LECTURE 3

Approximation methods III

WKB

This method works when we have a slow verying potential with changes no more than few wave lenghts.

In other words the system should have high kinetic energy and be in some high excited state.

Most often used for tunnelling across small and smooth potentials.

WKB is often used as the first step for semiclassical path integrals and instantons.

WKB's 3 steps

1. Eigenfunction is expanded in powers of $\hbar$.

   The approximation becomes wrong at x: $E = V(x)$

2. Construct a separate solution at x

3. Apply boundary conditions

Some details:

Start with Schrödinger eqn:

$$\hbar^2 \psi'' + 2m\,(E - V(x))\,\psi = 0$$

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

$A(x)$ and $S(x)$ are real.

$$\underline{\hbar^2 A''(x)} - 2iA\hbar S' \cdot A' + i\hbar A S'' \underline{- A S'^2} +$$

$$+ \underline{2m(E - V)A} = 0$$

Breaking it into real and imigenary parts:

$$\begin{cases} \hbar^2 A'' - A S'^2 + 2m(E - V)A = 0 \\ 2A'S' + AS'' = (A^2 S')' = 0 \end{cases}$$

$$A = c/\sqrt{S'} \qquad c \text{ is some constant}$$

This one is hard to solve.
intsead we assume that

$$\begin{cases} A = A_0 + \hbar^2 A_1 + \dots & \text{and} \\ S = S_0 + \hbar^2 S_1 + \dots \end{cases}$$

plug those into the 1st eqn.

$$\hbar^2 (A_0'' + \hbar^2 A_1'' + \dots) - (A_0 + \hbar^2 A_1 + \dots)$$
$$(S_0 + \hbar^2 S_1 + \dots)'^2 + \dots \text{ and so on}$$

Lets collect the terms with $\hbar^0$:

$$\hbar^0 \begin{cases} S_0'^2 = 2m(E - V) \Rightarrow S_0' = \pm[2m(E - V)]^{1/2} \\ A_0 = c/\sqrt{S_0'} \end{cases}$$

and for $\hbar^2$

$\hbar^2$: $A_0'' - 2S_0' S_1' A_0 = 0$

recall that $\hbar p(x) = \sqrt{2m(E-V)}$

then $S_0' = \pm\sqrt{2m(E-V)}' = \pm p(x)$

$\Rightarrow S_0 = \pm \int dx' p(x')$ and

$$A_0 = \frac{C}{\sqrt{p(x)}}$$

from $\hbar^2$: $S_1' = \frac{1}{(\sqrt{S_0'})''} \cdot \frac{1}{2\sqrt{S_0'}}$

In the lowest approximation: we only consider A_0 and S_0:

$$\psi(x) \equiv A_0(x) e^{iS_0/\hbar} = \frac{C_1}{\sqrt{p}} e^{iy_1} + \frac{C_2}{\sqrt{p}} e^{-iy_1}$$

where $y_1 = \frac{1}{\hbar}\int_0^x p(x')\,dx'$

b/c $p(x) = \sqrt{\dots}$ y_1 is real if $V<E$

and imaginary $V>E$

The solution will oscillate inside $V<E$ and decay for $E>V$

NB! Applicability: to converge $\hbar^2 S_1 < S_0$ or $|\hbar^2 S_1/S_0| < 1 \Rightarrow \hbar^2 S_1'/S_0'$ is small.

Since $S_0' = \hbar/p = \hbar/\lambda \Rightarrow |\lambda'^2 - 2\lambda\lambda''| \ll 32\pi$

here $\lambda' = \left(\frac{d\lambda}{dx}\right)/\lambda \Rightarrow$

$$\lambda\left|\frac{dp}{dx}\right|/p \ll 1 \quad \text{since } \lambda = \hbar/p$$

in other words

the change of momentum across λ should be very small

Now, once the quantum object is closer to $E - V(x_0) = 0$ the particle stopes at the turning point x_0 i.e. the $\lambda = 2\pi\hbar/p(x_0) \uparrow \infty$

x_0 is called the turning point

Ok what's the solution near x_0?
Lets assume $x = 0$ is turning point we expand around x_0

$$p^2(x) = \underset{n>0}{\rho x^n}\left(1 + \alpha x + \beta x^2 + \dots\right)$$

