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

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

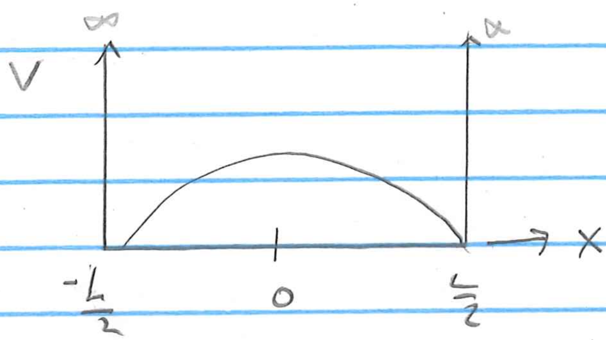
Boundary conditions:

$$\psi_E \xrightarrow[|x|\to\infty]{} 0$$

ψ continuous everywhere

ψ' continuous everywhere V finite

Particle in Box. Here $E > 0$



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

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

Box boundary $\quad \psi = 0 \quad x \geq \frac{L}{2}$ ~~ff~~ $x \leq -\frac{L}{2}$

discontinuous @ edges of box where $V \to \infty$

Energy quantized by boundary condition

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

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

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

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

P.D.F. $\quad |\psi_n^+(x)|^2 = |\psi_n^+(-x)|^2$

$\qquad |\psi_n^-(x)|^2 = |\psi_n^-(-x)|^2$

But Q.M. allows amplitude to be even (ψ_n^+) and odd (ψ_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

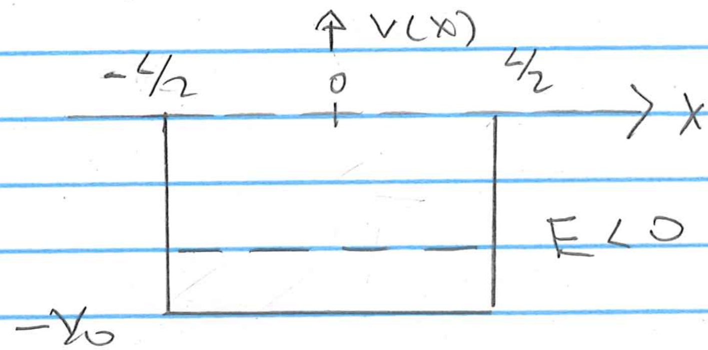
$$\langle \psi_n^+ | \psi_m^+ \rangle = \delta_{nm} \qquad \langle \psi_n^- | \psi_m^- \rangle = \delta_{nm}$$

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

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

⑤ measure E_n, state collapses
to energy eigenstate

Finite Square well



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

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

QM particle tunnels into classically forbidden region.

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

$x < -\frac{a}{2}$ $\psi_2 = Ce^{qx}$

$x > \frac{a}{2}$ $\psi_2 = De^{-qx}$

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

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

continuity $B \cos \frac{kL}{2} = De^{-qL/2}$

derivative $-kB \sin \frac{kL}{2} = -qDe^{-qL/2}$

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

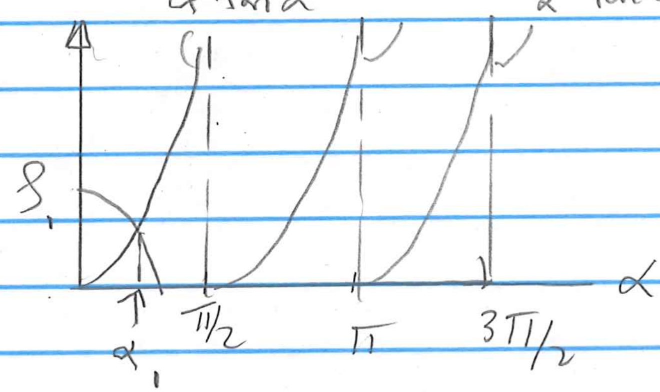
odd ψ_1 gives $\cot\left(\frac{ka}{2}\right) = -\frac{q}{k}$

