JWKB QUANTIZATION CONDITION

Last time:

1. $V(x) = \alpha x$ $\quad \phi(p) = N \exp\left[-\frac{i}{\hbar\alpha}\left(Ep - p^3/6m\right)\right]$

   $\psi(x) = \mathrm{Ai}(z)$
   * zeroes of Ai, Ai′
   * tables of Ai (and Bi)
   * asymptotic forms far from turning points

2. Semi-Classical Approximation for $\psi(x)$

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

   * $\psi(x) = \underbrace{|p(x)|^{-1/2}}_{\text{envelope}} \exp\left[\pm \underbrace{\frac{i}{\hbar}\int_c^x p(x')dx'}_{\text{wiggly-variable } k(x)}\right]$

   "classical wavefunction"

   modifies classical to make it QM wavefunction

   adjustable phase for boundary conditions

   ψ without differential equation

   qualitative behavior of integrals (stationary phase)

   * validity: $\frac{d\lambda}{dx} << 1$ —valid not too near turning point.

[One reason for using semi-classical wavefunctions is that we often need to evaluate integrals of the type $\int \psi_i^* \hat{O}_p \psi_j dx$. If $\hat{O}_p$ is a slow function of x, the phase factor is $\exp\frac{i}{h}\left[p_j(x') - p_i(x')\right]dx'$. Take $\frac{d}{dx}\left[\quad\right] = 0$ to find $x_{s.p.}$. δx is range about $x_{s.p.}$ over which phase changes by $\pm\pi/2$. Integral is equal to $I\left(x_{s.p.}\right)\delta x$.]

Logical Structure of pages 6-11 to 6-14 (not covered in lecture):

1. ψ_{JWKB} not valid (it blows up) near turning point — ∴ can't match ψ's on either side of turning point.

2. Near a turning point, $x_\pm(E)$, every well-behaved V(x) looks linear

$$V(x) \approx V\left(x_+(E)\right) + \left.\frac{dV}{dx}\right|_{x=x_+}\left(x - x_+\right)$$ first term in a Taylor series.

   This makes it possible to use Airy functions for *any* V(x) near turning point.

3. asymptotic-Airy functions have matched amplitudes (and phase) across validity gap straddling the turning point.

4. ψ_{JWKB} for a linear V(x) is identical to asymptotic-Airy!

<u>TODAY</u>

1. Summary of regions of validity for Airy, a-Airy, ℓ-JWKB, JWKB on both sides of turning point. This seems complicated, but it leads to a result that will be exceptionally useful!

2. WKB quantization condition: energy levels without wavefunctions!

3. compute dn_E/dE (for box normalization — can then convert to any other kind of normalization)

4. trivial solution of Harmonic Oscillator
   $E_v = \hbar\omega\,(v+1/2) \quad v = 0, 1, 2\ldots$

<u>Non-lecture</u> (from pages 6-12 to 6-14)

classical $$\psi_{\text{a-AIRY}} = \pi^{-1/12}\left(\frac{2m\alpha}{\hbar^2}\right)^{-1/12}(a-x)^{-1/4}\sin\left[\frac{2}{3}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}(a-x)^{3/2}+\frac{\pi}{4}\right]$$

forbidden $$\psi_{\text{a-AIRY}} = \frac{\pi^{-1/12}}{2}\left(\frac{2m\alpha}{\hbar^2}\right)^{-1/12}(x-a)^{-1/4}\exp\left[-\frac{2}{3}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}(x-a)^{3/2}\right]$$