Lets consider only the first term:

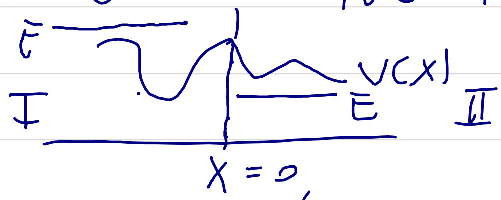
$$\hbar^2\psi'' + \underbrace{2m(E - V(x))}_{p^2}\psi = 0$$

$$\psi'' + \rho x^n \psi = 0$$ which has the solution

$$\psi(x) = A\sqrt{\frac{y}{p}}\, J_m(y) + B\sqrt{y/p}\, J_{-m}(y)$$

with $m = 1/(n+2)$ $\quad y = \int_0^x p(x')\,dx'$ $\quad J_m(y)$ Bessel

Now consider the turning point $x = 0$.



Lets start from $x < 0$: at $x = 0$
$E = V(x=0)$ so the kinetic term $= 0$
and at that point the particle should bounce back (in class. mech).
In QM it will tunnel; that is why often we call I – classical
II – non-class. regions

in other words in:

$$\mathrm{I}: \quad y_1 = \frac{1}{\hbar} \int_x^0 p(x')\,dx \quad \text{real}$$

$$\mathrm{II}: \quad y_2 = \frac{1}{\hbar} \int_x^0 p(x')\,dx \quad \text{imaginary}$$

and for ψ:

$$\begin{cases} \psi_1(x) = A_1 \sqrt{y_1/p}\, J_{1/3}(y_1) + B_1 \sqrt{\frac{y_1}{p}}\, J_{-1/3}(y_1) \\ \psi_2(x) = A_2 \sqrt{y_2/p}\, I_{1/3}(y_2) + I \sqrt{\frac{y_2}{p}}\, I_{-1/3} \end{cases}$$

Here I is the Bessel function with imaginary y.

At $x = 0$: $\psi_1(x) = \psi_2(x)$

for small x: $p^2(x) \approx px \Rightarrow$

$$y_1 = y_2 \approx \frac{2}{3} \sqrt{p}\, x^{3/2}$$

and thus $A_2 = -A_1 \quad B_1 = B_2$

What about the solution far away from $x=0$?

For this we can simply cite the asymptotic form of the Bessel function at $x \to \pm\infty$

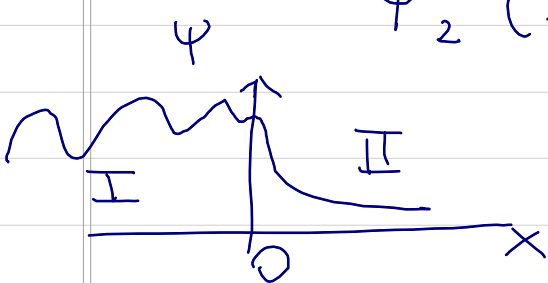
oscillates I: $\psi_1(x \to -\infty) \sim \frac{\alpha}{\sqrt{p}} \sin(y_1 + \pi/4)$

$\alpha = \sqrt{2/\pi}$

$$\psi_2(x \to \infty) \sim \frac{\alpha}{\sqrt{p}} \cos(y_1 + \pi/4)$$

decays II: $\psi_1(x \to \infty) \simeq \frac{\alpha}{2\sqrt{|p|}} e^{-y_2}$

$$\psi_2(x \to \infty) = \frac{\alpha}{\sqrt{|p|}} e^{y_2}$$



★ For several interesting appl. read pp: 409 - 414 and Section 15.3.3 on α-decay

<u>Few simple applications of WKB.</u>

Ex. 1 Energy levels of harmonic oscillator:

$V(x) = kx^2/2$, the turning point x is when $p(x) = 0$ or

$$p(x) = \sqrt{2m(E - V(x))} \rightarrow x^{\pm} = \pm\sqrt{\frac{2E}{k}}$$

$$\psi = \frac{1}{\hbar}\int_{x_-}^{x_T} p(x)\, dx =$$

$$= \frac{1}{\hbar}\int_{x_-}^{x^+} dx \sqrt{2m\left(E - \frac{kx^2}{2}\right)} =$$

$$= \sqrt{\frac{2mE}{\hbar}} \int_{x_-}^{x^+} \sqrt{1 - \frac{kx^2}{2E}}\, dx =$$

$$= \frac{2E}{\hbar}\sqrt{\frac{m}{k}} \int_{-1}^{1} dy \sqrt{1-y^2} = \frac{2E}{\hbar\omega}\int_{-\pi/2}^{\pi/2} \cos^2 z\, dz$$

$$= \frac{E\pi}{\hbar\omega} \Rightarrow$$

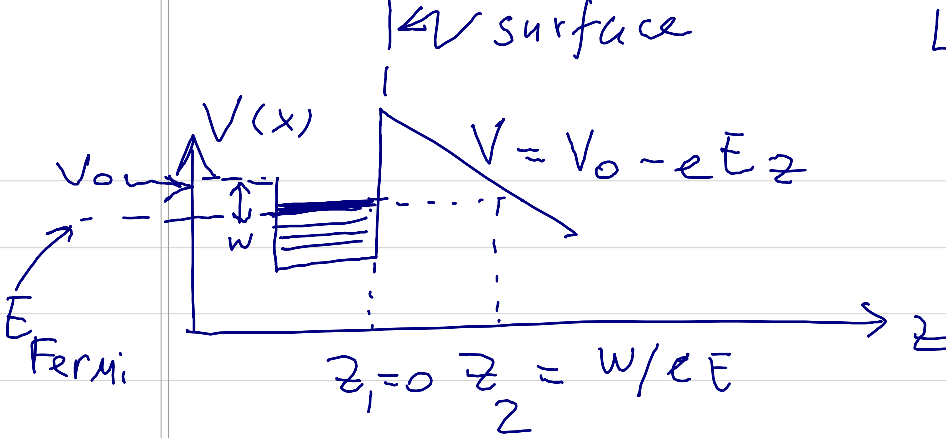
$$\frac{E\pi}{\hbar\omega} = \left(n + \frac{1}{2}\right)\pi \Rightarrow E = \left(\frac{1}{2} + n\right)\hbar\omega$$

$n = 0, 1, 2 \ldots$

see eqn. 15, 22 p 410

Ex. 2. <u>Cold EMISSION of e^- FROM A METAL</u>

Strong electric field may strip out an electron from an atom = this is called cold emission.



To remove electron from the metal we need to appy the electricic field (or potential) to we have 2 turning points

$$z_1 = 0 \quad \text{and} \quad W = eEz_2 \Rightarrow$$
$$z_2 = W/eE$$

$$V(z) = V_0 - eEz \quad \text{and}$$

$$E - V(z) = \underbrace{V_0 - eEz - E_F}_{} = W - eEz$$

W

Recall the transmittion probabitity is

$$T = \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2}\sqrt{2m(V(z) - E)}\,dz\right]$$

$$= \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2}\sqrt{-2m(eEz - W)}\,dz\right]$$

$$x_1 = z_1 \qquad x_2 = z_2$$

$$= \exp\left[-\frac{4}{3}\,\frac{\sqrt{2mW^3}}{3\hbar eE}\right]$$

$V_0 \rightarrow$ surface potential.

Large E can lower the barrier!

Assymtotic method:

To avoid different expressions for each region one can use the so-called ASYM. METHOD.

see pages 419 - 420 for this alternative treatment of the harmonic oscillator.

THE END. OF L3