Lecture 3

Wentzel - Kramer - Brillouin (WKB) Method

- **Heuristically:** Approximate soln by a "plane wave" in regions where kinetic energy >0, but with position-dependent wavevector $k(x)$ (wavelength). OK if potential $V(x)$ varies slowly on scale $\lambda(x)$, i.e. $\lambda\left(\frac{1}{V}\frac{\partial V}{\partial x}\right) << 1$ so that $V(x) \simeq V_0$ const.

$$\frac{\delta\lambda}{\lambda} = \frac{\frac{d\lambda}{dx}\lambda}{\lambda} = \frac{d\lambda}{dx} << 1$$

classical turning points.

In more detail:

$$\psi(x) = \psi(0)\, e^{\pm ikx}, \quad k = \left(\frac{2m(E-V)}{\hbar^2}\right)^{1/2}$$

exact for V - constant.

$V(x)$ varies slowly $\Rightarrow$ over small region over which $V(x) \simeq$ const.

$$\psi(x) \simeq e^{\pm i\phi(x)}, \quad k(x) = \sqrt{\frac{2m(E-V(x))}{\hbar^2}} = \frac{2\pi}{\lambda(x)}$$

$$\psi(x) = \psi(x_0)\, e^{\pm i \underbrace{\int_{x_0}^{x} k(x')\,dx'}}$$

$$\phi(x) = \frac{1}{\hbar} \underbrace{\int_{x_0}^{x} p(x')\,dx'}_{\text{classical action.}}$$

close analogy to ray optics approximation to E&M when dielectric constant $n(x)$ varies slowly in space

How slow is slow?

Need to have many oscillations before $V(x)$ changes appreciably, in order to have "position dependent wavelength" to make sense.

$$\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{d\lambda}{dx}\right| << 1$$

$$\approx \left|\lambda \frac{1}{V} \frac{\partial V}{\partial x}\right| << 1 .$$

- More formally:

$$\left[\frac{d^2}{dx^2} + \underbrace{\frac{2m}{\hbar^2}\left(E - V(x)\right)}_{p^2/\hbar^2}\right]\psi(x) = 0$$

(recall in Q.M-I used $\psi \sim |\psi| e^{iS(x)/\hbar}$

$\Longrightarrow$ Hamilton - Jacobi eqn $\Leftrightarrow$ C.M.)

$$\psi(x) = e^{i\phi(x)/\hbar}$$

$\phi(x)$ ← complex "phase"

← no approx.

$$-\left(\frac{\phi'}{\hbar}\right)^2 + \frac{i\phi''}{\hbar} + \frac{p^2(x)}{\hbar^2} = 0$$

expand $\phi(x)$ in powers of $\hbar$:

$$\phi = \phi_0 + \hbar\phi_1 + \hbar^2\phi_2 + \dots$$

note $\lambda(x) \simeq \frac{2\pi\hbar}{p} \to 0 \Rightarrow$ 

on this $\lambda(x) \to 0$ scale plane-wave approx. becomes better & better.

Corrections in powers of $\hbar$ to classical (ray) approximation

$$\text{Q.M.} \xrightarrow{\hbar \to 0} \text{C.M.}$$

semiclassical approximation: WKB - expansion about C.M. in powers of $\hbar$

analogy $\quad$ E & M $\xrightarrow{\lambda \to 0}$ Ray optics.

<u>lowest order approx:</u>

$$\underbrace{-\frac{(\phi_0')^2+p^2(x)}{\hbar^2}} + \frac{i\phi_0''-2\phi_1'\phi_0'}{\hbar}+O(\hbar^0)=0$$

<u>$\hbar^{-2}$:</u> $\downarrow \Rightarrow \phi_0' = \pm p(x)$

$$\phi_0(x) = \pm \int^x p(x')\,dx'$$

$$\Rightarrow \quad \underline{\psi(x) = \psi(x_0)\, e^{\pm \frac{i}{\hbar}\int_{x_0}^x p(x')\,dx'}}$$