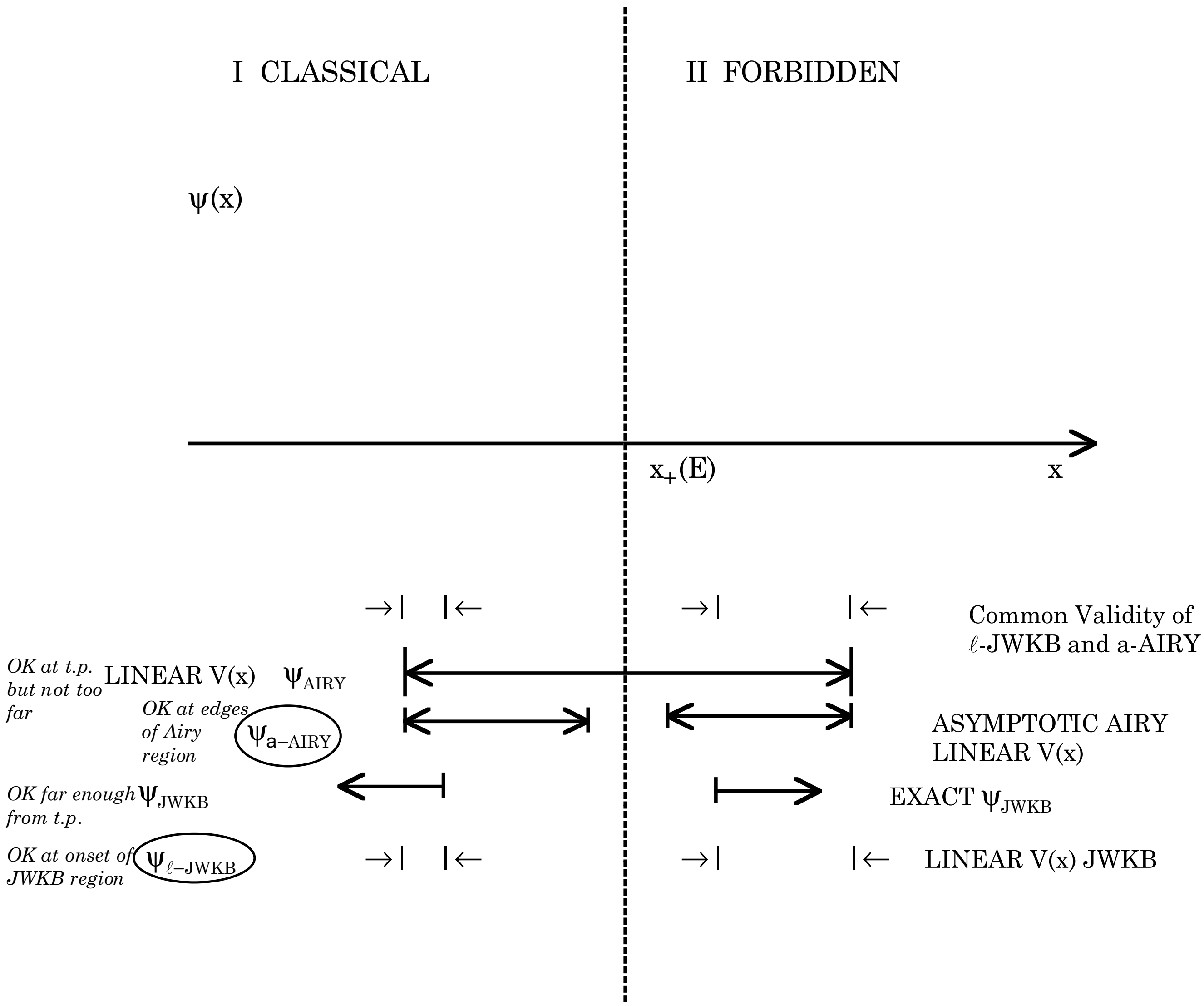
classical $$\psi_{\ell\text{-JWKB}} = C\,(a-x)^{-1/4}\sin\left[\frac{2}{3}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}(a-x)^{3/2}+\phi\right]$$

forbidden $$\psi_{\ell\text{-JWKB}} = D\,(x-a)^{-1/4}\exp\left[-\frac{2}{3}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}(x-a)^{3/2}\right]$$

C, D, and ϕ are determined by matching.

