6. Quantum Mechanics 2, 4

lecture 24, October 23, 2017

housekeeping

Exam 2

- Next Friday, October 27
- Thornton and Rex, Chapters 3,4,5, 6.1-6.3

today

more reality quantum mechanics

general solutions: $\psi = A \sin k_1 x \sin k_2 y \sin k_3 z$

$$k_i = \frac{n_i \pi}{L_i}$$

now 3 quantum numbers $n_1 n_2 n_3$.

when the total wavefunction is a product, the energies (eigenvalues) are sums:

(cube): $$E_{n_1 n_2 n_3} = \frac{\pi^2 \hbar^2}{2mL^2} \left(n_1^2 + n_2^2 + n_3^2 \right)$$

with ground state: $$E_{111} = \frac{3\pi^2 \hbar^2}{2mL^2}$$

First excited state $\quad E = \dfrac{6\pi^2\hbar^2}{2mL^2}$ which happens for

$$\left.\begin{array}{ccc} \underline{n_1} & \underline{n_2} & \underline{n_3} \\ 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{array}\right\} \text{3 states, each with same energy}$$

DEGENERACY: states with same energies but different quantum numbers

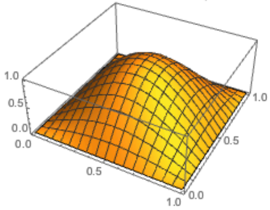
"Lift the degeneracy" .... by the introduction of some asymmetry.

electric or magnetic field

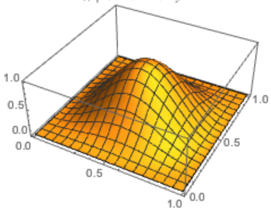
change size of box away from cubic

Two Dimensional, Infinite Well

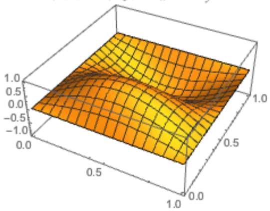
$\psi(x)$ vs $\psi(y)$; $n_x=1, n_y=1$



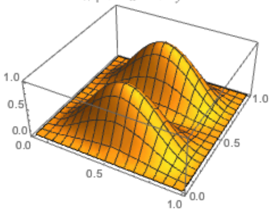
$|\psi|^2$; $n_x=1, n_y=1$



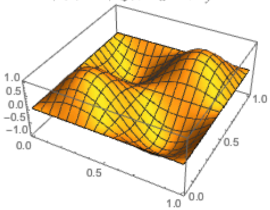
$\psi(x)$ vs $\psi(y)$; $n_x=1, n_y=2$



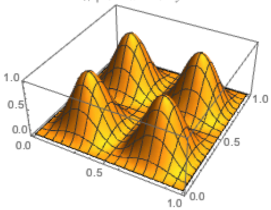
$|\psi|^2$; $n_x=1, n_y=2$



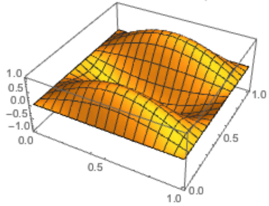
$\psi(x)$ vs $\psi(y)$; $n_x=2, n_y=2$



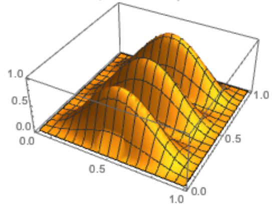
$|\psi|^2$; $n_x=2, n_y=2$



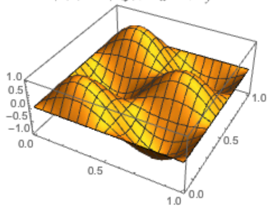
$\psi(x)$ vs $\psi(y)$; $n_x=1, n_y=3$



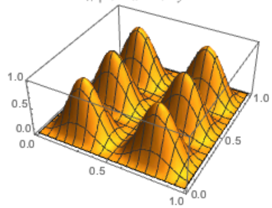
$|\psi|^2$; $n_x=1, n_y=3$



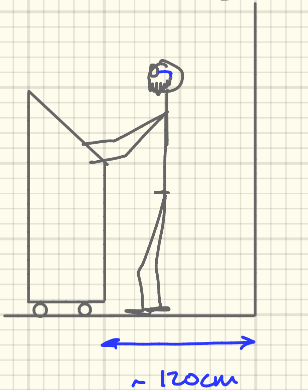
$\psi(x)$ vs $\psi(y)$; $n_x=2, n_y=3$



$|\psi|^2$; $n_x=2, n_y=3$



How about me? w/o my car.



