Quantum Physics (Intro to Quantum Physics)

1.4 Action

Define the action for a trajectory or path as:

$S = \int_A^B \underline{p} \cdot d\underline{x}$ $\quad ML^2T^{-2}$

Integral of momentum × position, unit of action same as for angular momentum.

$S = \int_{t_A}^{t_B} E\,dt$ $\quad J \cdot s \equiv kg\,m^2 s^{-1}$

Total action is $\int_A^B \underline{p} \cdot d\underline{x} + \int_{t_A}^{t_B} E\,dt$

2.1 Wave basics

$u(x,t) = a\cos(kx - wt + \phi)$

$k = \frac{2\pi}{\lambda}$ (wave vector)

$w = 2\pi\nu$ (angular frequency)

Complex representation

Recall $e^{i\theta} = \cos\theta + i\sin\theta$

$u(x,t) = \frac{a}{2}[\exp(i(kx - wt + \phi)) + \exp(i(-kx + wt - \phi))]$

$= Re(ae^{i\phi} e^{i(kx-wt)})$

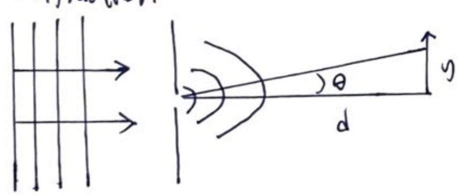
$= Re(Ae^{i(kx-wt)})$

Define intensity as the square of amplitude a:

$I = (ae^{i\phi})(ae^{-i\phi}) = AA^* = a^2$

2.2 Diffraction and Interference

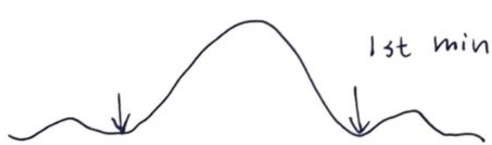
Diffraction



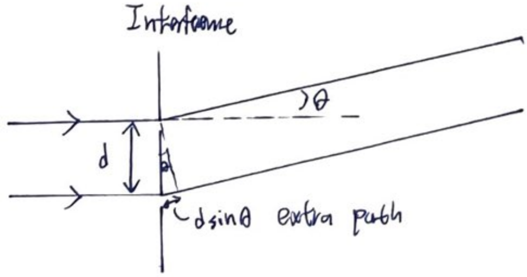
$\theta \simeq \frac{y}{d}$ (small angle)

$I(\theta) = I_0\left[\frac{\sin(\pi w \theta/\lambda)}{(\pi w \theta/\lambda)}\right]^2$

spread $\theta \sim \frac{\lambda}{w}$ since $\theta_{min} = \frac{\lambda}{w}$ gives $I(\theta) = 0$

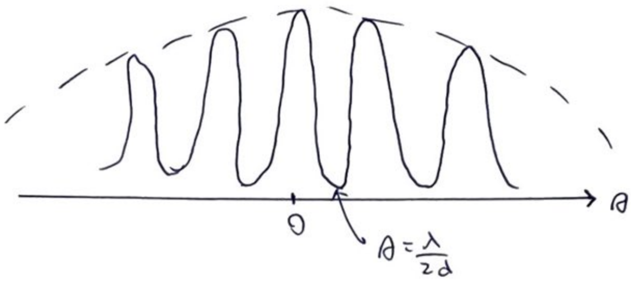


Interference



destructive: $\Delta L = \underbrace{m}_{odd} \frac{\lambda}{2} = d\sin\theta$

constructive: $\underbrace{m}_{even} \frac{\lambda}{2} = d\sin\theta$



envelope from single slit

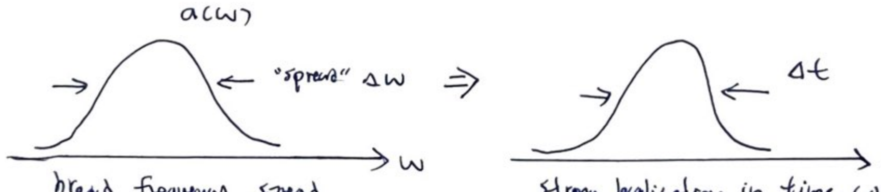
$$I = u \cdot u^* = 4a^2 \cos^2\left(\frac{kd\sin\theta}{2}\right)$$

