① A Reminder of the Basics of QM

The state of a system is described by its **wave function**

$\Psi(x,t)$ if 1D — continuous, integrable, single valued — contains all the info we can know about the system

Probability amplitude for position

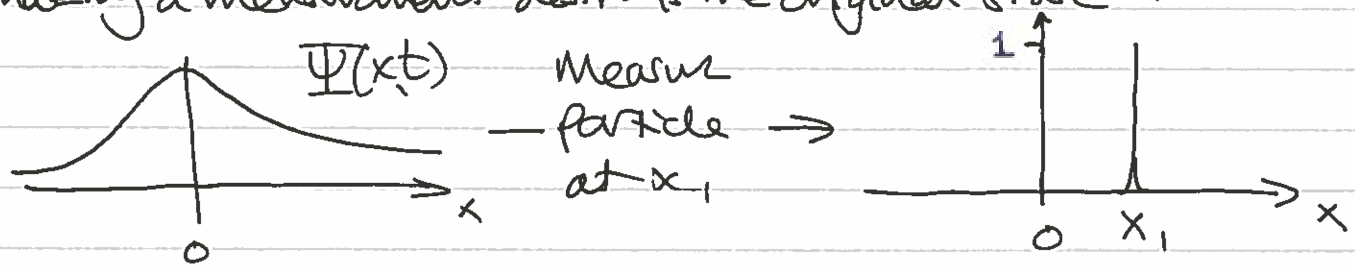
So square it to find prob of particle between x and $x+dx$: $|\Psi(x,t)|^2 . dx$

total prob. is unity $\int_{-\infty}^{\infty} \Psi(x,t) . dx = 1$ — make this so by adjusting a normalisation const. to make this integral unity

→ or expectation value of measurements on many identical copies of a system

QM: non deterministic — can only predict relative probs of outcomes of measurement

Making a measurement destroys the original state.



System left in a new state consistent with the outcome of the measurement — "collapse of wavefunction" irreversible change

The wavefunction obeys a dynamical equation
the time-dependent Schrödinger eq$^{\underline{n}}$ (TDSE)

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

the energy operator or Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r}) \text{ in 3D}$$

"KE + PE"

Q → how to solve it?

Just a PDE so could try to separate the variables
Try $\Psi(\underline{r},t) = \psi(\underline{r}).T(t)$
Substitute into eq$^{\underline{n}}$ and divide both sides by ψT

$$\rightarrow \frac{i\hbar}{T}\frac{dT}{dt} = \frac{1}{\psi}\hat{H}\psi \quad \text{if } \hat{H} \neq \hat{H}(t)$$

fnc of t only — fnc of $\underline{r}$ only

$\underline{r}$ and t are independent variables, make equal to a constant, E.

Get two eq$^{\underline{n}}$s:

$$\frac{dT}{dt} = \frac{-iE}{\hbar}T \qquad \text{Solution: } T = e^{-iEt/\hbar}$$

what's the sol$^{\underline{n}}$?

$$\hat{H}\psi = E\psi$$ the time independent Schrödinger eq$^{\underline{n}}$ (TISE)

This is an example of an "eigenvalue eq$^{\underline{n}}$":

$$\hat{A}\psi(\underline{r}) = a\,\psi(\underline{r})$$

operator — eigenvalue (a number) — eigenfunction

= the only possible outcomes of measuring an observable represented by $\hat{A}$.

In QM, physical observables represented by operators of a special kind called Hermitian.

$$\int \psi_1^* \hat{A}\psi_2 \, d^3\underline{r} = \int (\hat{A}\psi_2)^* \psi_1 \, d^3\underline{r}$$

(eigenvalues = the only outcomes of the measurement of an observable)

Hermitian property guarantees eigenvalues are real numbers.

TDSE is a linear PDE so superpositions of eigenfunctions are also solutions:

$$\Psi(\underline{r}, t) = \sum_n c_n \psi_n(\underline{r}) T_n(t)$$ is a general sol$^{\underline{n}}$.

c_n ← a number

ie. wavefunction is <u>not</u> necessarily an eigenfunction.