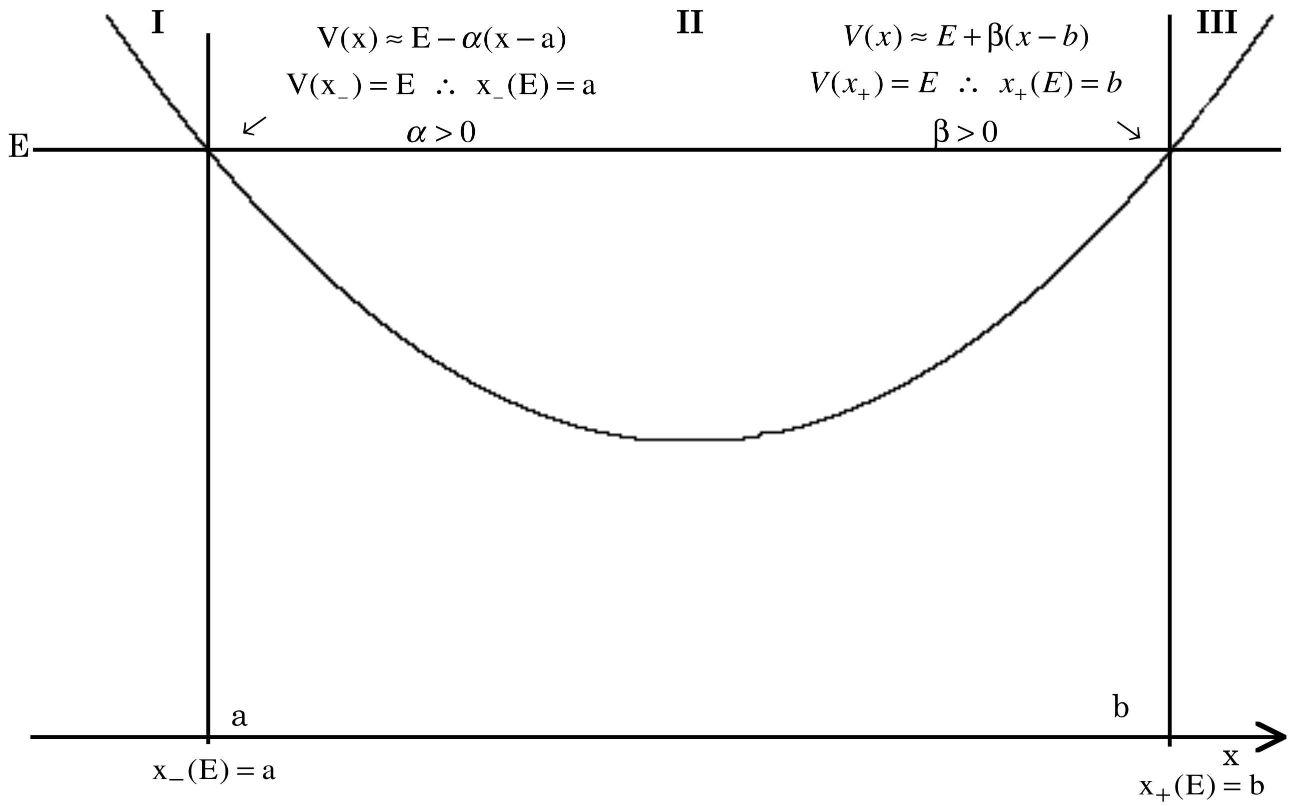
These Airy functions are not normalized, but each pair has correct relative amplitude on opposite sides of turning point. ℓ-JWKB has same functional form as a-Airy. This permits us to link pairs of JWKB functions across invalid region and then use JWKB to extend $\psi(x)$ into regions further from turning point where linear approximation to V(x) is no longer valid.

