Lecture 9

WKB Approximation

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

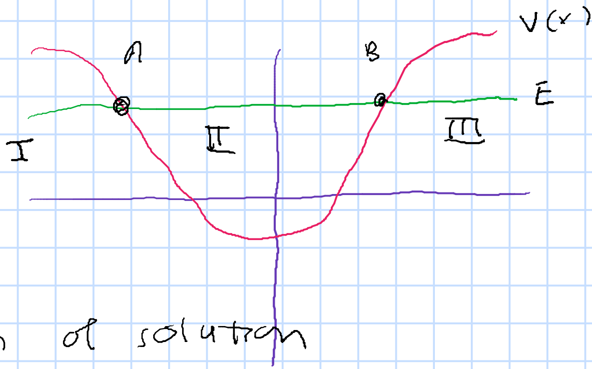
$$\psi(x) = A(x)\, e^{\frac{i}{\hbar}S(x)}$$

slow varying potential $\Rightarrow$

$$S(x) = \pm\int^{x} p_{cl}(x')\,dx'$$

$$p_{cl}^2(x) = 2m\,(E - V(x))$$

$$A(x) = \frac{1}{\sqrt{|p_{cl}(x)|}}$$



Form of solution

region I

$$\psi(x) = \frac{C_I}{\sqrt{|P_{cl}(x)|}} e^{-\int_x |P_{cl}(x')| dx'}$$

region II

$$\psi(x) = \frac{C_{II}}{\sqrt{|P_{cl}(x)|}} e^{\pm i \int^x P_{cl}(x') dx'}$$

region III

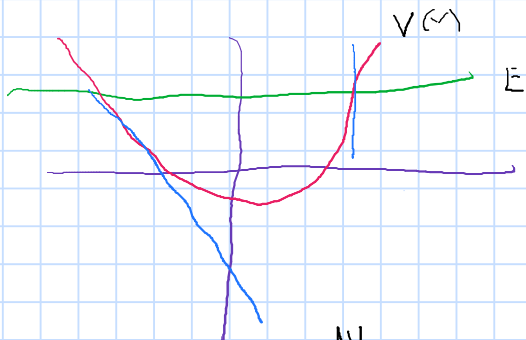
$$\psi(x) = \frac{C_{III}}{\sqrt{|P_{cl}(x)|}} e^{-\int^x |P_{cl}(x')| dx'}$$

Normally one would assume $\psi(x)$ and its first derivative are continuous at the classical turning points A and B.

The problem is that the condition for the approximation to be valid break down at the classical turning points.

In order to satisfy the boundary conditions

* approximate the potential near the classical turning points by a linear potential



$$V(x) \simeq V(x_A) + \frac{dV}{dx}(x_A)(x - x_A)$$
$$V(x) \simeq V(x_B) + \frac{dV}{dx}(x_B)(x - x_B)$$

* solve

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \left[V(x_A) + \frac{dV}{dx}(x_A)(x - x_A)\right]\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \left[V(x_B) + \frac{dV}{dx}(x_B)(x - x_B)\right]\psi = E\psi$$

Note for the turning points

$$E = V(x_A) = V(x_B)$$

We also use the notation

$$\frac{dV}{dx}(x_A) = -F_A$$

$$\frac{dV}{dx}(x_B) = -F_B$$

which represent constant forces.

* The third step is to match the WKB solutions to the solutions of

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}F_A(x-x_A)\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mF_B}{\hbar^2}(x-x_B)\psi$$

To solve equations of this general form

Let

$$\sigma = -\left(\frac{2mF}{\hbar^2}\right)^{1/3} (x - x_\pm)$$

$(\pm = A \text{ or } B)$

$$\frac{d}{dx} = \frac{d\sigma}{dx}\frac{d}{d\sigma} = -\left(\frac{2mF}{\hbar^2}\right)^{1/3}\frac{d}{d\sigma}$$

$$\frac{d^2}{dx^2} = \left(\frac{2mF}{\hbar^2}\right)^{2/3}\frac{d^2}{d\sigma^2}$$

with this change of variable the Schrodinger equation becomes

$$\left(\frac{2mF}{\hbar^2}\right)^{2/3}\frac{d^2}{d\sigma^2} = -\frac{2mF}{\hbar^2}\left(-\left(\frac{\hbar^2}{2mF}\right)^{1/3}\sigma\right)$$

$$= \left(\frac{2mF}{\hbar^2}\right)^{2/3}\sigma$$

canceling the $\left(\frac{2mF}{\hbar^2}\right)^{2/3}$ gives the following equation

