

## Lec 8: Simple one Dimensional problems

I. Bound states, Solutions are energy eigenstates,

$$\hat{H} \psi_E(x) = E \psi_E(x)$$

$$\Psi(x,t) = e^{-i\hat{H}t/\hbar} \psi_E(x) = e^{-iEt/\hbar} \psi_E(x)$$

then

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi$$

$$E e^{-iEt/\hbar} \psi_E(x) = \hat{H} \psi_E(x) e^{-iEt/\hbar}$$

time independent equation for energy eigenstate

$$\hat{H} \psi_E(x) = E \psi_E(x)$$

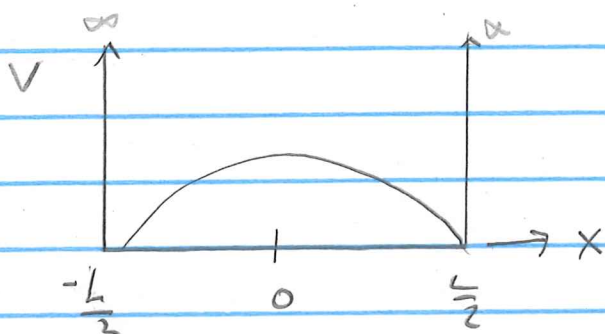
Boundary conditions:

$$\psi_E \rightarrow 0 \quad |x| \rightarrow \infty$$

$\psi$  continuous everywhere

$\psi'$  continuous everywhere  $\forall$  finite

Particle in Box. Here  $E > 0$



$$-\frac{\hbar^2}{2m} \psi'' = E \psi \quad \psi'' = -k^2 \psi$$

$$k = \frac{\sqrt{2mE}}{\hbar} \quad \text{real}$$

Box boundary  $\psi = 0$   $x \geq \frac{L}{2}$  &  $x \leq -\frac{L}{2}$   
 discontinuous @ edges of box where  $V \rightarrow \infty$   
 Energy quantized by boundary condition

$$\psi_n^+ = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) \quad n \text{ odd, even function}$$

$$\psi_n^- = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad n \text{ even, odd function}$$

$$k_n = \frac{n\pi}{L} \quad E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2$$

Reflection symmetry of  $V(x) = V(-x)$

$$\text{P.D.F.} \quad \begin{aligned} |\psi_n^+(x)|^2 &= |\psi_n^+(-x)|^2 \\ |\psi_n^-(x)|^2 &= |\psi_n^-(-x)|^2 \end{aligned}$$

But Q.M. allows amplitude to be even ( $\psi_n^+$ ) and odd ( $\psi_n^-$ )

Remarks

① Ground state has non-zero energy  
uncertainty principle

② Energy of bound state quantized

③ Energy eigenstates complete

$$\Psi(x,t) = \sum_{n=1}^{\infty} \left( C_n^+ e^{-iE_n t/\hbar} \psi_n^+ + C_n^- e^{-iE_n t/\hbar} \psi_n^- \right)$$

④ energy eigenstates are orthonormal

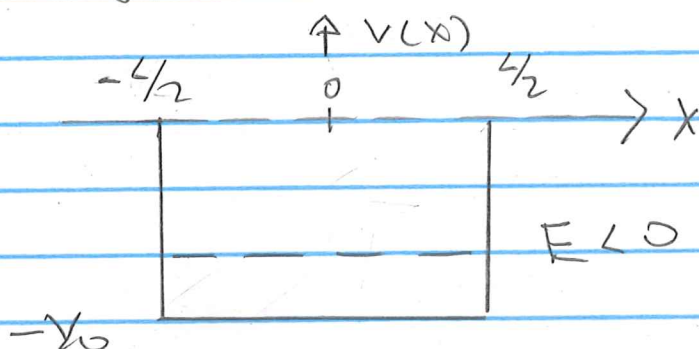
$$\langle \psi_n^+ | \psi_m^+ \rangle = \delta_{nm} \quad \langle \psi_n^- | \psi_m^- \rangle = \delta_{nm}$$

$$\langle \psi_n^+ | \psi_m^- \rangle = 0$$

Coefficients  $C_n^\pm$  are amplitudes  
to measure  $E_n$ .