If a system does have a wavefunction that is an eigenfunction of $\hat{A}$, a measurement of that quantity results in the corresponding eigenvalue. with 100% probability.

If it has some arbitrary initial wavefunction, a measurement resulting in one particular eigenvalue causes the wavefunction to collapse into the corresponding eigenfunction.

Solutions to TISE are eigenfunctions of $\hat{H}$ and if Ψ is one of these

$$\langle \hat{H} \rangle = \langle \Psi | \hat{H} | \Psi \rangle$$

= eigenvalue with no time dependence.

→ "stationary states"

(although wavefunc itself is time dep)

PROVE THIS!

what systems have these eigenvalues:

(i) $E_n \propto n^2$ where n integer — inf sq well

(ii) $E \propto n + 1/2$ — harm osc — what are conditions on n?

(iii) $E \propto -\frac{1}{n^2}$ — hydrogen atom

Introduction to
(2) Quantum Tunnelling

TISE: $\hat{H}\psi = E\psi$

Classically in 1D for a particle

$$H = \frac{p^2}{2m} + V(x)$$

replace with quantum operators

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

TISE: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$ a differential eq$^{\underline{n}}$.

Take simplest case: a constant potential $V(x) = V_0$

(i) classically allowed if $E > V_0$ [take care with signs, write in terms of positive quantities]

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\underbrace{(E-V_0)}_{\text{a positive \# as } E>V_0}\psi$$

$$= -k^2\psi$$

Sol$^{\underline{n}}$: $\psi(x) = Ae^{ikx} + Be^{-ikx}$ spatial parts of Right and left going waves
A and B constants of integration.

(ii) classically forbidden if $E < V_0$

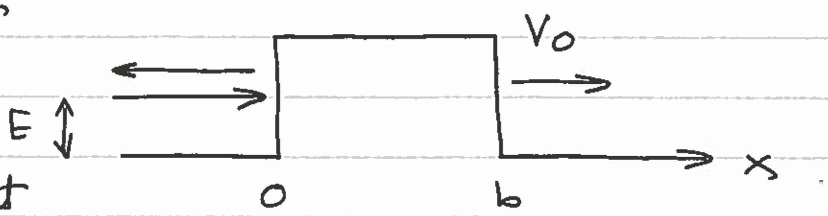
$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\underbrace{(V_0-E)}_{\text{a positive \# as } V_0>E}\psi$$

$$= \beta^2\psi$$

Sol$^{\underline{n}}$: $\psi(x) = Ce^{\beta x} + De^{-\beta x}$

i.e. probabilities are not zero and particles can sneak into this region.

Simple Square Barrier



Particles incident on a barrier of height V_0 with energies E where $E < V_0$

For $x < 0$: $\psi(x) = \underbrace{Ae^{ikx}}_{\text{incident}} + \underbrace{Be^{-ikx}}_{\text{reflected}}$ $\qquad k^2 = \frac{2mE}{\hbar^2}$

(classically all there is!)

For $0 < x < b$: $\psi(x) = Ce^{\beta x} + De^{\beta x}$ $\qquad \beta^2 = \frac{2m}{\hbar^2}(V_0 - E)$

(tunnel under)

For $x > b$: $\psi(x) = Fe^{ikx}$

(might emerge)

Boundary conditions: ψ continuous (part of unambiguous def^n of prob; ensures mom is well def^d)

$\frac{d\psi}{dx}$ continuous (unless infinite discontinuity in $V(x)$)

At $x = 0$ $\qquad \psi(0) = A + B = C + D \quad (e^{ik0} = ?)$

$$\left.\frac{d\psi}{dx}\right|_{x=0} = ik(A - B) = \beta(C - D)$$

At $x = b$ $\qquad \psi(b) = Ce^{\beta b} + De^{-\beta b} = Fe^{ikb}$

$$\left.\frac{d\psi}{dx}\right|_{x=b} = \beta(Ce^{\beta b} - De^{-\beta b}) = ikFe^{ikb}$$

