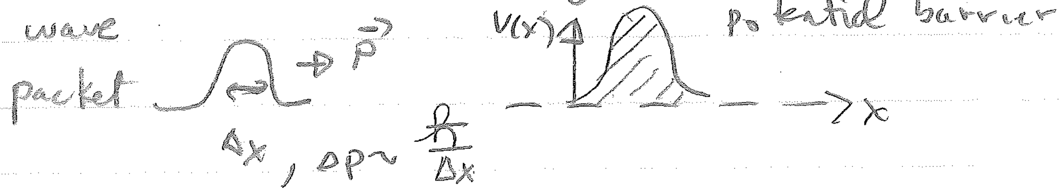
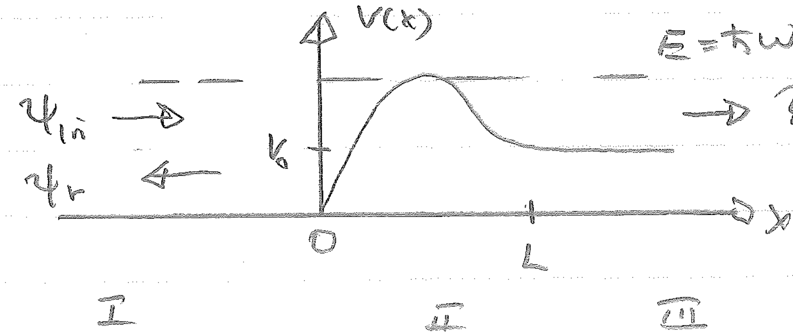
Lecture #9: Tunneling

One dimensional scattering:



Schrödinger equation is linear so we can solve for individual momentum plane wave and sum. Besides any macroscopic wave packet will be very nearly a plane wave.



Free particle in regions I, III.

$$\psi_I = \psi_{in} + \psi_{refl}$$

$$= A e^{i(kx - \omega t)} + B e^{i(-kx - \omega t)}$$

+x traveling -x traveling

time dependence $e^{-iEt/\hbar} = e^{-i\omega t}$

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

$$\psi_{III} = C e^{i(k' - \omega t)} \qquad k' = \sqrt{2m(E-V_0)}/\hbar$$

+x traveling

ψ, ψ' continuity at boundaries 0, L

Solve Schrödinger for $0 < x < L$

and match. Common factor $e^{-i\omega t}$ cancels.

probability flux $\quad j_x = \frac{\hbar}{m} \, \mathrm{Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right)$

$$j_{in} = |A|^2 \frac{\hbar k}{m} \qquad j_r = |B|^2 \frac{\hbar k}{m}$$

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

Reflected, transmitted probabilities:

$$R = \frac{j_r}{j_{in}} = \left|\frac{B}{A}\right|^2$$

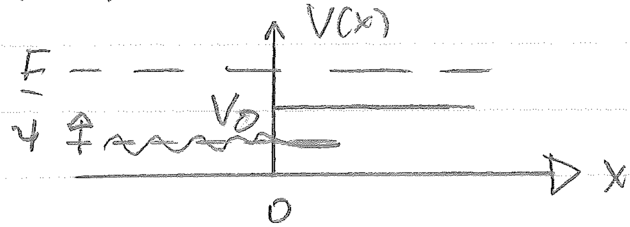
$$T = \frac{j_t}{j_{in}} = \left|\frac{C}{A}\right|^2 \frac{k'}{k}$$

probability conservation

$$R + T = 1$$

Can take $A = 1$

Step-up potential



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

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

$$\psi_- = e^{ikx} + Be^{-ikx} \qquad \psi_+ = Ce^{ik'x}$$

boundary matching:

$$\psi_-(0) = \psi_+(0) \qquad 1 + B = C$$

$$\psi_-'(0) = \psi_+'(0) \qquad ik(1-B) = ik'C$$

$$C = \frac{2k}{k+k'} \qquad B = \frac{k-k'}{k+k'}$$

For plane waves,

$$T = \frac{k'}{k}|C|^2 = \frac{4kk'}{(k+k')^2} \; ; \; R = \frac{(k-k')^2}{(k+k')^2}$$