$$\boxed{\frac{d^2}{d\sigma^2}A(x) = \sigma A(x)}$$

This equation is called Airy's equation. The solutions are called Airy functions. This is a second order linear differential equation. It has 2 independent solutions

$$\mathrm{Ai}(\sigma) \text{ and } \mathrm{Ai}(e^{2\pi i/3}\sigma)$$

where

$$\mathrm{Ai}(\sigma) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i(s\sigma+\frac{s^3}{3})}\,ds$$

$$= \frac{1}{\pi}\int_0^{\infty} \cos\left(s+\frac{s^3}{3}\right) ds$$

These are well defined functions like $\sin x$ $\cos x$ or Bessel functions

In fact

$$Ai(x) = \sqrt{\frac{x}{3\pi}}\, K_{1/3}\left(\frac{2}{3}x^{3/2}\right)$$

where $K_{1/3}$ is a Bessel function with $\nu = 1/3$

* some properties

① $$\int_{-\infty}^{\infty} Ai(\sigma)\, d\sigma = 1$$

② $$\int_{-\infty}^{\infty} Ai(\sigma - x)\, Ai(\sigma - y)\, d\sigma = \delta(x-y)$$

③ The important properties for the WKB approximation are

$$\lim_{\sigma \to \infty} Ai(\sigma) = \frac{1}{\sqrt{\pi}}\, \sigma^{-1/4}\, e^{-\frac{2}{3}\sigma^{3/2}}$$

$$\lim_{\sigma \to -\infty} Ai(\sigma) = \frac{1}{2\sqrt{\pi}}\, |\sigma|^{-1/4} \cos\left(\frac{2}{3}\sigma^{3/2} - \frac{\pi}{4}\right)$$

we want to compare the asymptotic solutions to the WKB solutions in the three regions

To do this we need to express σ in terms of the classical moments

$$P_{cl}^2(x) = 2m\Big(\underbrace{E - V(x_\pm)}_{0} + F_\pm (x - x_\pm)\Big)$$

$$\boxed{P_{cl}^2(x) = 2m F_\pm (x - x_\pm)}$$

where $F_\pm = -\frac{dV}{dx}(x_\pm)$ $\quad x_\pm = x_A$ a x_B

$$\sigma = -\left(\frac{2mF_\pm}{\hbar^2}\right)^{1/3}(x - x_\pm)$$

$$P_{cl}^2(x) = -2mF_\pm\left(\frac{\hbar^2}{2mF}\right)^{1/3}\sigma$$

$$= -(2mF_\pm\hbar)^{2/3}\sigma$$

$$\boxed{\sigma = -\frac{P_{cl}^2}{(2mF_\pm\hbar)^{2/3}}}$$

$$\frac{2}{3}\sigma^{3/2} = \frac{2}{3}\left(-\frac{p_{cl}^2}{(2mF_t\hbar)^{2/3}}\right)^{3/2}$$

$$= -\frac{2}{3}\frac{p_{cl}^3}{2mF_t\hbar}$$

$$\boxed{\frac{2}{3}\sigma^{3/2} = -\frac{p_{cl}^3}{3mF_t\hbar}}$$

note

$$\frac{1}{\hbar}\int^x p_{cl}(x) = \frac{1}{\hbar}\int^x \sqrt{2mF(x-x_A)}$$

$$= \frac{\sqrt{2mF}}{\hbar}\frac{2}{3}(x-x_A)^{3/2} + \text{const}$$

$$= \frac{2}{3}\frac{\sqrt{2mF}}{\hbar}\left(\frac{p_{cl}^2}{2mF}\right)^{3/2}$$

$$= \frac{2}{3}\frac{p_{cl}^{3/2}}{2mF\hbar} = \boxed{\frac{p_{cl}^3}{3mF\hbar}}$$

This means that the asymptotic forms of the Airy function can be expressed in terms of the classical momentum

$$\sigma^{1/4} = \left[\left(\frac{3}{2}\frac{p_{cl}^3}{3mF_t\hbar}\right)^{2/3}\right]^{1/4} =$$

$$= \text{const} \times p_{cl}^{1/4}$$

The asymptotic form in terms of the classical momenta become

$$\lim_{\sigma \to \infty} Ai(\sigma) \to \frac{const}{\sqrt{\pi}} \frac{1}{\sqrt{P_{cl}(x)}} e^{-\int^x P_{cl}(x)\, dx/\hbar}$$

$$\lim_{\sigma \to -\infty} Ai(\sigma) \to \frac{const}{2\sqrt{\pi}} \frac{1}{\sqrt{|P_{cl}(x)|}} \cos\left(\frac{\int^x P_{cl}(x)}{\hbar} + \frac{\pi}{4}\right)$$

The important properties are

(1) The constants are the same (they d on the turning point

(2) They have the same form as the WKB solutions

The relevant factors for matching are the factor of 2 and the phase.

