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

---

1. identities
2. $\psi_{\delta k}, \psi_{\delta p}, \psi_{\delta E}, \psi_{box}$
3. trick using box normalization

$$\underbrace{\left(\frac{\#\ \text{states}}{\delta\theta}\right)}_{\propto L}\underbrace{\left(\frac{\#\ \text{particles}}{\delta x}\right)}_{\propto 1/L}$$ for box normalization

4. $\frac{dn}{dE}$ often needed - alternate method via JWKB next lecture

1. $\boxed{V(x) = \alpha x \text{ linear potential}}$
   solve in momentum representation, $\phi(p)$, and take F.T. to $\psi(x) \to$ Airy functions
2. Semi-classical (JWKB) approx. for $\psi(x)$
   * $p(x) = [(E - V(x))2m]^{1/2}$
   * $\psi(x) = \underbrace{|p(x)|^{-1/2}}_{\text{envelope}} \exp\underbrace{\left[\pm\frac{i}{\hbar}\int_c^x p(x')dx'\right]}_{\text{variable}}$

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

**** splicing across classical (E > V)|| forbidden (E < V)] Next lecture

$\downarrow$

WKB Quantization Condition

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

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + \alpha \hat{x}$$

coordinate representation	momentum representation
$\hat{x} \to x$	$\hat{p} \to p$
$\hat{p} \to \frac{\hbar}{i}\frac{\partial}{\partial x}$	$\hat{x} \to i\hbar \frac{\partial}{\partial p}$
	(note $[\hat{x}, \hat{p}] = i\hbar$ in both representations - prove this?)
$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha x$	$\hat{H} = \frac{p^2}{2m} + i\hbar\alpha \frac{d}{dp}$
2nd order	1st order - easier!

Solve in momentum representation (a sometimes useful trick)

Schr. Eq. $\boxed{\frac{d\phi(p)}{dp} = -\frac{i}{\hbar\alpha}\left(E - p^2/2m\right)\phi(p)}$

solution $\phi(p) = N e^{ap + bp^3}$

$\boxed{\text{gives } p^2 \text{ times } \phi(p)}$

$\boxed{\text{gives constant times } \phi(p)}$

plug into Schr. Eq. and identify, term-by-term, to get $\boxed{\begin{aligned} a &= -\frac{iE}{\hbar\alpha} \\ b &= \frac{i}{6\hbar\alpha m} \end{aligned}}$

$$\boxed{\phi(p) = N \exp\left[-\frac{i}{\hbar\alpha}\left(Ep - p^3/6m\right)\right]}$$ easy?

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

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. NEVER exponentially increasing or decreasing!

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.

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

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

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

$$e^{i\theta} = \underbrace{\cos\theta}_{\text{even}} + i\underbrace{\sin\theta}_{\text{odd}} \qquad \int_{-\infty}^{\infty} \sin O(p)dp = 0$$

since O(p) is odd wrt $p \to -p$.

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

$$Ai(z) = \pi^{-1/2}\int_0^{\infty}\cos\left(s^3/3 + sz\right)ds$$

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

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

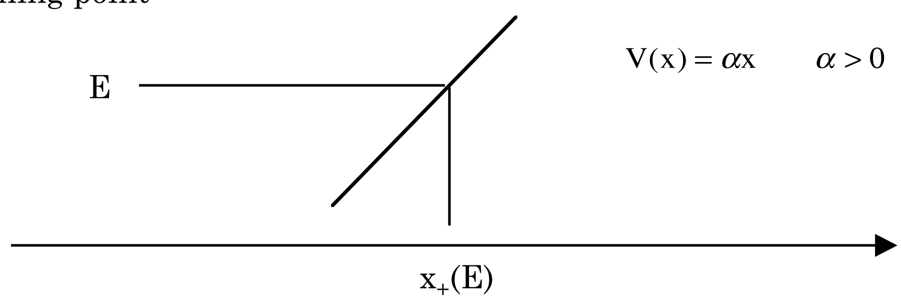
 useful for deriving f(q.n.) and for matching across boundaries.