Regions of Validity Near Turning Point $E = V(x_{\pm}(E))$



Common region of validity for $\psi_{\text{a-AIRY}}$ and $\psi_{\ell\text{-JWKB}}$ — same functional form, specify amplitude and phase for $\psi_{\text{JWKB}}(x)$ valid far from turning point for exact V(x)!

Quantization of E in Arbitrary Shaped Wells



Already know how to splice across I, II and II, III but how do we match ψ's in $a < x < b$ region?

Region I $\quad \psi^{I}_{JWKB}(x) = \frac{C}{2}|p(x)|^{-1/2} e^{-\frac{1}{\hbar}\int_x^a |p(x')dx'|}$ $\quad x < a \quad$ (forbidden region)

(real, no oscillations)

Note carefully that argument of exp goes to $-\infty$ as $x \to -\infty$, thus $\psi_I(-\infty) \to 0$.

Note also that (ψ^I/C) increases monotonically as x increases up to $x = a$.

When you are doing matching for the first time, it is very important to verify that the phase of ψ varies with x in the way you want it to.

Region II $\qquad \psi^{\mathrm{IIa}}_{\mathrm{JWKB}}(x) = C|p(x)|^{-1/2}\sin\left[\frac{1}{\hbar}\int_a^x p(x')dx' + \frac{\pi}{4}\right] \qquad a < x < b$

The first zero is located at an accumulated phase of $(3/4)\pi$ inside x=a because $(3/4 + 1/4)\pi = \pi$ and $\sin\pi = 0$.

It does not matter that ψ^{IIa} is invalid near x = a, x = b

Note that phase increases as x increases - as it must. The $\pi/4$ is the extra phase required by the AIRY splice across I,II. It reflects the tunneling of $\psi(x)$ into the forbidden region.

PHASE starts at $\pi/4$ in classical region and always increases as one moves (further into classical region) away from turning point. **NEVER FORGET!**

Region III $\qquad \psi^{\mathrm{III}}_{\mathrm{JWKB}}(x) = \frac{C'}{2}|p(x)|^{-1/2} e^{-\frac{1}{\hbar}\int_b^x |p(x')|dx'} \qquad x > b$

Note that phase advances (i.e. the phase integral gets more positive) as $x \to \infty$.

$\psi^{\mathrm{III}}_{\mathrm{JWKB}}$ decreases monotonically to 0 as $x \to +\infty$.

Region II again $\qquad \psi^{\mathrm{IIb}}_{\mathrm{JWKB}}(x) = C'|p(x)|^{-1/2}\sin\left[\frac{1}{\hbar}\int_x^b p(x')dx' + \frac{\pi}{4}\right]$

note: argument of sine <u>starts at $\pi/4$</u> and <u>increases</u> as one goes from x = b inward. In other words, opposite to ψ^{IIa}, the argument decreases from left to right!

But $\psi^{\mathrm{IIa}}(x) = \psi^{\mathrm{IIb}}(x)$ for all $a < x < b$!

2 ways to satisfy this requirement

1. $\sin(\underbrace{\theta(x)}_{\text{argument of }\psi^{\mathrm{IIa}}}) = \sin[\underbrace{(-\theta(x))}_{\text{argument of }\psi^{\mathrm{IIb}}} + (2n+1)\pi]$ AND $C = C'$

$$[\sin\theta = -\sin(-\theta), \qquad \sin(\theta + (2n+1)\pi) = -\sin\theta,$$
$$\therefore \sin\theta = \sin(-\theta + (2n+1)\pi)]$$

2. $\sin(\theta(x)) = -\sin[-\theta(x) + 2n\pi]$ if $C = -C'$

now look at what the 2 cases require for the arguments

1. $C = C'$ $\left[\frac{1}{\hbar}\int_a^x p dx + \frac{\pi}{4}\right] = -\left[\frac{1}{\hbar}\int_x^b p dx + \frac{\pi}{4}\right] + (2n+1)\pi$

$$\begin{array}{ll} \psi^{IIa} & \psi^{IIb} \\ \theta(x) & -\theta(x) + (2n+1)\pi \end{array}$$

$$\therefore \frac{1}{\hbar}\left(\int_a^x + \int_x^b p dx\right) = (2n+1)\pi - \frac{\pi}{4} - \frac{\pi}{4}$$

$$\boxed{\int_a^b p(x')dx' = \hbar\pi[2n + 1/2]}$$ Quantization.

