JWKB QUANTIZATION CONDITION

Last time:

1. \( V(x) = \alpha x \)  
   \( \phi(p) = N \exp \left[ -\frac{i}{\hbar \alpha} (Ep - p^3/6m) \right] \)  
   \( \psi(x) = Ai(z) \)  
   * zeroes of Ai, Ai'  
   * tables of Ai (and Bi)  
   * asymptotic forms far from turning points

2. Semi-Classical Approximation for \( \psi(x) \)
   
   "classical wavefunction"
   
   * \( p(x) = [(E - V(x))2m]^{1/2} \)  
   * \( \psi(x) = \left| \psi(x) \right|^{-1/2} \exp \left[ \pm \frac{i}{\hbar} \int_{x}^{x'} p(x')dx' \right] \)  
   * \( \psi \) without differential equation  
   * quality behavior of integrals (stationary phase)  
   * validity: \( \frac{dx}{dx} < < 1 \) — valid not too near turning point.

[One reason for using semi-classical wavefunctions is that we often need to evaluate integrals of the type \( \int_{x}^{x'} \psi_{i}^{*} \hat{O}_{p} \psi_{j} \ dx \). If \( \hat{O}_{p} \) is a slow function of \( x \), the phase factor is

\( \exp \left[ \frac{i}{\hbar} \left[ p_{i}(x') - p_{i}(x') \right] dx' \right] \). Take \( \frac{dx}{dx} = 0 \) to find \( x_{s.p.} \). \( \delta x \) is range about \( x_{s.p.} \) over which phase changes by \( \pm \pi/2 \). Integral is equal to \( I(x_{s.p.})\delta x \).]

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

1. \( \psi_{\text{JWKB}} \) not valid (it blows up) near turning point — \( \therefore \) can’t match \( \psi \)'s on either side of turning point.

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

   \( V(x) \approx V(x_{s}(E)) + \frac{dV}{dx_{x=x_{s}}} (x - x_{s}) \)  
   first term in a Taylor series.

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

updated 9/16/02 11:29 AM
3. asymptotic-Airy functions have matched amplitudes (and phase) across validity gap straddling the turning point.

4. $\psi_{\text{JWKB}}$ for a linear $V(x)$ is identical to asymptotic-Airy!

**TODAY**

1. Summary of regions of validity for Airy, a-Airy, $\ell$-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 $dn_{\epsilon}/dE$ (for box normalization — can then convert to any other kind of normalization)

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

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

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

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

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

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

C, D, and $\phi$ are determined by matching.

These Airy functions are not normalized, but each pair has correct relative amplitude on opposite sides of turning point. $\ell$-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.

*updated 9/16/02 11:29 AM*
Regions of Validity Near Turning Point \( E = V(x_+(E)) \)

I CLASSICAL

- \( \psi(x) \)

II FORBIDDEN

- Common Validity of \( \ell \)-JWKB and \( a \)-AIRY

- Linear \( V(x) \) Exact

- Asymptotic AIRY

- \( \Psi_{\text{AIKY}} \)

- \( \Psi_{\ell \text{-JWKB}} \)

- \( \Psi_{a \text{-AIRY}} \)

Common region of validity for \( \psi_{a \text{-AIRY}} \) and \( \psi_{\ell \text{-JWKB}} \) — same functional form, specify amplitude and phase for \( \psi_{\text{JWKB}}(x) \) valid far from turning point for exact \( V(x) \)!
5.73 Lecture #7
Quantization of E in Arbitrary Shaped Wells

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

Region I

\[
\psi_{\text{JWKB}}(x) = \frac{C}{2} [p(x)]^{-1/2} e^{-\frac{1}{\hbar} \int_{a}^{x} |p(x')dx'|} \quad x < a
\]

(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 \( (\psi/J) \) 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 \( \psi \) varies with \( x \) in the way you want it to.
Region II \[ \psi_{\text{JWKB}}^{\text{IIa}}(x) = C |p(x)|^{-1/2} \sin \left[ \frac{1}{\hbar} \int_a^x p(x')dx' + \frac{\pi}{4} \right] \quad a < x < b \]

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 \(\psi^{\text{IIa}}\) 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 \[ \psi_{\text{JWKB}}^{\text{III}}(x) = \frac{C'}{2} |p(x)|^{-1/2} e^{-\frac{1}{\hbar} \int_a^x p(x')dx'} \quad x > b \]

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

\(\psi_{\text{JWKB}}^{\text{III}}\) decreases monotonically to 0 as \(x \to +\infty\).