* 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 of potentials with definite even or odd symmetry.) [Two kinds of Airy functions, Ai and Bi.]

$$\boxed{\mathrm{Ai}(z) = \pi^{-1/2}\int_0^\infty \cos\left(\frac{s^3}{3} + sz\right)ds}$$

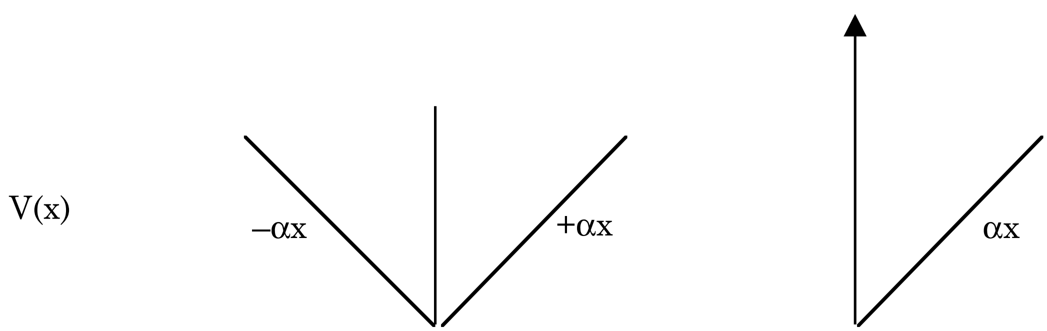
for our specific problem
$$s \equiv p(2m\hbar a)^{-1/3} \qquad (\text{if } \alpha > 0)$$
$$z \equiv \frac{(\alpha x - E)}{\alpha}\left[2m\alpha/\hbar^2\right]^{1/3}$$

Turning point



At turning point $E = V(x_+) = \alpha x_+ \quad \therefore \quad \boxed{x_+(E) = E/\alpha}$

Problems with linear potentials: boundary conditions

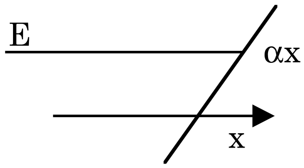


When there is symmetry (or 1/2 symmetry) we need to know where the zeroes of $\underbrace{\psi(x)}_{\text{for odd functions or } \infty \text{ barrier}}$ and $\underbrace{d\psi/dx}_{\text{for even functions}}$ are located.

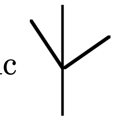
tables of zeroes of
Ai(z) and Ai′(z)
"z_n" "z'_n"

See Handout

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



This is not as bad as it seems because we are usually far from turning point at 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 nonclassical)

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

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

asymptotic form for $z << 0$.

* oscillatory, but wave vector, k, varies with x
* Ai vanishes as $x \to \pm\infty$ because of $(-z)^{-1/4}$ factor
* Bi is needed for case where Airy function must vanish as $x \to +\infty$ in classical region

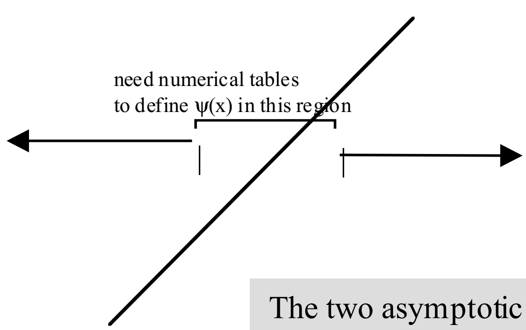
(ii) well behaved
$z >> 0$, $E < V(x)$ forbidden region

$$\mathrm{Ai}(z) \to \left(\pi^{-1/2}/2\right)\underbrace{z^{-1/4}}_{\text{positive}}\underbrace{e^{-(2/3)z^{3/2}}}_{\text{decreasing exponential}}$$

asymptotic form for $z >> 0$.

* not oscillatory, monotonic
* Ai vanishes as $x \to +\infty$
* Bi vanishes as $x \to \pm\infty$ in forbidden region

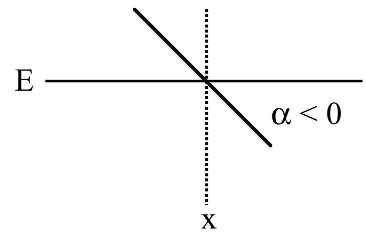
Cartoon



The two asymptotic forms of Ai(z) are not normalized, but their amplitudes (& phases) are matched. Links B.C. at $x \to +\infty$ to B. C. at $x \to -\infty$.