so $T + R = 1$

Barrier penetration $E < V_0$

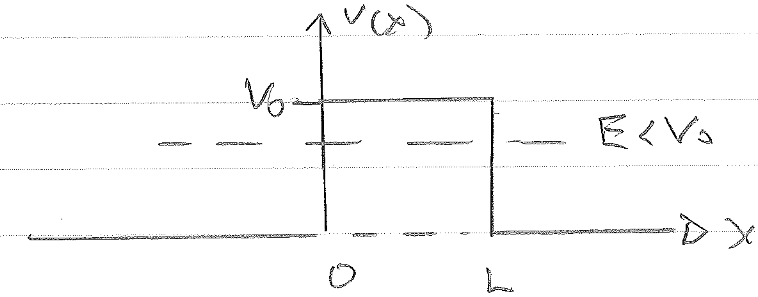
$$iq \equiv \sqrt{2m(E-V_0)}/\hbar = i\sqrt{2m(V_0-E)}/\hbar$$

$$\psi_+ = Ce^{-qx} \qquad \text{normalizable, real}$$

penetration depth $|\psi_+|^2 \propto e^{-2qx}$ $\qquad T = 0 ; R = 1$

$$\text{depth} = \frac{1}{2q} = \frac{\hbar}{\sqrt{8m(V_0-E)}}$$

Tunneling through rectangular barrier



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

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

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Fe^{qx} + Ge^{-qx} & 0 < x < L \\ C\,e^{ikx} & x > L \end{cases}$$

$$T = \frac{j_t}{j_{in}} = \left|\frac{C}{A}\right|^2 = \left[1 + \left(\frac{k^2+q^2}{2kq}\right)^2 \sinh^2 qL\right]^{-1}$$

typically $\underline{q}L \gg 1$

<u>macroscopic</u>: $V_0 - E = 1\,\text{erg}$ $L = 1\,\text{cm}$ $m = 1\,\text{g}$

$qL \sim 10^{27}$

<u>scanning tunneling microscope</u> –

e^- in metal $V_0 - E \sim 10\,\text{eV}$; $L = 1\,\text{nm}$

$$qL = \left[\frac{2mc^2(V_0 - E)}{(\hbar c)^2}\right]^{1/2} L = \left[\frac{10^6\,\text{eV}\cdot 10\,\text{eV}}{(200\,\text{eV}\cdot\text{nm})^2}\right]^{1/2} 1\,\text{nm}$$

$$= \frac{10}{2}\sqrt{10} = 16$$

$$\sinh qL = \frac{e^{qL} - e^{-qL}}{2} \underset{qL >> 1}{\approx} \frac{e^{qL}}{2}$$

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

More generally, $T = |A_T|^2 = e^{-2\gamma}$

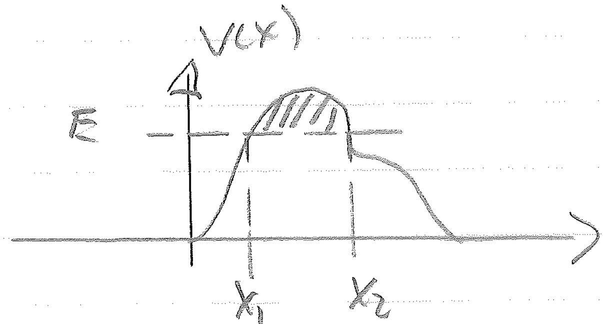
$$A_T \equiv e^{-\gamma} \cong \exp\left(-\int_{x_1}^{x_2} q(x)\,dx\right)$$

classically forbidden

$$q(x) = \sqrt{2m(V(x)-E)}\,/\hbar \quad = i\,p(x)$$

imaginary momentum

$$\gamma = \int_{x_1}^{x_2} q(x)\,dx$$



$x_1 < x < x_2$ classically forbidden

Gamow Theory of α decay

$$^{A=238}_{Z=92}U \rightarrow {}^{234}_{Z_d=90}Th + \alpha(4.18\,\text{MeV}) \qquad t_{1/2} = 4.5\times 10^{9}\,y$$