3.1 Synthesis of short pulses

Superposition $\sum_i a_i \cos(k_i x - \omega_i t + \phi_i)$

For many frequencies $\sum \rightarrow \int$

$$u(x,t) = \int_{-\infty}^{\infty} \underbrace{a(\omega)}_{\text{spectrum}} \cos(k(\omega)x - \omega t - \underbrace{\phi(\omega)}_{\text{spectral phase}})\, d\omega$$



broad frequency spread ⇒ strong localisation in time (short pulse)

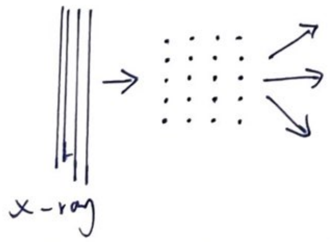
Rule from Fourier theory

$$\Delta t \Delta \omega \gtrsim \text{constant}$$

For gaussian form in t and ω in terms of full width at half-maximum.

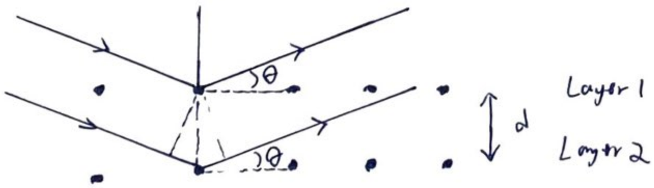
$$\Delta t \Delta \nu \gtrsim 0.44$$

3.3 X-ray diffraction



strong diffraction / interference.

To analyze this consider reflection of x-rays from crystal planes



extra path from layer 2 : $2d\sin\theta$

For reflectors to add constructively :

$n\lambda = 2d\sin\theta$ n is integer

4.1 Waves in a cavity

Cavity can support standing wave light modes that satisfy:

$$L = m\frac{\lambda}{2} \quad \text{or} \quad \lambda = \frac{2L}{m}$$

Concept of modes can be generalised to a 3-d cavity, density of modes $\propto \nu^2$

4.2 Blackbody radiation

Wien's displacement law

The wavelength at which emission maximised λ_{max}

$$\lambda_{max} = \frac{b}{T} \quad (\text{hotter} \to \text{bluer})$$

$b = 2.9 \times 10^{-3}\ mK$

Stefan's law

Total power radiated per unit area

$$P = \sigma T^4$$

$\sigma = 5.67 \times 10^{-8}\ W m^{-1} K^{-4}$ (hotter → much brighter)

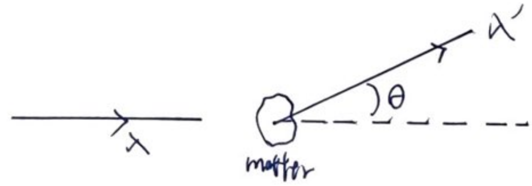
5.1 Photoelectric effect

- Light beam comprised of particles or packets of energy
- $E = h\nu$
- current depends on intensity once $\nu > \nu_0$ where $h\nu_0 = W_f$
- $E_{KE} = h\nu - W_f$

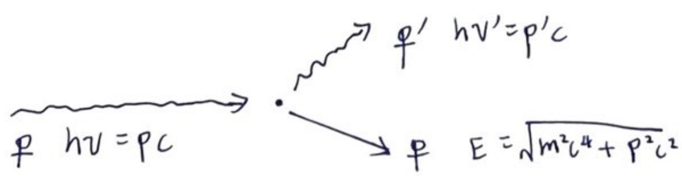
5.2 Compton Scattering

$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

- Found scattered X-rays at longer wavelength
- λ' depended on θ



- Assumed $E = h\nu = pc \to p = \frac{h}{\lambda}$ (photon momentum)