⑤ measure  $E_n$ , state collapses  
to energy eigenstate

## Finite Square well



$$|x| < \frac{L}{2} \quad \psi_1'' = -k^2 \psi_1 \quad k = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$|x| > \frac{L}{2} \quad \psi_2'' = \gamma^2 \psi_2 \quad \gamma = \frac{\sqrt{2m(-E)}}{\hbar}$$

$\psi$  particle tunnels into classically forbidden region.

$$k^2 + \gamma^2 = \frac{2m}{\hbar^2} [V_0 + E - E] = \frac{2mV_0}{\hbar^2}$$

$$x < -\frac{a}{2} \quad \psi_2 = C e^{\gamma x}$$

$$x > \frac{a}{2} \quad \psi_2 = D e^{-\gamma x}$$

$$\psi_1 = A \sin kx + B \cos kx$$

Consider Even case  $\psi_1 = B \cos kx$

continuity  $B \cos \frac{kL}{2} = D e^{-\gamma L/2}$

derivative  $-kB \sin \frac{kL}{2} = -\gamma D e^{-\gamma L/2}$

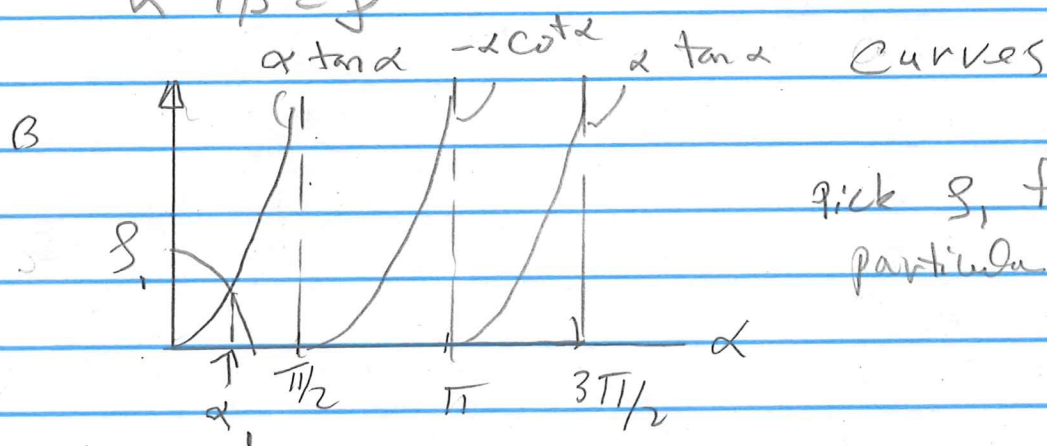
$$\tan\left(\frac{kL}{2}\right) = \frac{\gamma}{k}$$

odd  $\psi_1$  gives  $\cot\left(\frac{kL}{2}\right) = -\frac{\beta}{k}$

define dimensionless

$$\alpha = \frac{kL}{2} \quad \beta = \frac{\beta L}{2} \quad \beta = \frac{L}{2\hbar} \sqrt{2mV_0}$$

$$\alpha^2 + \beta^2 = \beta^2$$



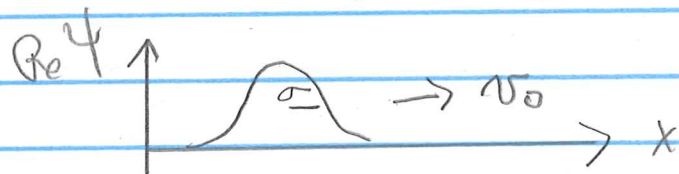
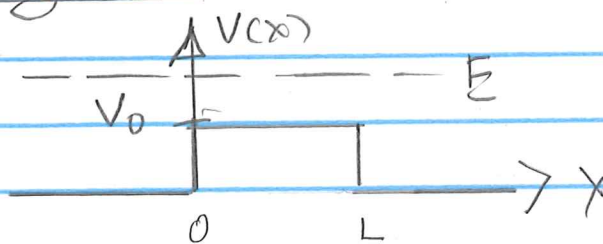
$\alpha_1$  determined graphically

