constant V(x).

*node spacing $\frac{\lambda(x)}{2} = \frac{h}{2p(x)}$

*

* gives easily identifiable stationary phase region for many wiggly integrands.

(Both ψ 's have same λ at stationary phase point $x_{s.p.}$)

Long Nonlecture derivation/motivation of the JWKB splice across the turning point, even though the JWKB functions are not valid near the turning point.

Try
$$\psi(x) = N(x) \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx'\right]$$

plug into Schr. Eq. and get a new differential equation that N(x) must satisfy

* derived
in box
below
$$0 = \left[N'' \pm \frac{2ip(x)}{\hbar} N' \pm \frac{ip'(x)}{\hbar} N \right] \exp \left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx' \right]$$

This is a new Schr. Eq. for N(x). Now make an approximation, to be tested later, that N'' is negligible everywhere. This is based on the expectation that a slowly varying V(x) will lead to a slowly varying N(x).

$$\frac{d\Psi}{dx} = \left[N' \pm \frac{i}{\hbar} p(x) \right] \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx' \right]$$

$$\frac{d^{2}\Psi}{dx^{2}} = \left[N'' \pm \frac{i}{\hbar} N' p \pm \frac{i}{\hbar} N p' \pm \frac{ip}{\hbar} \left(N' \pm \frac{i}{\hbar} N p \right) \right] \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx' \right]$$

$$= \left[N'' \pm \frac{2i}{\hbar} N' p \pm \frac{ip'}{\hbar} N - \frac{p^{2}}{\hbar^{2}} N \right] \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx' \right]$$

$$0 = \frac{d^{2}\Psi}{dx^{2}} + \frac{p^{2}}{\hbar^{2}} N \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx' \right]$$

$$0 = \left[N'' \pm \frac{2ip(x)}{\hbar} N' \pm \frac{ip'}{\hbar} N \right] \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx' \right]$$

so, if we neglect N", we get for the first term in [] 2pN'+p'N=0if $p \neq 0$, then $2p^{1/2} \left[p^{1/2}N' + \frac{1}{2}p^{-1/2}p'N \right] = 0$ $\frac{d(Np^{1/2})}{dx} = \left[N'p^{1/2} + \frac{1}{2}p^{-1/2}p'N \right]$ $\therefore \frac{d(Np^{1/2})}{dx} = 0$ $N(x)p^{1/2}(x) = \text{constant}$

$$\therefore N(x) = cp(x)^{-1/2}$$

OK, now we have a form for N(x) that we can use to tell us what conditions must be satisfied so that N''(x) is negligible everywhere.

$$N = cp^{-1/2}$$

$$\frac{dp^{-1/2}}{dx} = -\frac{1}{2}p^{-3/2}\frac{dp}{dx} \qquad p(x) = \left[2m(E - V(x))\right]^{1/2}$$

$$\frac{dp}{dx} = \frac{1}{2}\left[2m(E - V(x))\right]^{-1/2}(-2m)\frac{dV}{dx}$$

$$= \frac{1}{2}p^{-1}(-2m)\frac{dV}{dx} = -mp^{-1}\frac{dV}{dx}$$

$$\cdot\frac{dp^{-1/2}}{dx} = p^{-5/2}\frac{m}{2}\frac{dV}{dx}$$

$$\frac{d^2p^{-1/2}}{dx^2} = \frac{m}{2}\frac{dV}{dx}\left(-\frac{5}{2}\right)p^{-7/2}\left[-\frac{m}{p}\frac{dV}{dx}\right] + p^{-5/2}\frac{m}{2}\frac{d^2V}{dx^2}$$

$$U_{pd}$$

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But we have made several assumptions about N":

$$\left| N'' \right| \ll \left| \frac{2ip}{\hbar} N' \right| = \left| + \frac{icm}{\hbar} p^{-3/2} \frac{dV}{dx} \right|$$

$$\left| N'' \right| \ll \left| \frac{ip'}{\hbar} N \right| = \left| - \frac{icm}{\hbar} p^{-3/2} \frac{dV}{dx} \right|$$

$$\left| N'' \right| \ll \frac{p^2}{\hbar^2} N = \frac{c}{\hbar^2} p^{+3/2}$$
all of this is satisfied if
$$\left| 5 \ m\hbar \left(dV \right) \right| = \left| - \frac{c}{\hbar^2} p^{-3/2} \right|$$

 $\left|\frac{3}{4}\frac{mn}{i}\left(\frac{dv}{dx}\right)p^{-3}\right| \ll 1$

Is this the JWKB validity condition? If it is, what does it mean?