- Energy conservation: $pc + mc^2 = p'c + \sqrt{m^2c^4 + p^2c^2}$
- momentum conservation: $p^2 = (p - p')^2 + 2pp'(1 - \cos\theta)$

$$\frac{1}{p'} - \frac{1}{p} = \frac{1}{mc}(1 - \cos\theta)$$

6.2 Matter Waves

de Broglie postulate:

$$p = \frac{h}{\lambda} = \hbar k$$

$$k = \frac{2\pi}{\lambda} \quad \text{and} \quad \hbar = \frac{h}{2\pi}$$

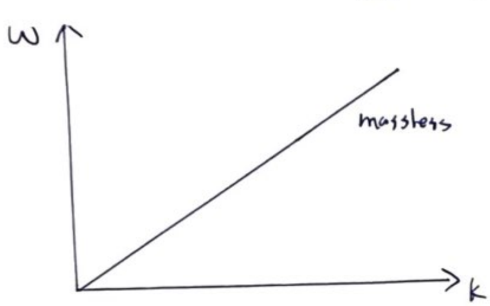
As for photons: $E = \hbar\omega = h\nu$

for matter waves: $E = \frac{p^2}{2m}$

so we have: $\hbar\omega = \frac{(\hbar k)^2}{2m}$

$$\omega = \frac{\hbar k^2}{2m} \quad \text{dispersion relation for finite mass particles}$$

$$\omega = ck \quad \text{For photons (massless particle)}$$



For a particle, since $E = \frac{p^2}{2m}$

$$p = \sqrt{2mE}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \qquad \lambda = \frac{c}{\nu} \text{ for photons}$$

energy / eV	wavelength / m		
	Photon	electron	neutron
1	1.24×10^{-6}	1.22×10^{-9}	2.86×10^{-11}
100	1.24×10^{-8}	1.22×10^{-10}	2.86×10^{-12}
10000	1.24×10^{-10}	1.22×10^{-11}	2.86×10^{-13}

Structure determination needs:

- high energy x-rays ($\gtrsim$ 10 keV)
- medium energy electrons ($\gtrsim$ 100 eV)
- 'thermal' neutrons ($\gtrsim$ 0.1 eV)

7.0 Matter waves

7.1 Free Particles

$$\psi(x,t) = a \exp[i(kx-\omega t)]$$

$$k = \frac{p}{\hbar} \qquad \omega = \frac{E}{\hbar}$$

$$\psi(x,t) = a \exp[i(px - Et)/\hbar]$$

$\psi(x,t)$ is called a wavefunction and such a particle is completely delocalised.

$$I = \psi(x)\psi^*(x) = a^2$$

7.2 Wave packets

We can build a superposition of waves with different $k(p)$

$$\psi(x,t) = \int a(k) \exp(i(kx - \omega(k)t))\,dk$$

To get high localisation, we need a large range of k vectors.

$$\Delta x\,\Delta k \gtrsim \frac{1}{2}$$

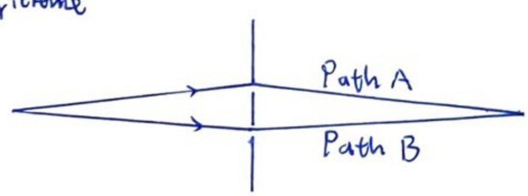
$$\Delta k = \frac{\Delta p}{\hbar} \rightarrow \Delta x\,\Delta p \gtrsim \frac{\hbar}{2}$$

7.3 Interpretation of $\psi(x,t)$

The wavefunction is a probability amplitude:

$$P(x,t) = |\psi(x,t)|^2 = \psi(x,t)\psi^*(x,t)$$

Interference



$$\psi(\theta) = \psi_A(\theta) + \psi_B(\theta)$$

$$P = |\psi_A(\theta) + \psi_B(\theta)|^2$$

If $\psi_A(\theta) = \psi_B(\theta)$ constructive interference

If $\psi_B(\theta) = -\psi_A(\theta)$ destructive interference.