In One Dimension, always at least one solution

$$E_n = -V_0 + \frac{\hbar^2}{2m} k^2 = -V_0 + \frac{\hbar^2}{2mL^2} (2\alpha_n)^2$$

recover infinite well in limit  $V_0 \rightarrow \infty$  (redefine zero of potential)

## II Scattering



macroscopic pulse  $\Delta x \cong \sigma$   
 very small  $\Delta p \cong \frac{\hbar}{2\sigma}$

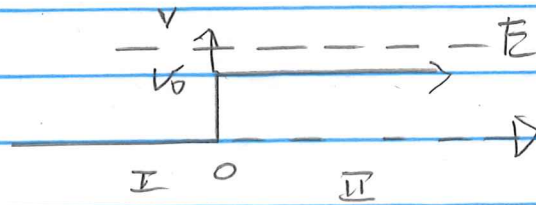
A careful treatment of pulse scattering was done by Goldberger & Watson "Collision Theory" but it is essentially irrelevant (important to show how it can be done)

For simulation, Fourier decompose wave packet, scatter individual plane waves, integrate to get scattered wave packet.

Plane waves  $\exp\left[\frac{i}{\hbar}(\pm px - Et)\right]$   $E = \frac{p^2}{2m}$   
 + +x traveling  
 - -x traveling

Time dependence cancels to give time independent solutions  $\exp(\pm i px/\hbar)$

Simplest example is step ( $L \rightarrow \infty$ )



$$\psi_I = A e^{ikx} + B e^{-ikx}$$

$$k = \sqrt{2mE}/\hbar$$

$$\psi_{II} = C e^{ik'x}$$

$$k' = \sqrt{2m(E-V_0)}/\hbar$$

without loss of generality, take  $A=1$

match boundary conditions at  $x=0$

$$\left. \begin{aligned} 1+B &= C \\ ik(1-B) &= ik'C \end{aligned} \right\} \Rightarrow \begin{aligned} C &= \frac{2k}{k+k'} \\ B &= \frac{k-k'}{k+k'} \end{aligned}$$

Physically measurable quantities are

$$R \equiv \frac{j_r}{j_i}$$

reflection coefficient

$$T = \frac{j_t}{j_i}$$

transmission coefficient

where  $j = \frac{\hbar}{m} \text{Im}(\psi^* \frac{\partial \psi}{\partial x})$  probability current

$$j_i = \frac{\hbar k}{m} ; j_r = |B|^2 \frac{\hbar k}{m}$$

$$j_t = |C|^2 \frac{\hbar k'}{m}$$

in this case  $T = \frac{4kk'}{(k+k')^2}$  ;  $R = \left(\frac{k-k'}{k+k'}\right)^2$

conservation of probability requires  $R+T=1$

Barrier penetration Analytically continue  
 Solution to imaginary  $k' = ig$  ( $g$  real)  
 corresponds to  $E < V_0$ ,

$$g = \sqrt{2m(V_0 - E)}/\hbar$$

Then  $\psi_2 = C e^{-\delta x}$  exponential decay in  
 classically forbidden region

What about  $T$ ?  $C = \frac{2k}{k+ig} \neq 0$

Go back to definition of  $j$ .  $\text{Im}(\psi_2 \frac{d\psi_2}{dx}) = 0$

penetration depth  $\lambda = \frac{1}{2g} = \frac{1}{2} \frac{\hbar}{\sqrt{2m(V_0 - E)}}$

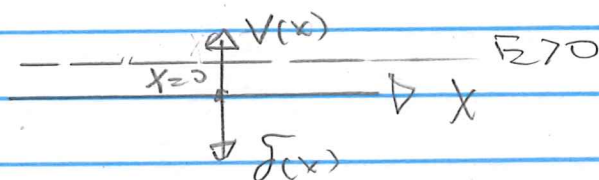


It is easy to show that conservation of probability implies that the S-Matrix is unitary.

