216 Handout

WKB Approximation

for One-Dimensional Problems

For stationary states,

$$\psi = u(x)\, e^{-iEt/\hbar}$$

$$u(x) = A \exp\left(i \frac{S(x)}{\hbar} \right)$$

$$\frac{1}{2m}\left(\frac{dS}{dx}\right)^2 - [E - V(x)] - \frac{i\hbar}{2m}\frac{d^2}{dx^2} S = 0$$

Idea: expand S in powers of $\hbar$

$$S = S_0 + \hbar S_1 + \ldots$$

Call $k(x) = \frac{1}{\hbar}\left[2m\left(E - V(x)\right)\right]^{1/2}$ $\quad E > V$

("allowed regions")

$\kappa(x) = \frac{1}{\hbar}\left[2m\left(V(x) - E\right)\right]^{1/2}$ $\quad E < V$

("forbidden regions")

Allowed region:

$\frac{1}{\hbar^2}\frac{1}{2m}(E-V)$

$$i\hbar S_0'' - S_0'^2 - 2\hbar S_0' S_1' + \hbar^2 k^2 = 0$$

$(+\, \mathcal{O}(\hbar^2))$

So

$$S_0'^2 = 2m(E - V(x))$$

$$i S_0'' - 2 S_0' S_1' = 0$$

$$S_0' = \pm \hbar k(x)$$

$$S_0 = \pm \int^x dx' \, k(x')$$

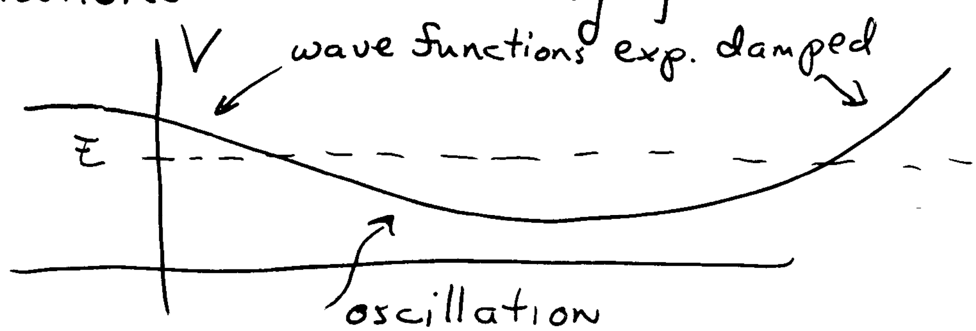
$$S_1' = \frac{1}{2i} \frac{S_0''}{S_0'} = \frac{1}{2i} \frac{d}{dx} \ln(S_0') = \frac{i}{2} \frac{d}{dx} \ln k(x)$$

or $\quad S_1 = \frac{i}{2} \ln k(x) + \text{const}$

$$u(x) = A k^{-1/2} \exp\left(\pm i \int^x k \, dx\right) \qquad V < E$$

$$u(x) = B K^{-1/2} \exp\left(\pm \int^x K \, dx\right) \qquad V > E$$

Our goal is to understand how to match solutions at "turning points"



First, where are approx. valid?

S_0: grows monotonically.

$\Rightarrow$ S_1/S_0 small if S_1'/S_0' small

$$\hbar \, S_1'/S_0' = \hbar \frac{S_1' S_0'}{S_0'^2} = \left| \hbar \frac{S_0''}{2S_0'^2} \right| << 1$$

or $$\frac{k'}{2k^2} << 1$$

$\lambda(x) = \frac{2\pi}{k(x)}$: local de Broglie wavelength.

Says wavelength doesn't change much over a wavelength.

Clearly violated at turning pts.

It turns out we can make progress by examining full eqn. near turning point in a different approximation.

Schrodinger eqn (allowed region)

$$\frac{d^2u}{dx^2} + k^2 u = 0$$

Suppose near turning point, $[x=0]$

$$k^2(x) = cx$$

So

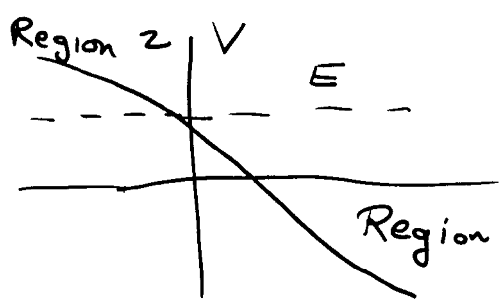
$$\frac{d^2u}{dx^2} + cxu = 0$$

This eqn. is a relative of Bessel's eqn.

(see, e.g., Arfken, Math. methods for physicists, chpt. 11

$$x^2 Z_n'' + x Z_n' + (x^2 - n^2) Z_n = 0$$

$$Z_n = J_n, N_n$$



Call $\xi_1(x) = \int_0^x dx\, k$

$u_\pm = A_\pm \xi_1^{1/2} k^{-1/2} J_{\pm 1/3}(\xi_1)$ solves;