<u>$\hbar^{-1}$:</u> require <u>also</u> $\frac{1}{\hbar}$ terms to vanish

$$i\phi_0'' = 2\phi_1'\phi_0'$$

$$\frac{\phi_0''}{\phi_0'} = -2i\phi_1'$$

$$\ln\phi_0' = -2i\phi_1 + c$$

$$\phi_1(x) = i\ln(\phi_0')^{1/2} + \frac{c}{2i}$$

$$\phi_1(x) = i\ln\sqrt{p(x)} + \bar{c}$$

$$\Rightarrow \quad \psi(x) = e^{i\phi(x)/\hbar} \simeq \frac{A}{\sqrt{p(x)}}\, e^{\pm\frac{i}{\hbar}\int^x p(x')\,dx'}$$

$$\underline{= \psi(x_0)\sqrt{\frac{p(x_0)}{p(x)}}\, e^{\pm\frac{i}{\hbar}\int_{x_0}^x p(x')\,dx'}}$$

$$\Psi(x) = \Psi(x_0)\sqrt{\frac{p(x_0)}{p(x)}}\, e^{\underbrace{\pm \frac{i}{\hbar}\int_{x_0}^{x} p(x')dx'}_{\text{phase change}}} \quad (3.5)$$

Physical interprettation:

$$\Psi \sim \frac{1}{\sqrt{p(x)}} \Rightarrow P = |\Psi|^2 \sim \frac{1}{p(x)} \sim \frac{1}{v}$$ as in classical physics.

For validity of expansion in $\hbar$:

$$\left|\frac{\phi_0''}{\hbar}\right| << \left|\frac{\phi_0'}{\hbar}\right|^2 \Rightarrow \hbar\left|\frac{d}{dx}\left(\frac{1}{\phi_0'}\right)\right| = \left|\frac{d}{dx}\left(\frac{\hbar}{p(x)}\right)\right|$$

$$= \left|\frac{d\lambda}{dx}\right| << 1 \quad \checkmark$$

• Path-integral formalism:

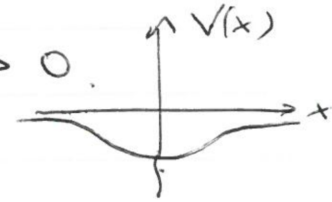
look at evolution operator

$$U_{cl}(x,t;x',0) = A\, e^{\frac{i}{\hbar} S_{cl}(x,t;x',0)}$$

connection to $\psi_n(x)$ & spectrum E_n

$$U(x,x';t) = \sum_n \psi_n(x)\psi_n^*(x')\, e^{-iE_n t/\hbar}$$

look at $E>0$ & $V(x\to\infty)\to 0$.



at $x\to\infty$ $\quad p_\infty = \pm\sqrt{2mE}$

use to label states.
right & left moving waves.

Extract $\psi_n(x)$ from $U(x,x';t)$

$$U(x,x';E+i\varepsilon) = \int_0^\infty dt\, U(x,x';t)\, e^{i(E+i\varepsilon)t/\hbar}$$

convergence factor $e^{-\varepsilon t/\hbar} \to 0$ as $t\to\infty$

$$= 2m\int_{-\infty}^{\infty}\frac{dp}{2\pi i}\,\frac{\psi_p(x)\psi_p^*(x')}{p^2-2mE-i\varepsilon} + \underbrace{\text{B.S.}}_{\text{bound states}\ \Rightarrow \text{drop.}}$$

continuum spectrum since $\frac{p^2}{2m}>0$. Because 1d nondegenerate $\Rightarrow \int dp = \int dE\, E^{1/2}$

$$= \frac{m}{\sqrt{2mE}}\int_{-\infty}^{\infty}\frac{dp}{2\pi i}\,\psi_p(x)\psi_p^*(x')\left[\frac{1}{p-\sqrt{2mE}-i\varepsilon} - \frac{1}{p+\sqrt{2mE}+i\varepsilon}\right]$$

use $\frac{1}{x\mp i\varepsilon} = \mathcal{P}\left(\frac{1}{x}\right) \pm i\pi\delta(x)$

$$\underbrace{U(x,x';E+i\varepsilon) + U(x',x;E+i\varepsilon)^*}_{\text{to kill principle parts so that } \int dp \text{ can be evaluated}} = \sqrt{\frac{m}{2E}}\Big[\psi_{\sqrt{2mE}}(x)\,\psi^*_{\sqrt{2mE}}(x') + \psi_{-\sqrt{2mE}}(x)\,\psi^*_{-\sqrt{2mE}}(x')\Big]$$