Spirit of JWKB: if initial JWKB approximation is not sufficiently accurate, iterate:

 $\begin{array}{ll} p(x) \rightarrow \psi_0(x) & (\text{ordinary JWKB}) \\ \psi_0(x) \rightarrow p_1(x) & \\ p_1(x) \rightarrow \psi_1(x) & (\text{first order JWKB}) \end{array}$

$$e.g. \quad \frac{d^2 \Psi_0}{dx^2} + \frac{p_1^2}{\hbar^2} \Psi_0 = 0 \rightarrow p_1(x) = \begin{bmatrix} -\frac{\hbar^2}{\Psi_0(x)} \frac{d^2 \Psi_0}{dx^2} \end{bmatrix}^{1/2} \qquad \text{see ** Eq.} \\ \text{on p. 6-8} \\ \Psi_1(x) = |p_1(x)|^{-1/2} \exp\left[\pm \frac{i}{\hbar} \int_c^x p_1(x') dx'\right] \qquad \text{iterative improvement} \\ \text{of accuracy} \end{cases}$$

 $p_1(x)$ is not smaller than $p_0(x)$, but it has more nearly correct wiggles in it. END OF NONLECTURE Resume Lecture

$$\psi(x) \approx |p(x)|^{-1/2} \exp\left[\pm \frac{i}{\hbar} \int_{c}^{x} p(x') dx'\right]$$
adjustable phase shift.
provided that $\frac{d^{2}V}{dx^{2}}$ is negligible
AND

$$\frac{\hbar m}{|p|^{3}} \frac{dV}{dx} \ll 1 \left(\text{ satisfied by } \lambda(x) \left| \frac{dp}{dx} \right| < |p(x)| \text{ or } \frac{d\lambda}{dx} \ll 1 \right)$$
required for $N''(x)$
to be negligible

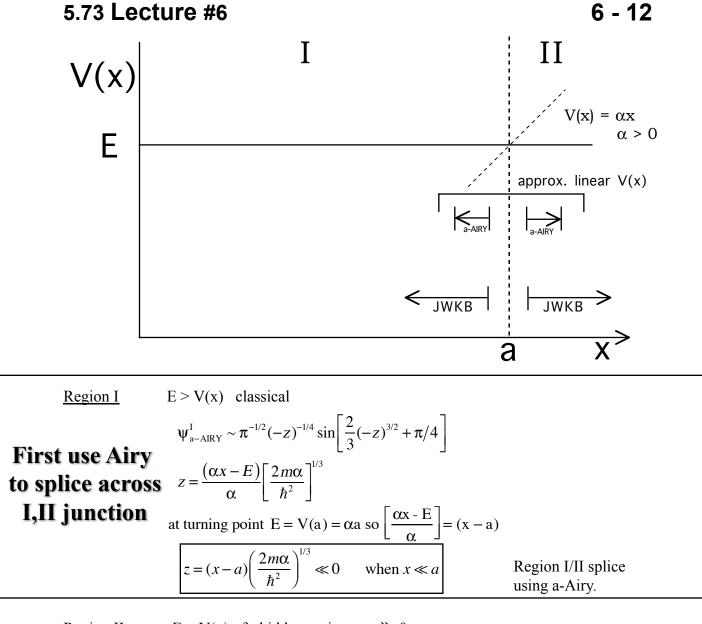
Next need to work out connection of $\Psi_{JWKB}(x)$ functions across region of x where the JWKB approx. breaks down (at turning points!).

$$\frac{d\lambda}{dx} \rightarrow \infty$$
 at turning point because $p(x) \rightarrow 0$ Looks BAD!

BUT ALL IS NOT LOST — near enough to a turning point <u>all potentials</u> V(x) look like $V(x)=\alpha x$! We have Airy functions that are solutions to the Schrödinger Equation for this linear potential.

Now our job is to show that <u>asymptotic – AIRY</u> and <u>JWKB</u> are identical for a small region not too close and not too far on both sides of each turning point.

THIS PERMITS ACCURATE SPLICING OF $\Psi(x)$ ACROSS TURNING POINT REGION!