As A determined by incoming intensity, four unknowns (B, C, D, F) and four linear eq^{n}s $\rightarrow$ solvable

"straightforward but tedious"

$$\frac{|F|^2}{|A|^2} = \left| \frac{4ik\beta e^{-ikb}}{e^{-\beta b}[2ik\beta - k^2 + \beta^2] + e^{\beta b}[2ik\beta - k^2 - \beta^2]} \right|^2$$

We're interested in prob of tunnelling

prob of incoming particle finding $|\Psi_{incident}(x<0)|^2 = |A|^2 \, |\cancel{e^{ikx}}|^2 = |A|^2$ $\quad e^{ikx} \cdot e^{-ikx}$

prob of finding tunnelled particle $|\psi(x>b)|^2 = |F|^2$

so probability of getting through $= \frac{|F|^2}{|A|^2}$ = hideous general expression. $[\beta_0^2 \propto V_0]$.

But if high, wide barrier $\beta b > 1$ and $e^{-\beta b} \ll 1$ and get a much simpler formula:

$$\frac{|F|^2}{|A|^2} = \underbrace{\frac{16k^2\beta^2}{(k^2+\beta^2)^2}}\ \underbrace{e^{-2\beta b}}$$

weak energy dependence $[\beta^2$ and k^2 linear in $E]$ in many practical situations is a factor of $\sim \frac{1}{10}$ to 10.

$$= \frac{16E(V_0 - E)}{V_0^2}$$

extremely strong energy dependence [eg. change exponent by $\times 5$ change exponential by $\times 100$]

Define a tunnelling factor $T = e^{-2\beta b}$

$$= \exp\left[-2b \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \right]$$

Gamow Factor

often used as an estimate in probabilities. (would need full expression if ~~very~~ accurate)

Example

to remove electron from metal need energy equal to the "work function", W

$$V_0 - E = W \sim \text{few eV say 4 eV typically}$$

$$\beta = \sqrt{\frac{2mW}{\hbar^2}} = \frac{1}{\hbar c}\sqrt{2mc^2 W}$$

Save mistakes and avoid SI units: put in factors of c and use rest masses in sensible units eg. $m_e = 0.511\ \text{MeV}/c^2$

W already in eV.

What about $\hbar c$? $\hbar c = 197\ \text{eV.nm} = 197\ \text{MeV.fm} = 200\ \text{TeV.zm}$

atoms nuclei particles

Prove from SI units then REMEMBER!

$$\beta = \frac{1}{\hbar c}\sqrt{2m_e c^2 . W} = \frac{1}{197}\sqrt{2 \times 0.511 \times 10^6 \times 4} = 10.3\ \text{nm}^{-1}$$

If the gap is $b = 5\text{nm}$ ($\sim$ 25 atoms)

$$T = e^{-2\beta b} \sim e^{-100} \sim 10^{-44}$$

Atom ~ 0.1 nm radii

If the gap is $b = 1\text{nm}$ ($\sim$ 5 atoms)

$$T = 2 \times 10^{-9}$$

Important:

(i) at nm scales electrons will leak through insulators
→ limitation on circuit miniturisation

(ii) scanning tunnelling microscope: tiny distances from probe to surface, even at fraction of atomic radius, give measurable current changes

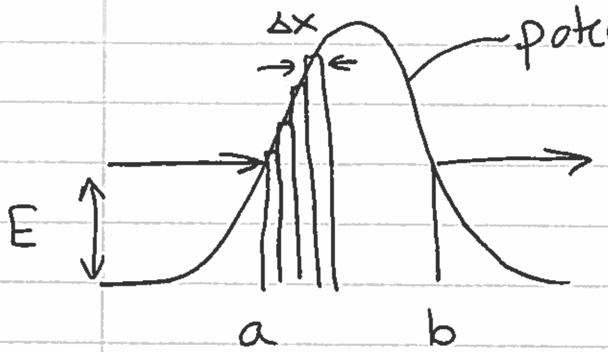
(iii) QM will be important in nanoscale physics

(iv) FLASH memory.