define dimensionless

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

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

$\alpha \tan\alpha$ $\quad -\alpha\cot\alpha$ $\quad \alpha\tan\alpha$ curves



pick ρ_1 for particular L, V_0

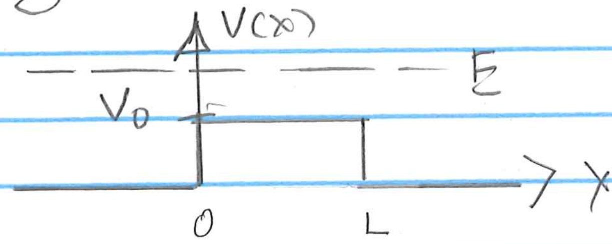
α_1 determined graphically

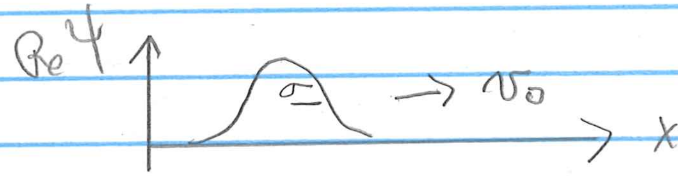
In <u>One Dimension</u>, always at least one solution

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

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

II Scattering





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

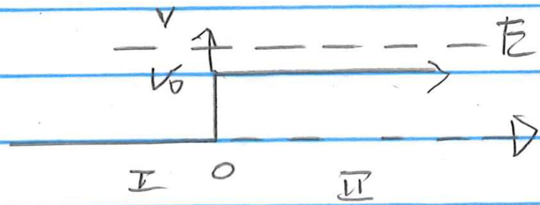
A carefull treatment of pulse scattering was done by Goldberger & Watson "Collision Theory" but it is essentially irrelevant
(important to show how it can be done)

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

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

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

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



$$\psi_I = Ae^{ikx} + Be^{-ikx} \qquad k = \sqrt{2mE}/\hbar$$

$$\psi_{II} = Ce^{ik'x} \qquad k' = \sqrt{2m(E-V_0)}/\hbar$$

without loss of generality, take $A=1$

match boundary conditions at $x=0$

$$\left.\begin{array}{l} 1+B=C \\ ik(1-B)=ik'C \end{array}\right\} \Rightarrow \quad C = \frac{2k}{k+k'} \qquad B = \frac{k-k'}{k+k'}$$

Physically measurable quantities are

$$R \equiv \frac{j_r}{j_i} \qquad \text{reflection coefficient}$$

$$T = \frac{j_t}{j_i} \qquad \text{transmission coefficient}$$

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

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

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

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

conservation of probability requires $R+T=1$

<u>Barrier penetration</u> Analytically continue solution to imaginary $k' = iq$ (q real) corresponds to $E < V_0$.

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

Then $\psi_2 = Ce^{-qx}$ exponential decay in classically forbidden region

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

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

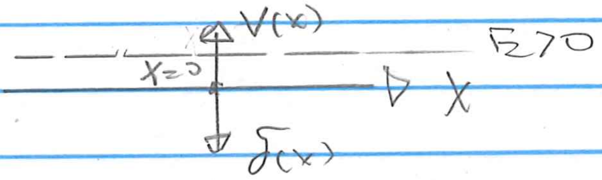
penetration depth $\lambda = \frac{1}{2q} = 1/2 \frac{\hbar}{\sqrt{2m(V_0-E)}}$

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 δ-function potential

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



time independent Schrödinger

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

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

$$\psi_- = Ae^{ikx} + Be^{-ikx} \qquad x<0$$
$$\psi_+ = Fe^{ikx} + Ge^{-ikx} \qquad x>0$$

Boundary conditions

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

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

multiply 2nd eq. by i/k becomes

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

then $$A\underbrace{\left(1+\frac{i}{kb}\right)}_{\equiv\alpha} - B\underbrace{\left(1-\frac{i}{kB}\right)}_{\alpha^*} = F-G$$

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

S-matrix takes initial to final.

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

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

The S matrix is an analytic function of the momentum (k). This is a consequence of causality.