S-Matrix key idea in general scattering theory introduced here in simple 1D context.

Consider  $\delta$ -function potential

$$V(x) = -\frac{\hbar^2}{2m} \left(\frac{1}{b}\right) \delta(x) \quad b \text{ is length}$$



time independent Schrödinger

$$\psi'' + \frac{1}{b} \delta(x) \psi = -k^2 \psi \quad k = \sqrt{2mE}/\hbar$$

Now we consider particle incident from both  $\pm x$ .

$$\begin{aligned} \psi_- &= A e^{ikx} + B e^{-ikx} & x < 0 \\ \psi_+ &= F e^{ikx} + G e^{-ikx} & x > 0 \end{aligned}$$

Boundary conditions

$$\psi_-(0) = \psi_+(0)$$

$$\frac{d\psi_+}{dx} - \frac{d\psi_-}{dx} = -\frac{1}{b} \psi_+(0) \quad \text{from integrating } \times \text{ over } x$$

$$A + B = F + G$$

$$ik(F - G) - ik(A - B) = -\frac{1}{b}(A + B)$$

multiply 2<sup>nd</sup> eq. by  $i/k$  become

$$(A - B) - (F - G) = \frac{-i}{kb} (A + B)$$

then 
$$A \left( 1 + \frac{i}{kb} \right) - B \left( 1 - \frac{i}{kb} \right) = F - G$$

$$\underbrace{\hspace{1.5cm}}_{\equiv \alpha} \quad \underbrace{\hspace{1.5cm}}_{\alpha^*}$$

then 
$$A + B = F + G$$

$$\alpha A - \alpha^* B = F - G$$

S-matrix takes initial to final.

$$\begin{pmatrix} B \\ F \end{pmatrix} = \begin{bmatrix} S \end{bmatrix} \begin{pmatrix} A \\ G \end{pmatrix}$$

re-arranging

$$\begin{pmatrix} 1 & -1 \\ \alpha^* & 1 \end{pmatrix} \begin{pmatrix} B \\ F \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ \alpha & 1 \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

recall 
$$[m] = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$

$$[m^{-1}] = \frac{1}{m_{11}m_{22} - m_{21}m_{12}} \begin{pmatrix} m_{22} & -m_{12} \\ -m_{21} & m_{11} \end{pmatrix}$$

So

$$[S] = \begin{pmatrix} 1 & -1 \\ \alpha^* & 1 \end{pmatrix}^{-1} \begin{pmatrix} -1 & 1 \\ \alpha & 1 \end{pmatrix}$$

with  $x = kb$

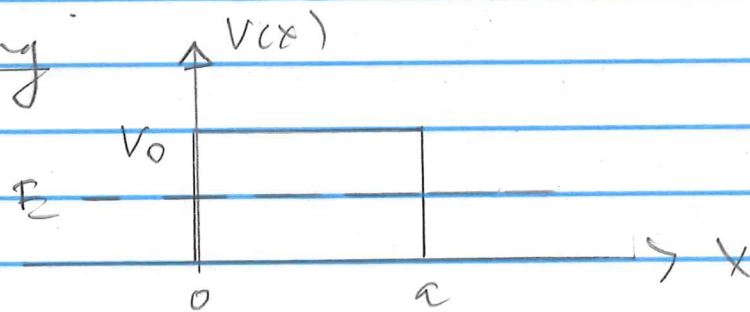
$$[S] = \frac{1}{2x - i} \begin{pmatrix} i & 2x \\ 2x & i \end{pmatrix}$$

particle incident from  $-x$ ,  $G=0$ ,  $A=1$

$$\begin{pmatrix} B \\ F \end{pmatrix} = [S] \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2x+i} \begin{pmatrix} 1 \\ 2x \end{pmatrix}$$

$$R = |B|^2 = \frac{1}{1+4x^2} \quad ; \quad T = |F|^2 = R^{-1} = \frac{4x^2}{1+4x^2}$$