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

Note: argument of sine starts at \(\pi/4\) and increases as one goes from \(x = b\) inward. In other words, opposite to \(\psi^{\text{IIa}}\), the argument decreases from left to right!

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

2 ways to satisfy this requirement

1. \(\sin(\theta(x)) = \sin \left[ (\theta(x)) + (2n + 1)\pi \right] \) AND \(C = C'\)

\[ \sin \theta = -\sin(-\theta), \quad \sin(\theta + (2n + 1)\pi) = -\sin \theta, \]
\[ \therefore \sin \theta = \sin(-\theta + (2n + 1)\pi) \]
2. \( \sin(\theta(x)) = -\sin[-\theta(x) + 2n\pi] \quad \text{if} \quad C = -C' \)

now look at what the 2 cases require for the arguments

1. \( C = C' \)
   \[
   \left[ \frac{1}{\hbar} \int_a^x p(x) \, dx + \frac{\pi}{4} \right] = - \left[ \frac{1}{\hbar} \int_x^b p(x) \, dx + \frac{\pi}{4} \right] + (2n + 1)\pi
   \]
   \[
   \psi^{IIa} \quad \psi^{IIb}
   \]
   \[
   \theta(x) \quad -\theta(x) + (2n + 1)\pi
   \]
   \[
   \therefore \frac{1}{\hbar} \left[ \int_a^x p(x) \, dx + \int_x^b p(x) \, dx \right] = (2n + 1)\pi - \frac{\pi}{4} \frac{\pi}{4}
   \]
   \[
   \int_a^b p(x') \, dx' = \hbar \pi [2n + 1] \quad \text{Quantization.}
   \]

2. \( C = -C' \)
   \[
   \int_a^b p(x') \, dx' = \hbar \pi [2n - 1/2]
   \]

combine the two:

\[
\int_a^b p(x') \, dx' = \hbar \pi (n + 1/2)
\]

**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.

<table>
<thead>
<tr>
<th>( n = 0 )</th>
<th>( n = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sin(\pi/4) \rightarrow \sin(3\pi/4) ) NO NODE!</td>
<td>( \sin(\pi/4) \rightarrow \sin(7\pi/4) ) 1 node.</td>
</tr>
</tbody>
</table>

Node count tells what level it is. \( dpdx \) at arbitrary \( E_{\text{probe}} \) tells how many levels there are at \( E \leq E_{\text{probe}} \).
Density of States $\frac{dn}{dE}$

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

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

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

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

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

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

you show that, for harmonic oscillator

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

\[ \omega = (k/m)^{1/2} \]

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

\[ x \quad x_+ = \text{LLL:} \]

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 $\psi_E$'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

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

(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, $V(x_t) = E$ and $p(x_t) = 0$,

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

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

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

Non-lecture: Dwight Integral Table 350.01

$t = \left[a^2 - x^2\right]^{1/2}$

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

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

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

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

use the nonlecture result:

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

$E_n = \hbar \left(\frac{k}{m}\right)^{1/2} \omega (n + 1/2)$
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**
  \[ V(x) = \frac{1}{2}kx^2 \]
  \[ E_n \propto (n + 1/2)^{1/2} \]

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

<table>
<thead>
<tr>
<th>power of x in V(x)</th>
<th>power of n in E(n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1</td>
<td>-2</td>
</tr>
<tr>
<td>1</td>
<td>2/3</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>4/3</td>
</tr>
</tbody>
</table>

Validity limits of WKB?

* **splicing** of \( \psi^{IIa}, \psi^{IIb} ? \)
  \[ \frac{d^2V}{dx^2} \] can't be too large near the splice region

* **\( \psi_{JWKB} \)** is bad when
  \[ \frac{d\lambda}{dx} \geq 1 \]
  \( (\lambda \text{ changes by more than itself for } \Delta x = \lambda) \)

  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...

* updated 9/16/02 11:29 AM