3.7

$$U_{cl}(x,x';E+i\varepsilon) = \int_0^\infty dt\, e^{\frac{i}{\hbar} S_{cl}(x,x';t)} \cdot e^{\frac{i}{\hbar}(E+i\varepsilon)t}$$

evaluate via stationary pnt t_*

$$\frac{\partial S}{\partial t} + E = -E_{cl}^{(t_*)} + E = 0$$

$$U_{cl}(x,x';E) = A' \sum_{\substack{\text{Right}\\\text{Left}}} e^{\frac{i}{\hbar}\underbrace{\left[S_{cl}(x,x';t^*) + Et^*\right]}_{\equiv W(x,x';E)}}$$

Legendre transform of S_{cl} from $t \to E = -\frac{\partial S}{\partial t}$

$$W = S_{cl}^* + Et^*$$

$$= \int_0^{t^*} (T-V)\,dt + Et^* \quad (\text{using } T+V=E)$$

$$T = \frac{p^2}{2m} = \frac{1}{2}p\dot{x}$$

$$= \int_0^{t^*} 2T\,dt = \int_0^{t^*} dt\; p\frac{dx}{dt}$$

$$W(x,x';E) = \int_{x'}^{x} p(x'')\,dx''$$

$$\Rightarrow \quad U_{cl}(x,x';E) \simeq A' \sum_{R,L} e^{\frac{i}{\hbar}\int_{x'}^{x} p(x'')dx''}$$

$$= \Theta(x-x')\, A' e^{\frac{i}{\hbar}\int_{x'}^{x}\sqrt{2m(E-V(x''))}\,dx''}$$

$$+ \Theta(x'-x)\, A' e^{-\frac{i}{\hbar}\int_{x'}^{x}\sqrt{2m(E-V(x''))}\,dx''}$$

$$\Rightarrow U_{cl}(x,x';E) + U_{cl}^*(x',x;E) = A' e^{\frac{i}{\hbar}\int_{x'}^{x} p'' dx''} + A' e^{-\frac{i}{\hbar}\int_{x'}^{x} p'' dx''}$$

$$\Rightarrow \boxed{\Psi_\pm(x) = \Psi(x_0)\, e^{\pm\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V(x''))}\,dx''}}$$

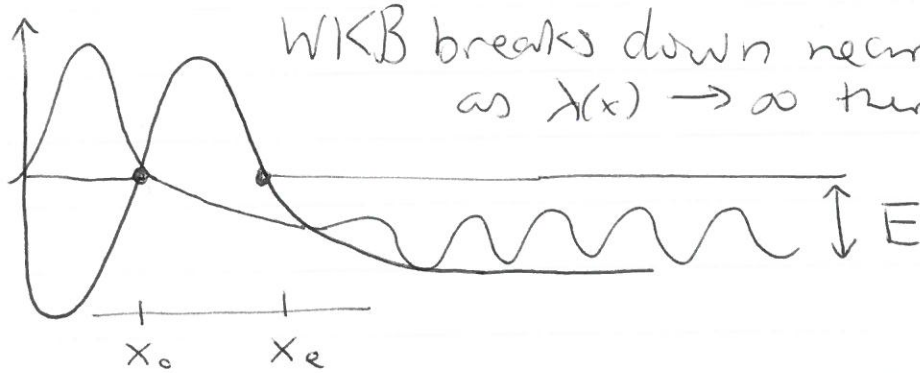
<u>Notes:</u> $\psi_{\pm}(x) = \psi(x_0)\, e^{\pm \frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V(x''))}\,dx''}$

▲ to get $\frac{1}{\sqrt{P}}$ prefactor need to go beyond lowest order saddle pnt. evaluation.