Tunneling



$$k = \sqrt{2mE}/\hbar \quad q = \sqrt{2m(V_0 - E)}/\hbar$$

$$T = \left[ 1 + \left( \frac{q^2 + k^2}{2kq} \right)^2 \sinh^2 qa \right]^{-1}$$

for  $qa \gg 1$   $\sinh qa \approx e^{qa/2}$

$$T \approx \left( \frac{4kq}{k^2 + q^2} \right)^2 e^{-2qa}$$

macroscopic

$$V_0 - E = 1 \text{ erg}; \quad a = 1 \text{ cm}; \quad m = 1 \text{ g}$$

$$qa \approx 10^{27}!$$

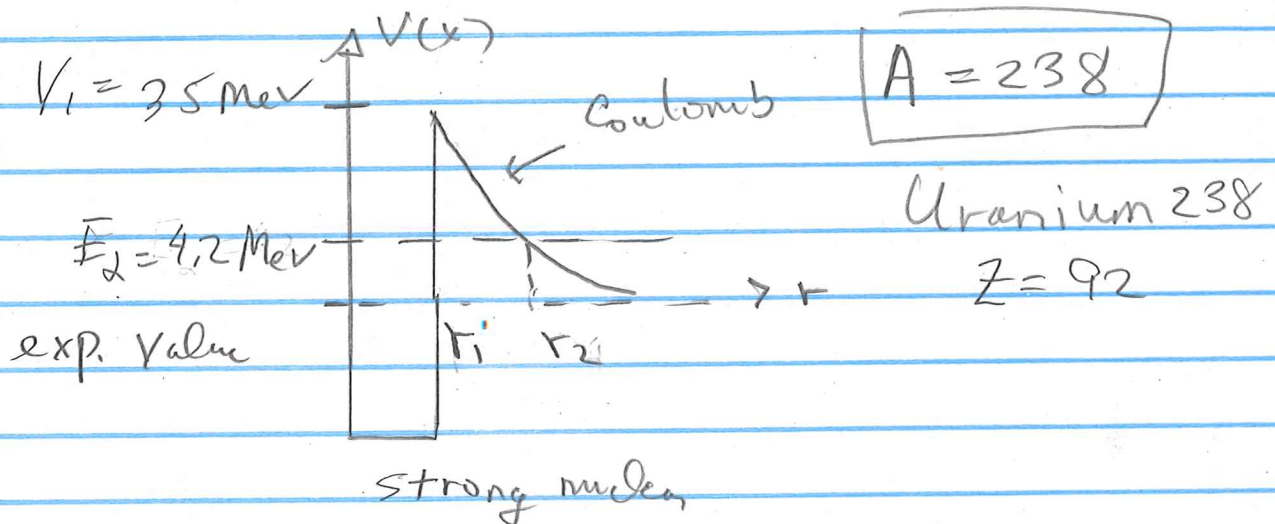
$e^-$  in metal  $V_0 - E \approx 10 \text{ eV}$   $a \approx 1 \text{ nm}$

$$\delta a = \frac{a}{\hbar c} \sqrt{2mc^2(V_0 - E)} = \frac{1 \text{ nm}}{200 \text{ eV} \cdot \text{nm}} \sqrt{10^6 (10 \text{ eV})}$$

$\approx 10$

basis for scanning, tunneling microscope.