2. $C = -C'$ get $\boxed{\int_a^b p(x')dx' = \hbar\pi[2n - 1/2]}$

combine the two:

$$\boxed{\begin{array}{l} \int_a^b p(x')dx' = \hbar\pi(n + 1/2) \\ n = 0,1,2,\ldots \\ C' = C(-1)^n \end{array}}$$

** WKB quantization condition. Most important result of this lecture.

n is # of internal nodes because argument always starts at $\pi/4$ and increases inward to $(n + 3/4)\pi$ at other turning point.

	inner t.p.		outer t.p.	
for $n = 0$	$\sin(\pi/4)$	$\rightarrow$	$\sin(3\pi/4)$	NO NODE!
$n = 1$	$\sin(\pi/4)$	$\rightarrow$	$\sin(7\pi/4)$	1 node.
	etc.			

Node count tells what level it is. $\int p dx$ at arbitrary E_{probe} tells how many levels there are at $E \leq E_{probe}$!

Density of States $\frac{dn}{dE}$ $\left[h\frac{dn}{dE}\text{ is the classical period of oscillation.}\right]$

$$n(E) = \frac{2}{h}\int_{x_-(E)}^{x_+(E)} p_E(x')dx' - \frac{1}{2}$$

$$\frac{dn}{dE} = \frac{2}{h}\left[p_E(x_+)\frac{dx_+}{dE} - p_E(x_-)\frac{dx_-}{dE} + \int_{x_-}^{x_+}\frac{dp_E}{dE}dx\right]$$ (must take derivatives of limits of integration as well as integrand)

but $p_E(x_\pm) \equiv 0$

$$\therefore \frac{dn}{dE} = \frac{2}{h}\int_{x_-}^{x_+}\frac{d}{dE}\left[2m(E - V(x'))\right]^{1/2}dx'$$

$$\frac{dn}{dE} = \frac{2}{h}\frac{1}{2}(2m)\int_{x_-}^{x_+}\left[2m(E - V(x'))\right]^{-1/2}dx'$$

you show that, for harmonic oscillator

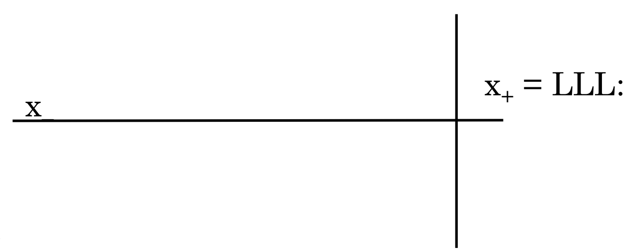
$$V(x) = \frac{1}{2}kx^2$$

$$\omega \equiv (k/m)^{1/2}$$

that $\frac{dn}{dE} = \frac{1}{\hbar\omega}$ independent of E, thus period of h.o. is independent of E.

Non-lecture

for general box normalization



can still use this to compute $\frac{dn}{dE}$ because

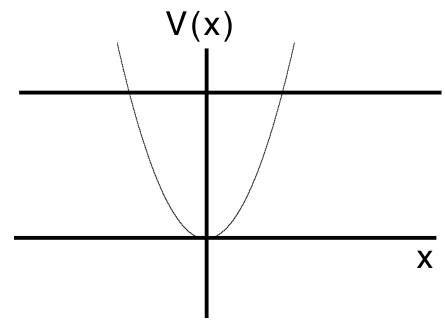
$\frac{dx_+}{dE} = 0$ (even though $p_E(x_+) \neq 0$).

location of right hand turning point is independent of E.