NonLecture

OTHER CASE: $\alpha < 0 \rightarrow z \equiv -\frac{(|\alpha| x + E)}{|\alpha|}\left[2m|\alpha| / \hbar^2\right]^{1/3}$



for this case, need Bi(z) instead of Ai(z)

$$\mathrm{Bi}(z) \rightarrow \left(\pi^{-1/2}/2\right) |z|^{-1/4} \exp\left[-\frac{2}{3}|z|^{3/2}\right] \quad \text{(forbidden region, } z << 0.)$$

$$\mathrm{Bi}(z) \rightarrow \pi^{-1/2} |z|^{-1/4} \cos\left[\frac{2}{3}|z|^{3/2} + \frac{\pi}{4}\right] \quad \text{(allowed region, } z >> 0.)$$

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

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

There are semi-classical JWKB $\psi(x)$'s — These 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.

(**J**EFFREYS)

WENTZEL

KRAMERS

BRILLOUIN

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

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} ♦ $V_J(R)$.
* semi-classical quantization.
* the link to classical mechanics is essential to wavepacket pictures.

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

$$\psi_{JWKB} = \underbrace{|p(x)|^{-1/2}}_{\text{classical envelope}} \exp\left[\pm\frac{i}{\hbar}\int_c^x p(x')dx'\right]$$

k(x) and p(x) are classical mechanical functions of x, not QM operators.

$$p(x) = [2m(E - V(x)]^{1/2}$$

phase factor: adjustable to satisfy boundary conditions

p(x) is pure real (classically allowed) or pure imaginary (classically forbidden). p(x) is not 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

$$\text{probability} \propto \frac{1}{v} \text{ so amplitude} \propto \sqrt{\frac{1}{v}}$$

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

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

* gives easily identifiable stationary phase region for many wiggly integrands. (Both ψ's have same λ at $x_{s.p.}$)

Long Nonlecture derivation/motivation.

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi = 0$$
$$\frac{d^2\psi}{dx^2} + \frac{1}{\hbar^2}p(x)^2\psi = 0 \qquad **$$

* 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 hope that a slowly varying V(x) will lead to a slowly varying N(x).

*

$$\frac{d\psi}{dx} = \left[N' \pm \frac{i}{\hbar}p(x)\right]\exp\left[\pm\frac{i}{\hbar}\int_c^x p(x')dx'\right]$$
$$\frac{d^2\psi}{dx^2} = \left[N'' \pm \frac{i}{\hbar}N'p \pm \frac{i}{\hbar}Np' \pm \frac{ip}{\hbar}\left(N' \pm \frac{i}{\hbar}Np\right)\right]\exp\left[\pm\frac{i}{\hbar}\int_c^x p(x')dx'\right]$$
$$= \left[N'' \pm \frac{2i}{\hbar}N'p \pm \frac{ip'}{\hbar}N - \frac{p^2}{\hbar^2}N\right]\exp\left[\pm\frac{i}{\hbar}\int_c^x p(x')dx'\right]$$
$$0 = \frac{d^2\psi}{dx^2} + \frac{p^2}{\hbar^2}N\exp\left[\pm\frac{i}{\hbar}\int_c^x p(x')dx'\right]$$
$$0 = \left[N'' \pm \frac{2ip(x)}{\hbar}N' \pm \frac{ip'}{\hbar}N\right]\exp\left[\pm\frac{i}{\hbar}\int_c^x p(x')dx'\right]$$

so, if we neglect N'', we get

$$2pN' + p'N = 0$$

if $p \neq 0$, then $2p^{1/2}\left[p^{1/2}N' + \frac{1}{2}p^{-1/2}p'N\right] = 0$

$$\frac{d\left(Np^{1/2}\right)}{dx} = \left[N'p^{1/2} + \frac{1}{2}p^{-1/2}p'N\right]$$

$$\therefore \frac{d\left(Np^{1/2}\right)}{dx} = 0$$

$$N(x)p^{1/2}(x) = \text{constant}$$

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

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

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

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

$$\frac{dp}{dx} = \left(-\frac{dV}{dx}\right)p^{-1}m$$

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

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

$$\therefore \boxed{N'' = c\frac{5}{4}m^2 p^{-9/2}\left(\frac{dV}{dx}\right)^2}$$

But we have made several assumptions about N″

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

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

$$* \quad |N''| << \frac{p^2}{\hbar^2}N = \frac{c}{\hbar^2}p^{+3/2}$$

all of this is satisfied if

$$\left|\frac{5}{4}\frac{m\hbar}{i}\left(\frac{dV}{dx}\right)p^{-3}\right| << 1$$

Is this the JWKB validity condition?