210 lbs dripping wet $\Rightarrow$ $m = 95\,kg$.

3 mph $\Rightarrow$ $v = 1.34\ m/s$

$$E = \tfrac{1}{2} m v^2 = \tfrac{1}{2}(95)(1.34)^2$$

$$E \hat{=} 85\ J$$

What's my quantum number?

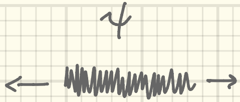
$$E_n = \frac{n^2 \hbar^2 \pi^2}{2 m L^2}$$

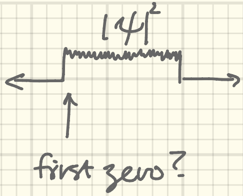
$$n = \sqrt{\frac{2 m L^2}{\hbar^2 \pi^2}} = \sqrt{\frac{2 m L^2 E_n}{(1.05 \times 10^{-34})^2 \pi^2}}$$

$$= \sqrt{\frac{(2)(95)(0.12)^2(85)}{(1.05 \times 10^{-34})^2 \pi^2}}$$

Remember the Correspondence Principle? $\longrightarrow$ $n = 4.6 \times 10^{34}$

my ψ_n ?





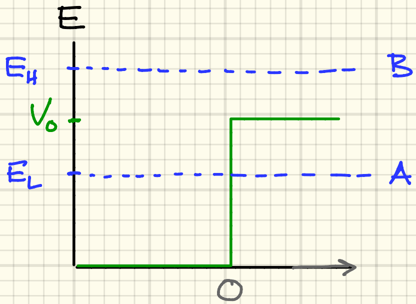
$$\psi_n = \sqrt{\frac{2}{L}}\,\sin\left(\frac{n\pi x}{L}\right)$$

$$|\psi_n|^2 \sim \frac{2}{L}\,\sin^2\left(\frac{4.6\times10^{34}}{0.12}\cdot\pi x\right) = \frac{2}{L}\,\sin^2\left(1.2\times10^{36}\,x\right)$$

1^{st} zero at $x \cong 3\times10^{-36}$ m

so, $|\psi|^2$ is effectively smooth

POTENTIAL BARRIER



2 situations:

A. $E < V_0$
$\shortparallel$
E_L

B. $E > V_0$
$\shortparallel$
E_H

A. Energy less than the barrier

Total energy. $E = \frac{p^2}{2m} + V_0 = \text{constant}$.

if $E < V_0$ then $E - V_0 = \frac{p^2}{2m} < 0 \Rightarrow p$ imaginary.

can't happen classically.

Classically: bounce off, so $|p_{before}| = |p_{after}|$

Solve S.E.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x) \qquad x<0$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\,\psi(x) = E\,\psi(x) \qquad x>0$$

$\boxed{x<0}$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}E\,\psi(x)$$

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

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$$

general solution:

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

$\boxed{x > 0}$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x) \qquad x > 0$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E - V_0)\psi(x)$$

$$\frac{d^2}{dx^2}\psi(x) = \underbrace{\frac{2m}{\hbar^2}(V_0 - E)}_{\alpha^2}\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} = \alpha^2\psi(x)$$

general solution: $\psi(x) = Ce^{\alpha x} + De^{-\alpha x} \qquad x > 0$

$$\psi(x) = A e^{ikx} + B e^{-ikx} \qquad x < 0$$

$$\psi(x) = C e^{\alpha x} + D e^{-\alpha x} \qquad x > 0$$

The boundary conditions allow us to solve for A, B, C, and D

$\psi(x)$ must be continuous

$\frac{d\psi(x)}{dx}$ must be continuous

$\psi(x) \to 0$ as $x \to \infty$ $\longrightarrow$ for $x > 0$ $\psi(x) \to \infty$ unless $C = 0$