▲ $U^*(x', x; t)$ is time reversal of $U(x, x'; t)$

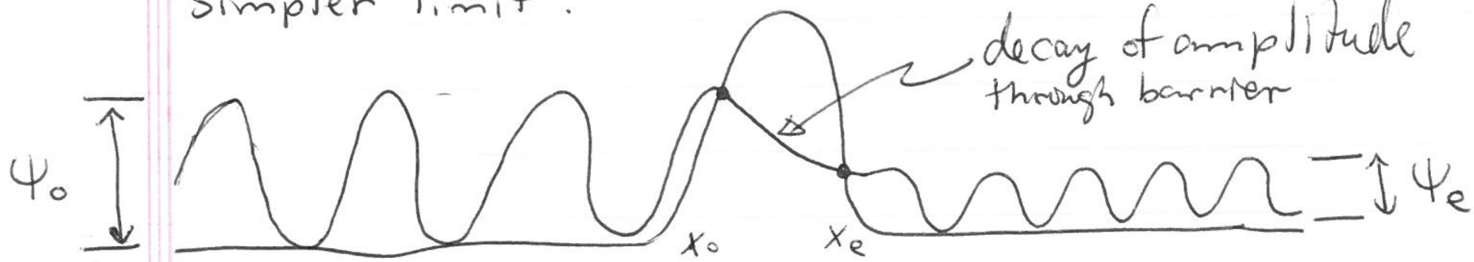
• Application to tunneling:

WKB breaks down near turning pnts as $\lambda(x) \to \infty$ there!



(see 5.4, Shankar)

simpler limit:



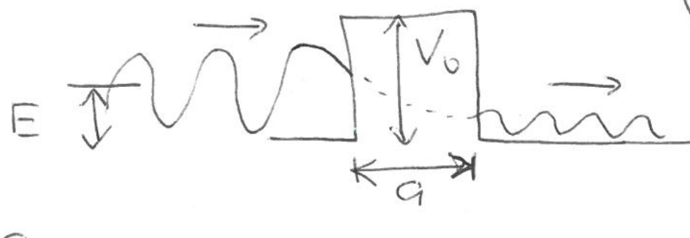
$$\psi(x) = \begin{cases} e^{ikx} + R e^{-ikx}, & x < x_0 \\ A e^{\kappa x} + B e^{-\kappa x}, & x_0 < x < x_e \\ T e^{ikx}, & x_e < x \end{cases}$$

match $\psi, \psi' \Rightarrow A, B, R, T$

R, T reflection & transmission amplitudes.

$|T|^2$ – probability of tunneling through barrier = ratio of $\frac{|\psi_e|^2}{|\psi_0|^2}$

$|T|^2 \simeq e^{-2\kappa a}$



$\kappa a = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}\, a$

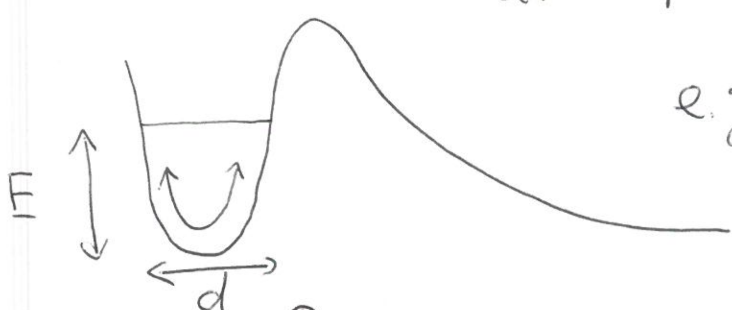
If slowly varying barrier

$$\frac{\gamma}{2} = \kappa a \longrightarrow \int_{x_0}^{x_e} \kappa(x)\,\Delta x = \frac{1}{\hbar}\int_{x_0}^{x_e} \sqrt{2m(V(x) - E)}\, dx$$

$$A_{tunnel} \sim e^{-\gamma/2}$$

$$P_{tunnel} \simeq \omega_0\, e^{-\gamma}$$ prob. of tunneling through

attempt frequency



e.g. Alpha decay He_4^{2+} (Helium nucleus)