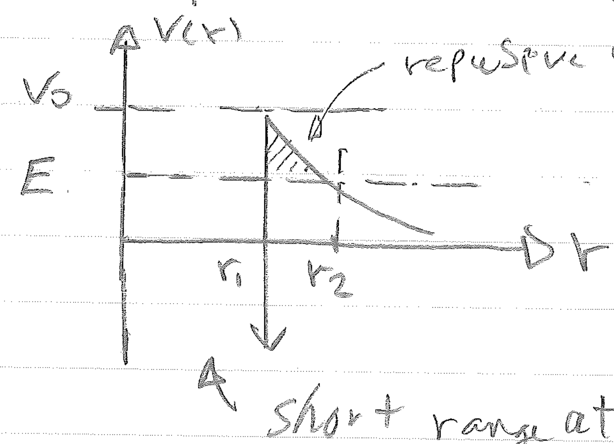
Z_d = daughter nuclear charge

$$^{212}Po \rightarrow {}^{208}Pb + \alpha(8.78\,\text{MeV}) \qquad t_{1/2} = 0.3\,\mu s$$

An enormous range of lifetimes
lifetime exponentially sensitive to kinetic energy.

Unlike β decay, α is confined inside nucleus prior to decay. Decays by tunneling

Sketch of potential seen by α particle



hatched area is $V(r)-E$ in forbidden region

Note: since $E > 0$, these heavy nuclei cannot be formed by fusion in stars. Supernovae, neutron star collisions (?)

Z_d: charge of daughter nucleus

$$E = \frac{2 Z_d \alpha \hbar c}{r_2} \; ; \; V_0 = \frac{2 Z_d \alpha \hbar c}{r_1}$$

then $\gamma = \frac{\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{V(r)}{E}-1}\,dr$

$$\gamma = \frac{\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{r_2}{r}-1}\,dr$$

$$= \frac{\sqrt{2mE}}{\hbar}\left[r_2\cos^{-1}\left(\frac{r_1}{r_2}\right) - \sqrt{r_1(r_2-r_1)}\right]$$

for $r_1 \ll r_2$

$$\gamma \cong \frac{\sqrt{2mE}}{\hbar}\left[\frac{\pi}{2}r_2 - \sqrt{r_1 r_2}\right]$$

$$= \frac{C_1 Z_d}{\sqrt{E}} - C_2\sqrt{Z_d r_1}$$

$C_1 = 1.980\ \sqrt{\mathrm{MeV}}$, $C_2 = 1.485\ (\mathrm{fm})^{-1/2}$

nuclear radius $r_1 \cong 1.5 A^{1/3}$ fm
for heavy nuclei, $A \approx 2Z$ so $r_1 \propto Z_d^{1/3}$
and $\sqrt{Z_d Z_d^{1/3}} = Z_d^{2/3}$
$C_2' = 1.485 \frac{1}{\sqrt{\mathrm{fm}}}\ \sqrt{1.5\ \mathrm{fm}} = 1.786$