$$\psi(x) = A e^{ikx} + B e^{-ikx} \qquad x<0$$

$$\psi(x) = C e^{\alpha x} + D e^{-\alpha x} \qquad x>0$$

$$\psi(0)_{x<0} = \psi(0)_{x>0}$$

$$A e^{ik0} + B e^{ik0} = D e^{-\alpha 0}$$

① $$A + B = D$$

$$\frac{d\psi(0)_{x<0}}{dx} = \frac{d\psi(0)_{x>0}}{dx}$$

$$A(ik) e^{ik0} + B(-ik) e^{-ik0} = D(-\alpha) e^{-\alpha 0}$$

$$-D \frac{\alpha}{ik} = A - B$$

② $$D \frac{i\alpha}{k} = A - B$$

① + ②

$$A + B = D$$

$$A - B = \frac{i\alpha}{k} D$$

$$2A = D\left(1 + \frac{i\alpha}{k}\right)$$

① − ②

$$2B = D\left(1 - \frac{i\alpha}{k}\right)$$

So, A and B in terms of D:

$x \le 0$: $\psi(x)_< = \frac{D}{2}\left(1 + \frac{i\alpha}{k}\right) e^{ikx} + \frac{D}{2}\left(1 - \frac{i\alpha}{k}\right) e^{-ikx}$

$x \ge 0$ $\psi(x)_> = D e^{-\alpha x}$

Could go through a normalization process.

We can put back time-dependence

$$\Psi(x,t)_< = A e^{ikx} e^{-iEt/\hbar} + B e^{-ikx} e^{-iEt/\hbar}$$

$$= A e^{i(kx - Et/\hbar)} + B e^{i(-kx - iEt/\hbar)}$$

$\longrightarrow$ wave increasing x

incident wave

$\longleftarrow$ wave decreasing x

reflected wave

reflected

form: $\frac{B}{A} = \frac{\left(1 - \frac{i\alpha}{k}\right)}{\left(1 + \frac{i\alpha}{k}\right)}$

incident

the "Reflection coefficient" $\rightarrow$ must refer to probabilities:

$$R = \frac{B^* B}{A^* A} = \frac{\left(1 + \frac{i\alpha}{k}\right)\left(1 - \frac{i\alpha}{k}\right)}{\left(1 - \frac{i\alpha}{k}\right)\left(1 + \frac{i\alpha}{k}\right)} = 1$$

∞ barrier:
always reflected
like classical.

But:

$$\psi(x)_> = D e^{-\alpha x}$$

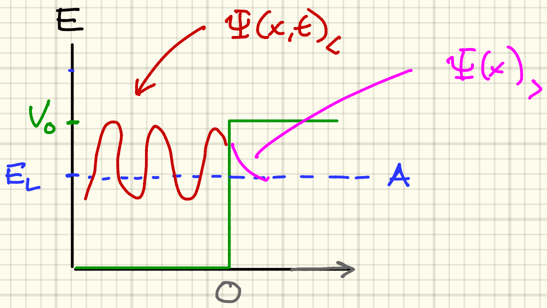
exponentially decreasing.

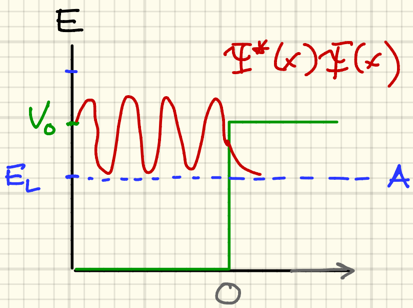
after some work:

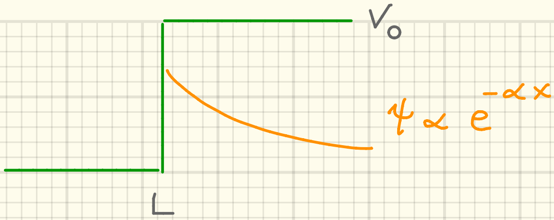
$$\psi(x)_< = D\cosh kx - D\frac{\alpha}{k}\sinh kx$$

