JWKB QUANTIZATION CONDITION

Last time:

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

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

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

   * $p(x)=[(E-V(x))2m]^{1/2}$ — modifies classical to make it QM wavefunction (oscillatory)

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

   "classical wavefunction" (nodeless) → $|p(x)|^{-1/2}$ envelope; $\pm\frac{i}{\hbar}\int_c^x p(x')dx'$ wiggly-variable $\lambda(x)$; c: adjustable phase to satisfy boundary conditions

   * ψ without differential equation
   * qualitative behavior of integrals (stationary phase)

   * *validity*: $\frac{d\lambda}{dx}\ll 1$ *valid* when not too near a 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 the stationary phase point $x_{s.p.}$. 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} is not valid (it blows up) near turning point — ∴ we can't use ψ_{JWKB} to match ψ's on either side of turning point.

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

$$V(x)\approx V\left(x_\pm(E)\right)+\left.\frac{dV}{dx}\right|_{x=x_\pm}\left(x-x_\pm\right)$$

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 the JWKB validity-gap that straddles the turning point.

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

It may be grubby, but it works!

TODAY

1. Summary of regions of validity for Airy, a-Airy, ℓ-JWKB, and 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 density of states dn_E/dE: (for box normalization — can then convert to any other kind of normalization)

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

Non-lecture (from pages 6-12 to 6-14)

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

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

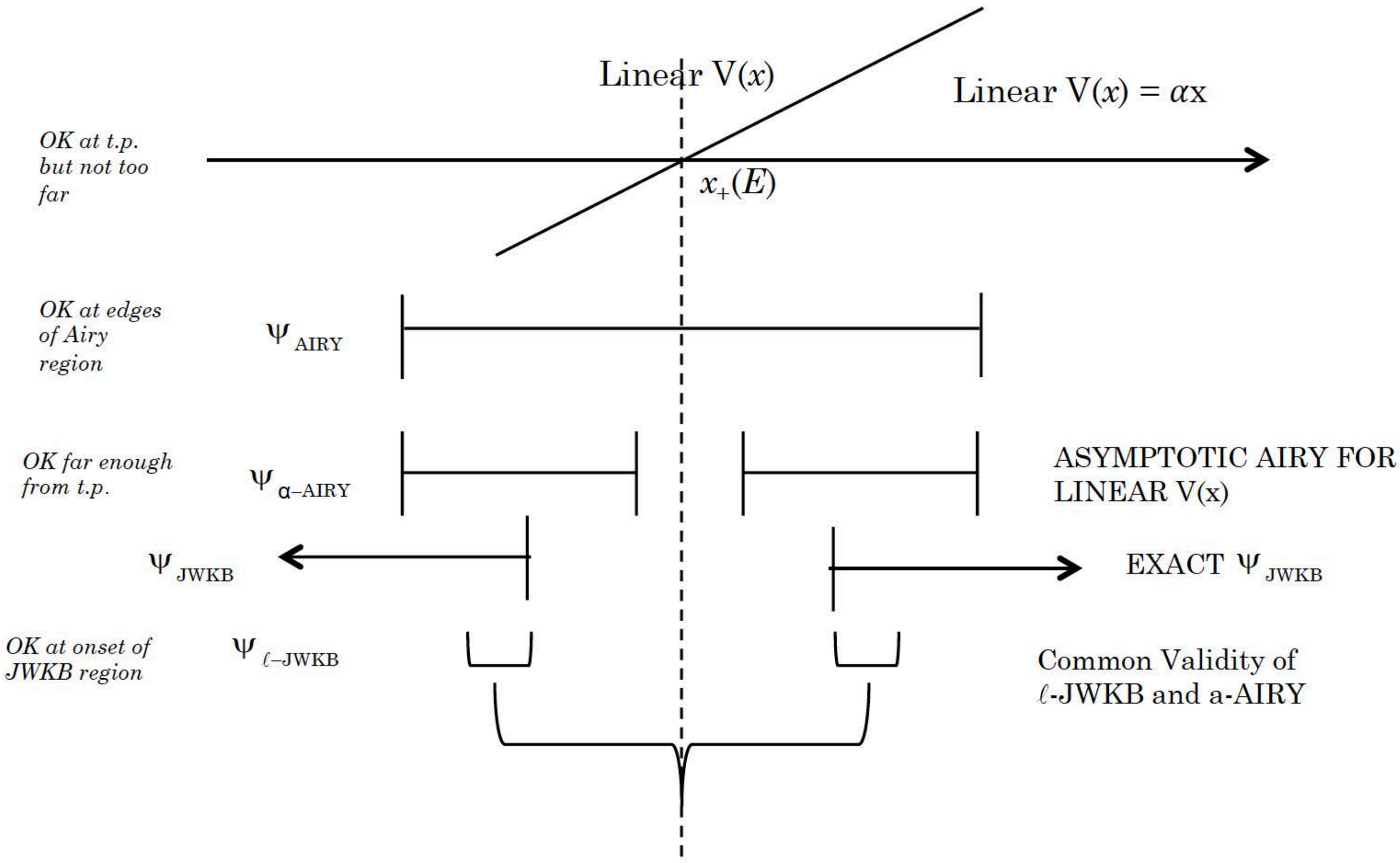
classical $$\psi_{\ell-\text{JWKB}} = C\ (a-x)^{-1/4}\sin\left[\frac{2}{3}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}(a-x)^{3/2}+\phi\right]$$

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.