Can always use WKB quantization to compute density of box normalized ψ_E's, provided that $E > V(x)$ everywhere except the 2 turning points.

Use WKB to solve a few "standard" problems. Since WKB is "semi-classical", we expect it to work in the $n \to \infty$ limit. Could be some errors for a few of the lowest-n E_n's.

Harmonic Oscillator $V(x) = kx^2/2$ (k is force constant, not wave vector)



$$p(x) = \left[2m\left(E - \frac{1}{2}kx^2\right)\right]^{1/2}$$

At turning points, $V\left(x_{tp}\right) = E$ and $p\left(x_{tp}\right) = 0$,

thus, at turning points $x_{\pm} = \pm\left[2E_n/k\right]^{1/2}$

because $E_n = \frac{1}{2}kx_{\pm}^2$

$$\hbar\pi(n + 1/2) = \int_{x_- = -[2E_n/k]^{1/2}}^{x_+ = [2E_n/k]^{1/2}} \left[2m\left(E_n - kx^2/2\right)\right]^{1/2} dx$$

Non-lecture: Dwight Integral Table 350.01 $t \equiv \left[a^2 - x^2\right]^{1/2}$

$$\int t\,dx = \frac{xt}{2} + \frac{a^2}{2}\sin^{-1}(x/a)$$

here $t = 0$ at both x_+ and x_-

$$I = (2mk/2)^{1/2} \int_{-[2E_n/k]^{1/2}}^{[2E_n/k]^{1/2}} \left[2E_n/k - x^2\right]^{1/2} dx$$

$$I = (2mk/2)^{1/2}\left(\frac{2E_n}{k}\right)\left[\sin^{-1}1 - \sin^{-1}(-1)\right]$$

$$I = \left(\frac{m}{k}\right)^{1/2} E_n\left((\pi/2) - (-\pi/2)\right) = \pi\left(\frac{m}{k}\right)^{1/2} E_n$$

use the nonlecture result: $$\hbar\pi(n + 1/2) = \pi\left(\frac{m}{k}\right)^{1/2} E_n$$

$$E_n = \hbar\underbrace{\left(\frac{k}{m}\right)^{1/2}}_{\omega}(n + 1/2)$$

I suggest you apply WKB Quantization Condition to the following problems: See Shankar pages 454-457.

Vee	$V(x) = a\|x\|$	$E_n \propto (n + 1/2)^{2/3}$
quartic	$V(x) = bx^4$	$E_n \propto (n + 1/2)^{4/3}$
$\ell = 0$, H atom	$V(x) = cx^{-1}$	$E_n \propto n^{-2}$
harmonic	$V(x) = \frac{1}{2}kx^2$	$E_n \propto (n + 1/2)^1$

What does this tell you about the relationship between the exponents m and α in $V_m \propto x^m$ and $E_n \propto n^\alpha$?

power of x in V(x)	power of n in E(n)
–1	–2
1	2/3
2	1
4	4/3

Validity limits of WKB?

* splicing of ψ^{IIa}, ψ^{IIb} ? $\frac{d^2V}{dx^2}$ can't be too large near the splice region

* ψ_{JWKB} is bad when $\frac{d\lambda}{dx} \gtrsim 1$ (λ changes by more than itself for $\Delta x = \lambda$)

  near turning points and near the minimum of V(x)

* can't use WKB QC if there are more than 2 turning points

* near bottom of well $\frac{d^2V}{dx^2}$ is not small and $\frac{d\lambda}{dx} > 1$
  (near both turning points). However, most wells look harmonic near minimum and WKB gives exact result for harmonic oscillator - should be more OK than one has any right to expect.

* semi-classical: should be good in high-n limit. If exact E_n has same form as WKB QC at low-n, WKB E_n is valid for all n.

H.O., Morse Oscillator…