Region II

E < V(x) forbidden region, $z \gg 0$

$$\Psi^{II}_{a-AIRY} \sim \frac{\pi^{-1/2}}{2} z^{-1/4} e^{-(2/3)z^{3/2}}$$

Now consider ψ_{JWKB} for a linear potential and show that it is identical to a-Airy!

$$\Psi_{JWKB} \sim c_{\pm} |p(x)|^{-1/2} \exp\left[\pm \frac{i}{\hbar} \int_{a}^{x} p(x') dx'\right]$$

Then both c_+ and c_- additive terms could be present use WKB p

$$\mathbf{x} \equiv \left[2m(\mathbf{E} - \mathbf{V}(\mathbf{x}))\right]^{1/2}$$

x < a classical , p is real ,
$$\psi_{JWKM}$$
 oscillates
x > a forbidden , p is imaginary , ψ_{JWKB} is exponential
pretend V(x) looks linear near x = a $(\ell - JWKB)$
 $p(x) = [2m\alpha(a - x)]^{1/2}$
 $\int_{a}^{x} p(x') dx' = (2m\alpha)^{1/2} \int_{a}^{x} (a - x')^{1/2} dx'$
 $= (2m\alpha)^{1/2} \left(-\frac{2}{3}\right) (a - x')^{3/2} \Big|_{a}^{x}$
 $= -(2m\alpha)^{1/2} \frac{2}{3} (a - x)^{3/2}$
 $Region I$
 $\psi_{1-JWKB}^{I}(x) \sim |p(x)|^{-1/2} [Ae^{i\theta} + Be^{-i\theta}]$
 $= |p(x)|^{-1/2} C \sin(\theta + \phi)$
Define the JWKB phase factor, $\theta(x)$:
 $\theta = \frac{1}{\hbar} \int_{a}^{x} p(x') dx' = -\left(\frac{2m\alpha}{\hbar^{2}}\right)^{1/2} \frac{2}{3} (a - x)^{3/2}$
Now compare $\theta(x)$ to $z(x)$
but, earlier, $z = (x - a) \left(\frac{2m\alpha}{\hbar^{2}}\right)^{1/3}$ $\therefore \theta = -\frac{2}{3} (-z)^{3/2}$
 $\therefore p = (2m\alpha\hbar)^{1/3} (-z)^{1/2}$ for exponential factor
 $|p|^{-1/2} = (2m\alpha\hbar)^{-1/6} (-z)^{-1/4}$ for pre-exponential factor

Thus, putting all of the pieces together

$$\psi_{\ell-JWKB}^{I} = \overline{-(2m\alpha\hbar)^{-1/6}(-z)^{-1/4}} C \sin\left[\frac{-\theta}{2(-z)^{3/2}} - \phi\right]$$
$$= \psi_{a-AIRY}^{I} \quad \text{If } C = -(2m\alpha\hbar)^{1/6}\pi^{-1/2}$$
$$\phi = -\pi/4$$

 $\psi_{\ell-JWKB}^{I}$ exactly splices onto ψ_{a-AIRY}^{I} with a $\pi/4$ phase factor (shifted from what the argument of sine would have been if one had started the phase integral at x = a

Similar result in Region II

$$\begin{split} \psi_{JWKB}^{II} &\sim Ae^{-f(x)} + Be^{+f(x)} \\ \text{at } x \to +\infty \qquad f(x) \to \infty \qquad \therefore B = 0 \\ \therefore \psi_{\ell-JWKB}^{II} &= A(2m\alpha)^{-1/4} (x-a)^{-1/4} \exp\left[-\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2} \frac{2}{3} (x-a)^{3/2}\right] \\ \text{which is equal to } \psi_{a-AIRY}^{II} \text{ if } A &= (2m\alpha\hbar)^{+1/6} \pi^{-1/2}/2 \end{split}$$

Final step:
$$\psi^{I}_{JWKB} \leftrightarrow \psi^{I}_{a-AIRY}$$
, $\psi^{II}_{JWKB} \leftrightarrow \psi^{II}_{a-AIRY}$

require A = -C/2

perfect match on opposite sides of turning point.

Ai(z) is valid in region where Ψ_{JWKB} is invalid.

The logic is complicated, but the analysis assures that matching of Ψ^{I}_{JWKB} to Ψ^{II}_{JWKB} is valid and that one gets an extra $\pi/4$ phase factor at each turning point in the classically allowed region. This corresponds to the extra phase accumulated in the non-classical region so that $\Psi(\pm \infty) \rightarrow 0$. The energy levels are lowered below where they would have been if the wavefunctions in the classically allowed region were zero at turning points.

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