Less "Simple"

(3) Tunnelling through Barriers.

What about barriers which are not finite sq?



Approximate with a series of sq barriers across the classically forbidden zone ($E<V$) with width Δx.

Provided each is high enough to apply approx used last time probability of tunnelling through one of them is:

$$T(x_n) \sim \exp\left[-2\Delta x\sqrt{\frac{2m}{\hbar^2}\left[V(x_n)-E\right]}\right]$$

Total probability of getting out is the product of these

$$T = T(x_1)\,T(x_2)\ldots T(x_n)$$

$$= \exp\left[-2\sum_{n=1}^{N}\sqrt{\frac{2m}{\hbar^2}\left[V(x_n)-E\right]}\,.\,\Delta x\right]$$

(Product of exponentials = exponential of sum)

As $\Delta x \to 0$, sum becomes an integral

$$T = \exp\left[-2\int_a^b\sqrt{\frac{2m}{\hbar^2}\left[V(x_n)-E\right]}\,dx\right]$$

Wentzel-Kramers-Brillouin (WKB) approximation
Good for tunnelling through smoothly varying barriers at energies well below the top.

[Would need corrections for region at ends where approximation of wavefunction fails and $E \sim V$]

why does the sun shine?

Example: thermonuclear fusion

Sun = ionised gas of electrons, protons and light nuclei @ 10^7 K

fuse to produce energy

Consider two protons:

thermal KE $\sim kT \sim 1$ keV

distance of closest approach when

$$KE = \text{Coulomb PE} = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_c}$$

fine structure constant dimensionless.

$$r_c = \frac{e^2}{4\pi\varepsilon_0}\ \frac{1}{KE}$$

NB// $\alpha = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{\hbar c} = \frac{1}{137}$

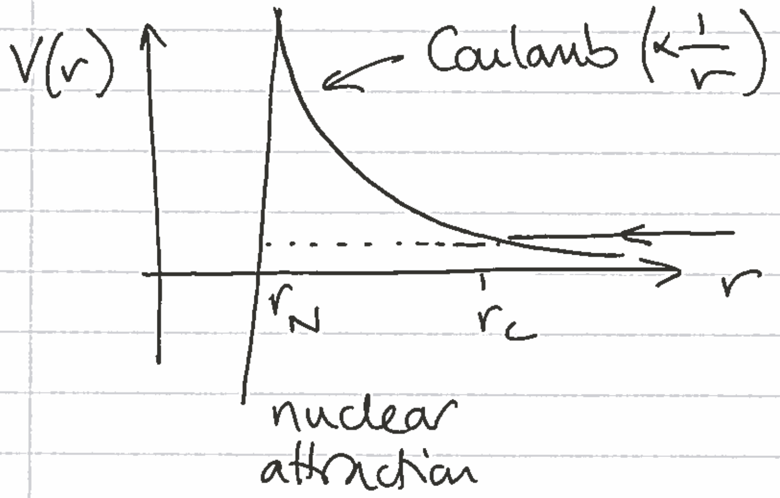
$\hbar c = 197$ MeV fm

$\frac{e^2}{4\pi\varepsilon_0} = \frac{197}{137}$ MeV fm

$$= \frac{197}{137} \times \frac{1}{10^{-3}} \text{ fm}$$

~ 1000 fm except range of nuclear forces is ~ 1 fm

how do they ever get close enough to react?



$r_c \gg r_N$

NB// relative motion of two identical particles use reduced mass $\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{m}{2}$

Tunnelling factor $T = \exp\left[-2\int_{r_N}^{r_c}\sqrt{\frac{2\mu}{\hbar^2}\left(V(r)-E\right)}\,dr\right]$

$$= \exp\left[-2\left\{\frac{2\mu e^2}{4\pi\epsilon_0\hbar^2}\right\}^{1/2}\int_{r_N}^{r_c}\left(\frac{1}{r}-\frac{1}{r_c}\right)^{1/2}dr\right]$$

using $E = V(r_c)$
and $V(r) = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$