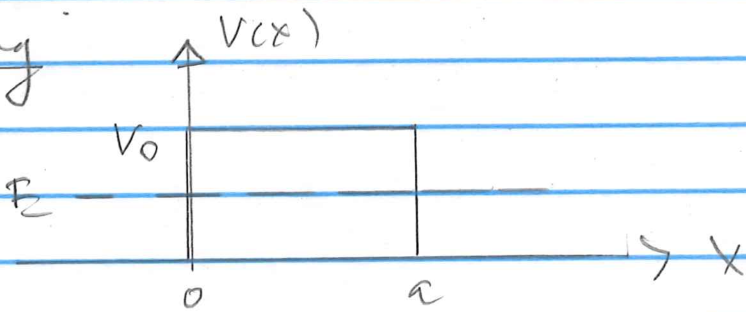
particle incident from $-x$, $G=0$, $A=1$

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

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

$$= \frac{4X^2}{1+4X^2}$$

Tunneling



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

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

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

$$T \underset{qa\gg 1}{\approx} \left(\frac{4kq}{k^2+q^2}\right)^2 e^{-2qa}$$

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

$qa \cong 10^{27}$!

e^- in metal $V_0 - E \simeq 10\,eV$ $a \simeq 1\,nm$

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

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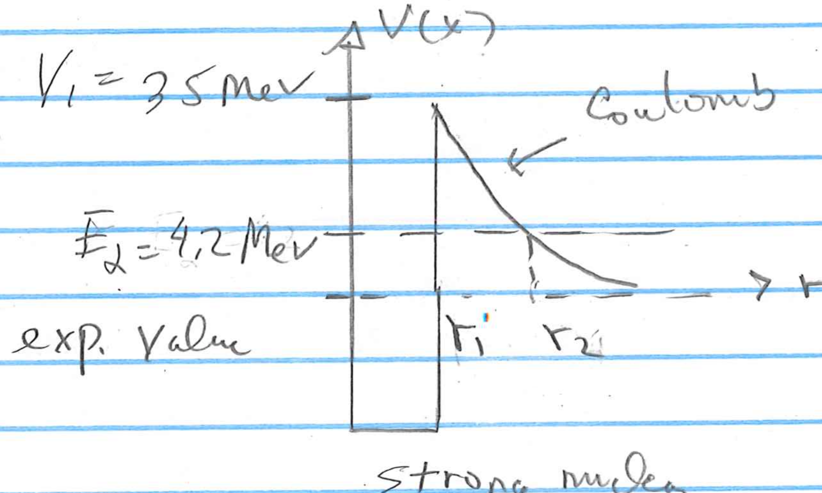
basis for scanning, tunneling microscope.

Arguably most important physical example, Gamov's theory of α decay



$\boxed{A = 238}$

Uranium 238

$Z = 92$

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

$$V_c(r) = 2 Z_d\, e^2/r$$

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

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

$\simeq 35$ MeV

Calculate r_2 from experimental E_α

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

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

Simplest approximation square well barrier:

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

$a = \frac{1}{2}(r_2 - r_1) = 26.5$ 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 ≈ 1.

$$q = \frac{\sqrt{2m_\alpha c^2(V_0-E)}}{\hbar c} = \left[\frac{2\cdot 4\cdot \overset{\text{amu}}{\overset{\downarrow}{(931.5\text{ MeV})}}(13.5\text{ MeV})}{197\text{ MeV fm}}\right]^{1/2}$$

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

$$qa = \frac{26.5\text{ fm}}{0.62\text{ fm}} = 42.7$$

$$T = \exp(-2(42.7)) = 10^{-85.4\log_{10}e}$$

$$= 10^{-37}$$

Experimental quantity is decay rate $= \tau^{-1}$
We need characteristic frequency.
Gamov made a classical estimate
based on frequency with which α
particle strikes the barrier.