We see $C_1 \approx C_2'$ so

$$\gamma \cong \frac{Z_d}{\sqrt{E}} - Z_d^{3/2}$$

plot $\log\tau$ versus γ

9-8

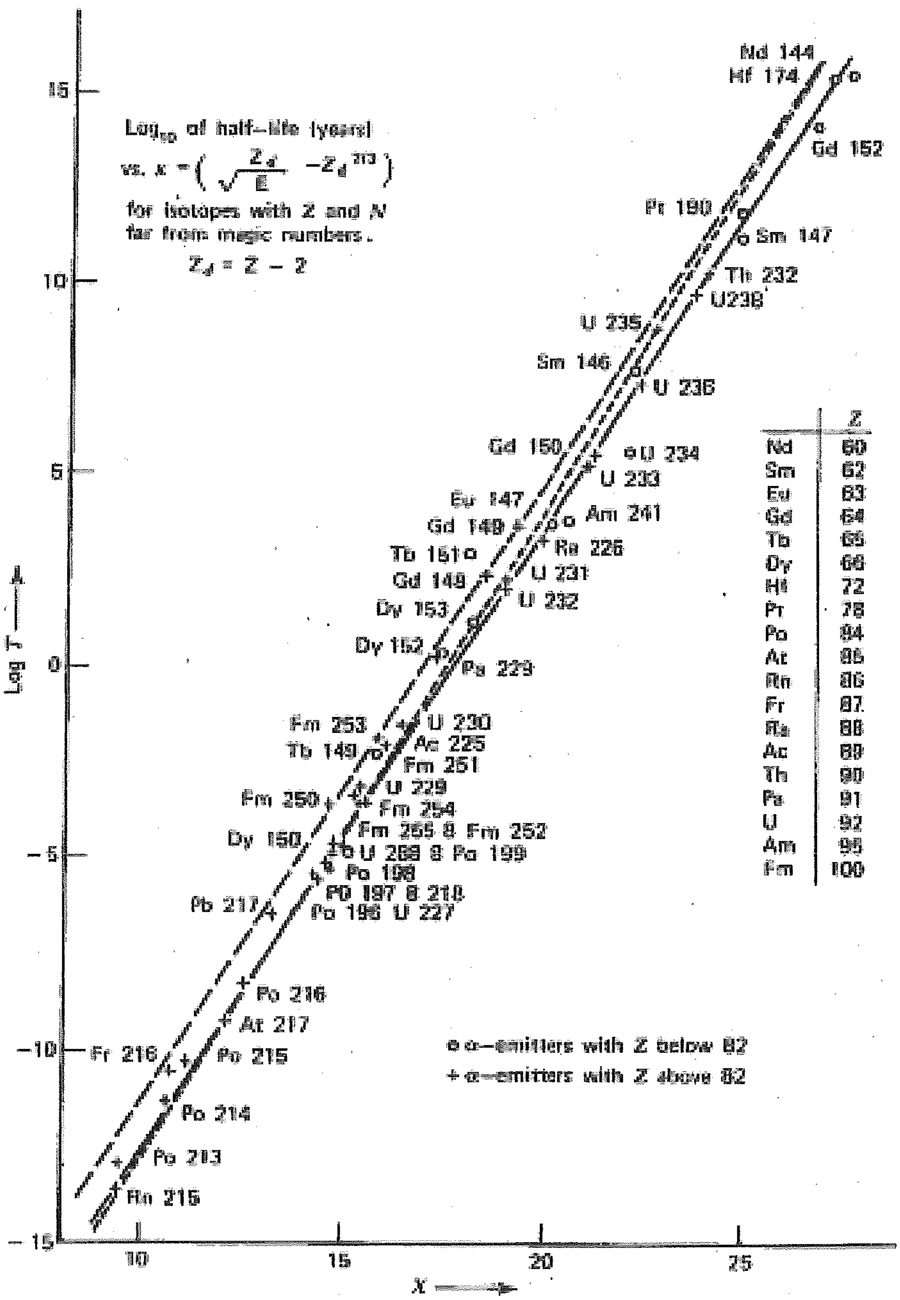


Figure 5-9. Plot of $\log_{10} 1/\tau$ versus $C_2 - C_1 Z_1/\sqrt{E}$ with $C_1 = 1.61$ and a slowly varying $C_2 = 28.9 + 1.6 Z_1^{2/3}$. (From E. K. Hyde, I. Perlman, and G. T. Seaborg, *The Nuclear Properties of the Heavy Elements,* Vol. 1, Prentice-Hall, Englewood Cliffs, N.J. (1964), reprinted by permission.)

α-decay lifetime. $\tau = \frac{T}{f}$

Where f is a frequency, the frequency that α particle "strikes" the barrier.