$\rightarrow$ a standing wave fn $\Psi(x,t)$

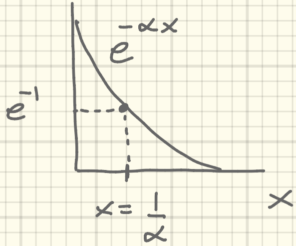
Probability: $\Psi^*(x,t)\,\Psi(x,t)$







characterize "penetration-depth" standard way:



$e^{-1} = 0.368$

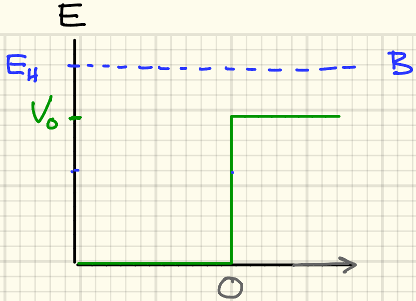
Here $\alpha = \sqrt{\dfrac{2m(V_0 - E)}{\hbar}}$

wave function leaks into the classically-forbidden regions

$$\Delta x = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

for classically-sized objects Δx tiny.

How about B?



Think about it. Since $E_H > V_0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}V\psi = -\frac{2m}{\hbar^2}E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E-V)$$

$x \leq 0$, $V=0$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}E\psi = -k_1^2\psi$$

$x \geq 0$, $V=V_0$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E-V_0)\psi = -k_2^2\psi$$

both waves

$$k_1 = \sqrt{\frac{2m}{\hbar^2}E} = \frac{P_1}{\hbar}$$

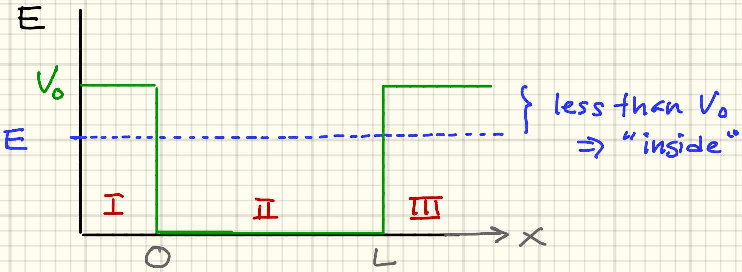
$$k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = \frac{P_2}{\hbar} \Rightarrow P_2 < P_1$$

$$\lambda_2 > \lambda_1$$

MATHEMATICA

FINITE SQUARE WELL

... inside ...



Put classical particle in Region II $\rightarrow$ trapped & confined: $E < V_0$

REGION II

S.E. $\quad V(x) = 0 \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) = \frac{\hbar^2 k^2}{2m}\psi(x)$

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \qquad \frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$$

general solutions:

$$\psi_{II}(x) = Ce^{ikx} + De^{-ikx}$$

standing waves again

REGIONS I & II ?

$V = V_0 \qquad x < 0 \;\&\; x > L$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E - V_0)\psi(x)$$

$$\frac{d^2}{dx^2}\psi(x) = +\alpha^2\psi \qquad \alpha^2 = \frac{2m}{\hbar^2}\underbrace{(V_0 - E)}_{>0}$$

NOTE! There is a solution: → not a classical thing.

General solutions:

$$\psi_I(x) = Ae^{\alpha x} + Be^{-\alpha x}$$ as $x \to -\infty$ $\psi_I \to 0$

$B = 0$

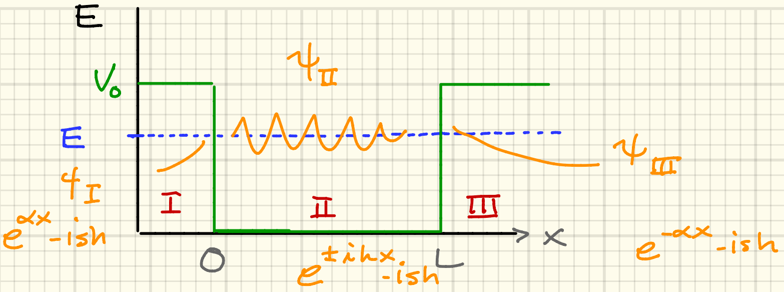
$$\psi_I(x) = Ae^{\alpha x} \qquad x < 0 \; *$$

$$\psi_{III}(x) = Ae^{\alpha x} + Be^{-\alpha x}$$ as $x \to \infty$ $\psi_{III} \to 0$