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

$p(x) \to \psi_0(x)$ (ordinary JWKB)

$\psi_0(x) \to p_1(x)$

$p_1(x) \to \psi_1(x)$ (first order JWKB)

$$e.g. \quad \frac{d^2\psi_0}{dx^2} + \frac{p_1^2}{\hbar^2}\psi_0 = 0 \to p_1(x) = \left[-\frac{\hbar^2}{\psi_0(x)}\frac{d^2\psi_0}{dx^2}\right]^{1/2}$$

see ** Eq. on p. 6-8

$$\psi_1(x) = |p_1(x)|^{-1/2}\exp\left[\pm\frac{i}{\hbar}\int_c^x p_1(x')dx'\right]$$

iterative improvement of accuracy

$p_1(x)$ is not smaller than $p_0(x)$. It has more of the correct wiggles in it.

END OF NONLECTURE

Resume Lecture

$$\psi(x) \approx \underbrace{|p(x)|}_{\text{envelope}}^{-1/2} \exp\left[\pm \frac{i}{\hbar}\int_{\underset{\uparrow}{c}}^{x} p(x')dx'\right]$$

adjustable phase shift.

provided that $\frac{d^2V}{dx^2}$ is negligible

AND

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

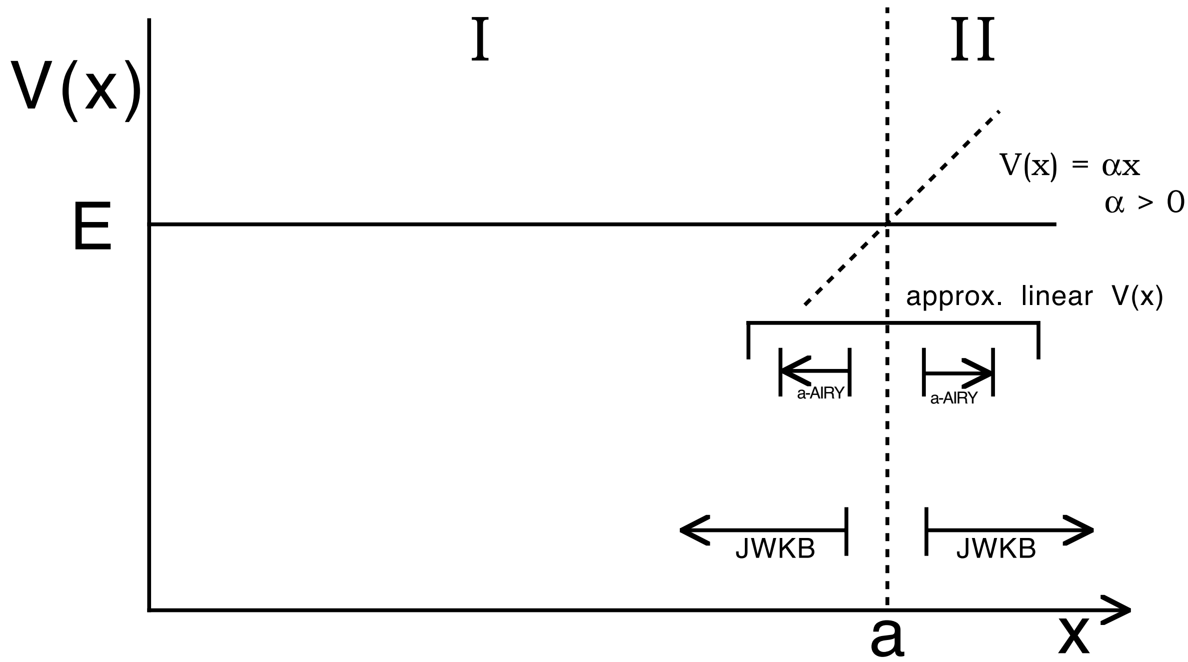
Next need to work out connection of $\psi_{JWKB}(x)$ across region where JWKB approx. breaks down (at turning points!).

$$\left|\frac{d\lambda}{dx}\right| \to \infty \text{ at turning point because } p(x) \to 0$$

BUT ALL IS NOT LOST — near enough to a turning point all potentials V(x) look like V(x)=αx!