[WKB invariably results in horrid integrals.]
Use "standard integral"

$$\int\left(\frac{1}{x}-1\right)^{1/2}dx = \sqrt{x(1-x)} - \cos^{-1}\sqrt{x} + C$$

[subs. $x = \cos^2\theta$ if you want to check it]

$$\int_{r_N}^{r_c}\left(\frac{1}{r}-\frac{1}{r_c}\right)^{1/2}dr$$

change $x = \frac{r}{r_c}$

upper limit $= \frac{r_c}{r_c} = 1$

lower limit $= \frac{r_N}{r_c} \sim 0$ $r_N \ll r_c$

$dr = r_c\,dx$

$r = r_c x$

$$= \int_0^1\left(\frac{1}{x r_c}-\frac{1}{r_c}\right)^{1/2} r_c\,dx$$

$$= r_c^{1/2}\int_0^1\left(\frac{1}{x}-1\right)^{1/2}dx$$

$$\left[= r_c^{1/2}\left[\sqrt{1(1-1)} - \cos^{-1}\sqrt{1} - \sqrt{0} + \cos^{-1}\sqrt{0}\right]\right]$$ skip.

$$= r_c^{1/2}\cdot\frac{\pi}{2}$$

So $T = \exp\left[-\left\{\frac{2\pi^2\mu e^2 r_c}{4\pi\varepsilon_0\hbar^2}\right\}\right] = \exp\left[-\left(\frac{r_c}{R_q}\right)^{1/2}\right]$

where $R_q = \frac{4\pi\varepsilon_0}{e^2}\,\frac{\hbar^2}{2\pi^2\mu}$ again use $\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} = \frac{1}{137}$

$\hbar c = 197\ \text{MeV fm}$

$= \frac{4\pi\varepsilon_0\hbar c}{e^2} \times \frac{1}{2\pi^2\mu c^2} \times \hbar c$

reduced rest mass $= \frac{938}{2}\frac{\text{MeV}}{c^2} \times c^2$

$= 137 \times \frac{1}{\pi^2 \times 938\ \text{MeV}} \times 197\ \text{MeV fm} = 2.9\ \text{fm}$

So $T = \exp\left[-\left(\frac{1400}{3}\right)^{1/2}\right] = e^{-22} \sim 4\times10^{-10}$

A pair of protons has a 1 in 3 billion chance of tunnelling through the Coulomb barrier; ~~having a chance of fusing and releasing thermonuclear energy.~~ within the range of nuclear forces – except they are not actually strong enough to bind two protons!

$p + p \rightarrow {}^2He$? no, diproton isn't bound and falls apart immediately (well in 10^{-22} s)

two protons don't stick so no energy released either!

Hans Bethe 1939 : $p + p \rightarrow {}^2H + e^+ + \nu_e + 0.42\ \text{MeV}$

weak interaction

" diproton β^+ decays during brief moment of fusion " (Nobel Prize 1967)

chances of reaction very low even if fused

"main" reactions of hydrogen burning

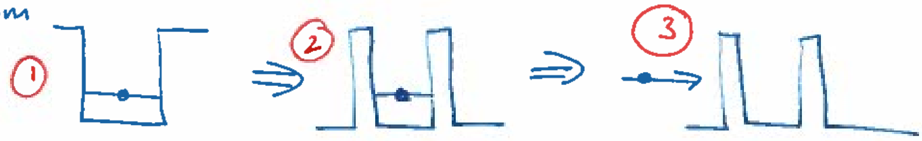
Deuterons then go into other stages: ${}^2H + p \rightarrow {}^3He + 5.49\ \text{MeV}$

and ${}^3He + {}^3He \rightarrow \alpha + 2p$

Overall: 6 protons in and alpha and 2 protons out : 4 protons used to make He.

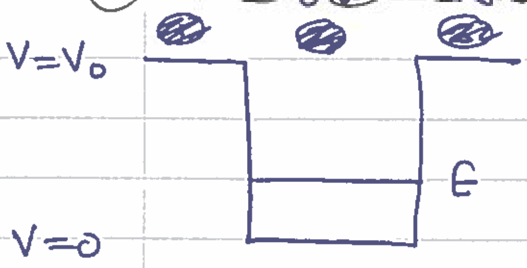
Tunnelling thru two barriers important for loading Qdots with electrons.