Classically, $f = \frac{v}{r_1} = \frac{1}{r_1}\sqrt{\frac{2E}{m_\alpha}}$

for ^{238}U $\quad E = 4.18$ MeV (α energy)

$r_1 = 1.5\,fm\,(238)^{1/3} = 9.3\,fm$

$$f \cong \frac{c}{r_1}\sqrt{\frac{2E}{m_\alpha c^2}} = \frac{3\times10^{8+15}\,fm/s}{9.3\,fm}\sqrt{\frac{2.4\,MeV}{4\times10^{3}\,MeV}}$$

$$= \frac{3}{9.3}\frac{1}{\sqrt{5}}\,10^{18+15-1}\,s^{-1}$$

$f^{-1} = 7\times10^{-22}\,s \qquad \gamma = \frac{c_1 Z_d}{\sqrt{E}} - c_2\sqrt{Z_d r_1}$

$Z_d = 90$

$$\gamma = \frac{1.980(90)}{\sqrt{4.18}} - 1.485\sqrt{90(9.3)}$$

$= 44.20$

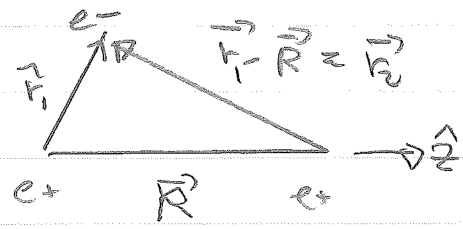
$$\log_{10}(\tau) = \log_{10}(T) - 22 + \frac{2(44.2)}{\log(10)} = 17.3$$

$$\tau = 10^{17.3}\,s = 10^{0.3}\,\frac{10^{17}\,s}{3.2\times10^{7}\,s/y} = 6\times10^{9}\,y$$

pretty good!

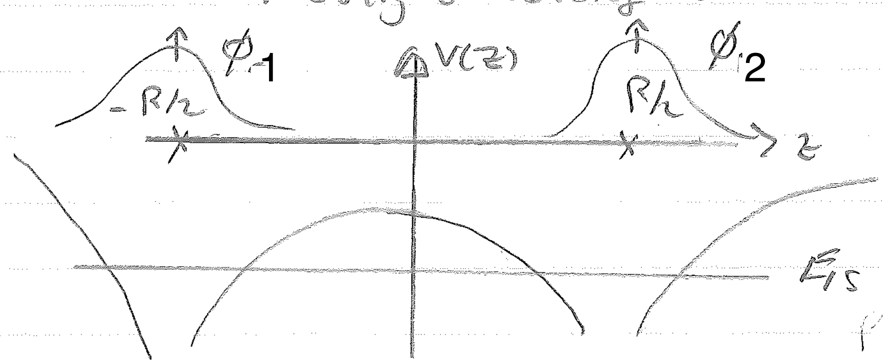
Covalent bond

Simplest example is H_2^+ hydrogen molecular ion. (See Feynman, Pauling & Wilson)



no classical bound state!

Potential moving e⁻ along z axis



Potential is symmetric $V(-z) = V(z)$

Consider ground state wave function
Energy eigenstates for H-atom (1s states)

$$\phi_i^{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r_i} \qquad i = 1, 2 \qquad E_{1s} = -13.6\,eV$$

solutions for $R \gg a_0$, but as protons come together, e⁻ can tunnel from one state to the other.