8.0 Probability Distributions & Expected Value

8.1 Probability of discrete events

e.g. coin toss

P_i = probability of ith outcome

$\sum_i P_i = 1$ normalisation

In Quantum Physics: electron spins: up ↑, down ↓

State is represented by α_i

Probability amplitude is c_i

$u = \sum_i c_i \alpha_i \qquad u = \frac{1}{\sqrt{2}}\alpha(\uparrow) + \frac{1}{\sqrt{2}}\alpha(\downarrow)$

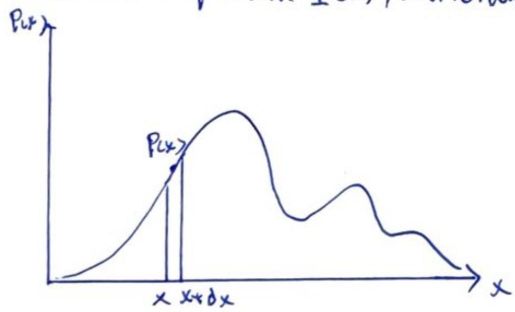
$\sum c_i^2 = 1$

$\sum = \frac{1}{2} + \frac{1}{2} = 1$ so state is normalised.

8.2 Probability Distributions

Classical: Height and weight of people

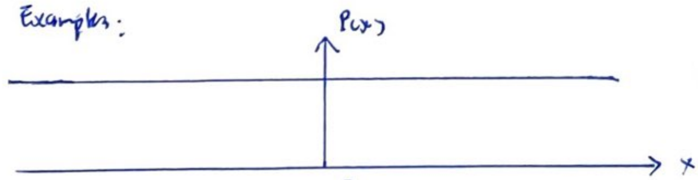
Quantum: position $\underline{r}(x)$, momentum $\underline{p}(p)$



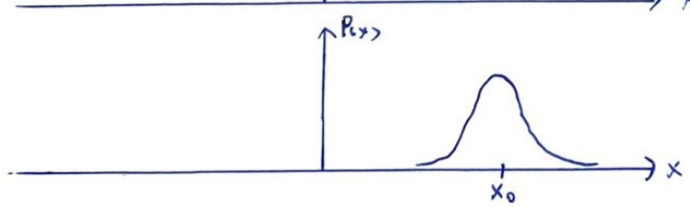
$P(x)dx$ is the probability of finding a particle in the interval x to $x+dx$

$\int_{-\infty}^{\infty} P(x)\,dx = 1$ (particle must be somewhere)

Examples:



free particle
Equal probability everywhere
Hard to normalise



localised particle
Gaussian distribution

8.3 Wavefunctions and Normalisation

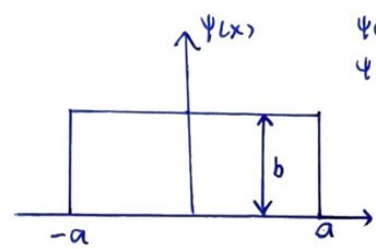
If a wave function describes the position state of a system:

$$P(\underline{r}) = |\psi(\underline{r})|^2$$

and since $\int_{\text{all space}} |\psi(\underline{r})|^2 d\underline{r} = 1$

$\psi(x) = 0 \quad |x| > a$

$\psi(x) = b \quad -a < x < a$



$$\int |\psi(x)|^2 dx = \int_{-a}^{a} b^2\,dx = 1$$

$$b = \frac{1}{\sqrt{2a}}$$

5.4 Expected Value

Discrete case : $\langle x \rangle = \sum_i x_i P_i$

For a distribution : $\langle x \rangle = \int_{-\infty}^{\infty} x \, P(x) \, dx$

For a wavefunction $\psi(x)$

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi(x) \, x \, \psi^*(x) \, dx = \int_{-\infty}^{\infty} x \, |\psi(x)|^2 dx$$