Approach by going from



4) Multiple Barriers and Resonant Tunnelling

1) ~~Some reminders about levels in wells~~: Particle in a Sq Well



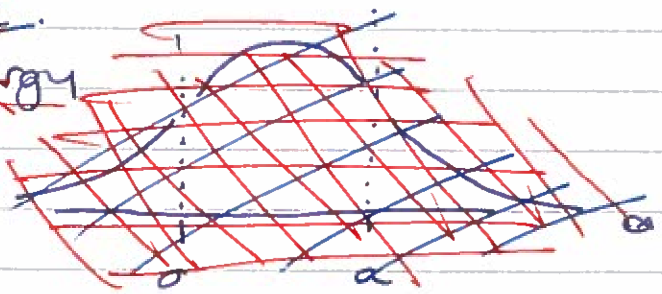
Particle with energy $E < V_0$ in sq. well potential.

$$\psi(x) = Ae^{\beta x} + Be^{-\beta x} \quad x<0$$
$$= Ce^{ikx} + De^{-ikx} \quad 0<x<a$$
$$= Fe^{\beta x} + Ge^{-\beta x} \quad x>a$$

$$\beta^2 = \frac{2m}{\hbar^2}(V_0 - E) \qquad k^2 = \frac{2mE}{\hbar^2}$$

To be normalisable, keep ψ finite so $F=0$ and $B=0$

~~Then looks like~~
~~For lowest energy~~



$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

Apply continuity of ψ and $d\psi/dx$ $\Rightarrow$ 4 eqⁿs plus normalisation condⁿ
5 conditions
but only 4 unknowns!

Solvable if E has special values (eigenvalues).
After tedious algebra, two sets of solⁿs with:

$$k\tan\frac{ka}{2} = \beta \quad \text{or} \quad -k\cot\frac{ka}{2} = \beta$$
$\Rightarrow$ solve numerically for k $\rightarrow$ eigenvalues of E

If $V_0 \gg E$, β gets large, $\tan\frac{ka}{2} \rightarrow \infty$

$$\frac{ka}{2} = \frac{n\pi}{2} \quad n = 1, 3, \ldots$$
[$\tan\theta \Rightarrow \infty$ at $\theta = \pi/2, 3\pi/2 \ldots$]

Similarly for cot
$$\frac{ka}{2} = \frac{n\pi}{2} \quad n = 2, 4 \ldots$$
[infinite when $\tan\theta = 0$ at $\theta = \pi, 2\pi$]

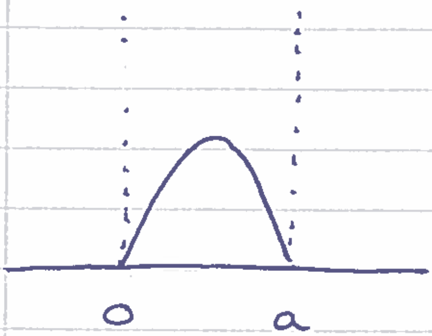
For well with v. high walls : $k = \frac{n\pi}{a}$ $n = 1, 2, 3 \ldots$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

ie. levels in infinite sq well.

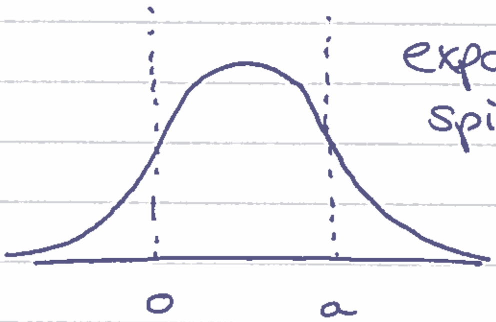
Sketching the gs. wavefunction:

Large V_0



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

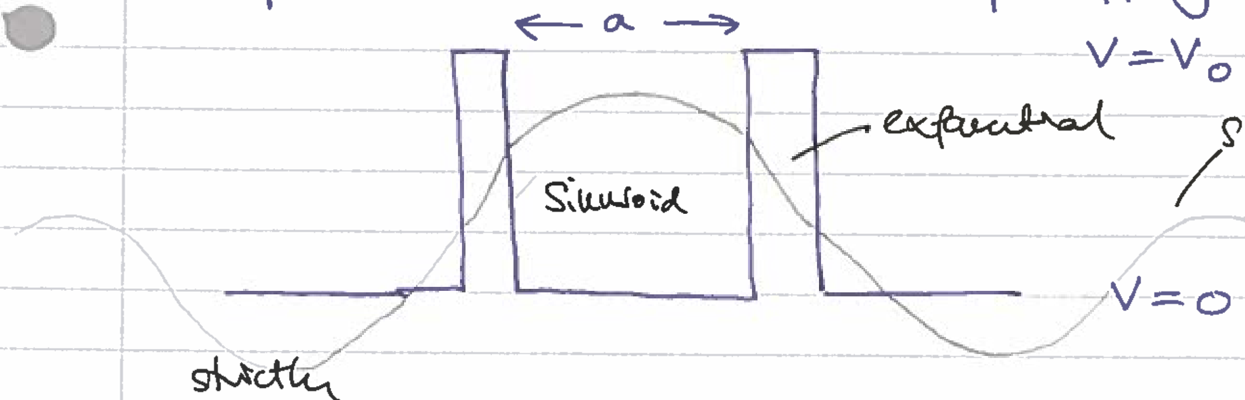
Small V_0



function less curved
"wavelength" longer, $p = h/\lambda$
→ energy levels lower

(ii) Particle inside a double barrier:

Now produce a double barrier by dropping sides:



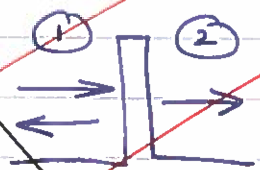
Particle can now leak out the sides by tunnelling.
No stationary states
Wave packet inside will decay away with lifetime τ
(related to tunnelling prob)
Gives an uncertainty in energy via $\Gamma \sim \hbar/\tau$
ie. a "width" a bit like a classically damped resonance

If $E < V_0$, tunnelling prob might be small
τ might be long } talk about quasi bound
Γ small } states.
ie. states with energies similar to infinite sq well but with a finite width.

—//—

Now fire particles at a double barrier:
particles will partially reflect from each barrier → QM Fabry-Perot etalon.

For single barrier:



$$\psi_1(x) = e^{ikx} + r e^{-ikx}$$

incident   fraction reflected

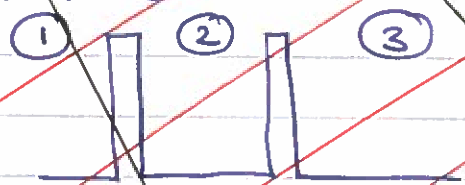
$$\psi_2(x) = t e^{ikx}$$

fraction transmitted.

] unit flux incident
$r = \frac{B}{A}$
$t = \frac{F}{A}$.

Prob reflection $R = |r|^2$ } $R + T = 1$
transmission $T = |t|^2$ }

For double barrier:



NB, Hiding some assumptions that only work for $E < V_0$, but outcomes still valid.

$$\psi_3(x) = |t|^2 \left[1 + |r|^2 e^{2ika} + |r|^4 e^{4ika} + \dots \right] e^{ikx}$$

everything that gets thru tunnels twice

str8 thru

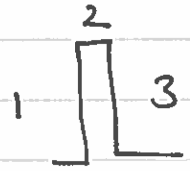
reflects twice before escape travels extra dist 2a

reflects four times

more terms

(iii) Particle incident on double barrier.