This leads to coupled equations

(1) $\hat{H}\phi_1 = E_0\phi_1 - K\phi_2$ $\quad K>0$ minus sign for tunneling

(2) $\hat{H}\phi_2 = E_0\phi_2 - K\phi_1$

$ke^2 = \hbar c\alpha$

$$E_0 = \underset{\text{ground state}}{E_{1s}} + \underset{\text{proton repulsion}}{\frac{ke^2}{R}} - J$$

$J>0$ energy associated with not tunneling

$$J = \int \phi_1 \left(\frac{+e^2}{r_2}\right)\phi_1\, d^3v = \frac{ke^2}{a_0}\left(\frac{a_0}{R} - e^{-2R/a_0}\left(1+\frac{a_0}{R}\right)\right)$$

$$K = \int \phi_2 \left(\frac{+e^2}{r_2}\right)\phi_1\, d^3v = \frac{ke^2}{a_0} e^{-R/a_0}\left(1+\frac{R}{a_0}\right)$$

Add and subtract (1), (2) to decouple:

$$E_0(\phi_1+\phi_2) - K(\phi_1+\phi_2) = E_S(\phi_1+\phi_2)$$

$$E_0(\phi_1-\phi_2) + K(\phi_1-\phi_2) = E_A(\phi_1-\phi_2)$$

E_S, E_A are symmetric, antisymmetric eigenvalues

$$\phi_S = \frac{1}{\sqrt{2}}(\phi_1+\phi_2)$$

$$\phi_A = \frac{1}{\sqrt{2}}(\phi_1-\phi_2)$$

Energy eigenvalues:

$$E_S = E_0 - K = E_{1s} + \frac{e^2}{R} - J - K$$

$$E_A = E_0 + K = E_{1s} + \frac{e^2}{R} - J + K \qquad E_A > E_S$$

minimize E_s with respect to separation R.

Molecular binding energy (energy required to pull molecule apart, leaving neutral H + proton)

$-E_b = E - E_{1s} = \frac{e^2}{R} - J \mp K$ (plotted on next page)

		exp
$R_{min} =$	$1.32\,\mathring{A}$	$1.06\,\mathring{A}$
$-E_b =$	$-1.77\,eV$	$-2.7\,eV$

state ϕ_A is unbound for any separation R.

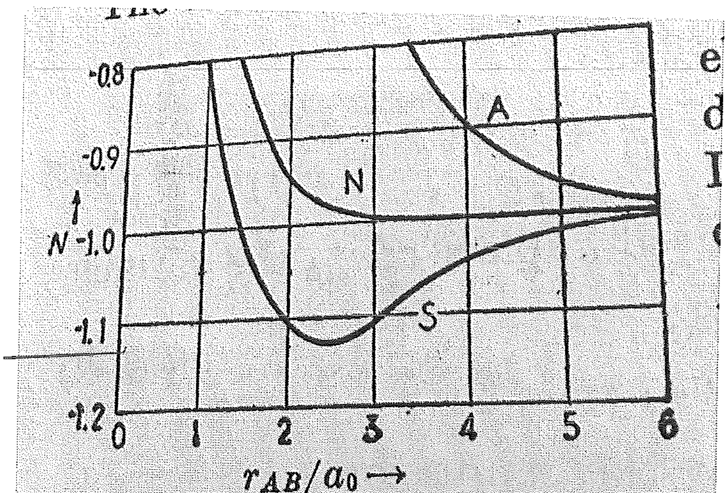
Binding state ϕ_s due to tunneling "sharing" of electron

Date: March 4, 2020 at 11:15 AM
Topic: h-ion-energy

From Pauling and Wilson <u>Introduction to Quantum Mechanics</u>

$\frac{E}{|E_{1s}|}$

E_{min} -1.13



Min of Symmetric state is

$E_{min} = -1.13\,(13.6\,eV)$

$-E_b = E_{min} - (-13.6\,eV)$

$= 0.13\,(-13.6\,eV)$

$= -1.77$ eV

FIG. 42–2.—Energy curves for the hydrogen molecule-ion (in units $e^2/2a_0$), calculated for undistorted hydrogen atom wave functions.

The separation between hydrogen atoms is here R=r_AB.
Curve A is for the anti-symmetric state energy, curve S is for the symmetric state energy and curve N is for the energy state
if the tunneling energy K is set to zero. Only the curve S has a stable minimum, curves N,A show repulsion for all values of the separation.

The corresponding frequency for which the electron "jumps" back and forth between the 2 atoms is 2K/h (h=Planck's constant).