$\omega_0 = ? \longrightarrow$ typical v / typical length of well

$$\omega_0 = \frac{p_{well}}{md} = \frac{\sqrt{2mE}}{md}$$

e.g. Harmonic oscillator: $p = \sqrt{2m(E)}$

$$d \simeq ? \Rightarrow \frac{1}{2} m\omega^2 d^2 \simeq E \Rightarrow d = \sqrt{\frac{2E}{m\omega^2}}$$

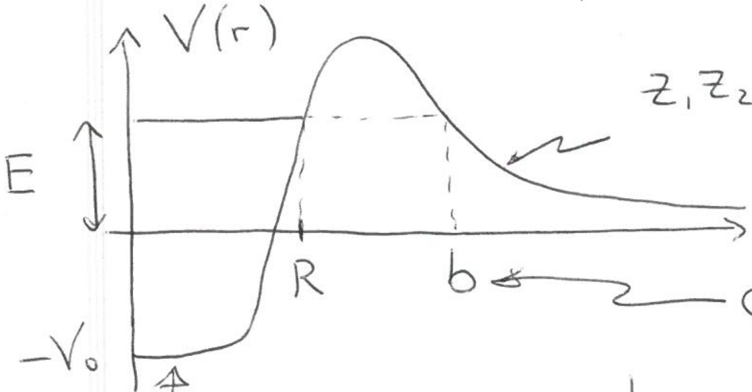
$$\Rightarrow \underline{\omega_0} \simeq \frac{p_{well}}{md} \simeq \frac{\sqrt{2mE}\,\sqrt{m\omega^2}}{m\sqrt{2E}} = \underline{\omega}$$

(tunneling can be derived via path integral in imaginary time; see S. Coleman's "Aspects of Symmetry" & Shankar Ch. 21, pg 616.

Applications:

- **Nuclear physics**: alpha decay (see prob. 16.2.4)

= ejection of α-particle (He nucleus $Z=2$) by a nucleus $A^{N}_{Z_1+2} \rightarrow B^{N-4}_{Z_1} + \alpha^{4}_{++}$



$$\gamma = 2\left(\frac{2m}{\hbar^2}\right)^{1/2} \int_R^b dr \left(\frac{Z_1 \overset{+2}{Z_2} e^2}{r} - E\right)^{1/2}$$

Z_1: daughter nucleus charge

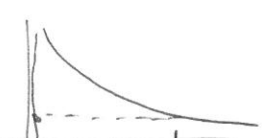
s.r. nuclear potential

use $\displaystyle\int_R^b dr\left(\frac{1}{r}-\frac{1}{b}\right)^{1/2} = \sqrt{b}\Big[\underbrace{\cos^{-1}\left(\frac{R}{b}\right)^{1/2} - \left(\frac{R}{b}-\frac{R^2}{b^2}\right)^{1/2}}_{b \gg R \Rightarrow \frac{\pi}{2} - \left(\frac{R}{b}\right)^{1/2}}\Big]$

$\underset{b \gg R}{\simeq}$

$$\Rightarrow \gamma \simeq 2\sqrt{\frac{2m Z_1 Z_2 e^2 b}{\hbar^2}}\left(\frac{\pi}{2} - \left(\frac{R}{b}\right)^{1/2}\right)$$

roughly: $\displaystyle\int_R^b \left(\frac{a}{r} - E\right)^{1/2} dr \simeq \int_R^b \left(\frac{a}{r}\right)^{1/2} = 2a^{1/2}\left(b^{1/2} - R^{1/2}\right) = 2(ab)^{1/2}\left(1 - \left(\frac{R}{b}\right)^{1/2}\right)$