Variance is a measure of spread of the probability distribution

$$\Delta x^2 = \langle (x - \langle x \rangle)^2 \rangle$$

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$

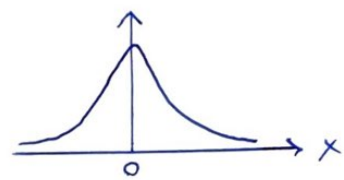
$$\Delta x^2 = \int (x - \langle x \rangle)^2 P(x) \, dx = \langle x^2 \rangle - \langle x \rangle^2$$

example : For a symmetric distribution

$$\langle x \rangle = 0$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx$$

$$\Delta x^2 = \int x^2 P(x) \, dx$$



9.0 Confined Particle

9.1 Particle in a box

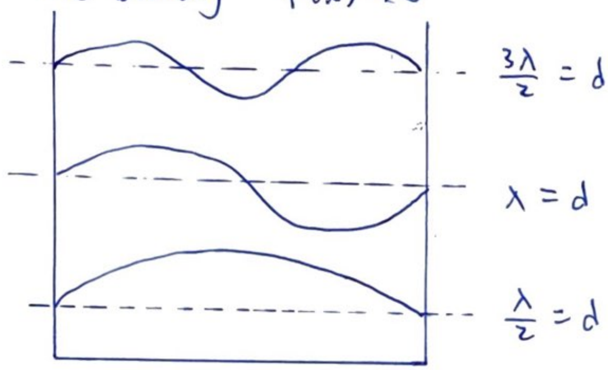
Consider a potential ∞ everywhere except in a region of width d.

In box (Ignoring time dependence)

$$\psi(x) = a \exp\left(i \frac{p}{\hbar} x\right)$$

or $a' \cos\left(\frac{p}{\hbar} x\right)$ or $a' \cos\left(\frac{2\pi}{\lambda} x\right)$

At boundary $\psi(x) \to 0$



Only discrete sets of de Broglie wavelengths exists inside box

$$d = \frac{n\lambda}{2}$$

$$\lambda_{deB} = \frac{2d}{n}$$

But since $p = \frac{h}{\lambda_{deB}}$

$$p = \frac{nh}{2d}$$ (actually $p = \pm \frac{nh}{2d}$) quantisation of momentum

9.2 Energy Quantisation

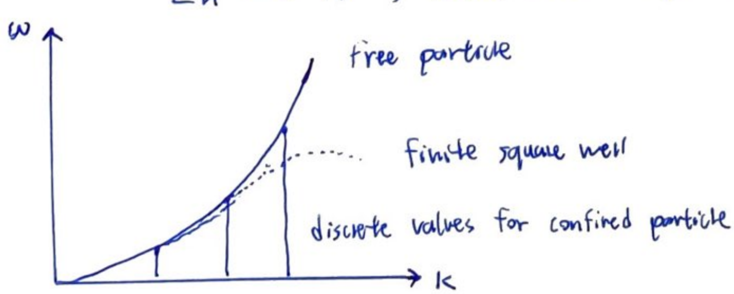
Energy of a particle: $E = V + T$ (V is Potential, T is kinetic)

$V = 0$ inside the box

$$T = \frac{p^2}{2m}$$

$$E_n = \frac{p_n^2}{2m} = \left(\frac{nh}{2d}\right)^2 \frac{1}{2m} = \frac{h^2 n^2}{8md^2}$$ (Energy quantisation)

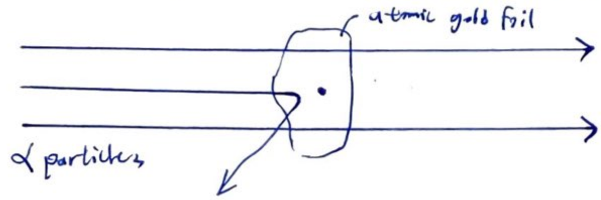
$E_n \propto n^2$, same outcome qualitatively for 3d box



10. The Hydrogen Atom

10.1 Evidence for atoms

Structure of atoms from Rutherford's scattering experiment (1911)

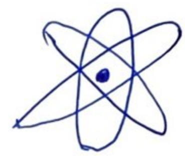


- A few very strong backscattered particles, most passed straight through
- ~~Proved~~ Supported a small massive nucleus.

