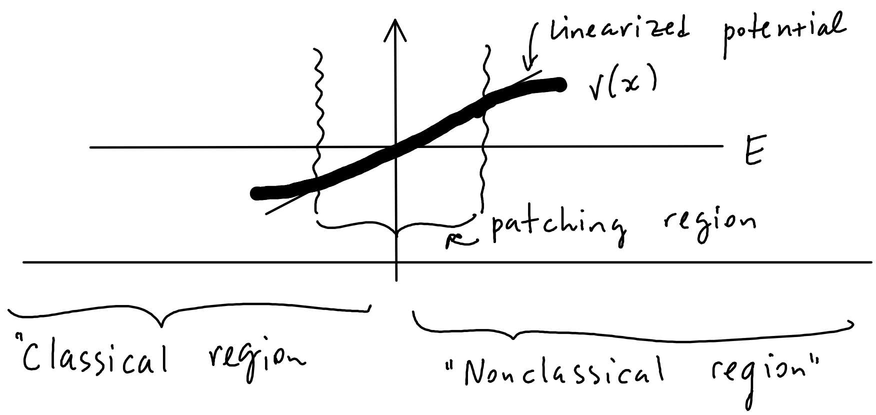
Lecture 17

WKB approximation, connection formulas

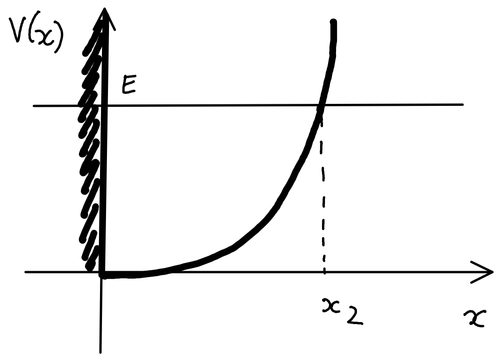


$$\psi(x) \cong \begin{cases} \dfrac{2D}{\sqrt{p(x)}} \sin\left[\dfrac{1}{\hbar}\displaystyle\int_x^{x_2} p(x')\,dx' + \dfrac{\pi}{4}\right] & x < x_2 \\[2ex] \dfrac{D}{\sqrt{|p(x)|}} \exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{x_2}^{x} |p(x')|\,dx'\right] & x > x_2 \end{cases}$$

x_2 is a turning point

Example 1

Consider the "half-harmonic oscillator".



$$V(x) = \begin{cases} \frac{1}{2} m\omega^2 x^2, & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$$

Use WKB approximation to get the energy levels.

Solution

We use the formula that we derived in the previous lecture:

$$\psi(x) \approx \frac{2D}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_x^{x_2} p(x')\, dx' + \frac{\pi}{4} \right) \qquad x < x_2$$

(we only need this region, $E > V$)

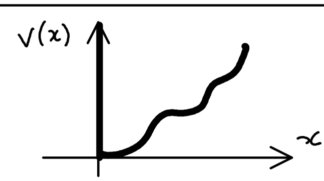
$$\psi(0) = 0 \Rightarrow \qquad \sin\left(\frac{1}{\hbar} \int_0^{x_2} p(x')\, dx' + \frac{\pi}{4} \right) = 0 \quad \Rightarrow$$

$x = 0$ note that it is x', not x.

$$\frac{1}{\hbar} \int_0^{x_2} p(x')\, dx' + \frac{\pi}{4} = \pi n \quad , \quad n = 1, 2, 3, \ldots$$

$$\boxed{\int_0^{x_2} p(x')\, dx' = \left(n - \frac{1}{4}\right) \pi\hbar} \qquad (1)$$

Note that this is true for any potential of the form:



$$p(x) = \sqrt{2m[E - \underbrace{\tfrac{1}{2} m\omega^2 x^2}_{V(x)}]} = m\omega \sqrt{x_2^2 - x^2}$$

$E = V(x_2) = \frac{1}{2} m\omega^2 x_2^2$

(see picture)

Therefore, $$\int_0^{x_2} p(x)\,dx = m\omega \underbrace{\int_0^{x_2} \sqrt{x_2^2 - x^2}\,dx}_{= \frac{x^2 \pi}{4}} = \frac{\pi}{4} m\omega x_2^2 = \frac{\pi E}{2\omega}$$

$$x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$$

substitute here to get formula for E

We now plug our result info Eq. (1):

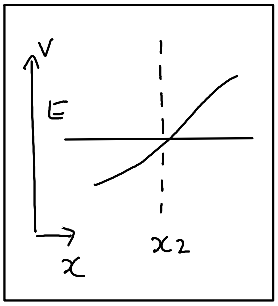
$$\int_0^{x_2} p(x)\,dx = \frac{\pi E}{2\omega} = \left(n - \frac{1}{4}\right)\pi\hbar \Rightarrow$$

$$E_n = 2\omega\left(n - \frac{1}{4}\right)\hbar = \left(2n - \frac{1}{2}\right)\hbar\omega = \left(\frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \dots\right)\hbar\omega$$

This just happened to be exact result (odd energies of the full harmonic oscillator).