$A = 0$

$$\psi_{III}(x) = Be^{-\alpha x} \qquad x > 0 \; *$$

* BOTH – exponential



$$\psi_{II}(x) = Ce^{ikx} + De^{-ikx}$$

$$\psi_I(x) = Ae^{\alpha x}$$

$$\psi_{III}(x) = Be^{-\alpha x}$$

Actually, hard to solve

Energy

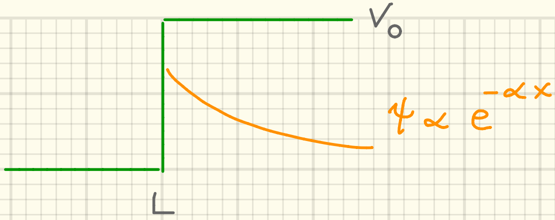
$$E_n = \frac{n^2\pi^2\hbar^2}{2m(L + 2/\alpha)^2}$$

$$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

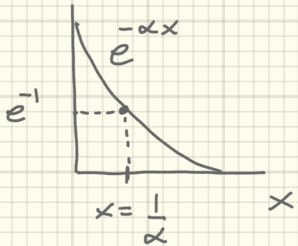
is energy-dependent*

iterate:

1) estimate E
2) calculate α
3) plug into E_n
4) get new E
5) recalculate α
6) .. etc until precision is acceptable



characterize "penetration-depth" standard way:

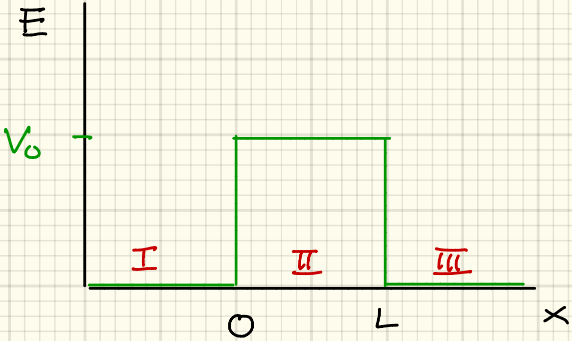


$e^{-1} = 0.368$

Here $\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

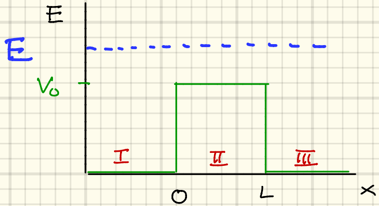
wave function <u>leaks</u> into the classically-forbidden regions

BARRIERS AND TUNNELING

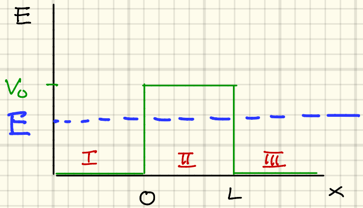


TWO CIRCUMSTANCES:

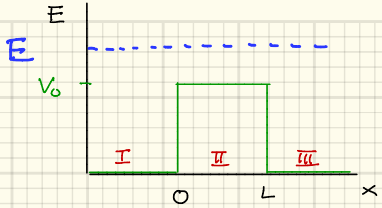
A. $E > V_0$



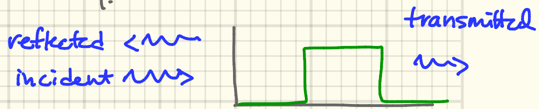
B. $0 < E < V_0$



A.



Assume particles move $\longrightarrow$ initially.



I. $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_I(x) = E\psi_I \qquad u=0$$

$$\frac{d^2}{dx^2}\psi_I = -k^2\psi_I(x) \longrightarrow \psi_I(x) = Ae^{ikx} + Be^{-ikx} \qquad k^2 = \frac{2mE}{\hbar^2}$$

II $$\frac{d^2}{dx^2}\psi_{II}(x) + \frac{2m(E-V_0)}{\hbar^2}\psi_{II}(x) = 0 \qquad q^2 \equiv \frac{2m(E-V_0)}{\hbar^2} > 0$$

$$\frac{d^2\psi(x)}{dx^2} = -q^2\psi(x) \longrightarrow \psi_{II}(x) = Ge^{iqx} + Fe^{-iqx}$$