Arguably most important physical example, Gamov's theory of  $\alpha$  decay



$\alpha = \text{He}^{++}$  daughter  $Z_d = Z - 2 = 90$

$$V_c(r) \approx 2Z_d e^2 / r$$

$$r_1 \approx (1.2 \text{ fm}) A^{1/3} = 7.4 \text{ fm}$$

$$V_1 \approx 2(90) \left( \frac{e^2}{\hbar c} \right) \frac{\hbar c}{r_1} = 2(90) \frac{1}{137} \frac{197 \text{ MeV} \cdot \text{fm}}{7.4 \text{ fm}}$$

$$\approx 35 \text{ MeV}$$

Calculate  $r_2$  from experimental  $E_\alpha$

$$V(r_2) = E_\alpha = 2Zd \left( \frac{\hbar c}{r_2} \right) =$$

$$r_2 = 2Zd \left( \frac{\hbar c}{E_\alpha} \right) = 61.6 \text{ fm}$$

Simplest approximation square well barriers

$$\text{Take } V_0 = \frac{1}{2} V_1 = 17.5 \text{ MeV}$$

$$a = \frac{1}{2} (r_2 - r_1) = 26.5 \text{ fm}$$

$$\frac{4E(V_0 - E)}{V_0^2} = \frac{4(4.5 \text{ MeV})(13.5 \text{ MeV})}{(17.5 \text{ MeV})^2} = 0.79 \approx 1$$

typically prefactor  $\approx 1$ .

$$g = \frac{\sqrt{2m_e c^2 (V_0 - E)}}{\hbar c} = \left[ \frac{2 \cdot 4 \cdot (931.5 \text{ MeV})(13.5 \text{ MeV})}{197 \text{ MeV} \cdot \text{fm}} \right]^{1/2}$$

$$= (0.62 \text{ fm})^{-1}$$

$$g a = \frac{26.5 \text{ fm}}{0.62 \text{ fm}} = 42.7$$

$$T = \exp(-2(42.7)) = 10^{-85.4} \approx 10^{-37}$$

Experimental quantity is decay rate =  $\lambda^{-1}$   
 We need characteristic frequency.

Gamov made a classical estimate based on frequency with which  $\alpha$  particle strikes the barrier.

$$f = \frac{v}{2r} = \frac{v}{2r} \sqrt{\frac{2E\alpha}{m\alpha c^2}} = \frac{c}{2r} \sqrt{\frac{2(4.2 \text{ MeV})}{4(931.5 \text{ MeV})}}$$

$$= 0.0475 \frac{c}{2(7.4 \text{ fm})} = 3 \times 10^{23} \frac{\text{fm/s}}{2(7.4 \text{ fm})} (0.0475)$$

$$f = 9.6 \times 10^{20} \text{ s}^{-1}$$

$$\% \text{ lifetime } \lambda = (fT)^{-1} = 10^{16} \text{ s}$$

$$= \frac{10^{16} \text{ s}}{\pi \times 10^7 \text{ s/y}} = 0.3 \text{ Gy}$$

exp Value 6.45 Gy

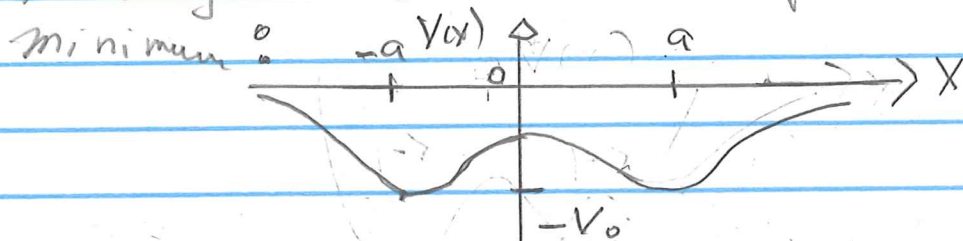
$$\lambda_{1/2}^{\text{exp}} = \ln(2\pi) = 4.47 \text{ Gy}$$

Can do much better with WKB approximation but this gets essence of physics correct - huge range of  $\alpha$ -decay lifetime -

$${}_{84}^{212}\text{Po} \quad T_{1/2} = 0.3 \mu\text{s}$$

Theorem: Cahill

Given symmetric attractive potential with two minimum



ground state is symmetric

$$\langle x | \pm \rangle = \exp(-|x \mp a|) \quad \langle + | - \rangle \neq 0$$