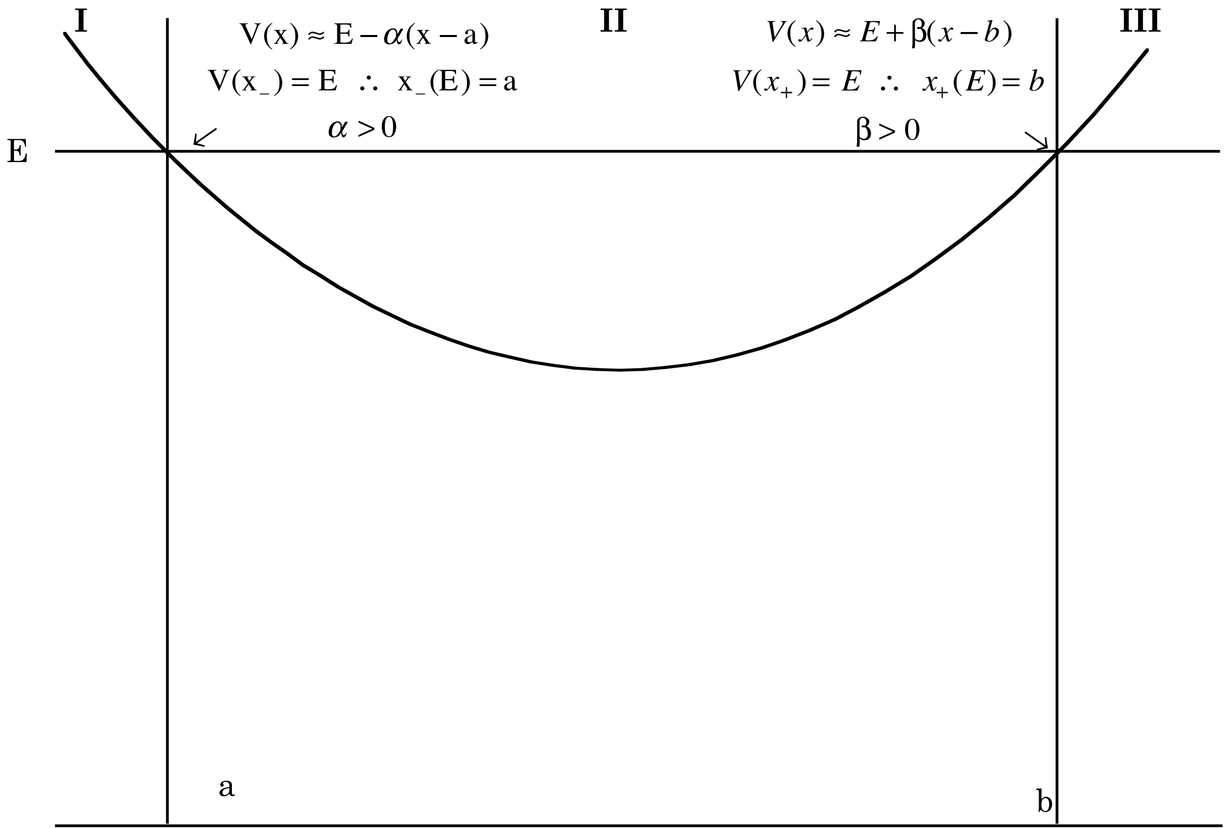
These Airy functions are not normalized, but each pair has the correct relative amplitude on opposite sides of the turning point. ℓ-JWKB has same functional form as a-Airy. This permits us to link pairs of JWKB functions across invalid-JWKB region and then use JWKB to extend $\psi(x)$ into regions further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

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



Common regions 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



We already know how to splice across I, II and II, III regions, but how do we match ψ's in the entire $a < x < b$ region? (ψ propagated inward from $x_-(E)$ must join smoothly onto ψ propagated inward from $x_+(E)$.)

Region I $$\psi^I_{JWKB}(x) = \frac{C}{2}|p(x)|^{-1/2} e^{-\frac{1}{\hbar}\int_x^a |p(x')dx'|} \qquad x < a$$ (forbidden region) (ψ real, no oscillations)

Note carefully that the argument of $\exp\left[-\frac{1}{\hbar}\int_x^a |p(x')| dx'\right]$ goes to $-\infty$ as $x \to -\infty$, thus $\psi_I(-\infty) \to 0$.

Note also that $|\psi^I/C|$ 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 expect it to vary.

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

The *first* zero is located at an accumulated phase of (3/4)π inside x = a because (3/4 + 1/4)π = π and sin π = 0. Why is this the first zero?

It does not matter that is invalid near x = and x = b.