$X < X_A$

$$\psi(x) = \frac{C_A}{\sqrt{|P_{cl}(x)|}} e^{-\int_x^{x_A} |P_{cl}(x')| dx'/\hbar}$$

$X_A < X < X_B$

$$\psi(x) = \frac{C_A}{2\sqrt{P_{cl}(x)}} \cos\left(\frac{1}{\hbar}\int_{x_A}^{x} P_{cl}(x')dx' - \frac{\pi}{4}\right.$$

$$= \frac{C_B}{2\sqrt{P_{cl}(x)}} \cos\left(\frac{1}{\hbar}\int_{x}^{x_B} P_{cl}(x')dx' - \frac{\pi}{4}\right)$$

$X > X_B$

$$\psi(x) = \frac{C_B}{\sqrt{|P_{cl}(x)|}} e^{-\int_{x_B}^{x} |P_{cl}(x')| dx'/\hbar}$$

In order to get the quantization we need to use the two equations for $X_A < X < X_B$

clearly we must have

$$\boxed{\begin{gathered} C_B = \pm C_A \quad \text{and} \\ \cos\left(\frac{1}{\hbar}\int_{x_A}^{x} P_{cl}(x')dx' - \frac{\pi}{4}\right) = \pm \cos\left(\frac{1}{\hbar}\int_{x}^{x_B} P_{cl}(x')dx' - \frac{\pi}{4}\right) \end{gathered}}$$

In order to compare them we note

$$\cos\left(\frac{1}{\hbar}\int_{x}^{x_B} P_{cl}(x')\,dx' - \frac{\pi}{4}\right) =$$

$$\cos\left(\frac{1}{\hbar}\int_{x_A}^{x_B} P_{cl}(x')\,dx' + \int_{x}^{x_A} \frac{1}{\hbar} P_{cl}(x')\,dx' - \frac{\pi}{4}\right) =$$

$$\cos\left(-\int_{x_A}^{x_B} P_{cl}(x')\,dx' - \frac{1}{\hbar}\int_{x}^{x_A} P_{cl}(x') + \frac{\pi}{4}\right) =$$

$$\cos\left(-\frac{1}{\hbar}\int_{x_A}^{x_B} P_{cl}(x')\,dx' + \underline{\frac{1}{\hbar}\int_{x}^{x_A} P_{cl}(x')\,dx'} + \frac{\pi}{4}\right)$$

$$= \pm \cos\left(\underline{\int_{x}^{x_A} \frac{1}{\hbar} P_{cl}(x')\,dx'} - \frac{\pi}{4}\right)$$

The x dependence is in the red underlined factors

$$\Rightarrow \pm = \cos\left(-\frac{1}{\hbar}\int_{x_A}^{x_B} P_{cl}(x')\,dx' + \frac{\pi}{4} - \left(-\frac{\pi}{4}\right)\right)$$

$$\boxed{\begin{aligned}\int_{x_A}^{x_B} P_{cl}(x')\,dx' &= \hbar\left(n\pi + \frac{1}{2}\pi\right)\\ &= \hbar\left(n+\frac{1}{2}\right)\pi\end{aligned}}$$

This is the WKB quantization condition.

Application - Harmonic oscillator

$$P_{cl}^2 = 2m\left(E - \tfrac{1}{2}kx^2\right)$$

$$P_{cl} = 0 \Rightarrow x_T = \pm\sqrt{\frac{2E}{k}}$$

$$\left(n+\tfrac{1}{2}\right)\hbar\pi = \int_{-\sqrt{\frac{2E}{k}}}^{\sqrt{\frac{2E}{k}}} \sqrt{2m\left(E-\tfrac{1}{2}kx^2\right)}\,dx$$

$$= \sqrt{2mE}\int_{-\sqrt{\frac{2E}{k}}}^{\sqrt{\frac{2E}{k}}} \sqrt{1-\frac{k}{2E}x^2}\,dx$$

Let $u = \sqrt{\frac{k}{2E}}\,x \qquad du = \sqrt{\frac{k}{2E}}\,dx$

$$= \sqrt{2mE} \times \sqrt{\frac{2E}{k}}\ \underbrace{\int_{-1}^{1}\sqrt{1-u^2}\,du}_{\text{area of semicircle}}$$

$$= \frac{\pi}{2}$$

$$= \sqrt{\frac{m}{k}}\,E\,\pi$$

$$\boxed{E = \sqrt{\frac{k}{m}}\left(n+\tfrac{1}{2}\right)}$$

which is the exact oscillator eigenvalues.