Symmetric, anti-symmetric combinations are:

$$|\Psi_{S,A}\rangle = \frac{1}{\sqrt{2}} (|+\rangle \pm |- \rangle)$$

Energy of ground state dominated by potential energy

$$\langle V \rangle_{S,A} = \frac{1}{2} (\langle + | \pm \langle - | |) V (|+\rangle \pm |- \rangle)$$

$$= \langle + | V | + \rangle \pm \langle - | V | - \rangle$$

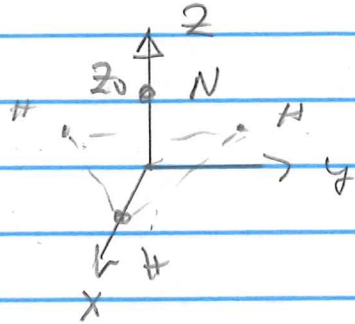
with  $\langle \pm | V | \pm \rangle < 0$

Ground state is symmetric

## Example Ammonia Molecule

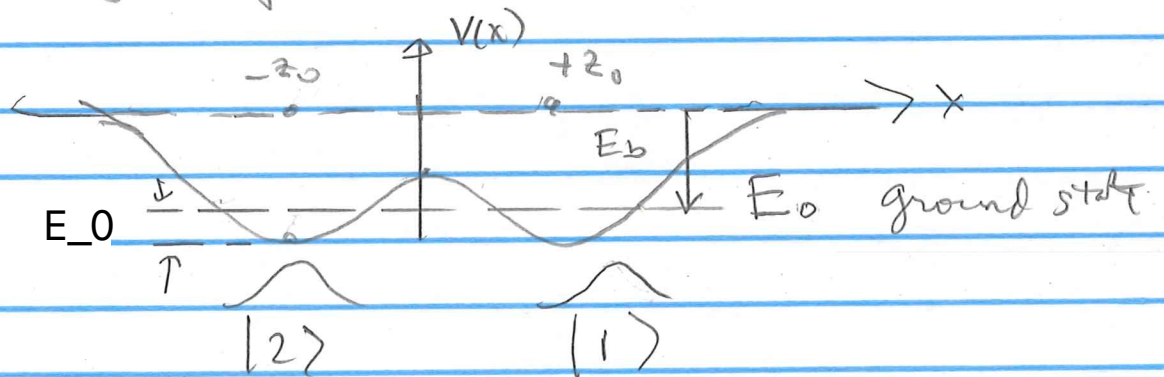
refer to Feynman Lectures

Ammonia has 3 hydrogens in equilateral planar triangle and symmetric nitrogen



hydrogens in  $x-y$  plane

by symmetry there are 2 stable states at  $z = \pm z_0$ . Potential of N moving along  $z$  axis



$E_0 > 0$  measured from minimum of potential

Nitrogen will tunnel across barrier



$$[H]_{1,2} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

A tunneling exchange energy. Negative from theory given later, or from Cahill theorem.

diagonalizing

$$E_{\pm} = E_0 \pm A$$

Ground state  $|I\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle)$   
 and  $|II\rangle = \frac{1}{\sqrt{2}} (|1\rangle - |2\rangle)$

Time dependence is simple in this basis.

$$(|I\rangle, |II\rangle) = (|1\rangle, |2\rangle) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ \equiv [S]$$

components transform as

$$\begin{pmatrix} c_I \\ c_{II} \end{pmatrix} = [S^{\dagger}] \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} c_1 + c_2 \\ c_1 - c_2 \end{pmatrix}$$

take  $|\psi(0)\rangle = |1\rangle$ . Probability

On HW you will show,

$$P_{1 \rightarrow 2}(t) = |\langle 2 | \psi(t) \rangle|^2 = \sin^2 \left( \frac{At}{\hbar} \right)$$