A 'planetary' model was envisioned

electrons orbiting +ve charged heavier nucleus

Subject to coulomb interaction



$$V(r) = -\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}$$

10.2 Atomic Spectra

Spectra of emission or absorption from atoms in a gas show discrete lines only.

Rydberg fitted the following formula for Hydrogen

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n^2} - \frac{1}{m^2}\right) \qquad n \text{ and } m \text{ are integers}$$

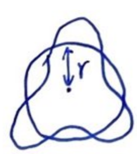
$$R_H = 1.097 \times 10^7 \ m^{-1}$$

10.3 Bohr atom

Both spectra and stability against radiation explained energy quantisation

Bohr proposed: (a theory for confined electron orbit that assumed)

(1) Circular orbits



(2) electron waves, where λ must be an integer multiple of circumference eg. $n\lambda = 2\pi r$

This leads to momentum quantisation

$$p = \frac{h}{\lambda} = \frac{hn}{2\pi} = \frac{n\hbar}{r}$$

Angular momentum

$$L = mvr = n\hbar$$

[Not correct quantisation, but here it doesn't matter]

For orbit, Coulomb force F balanced against centripetal force:

$$F = \frac{e^2}{4\pi\varepsilon_0 r^2} = \frac{mv^2}{r} = \frac{(mvr)^2}{mr^3} = \frac{(n\hbar)^2}{mr_n^3}$$

$$r_n = \frac{4\pi\varepsilon_0 (n\hbar)^2}{m_e e^2}$$

Smallest radius orbit: (n=1)

$$r_1 = a_0 = 5.3 \times 10^{-11}\,m$$

Energy: $E_{total} = T + V$

$$= \frac{1}{2}mv^2 - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$= \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 r} - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$= -\frac{e^2}{2(4\pi\varepsilon_0)r_n} \quad \text{(sub } r_n\text{)}$$

$$E_n = \frac{-me^4}{2(4\pi\varepsilon_0\hbar)^2 n^2}$$

$$E_n = -\frac{13.6}{n^2}\,eV$$ For hydrogen like atoms

11.0 Observables and Operators

11.1 Playing with the maths

1-d free particle

$$\psi(x,t) = a \exp\left[\frac{i}{\hbar}(px - Et)\right]$$

P and E are possible physicals observables. What mathematical operation could be used to extract these quantities from $\psi(x,t)$?

Define an operator associated with a physical observable, A:

$$\hat{A}\psi = A\psi$$

$\hat{A}$ is an operator, just a mathematical operation that acts on a function ψ.

(ψ is an eigenstate/eigenfunction, A is an eigenvalue)

An operator for p (not just for free-particles)

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

Similarly,

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

11.2 Wavefunction: Momentum representation

We could equally have worked in momentum space with a wavefunction $\psi(p)$

$$P(p)\,dp = |\psi(p)|^2 dp$$

Probability that momentum range p to $p+dp$

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

$$\hat{p}\psi(p) = p\psi(p)$$

minimal solution: $\hat{p} = p$, $\hat{x} = x$

11.3 Expectation Values

$$\langle x\rangle = \int_{-\infty}^{\infty} x P(x)\,dx = \int_{-\infty}^{\infty} x\,\psi(x)\,\psi^*(x)\,dx = \int_{-\infty}^{\infty}\psi^*(x)\,\hat{x}\,\psi(x)\,dx$$

Generally for an operator $\hat{A}$, the expection value of observable A:

$$\langle A\rangle = \int_{-\infty}^{\infty}\psi^*(x)\,\hat{A}\,\psi(x)\,dx$$

* Ordering important

example: $\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi(x)\, dx$

11.4 Variance and Uncertainty Relations

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$

$$\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

Similar measures for variance in p:

$$\Delta x \Delta p \gtrsim \frac{\hbar}{2} \quad \text{(position - momentum uncertainty relation)}$$

$\hat{x}$ and $\hat{p}$ are said to be incompatible observables

For infinite square well centered at $x=0$, lowest confined state

$$\Delta x = \sqrt{\langle x^2 \rangle}, \quad \Delta p = \sqrt{\langle p^2 \rangle}$$