Now our job is to show that asymptotic – AIRY and JWKB 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 ψ(x) ACROSS TURNING POINT REGION!



Region I $\quad E > V(x)$ classical

$$\psi^{I}_{a-AIRY} \sim \pi^{-1/2}(-z)^{-1/4}\sin\left[\frac{2}{3}(-z)^{3/2} + \pi/4\right]$$

$$z = \frac{(\alpha x - E)}{\alpha}\left[\frac{2m\alpha}{\hbar^2}\right]^{1/3}$$

at turning point $E = V(a) = \alpha a$ so $\left[\frac{\alpha x - E}{\alpha}\right] = (x - a)$

$$\boxed{z = (x-a)\left(\frac{2m\alpha}{\hbar^2}\right)^{1/3} << 0 \qquad \text{when } x << a}$$

Region I/II splice using a-Airy.

Region II $\quad E < V(x)$ forbidden region, $\quad z >> 0$

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

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

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

both c_+ and c_- additive terms could be present

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

$x < a$	classical ,	p is real ,	ψ_{JWKM}	oscillates
$x > a$	forbidden ,	p is imaginary ,	ψ_{JWKB}	is exponential

pretend V(x) looks linear near x = a (ℓ-JWKB)

linear

$$p(x) = \left[2m\alpha(a-x)\right]^{1/2}$$

$$\int_a^x p(x')dx' = (2m\alpha)^{1/2}\int_a^x (a-x')^{1/2}dx'$$

$$= (2m\alpha)^{1/2}\left(-\frac{2}{3}\right)(a-x')^{3/2}\Big|_a^x$$

$$= -(2m\alpha)^{1/2}\frac{2}{3}(a-x)^{3/2}$$

Region I

$$\psi^{I}_{\ell-JWKB}(x) \sim |p(x)|^{-1/2}\left[Ae^{i\theta} + Be^{-i\theta}\right]$$

$$= |p(x)|^{-1/2}C\ \sin(\theta+\phi)$$

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, $z = (x-a)\left(\dfrac{2m\alpha}{\hbar^2}\right)^{1/3}$ $\quad \therefore \theta = -\dfrac{2}{3}(-z)^{3/2}$

$$\therefore p = (2m\alpha\hbar)^{1/3}(-z)^{1/2}$$ 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

$$\psi^{I}_{\ell-JWKB} = \overbrace{-(2m\alpha\hbar)^{-1/6}(-z)^{-1/4}}^{-|p|^{-1/2}} C \ \sin\left[\overbrace{\frac{2}{3}(-z)^{3/2}}^{-\theta} - \phi\right]$$

$$= \psi^{I}_{a-AIRY} \qquad \text{If } C = -(2m\alpha\hbar)^{1/6}\pi^{-1/2}$$
$$\phi = -\pi/4$$

$\psi^{I}_{\ell-JWKB}$ exactly splices onto ψ^{I}_{a-AIRY}

with a $\boxed{\pi/4 \text{ phase factor}}$ (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

$$\psi^{II}_{JWKB} \sim Ae^{-f(x)} + Be^{+f(x)}$$

at $x \to +\infty \qquad f(x) \to \infty \qquad \therefore B = 0$

$$\therefore \psi^{II}_{\ell-JWKB} = A(2m\alpha)^{-1/4}(x-a)^{-1/4}\exp\left[-\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}\frac{2}{3}(x-a)^{3/2}\right]$$

which is equal to ψ^{II}_{a-AIRY} if $A = (2m\alpha\hbar)^{+1/6}\pi^{-1/2}/2$

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) valid in region where ψ_{JWKB} is invalid.