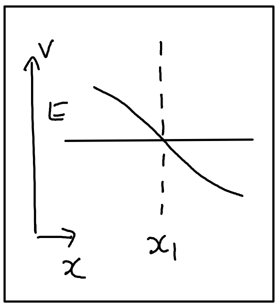
Example 2: potential well with no vertical walls

The formulas that we derived connects the WKB formulas where potential slopes upward:



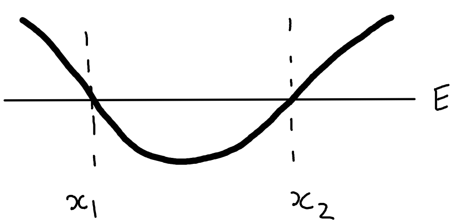
$$\psi(x) \cong \begin{cases} \dfrac{2D}{\sqrt{p(x)}} \sin\left[\dfrac{1}{\hbar}\displaystyle\int_x^{x_2} p(x')\,dx' + \dfrac{\pi}{4}\right] & x < x_2 \quad (1) \\[2ex] \dfrac{D}{\sqrt{|p(x)|}} \exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{x_2}^{x} |p(x')|\,dx'\right] & x > x_2 \quad (2) \end{cases}$$

If the potential slopes downward, we get in a similar way:



$$\psi(x) \cong \begin{cases} \dfrac{D'}{\sqrt{|p(x)|}} \exp\left[-\dfrac{1}{\hbar}\displaystyle\int_x^{x_1} |p(x')|\,dx'\right] & x < x_1 \quad (3) \\[2ex] \dfrac{2D}{\sqrt{p(x)}} \sin\left[\dfrac{1}{\hbar}\displaystyle\int_{x_1}^{x} p(x')\,dx' + \dfrac{\pi}{4}\right] & x > x_1 \quad (4) \end{cases}$$

Therefore, we can write for the intermediate region of the potential with both downward and upward-sloping points:



I. $\psi(x) \simeq \dfrac{2D}{\sqrt{p(x)}} \sin\theta_2(x)$

$$\theta_2(x) = \frac{1}{\hbar}\int_x^{x_2} p(x')\,dx' + \frac{\pi}{4}$$

from upward-sloping point, Eq. (1)

II. $\psi(x) \simeq \dfrac{-2D'}{\sqrt{p(x)}} \sin[\theta_1(x)]$; $\theta_1(x) = -\dfrac{1}{\hbar}\displaystyle\int_{x_1}^{x} p(x')\,dx' - \dfrac{\pi}{4}$

put "–" sign twice

from downward-sloping point, Eq. (3).

The arguments of the **sin** functions must be equal since both of the formulas apply for this region:

$$\theta_2 = \theta_1 + \pi n \quad \Rightarrow$$

$$\underbrace{\frac{1}{\hbar}\int_{x}^{x_2} p(x')\,dx'}_{} + \frac{\pi}{4} = \underbrace{-\frac{1}{\hbar}\int_{x_1}^{x} p(x')\,dx'}_{} - \frac{\pi}{4} + \pi n$$

put both integrals together

$$\boxed{\frac{1}{\hbar}\int_{x_1}^{x_2} p(x')\,dx' = \left(n - \frac{1}{2}\right)\pi\hbar \,, \quad n = 1, 2, 3, \ldots}$$

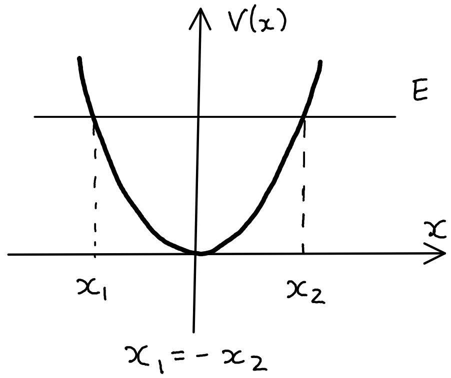
WKB approximation lets us get approximate energy levels without ever calculating the Schrödinger equation! All we need to do is to evaluate one integral!

Note that we got the same formula as before for both or one vertical wall, only the subtraction term differs:

0 for two vertical walls
1/4 for one vertical wall
1/2 for no vertical wall.

Class exercise

Use WKB approximation to find allowed energies of the harmonic oscillator.



Hint: use formula for potential with no vertical walls derived on previous page.

Note that $E = V(x_2) = \frac{1}{2} m\omega^2 x_2^2$.

$$\int_0^a \sqrt{a^2 - x^2}\, dx = \frac{a^2 \pi}{4}$$

Also note that WKB numbering starts from n=1 but usual numbering for harmonic oscillator energy levels starts from n=0.

Solution:

$$\int_{x_1}^{x_2} p(x)\, dx = \left(n - \frac{1}{2}\right)\pi\hbar$$

$$p(x) = \sqrt{2m(E - V)} = \sqrt{2m\left(E - \frac{1}{2}m\omega^2 x^2\right)}$$

$$E = V(x_2) = \frac{1}{2} m\omega^2 x_2^2 \quad \Rightarrow \quad p(x) = \sqrt{2m\left(\frac{1}{2}m\omega^2 x_2^2 - \frac{1}{2}m\omega^2 x^2\right)}$$

$$p(x) = m\omega\sqrt{x_2^2 - x^2}$$

$$\int_{x_1}^{x_2} m\omega\sqrt{x_2^2 - x^2}\, dx = 2m\omega \underbrace{\int_0^{x_2} \sqrt{x_2^2 - x^2}\, dx}_{\frac{x_2^2 \pi}{4}} = \frac{\cancel{2} m\omega \pi x_2^2}{\cancel{4}\ 2}$$

plug in

$$E = \frac{1}{2} m\omega^2 x_2^2$$

$$\frac{\cancel{\pi} m\omega x_2^2}{2} = \left(n - \frac{1}{2}\right)\cancel{\pi}\hbar$$

$$\frac{\cancel{2}E}{\cancel{m}\omega^{\cancel{2}}}\frac{\cancel{m\omega}}{\cancel{2}} = \left(n - \frac{1}{2}\right)\hbar \quad \Rightarrow \quad E = \hbar\omega\left(n - \frac{1}{2}\right), \quad n = 1, 2, 3, \ldots$$

Shifting $n \rightarrow n+1$ we get $\boxed{E = \hbar\omega\left(n + \frac{1}{2}\right)}$ Exact result!