III same S.E. as I.

$$\psi_{III}(x) = Ce^{ikx} + De^{-ikx}$$

$\hookrightarrow$ $D=0$ (nothing incident from RHS)

Boundary Conditions:

$\psi(x)$ and $\frac{d\psi(x)}{dx}$ must be continuous

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$
$$\psi_{II}(x) = Ge^{iqx} + Fe^{-iqx}$$
$$\psi_{III}(x) = Ce^{ikx}$$

at $x=0$ $\qquad \psi_I(0) = \psi_{II}(0)$

$$A + B = G + F$$

$x=a$ $\qquad \psi_I(a) = \psi_{II}(a)$

$$Ge^{iqa} + Fe^{-iqa} = Ce^{ika}$$

$x=0$ $\qquad \frac{d\psi(0)_I}{dx} = \frac{d\psi_{II}(0)}{dx}$

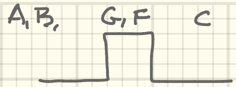
$$Aik\,e^{ik0} + B(-ik)e^{-ik0} = iqGe^{iq0} + F(-iq)e^{-iq0}$$

$$k(A-B) = q(G-F)$$

$x=a$ $\qquad \frac{d\psi(a)_I}{dx} = \frac{d\psi(a)_{II}}{dx}$

$$iqGe^{iqa} - iqFe^{-iqa} = ikCe^{ika}$$

4 equations, 5 unknowns $\quad A, B, G, F, C$



Make ratios: $\left|\frac{C}{A}\right|^2 \rightarrow$ like a transmission past the barrier

$$\vdots$$

$$T = \left|\frac{C}{A}\right|^2 = \frac{4E(E-V_0)}{V_0^2\sin^2 qa + 4E(E-V_0)}$$

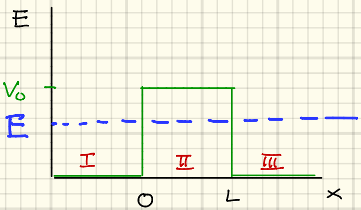
$$\left|\frac{B}{A}\right|^2 = R \quad \text{like reflection}$$

$$R = \frac{V_0^2\sin^2 qa}{V_0^2\sin^2 qa + 4E(E-V_0)} \qquad \neq 0 \quad \text{if } V_0 \neq 0$$

if $V_0 \to 0$ $\quad T \to 1$ and $R \to 0$

now... for the fun part $\longrightarrow$

B.



I. $\psi_I(x) = Ae^{ikx} + Be^{-ikx}$ ✓

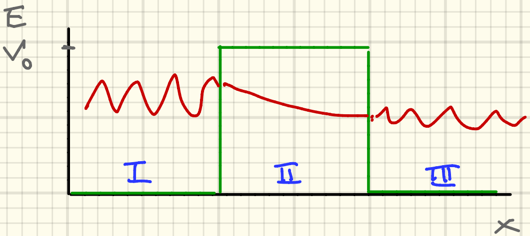
II. define: $q^2 \equiv \dfrac{2m(E-V_0)}{\hbar^2} > 0$

like the step, $E - V_0 < 0$ so $q = \sqrt{\dfrac{2m(E-V_0)}{\hbar^2}}$ is imaginary

$q = \dfrac{i}{\hbar}\sqrt{2m(V_0-E)}$ $\quad q \equiv \dfrac{i}{2\delta}$; $\delta = \dfrac{\hbar}{\sqrt{8m(V_0-E)}}$

$\psi_{II} = Ge^{-\frac{x}{2\delta}} + Fe^{\frac{x}{2\delta}}$

III. $\psi_{III}(x) = Ce^{ikx}$ as before.



same energy / frequency I & III

reduced probability III vs I

$$T = \frac{4E(V_0 - E)}{V_0^2 \sinh^2 \frac{L}{2\delta} + 4E(V_0 - E)}$$

if $\neq 0$ transmission happens

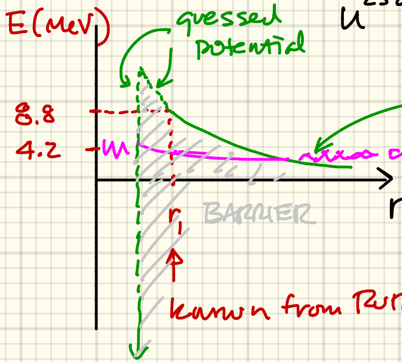
$$R = \frac{V_0^2 \sinh^2 L/2\delta}{V_0^2 \sinh^2 \frac{L}{2\delta} + 4E(V_0 - E)}$$

TUNNELING $\longrightarrow$ huge application and explanatory power

α DECAY — 1928 George Gamow.