Note that phase increases as x increases – as it must. The π/4 is the extra phase required by the AIRY splice across I,II. It reflects the tunneling of $\psi(x)$ into the forbidden region. *This means the real state with tunneling lies at lower energy than one that satisfies the incorrect* $\psi(x_\pm) = 0$ *boundary condition.*

|PHASE| starts at π/4 in classical region and always increases as one moves (further into the classical region) away from the turning point.

NEVER FORGET THIS!

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

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

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

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

note: the argument of sine <u>starts at π/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 it must be true that $\psi^{IIa}(x) = \psi^{IIb}(x)$ for all a < x < b !

There are 2 ways, C = C′ and C = –C′, to satisfy this requirement.

1. $\sin(\underbrace{\theta(x)}_{\text{argument of } \psi^{IIa}}) = \sin[(\underbrace{-\theta(x)}_{\text{argument of } \psi^{IIb}}) + (2n+1)\pi]$ AND C = C′ $\left[\psi^{I} \text{ and } \psi^{II} \text{ have the same sign.}\right]$

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

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2. $\sin(\theta(x)) = -\sin[-\theta(x) + 2n\pi]$ *if* $C = -C'$ $[\psi^{\mathrm{I}}$ and ψ^{II} have opposite signs$]$

now look at what the 2 cases require for the arguments

1. For $C = C'$ $\left[\frac{1}{\hbar}\int_a^x p\,dx + \frac{\pi}{4}\right] = -\left[\frac{1}{\hbar}\int_x^b p\,dx + \frac{\pi}{4}\right] + (2n+1)\pi$ $n = 0,1,2\ldots$

ψ_a^{II} ψ_b^{II}

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

$$\int_a^b p(x')dx' = \hbar\pi[2n + 1/2]$$ Quantization: $\frac{1}{2}, \frac{5}{2}, \frac{9}{2}, \ldots$

2. For $C = -C'$ we get $\int_a^b p(x')dx' = \hbar\pi[2n - 1/2]$ Quantization: $\frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \ldots$

$\boxed{\hbar\pi = h/2}$

combine the two:

$$\int_a^b p(x')\,dx' = h/2(n + 1/2)$$
$$n = 0,1,2,\ldots$$
$$C' = C(-1)^n$$

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

note: n = 0 is lowest possible value

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

		inner t.p.	outer t.p.	
for	n = 0	sin(π/r)	⟶ sin(3π/4)	NO INTERNAL NODE
	n = 1	sin(π/4)	⟶ sin(7π/4)	1 internal node
		etc.		

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

updated 8/13/20 8:21 AM

"Density of States" $\frac{dn}{dE}$ Always a crucial quantity $\left[h\frac{dn}{dE}\right.$ is the classical mechanical period of oscillation.$\left.\right]$ large $\frac{dn}{dE}$, slow oscillation

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

$$\frac{dn}{dE}=\frac{2}{h}\left[p_E(x_+)\frac{dx_+}{dE} - p_E(x_-)\frac{dx_-}{dE} + \int_{x_-}^{x_+}\frac{dp_E}{dE}dx\right]$$

(must take derivatives of the limits of integration as well as the integrand)

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

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

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

A very widely useful quantity!

you show that, for harmonic oscillator,

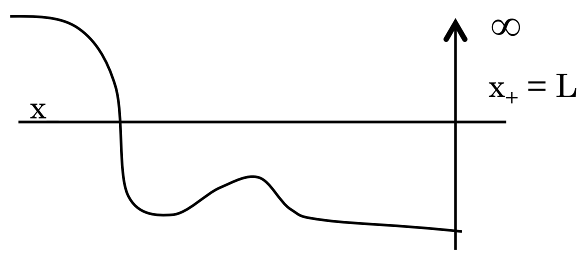
$$V(x)=\frac{1}{2}kx^2$$

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

that $\frac{dn}{dE}=\frac{1}{\hbar\omega}$ independent of E, thus the oscillation period of the Harmonic Oscillator 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 at the 2 turning points.

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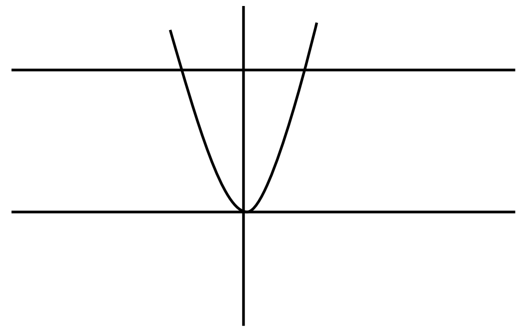
Use WKB to solve a few "standard" problems. Since WKB is "semi-classical", we expect it to work in the $n \to \infty$ limit. There could be some errors for a few of the lowest-n E_n's.

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, $V(x_{tp}) = E$ and $p(x_{tp}) = 0$,

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

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_-

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

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

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

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

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

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

Vee	$V(x)=a\lvert x\rvert$	$E_n \propto (n+1/2)^{2/3}$
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	$\ell = 0$ H atom
1	2/3	Vee
2	1	Harmonic oscillator
4	4/3	Quartic oscillator

As power of x increases, power of n increases but slower.

Validity limits of WKB? surprisingly robust!

* 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 $\Delta x = \lambda$)

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

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

* bad 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 near the minimum of V(x) 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…