$$f = \frac{v}{2r_1} = \frac{c}{2r_1}\sqrt{\frac{2E_\alpha}{m_\alpha c^2}} = \frac{c}{2r_1}\sqrt{\frac{2(4.2\,\text{MeV})}{4(931.5\,\text{MeV})}}$$

$$= 0.0475\,\frac{c}{2(7.4\,\text{fm})} = 3\times10^{23}\,\text{fm/s}\,\frac{(0.0475)}{2(7.4\,\text{fm})}$$

$$f = 9.6\times10^{20}\,\text{s}^{-1}$$

1/e lifetime $\tau = (fT)^{-1} = 10^{16}\,\text{s}$

$$= \frac{10^{16}\,\text{s}}{\pi\times10^{7}\,\text{s/y}} = 0.3\,\text{Gy}$$

exp Value 6.45 Gy

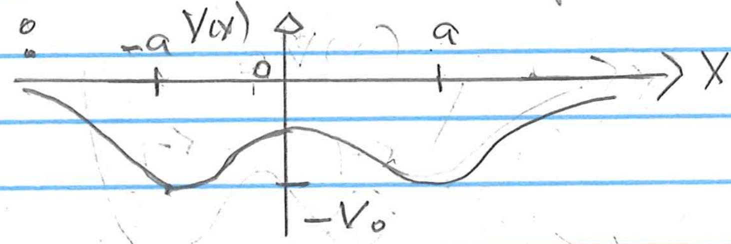
$$\tau_{1/2}^{exp} = \ln(2\tau) = 4.47\,\text{Gy}$$

Can do much better with WKB approximation
but this gets essence of physics
correct - huge range of α-decay lifetimes -

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

Theorem: Cahill

Given symmetric attractive potential with two minimum:



ground state is symmetric

$$\langle x|\pm\rangle = \exp\left(-(x\mp a)^2\right) \qquad \langle +|-\rangle \simeq 0$$

symmetric, anti-symmetric combinations are:

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

Energy of ground state dominated by potential energy

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

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

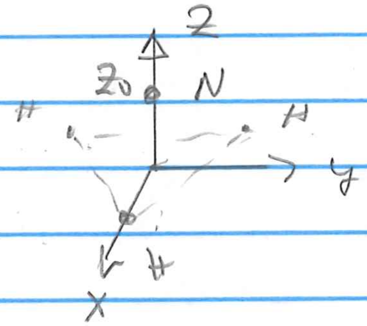
with $\langle \pm|V|\pm\rangle < 0$

Ground state is symmetric

Example Ammonia Molecule

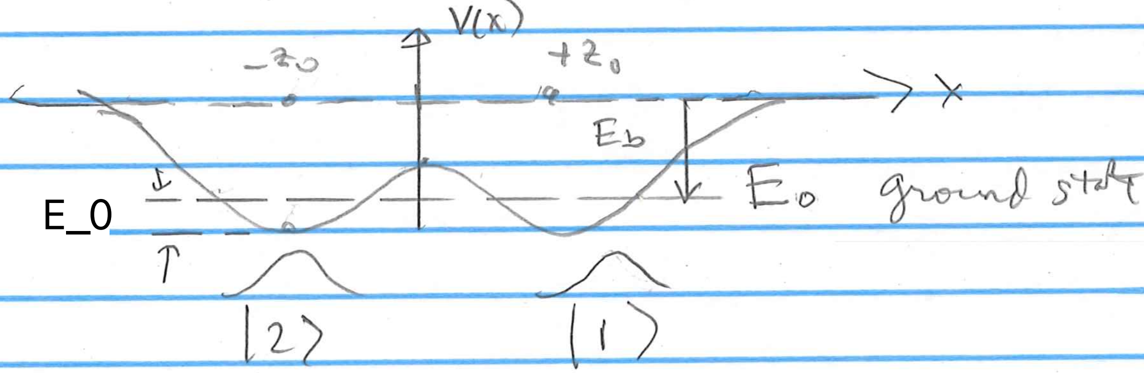
refer to Feyman Lectures

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

Time dependence is simple in this basis.

$$\left(|I\rangle, |II\rangle\right) = \left(|1\rangle, |2\rangle\right)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\equiv [S]$$

components transform as

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

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

On HW you will show,

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