U^{238} → α decay with 4.2 MeV α

guessed potential



measured Coulomb-like potential repulsion (+)

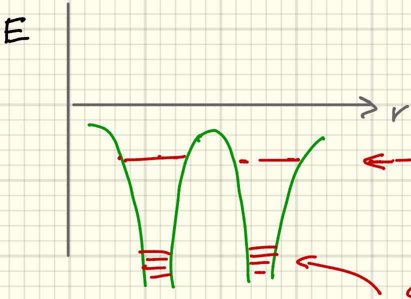
α decay is a tunneling phenomenon

known from Rutherford scattering with 8.8 MeV α

Fusion

$$\underbrace{{}^2H + {}^2H}_{\text{Coulomb barrier} \to \text{D-D apart until they tunnel}} \to {}^3H + n + 6.4\times 10^{-13}\ J$$

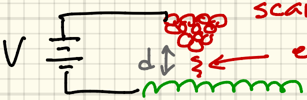
Molecules



← outer electrons can tunnel from one atom to another – shared

deeply bound electrons

Scanning Tunnel Microscopy (STM)



scan tip

electrons tunnel

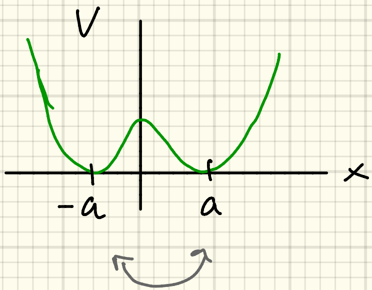
atomic surface

tiny current sensitive to distance, d

- measure potential peaks & valleys
- can deposit electrons

Inversion NH_3 ammonia

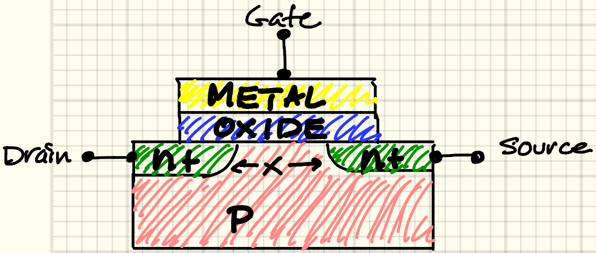
3 H atoms in plane



tunnels from one to the other → radiation emitted

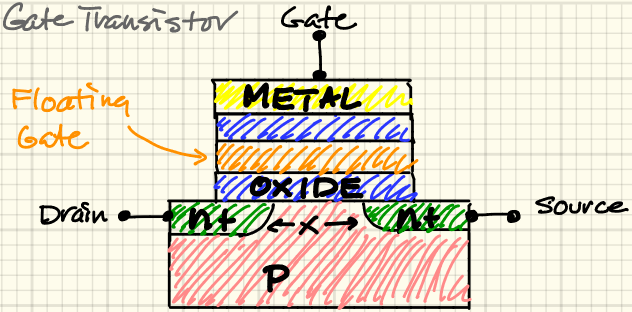
Flash memory.

MOSFET* transitor

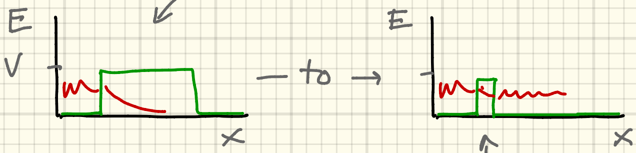


power-off... no charge

Floating Gate Transistor



Gate potential effectively takes!



tunneling into floating gate

power off... floating gate still charged — decades

*Metal oxide field effect transistor