Forbidden region: $B_\pm \xi_2^{1/2} \kappa^{-1/2} I_{\pm 1/3}(\xi_2)$

$$\xi_2 = \int_x^0 \kappa\, dx$$

We need the behavior of I, J near the origin, ∞:

$$J_{\pm 1/3}(\xi_1) \underset{x\to 0}{\to} \frac{(\frac{1}{2}\xi_1)^{\pm 1/3}}{\Gamma(1\pm 1/3)}$$

$$\underset{x\to\infty}{\to} (\tfrac{1}{2}\pi\xi_1)^{-1/2}\cos(\xi_1 \mp \pi/6 - \pi/4)$$

$$I_{\pm 1/3}(\xi_2) \to \frac{(\frac{1}{2}\xi_2)^{\pm 1/3}}{\Gamma(1\pm 1/3)}$$

$$\to (2\pi\xi_2)^{-1/2}\left(e^{\xi_2} + e^{-\xi_2} e^{-(\frac{1}{2}\pm\frac{1}{3})\pi i}\right)$$

Calling $u_{1\pm}$ the two solutions in region 1, $u_{2\pm}$ the solutions in region 2, we need first to match wave functions and derivatives at $x=0$. Note

$$\xi_1 = \frac{2\sqrt{c}}{3}x^{3/2}\ ; \quad \xi_2 = \frac{2c}{3}|x|^{3/2}$$

so, near $x=0$

$$u_1^+ = A_+ \frac{\left(\tfrac{2}{3}\right)^{1/2}\left(\tfrac{1}{3}c\right)^{1/3}}{\Gamma(4/3)}\, x \qquad u_1^- = \frac{A_- \left(\tfrac{2}{3}\right)^{1/2}\left(\tfrac{1}{3}c\right)^{-1/3}}{\Gamma(2/3)}$$

$$u_2^+ = B_+ \frac{\left(\tfrac{2}{3}\right)^{1/2}\left(\tfrac{1}{3}c\right)^{1/3}}{\Gamma(4/3)}\,|x| \qquad u_2^- = B_- \frac{\left(\tfrac{2}{3}\right)^{1/2}\left(\tfrac{1}{3}c\right)^{-1/3}}{\Gamma(2/3)}$$

So $A_- = B_-$; $A_+ = -B_+$

Call the two resulting solutions $u_\pm$.

u^+ vanishes at origin; u^- does not.

Asymptotically:

Note matching to WKB soln.

$$\begin{cases} u^+_{x\to\infty} \to \left(\tfrac{1}{2}\pi k\right)^{-1/2} \cos\left(\xi_1 - 5\pi/12\right) \\ u^+_{x\to-\infty} \to -(2\pi k)^{-1/2}\left(e^{\xi_2} + e^{-\xi_2 - 5\pi i/6}\right) \\ u^- \to \left(\tfrac{1}{2}\pi k\right)^{-1/2} \cos\left(\xi_1 - \pi/12\right) \\ \quad\; \to (2\pi k)^{-1/2}\left(e^{\xi_2} + e^{-\xi_2 - \pi i/6}\right) \end{cases}$$

Now suppose region 2 extends to ∞.

Then need linear comb. of u^+, u^- which vanishes at ∞; this is $u^+ + u^-$.

In region 1,

$$u^+ + u^- \sim k^{-1/2}\left[\cos\left(\xi_1 - 5\pi/12\right) + \cos\left(\xi_1 - \pi/12\right)\right]$$

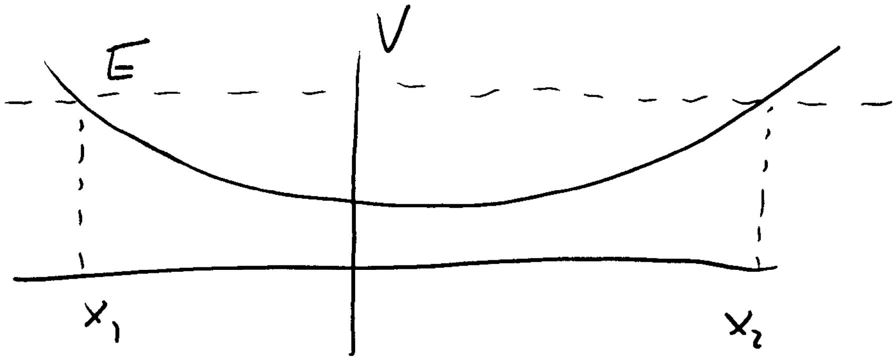
$$\propto k^{-1/2}\cos\left(\xi_1 - \pi/4\right)$$

So

$$\underset{\text{Region 2}}{K^{-1/2} e^{-\xi_2}} \Longleftrightarrow \underset{\text{Region 1}}{k^{-1/2}\cos\left(\xi_1 - \tfrac{1}{4}\pi\right)}$$

"Connection formula"

Application: Bohr-Sommerfeld quantization condition



The solution to right of turning pt. at x_1 is

$$k^{-1/2}\cos\left(\int_{x_1}^{x} k\,dx - \tfrac{1}{4}\pi\right)$$

To left of x_2:

$$k^{-1/2}\cos\left(\int_{x}^{x_2} k\,dx - \tfrac{1}{4}\pi\right)$$

$$= k^{-1/2}\cos\left(\int_{x_1}^{x} k\,dx - \tfrac{1}{4}\pi - \eta\right)$$

$$\eta = \int_{x_1}^{x_2} k\,dx - \pi/2$$

In order that wave functions join smoothly

$$\int_{x_1}^{x_2} k\,dx = (n+\tfrac{1}{2})\pi \qquad n = 0, 1, 2, \ldots$$

or $$2\int_{x_1}^{x_2} \{2m(E-V(x)\}^{1/2}\,dx = (n+\tfrac{1}{2})(2\pi\hbar)$$