Now for a double barrier:
deal with partial reflections between barriers $\Rightarrow$ QM Fabry Perot
Notation:
For single barrier:

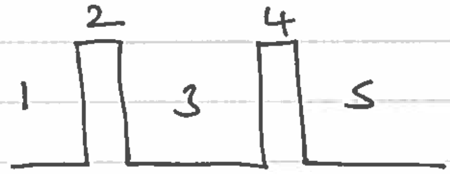


unit flux incident
$r = \frac{B}{A} \quad t = \frac{F}{A}$

$\psi_1(x) = e^{ikx} + r_{13} e^{-ikx}$
$\psi_3(x) = t_{13} e^{ikx}$

subscripts give indication of direction
(which matters for phases – won't go into explicitly)

For double barrier:



$$\psi_5(x) = t_{13}\left[1 + r_{35}r_{31}e^{2ika} + (r_{35}r_{31})^2 e^{4ika} + \dots\right] t_{35} e^{ikx}$$

str8 thru — reflects twice then escapes, travels extra 2a — reflects four times — higher terms

$$= t_{13} \sum_{n=0}^{\infty} \left(r_{35}r_{31} e^{2ika}\right)^n t_{35} e^{ikx} \quad \text{geometric series}$$

$\sum^{\infty} aR^n = \frac{a}{(1-R)}$

$$= \frac{t_{13}t_{35}e^{ikx}}{(1 - r_{35}r_{31}e^{2ika})}$$

CRAZINESS

Tunnelling prob $= \left|\frac{t_{13}t_{35}}{1 - r_{35}r_{31}e^{2ika}}\right|^2$

Max if $e^{2ika} = 1$

For symmetric barriers: $|t_{13}| = |t_{35}|$, $|r_{35}| = |r_{31}|$; $t_{13}t_{35} = T$, $r_{35}r_{31} = R$

Tunnelling prob $= 100\% \leftarrow T + R = 1 \leftarrow$ probs for single barrier

For this "resonance tunnelling" condition:

$e^{2ika} = 1$ ie. $\cos 2ka = 1$

$2ka = n.2\pi \quad n = 1, 2, \ldots$

$k = \frac{n\pi}{a}$ ie. occurs at energies where ½ wavelength fits in well.

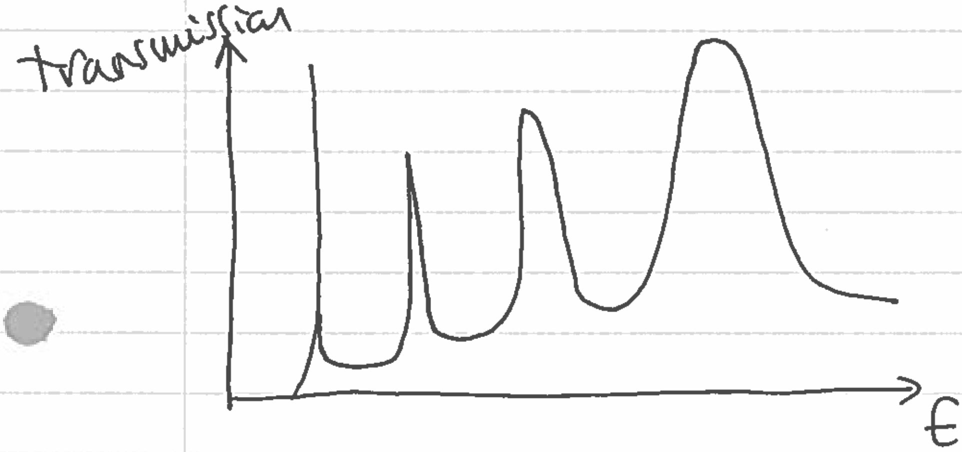
Internally reflected waves travel extra distance which is multiple of wavelength → constructive interference

↓

Large probability of finding particle in the well.

(a route to filling quantum wells)

Corresponds to matching incoming energy to that of quasi-bound states in the well.



Increasing widths towards higher energy

as tunnelling out is easier

so quasibound levels decay quicker

so widths larger.

Examples: quantum dots

resonant tunnelling diodes

graphene – BN – graphene atomic layers

resonances in nuclear fission.