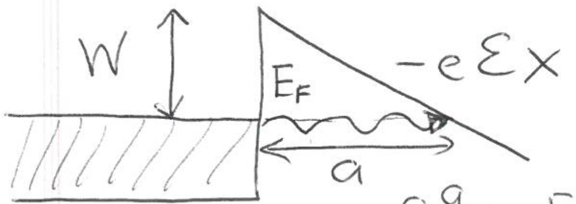
$$b = \frac{Z_1 Z_2 e^2}{E}$$

$$\Rightarrow \underline{\gamma} \simeq \frac{2\pi Z_1 Z_2 e^2}{\hbar v} = \underline{2\pi\alpha Z_1 Z_2 \frac{c}{v}}$$

v: velocity of emitted α-particle

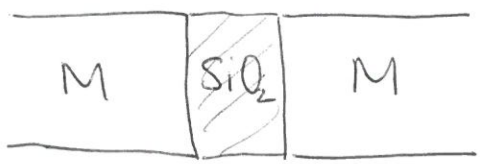
▲ solid state physics

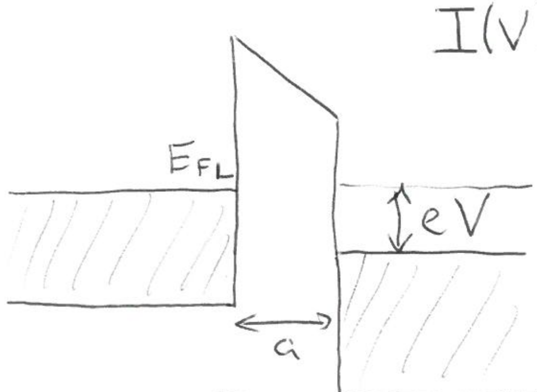
"cold emission"



$$e^{-\gamma} = e^{-2\int_0^a dx\,[2m(W-e\mathcal{E}x)/\hbar^2]^{1/2}}$$
$$\simeq e^{-\frac{c}{\hbar}\sqrt{mW}\underbrace{\left(\frac{W}{e\mathcal{E}}\right)}_{a}}$$

also tunneling between two metals or s.c. through an insulating film.



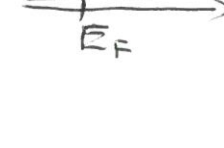


$$I(V) = I_{\rightarrow} - I_{\leftarrow}$$
$$= \sum_k |T|^2 [f_L(1-f_R) - f_R(1-f_L)]$$
$$\simeq |T|^2 \sum_k (f_L(\epsilon_k) - f_R(\epsilon_k))$$

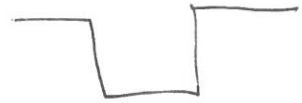
$$I(V) \simeq e^{-2\sqrt{2mW/\hbar^2}\,a} \sum_k (f(\epsilon_k + eV) - f(\epsilon_k))$$
$$\simeq e^{-\frac{2}{\hbar}\sqrt{2mW}\,a} \int_0^\infty d\epsilon\, N(\epsilon)\, \partial_\epsilon f\, eV$$

density of states

$$I(V) = \Big(\underbrace{e^{-\gamma} N(\epsilon_F)\, e}_{\text{Resistance}}\Big) V$$



- **Bound states via WKB:**

Analogous to square well 
but now match WKB oscillatory & decaying $\psi(x)$ (solve near turning pts exactly) approx by linear potential $V(x) \simeq a(x-x_0)$.

$\Rightarrow$ improved Bohr - Sommerfeld quantization (via matching)

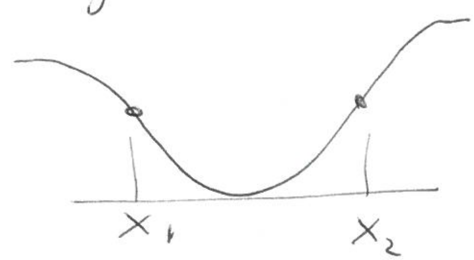
$$\int_{x_1}^{x_2} p(x)\,dx = \left(n + \frac{1}{2}\right)\pi\hbar$$

can vary depending on $V(r)$.

from match near turning pts.

$\Rightarrow$
- n nodes in ψ
- $p = \sqrt{2m(E - V(x))}$

  $\Rightarrow$ E_n quantization.



- best for n, E_n large (since $\lambda \to 0 \Rightarrow$ WKB ok.)

  $\Rightarrow$ complements variational approach good for small n (e.g. g.s. $n=0$)