Since $\langle x \rangle = 0$ and for a confined particle net momentum $= 0$

Likewise ΔE will be finite since

$$\langle \hat{E} \rangle = \frac{\langle \hat{p}^2 \rangle}{2m} = \frac{\Delta p^2}{2m} = \frac{\hbar^2}{4m\Delta x^2}$$

Zero point energy (more confined, smaller $\Delta x \rightarrow$ higher zero point energy)

Also an energy-time uncertainty relation arises from the bandwidth theorem $\Delta t \Delta \omega \gtrsim \frac{1}{2}$

$$\Delta E \Delta t \gtrsim \frac{\hbar}{2}$$

A very short lived state has a large energy uncertainty.

12 An Operator for Energy of the Schrödinger Equation

12.1 An Operator for energy

Let $\hat{H}$ be the operator that 'measures' the value of the energy observable called the Hamiltonian:

$$\hat{H} \Psi_n = E_n \Psi_n$$

where Ψ_n is the energy eigenstate, E_n is the energy eigenvalue

Classical Physics:

$$E_{Tot} = T + V(\underline{r})$$

we involve the Correspondence Principle

The equivalent of classic and quantum physics under appropriate limit

$$T = \frac{p^2}{2m} \rightarrow \frac{\hat{p}^2}{2m}$$

$$V(x,y,z) \rightarrow \hat{V}(x,y,z)$$

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

In 3d $\frac{\partial}{\partial x} \rightarrow \underline{\nabla}$ (del)

$$\underline{\nabla} = \underline{i}\frac{\partial}{\partial x} + \underline{j}\frac{\partial}{\partial y} + \underline{k}\frac{\partial}{\partial z}$$

$$\hat{p} = -i\hbar\underline{\nabla}$$

$$\frac{\hat{p}^2}{2m} = \frac{(-i\hbar\underline{\nabla})^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ (Cartesian coordinate)

12.2 Time-Independent Schrödinger Equation

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

Consider only 1-d:

$$\hat{H}\psi_n(x) = E_n\psi_n(x)$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}(x)\right]\psi_n(x) = E_n\psi_n(x)$$

Often we can write $\hat{V}(x) = V(x)$, true if $V(x) = f(x^a)$ since $\hat{x} = x$

e.g. $V(x) \propto x^2$ for harmonic oscillator

$V(x) \propto \frac{1}{x}$ for Coulomb potential.

then, $\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi_n(x) = E_n\psi_n(x)$

12.3 Time-Independent Schrödinger equation

Recall
$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = E\psi(x,t)$$

$$\hat{H}\psi(x,t) = E_n\psi(x,t)$$

Equating these we obtain

$$i\hbar\frac{\partial}{\partial t}\psi_n(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}(x,t)\right]\psi_n(x,t)$$

- Solutions of this equation $\Psi_n(x,t)$ are the wavefunctions of states of definite energy
- An energy eigenvalue equation
- Also the wave-equation for matter waves
- $\Psi_n(x,t)$ probability amplitude for position measurements

$\hat{H}$ acts on only spatial part (if $V(x)$ time-independent)

factor $\Psi(x,t) = u(x)\exp(-i\frac{E}{\hbar}t)$ $u(x)$ is spatial dependent part

$$\hat{H}\Psi_n(x,t) = e^{-i\frac{E_n}{\hbar}t}\hat{H}u_n(x)$$
$$= E_n u_n(x) e^{-i\frac{E_n}{\hbar}t}$$

$\exp(-i\frac{E}{\hbar}t)$ is the simplest solution that satisfies the time dependent part.

- An energy eigenstate has simple temporal dependence $\sim e^{-i\frac{E_n}{\hbar}t}$

13 The infinite Square Well

13.1 Applying Schrodingers Equation — Free Particle TISE

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

In region where $V(x)=0$, or 'free space'

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

$$\frac{d^2}{dx^2}\Psi(x) = -\frac{2mE}{\hbar^2}\Psi(x) = -\left(\frac{p}{\hbar}\right)^2\Psi(x)$$

General Solutions:

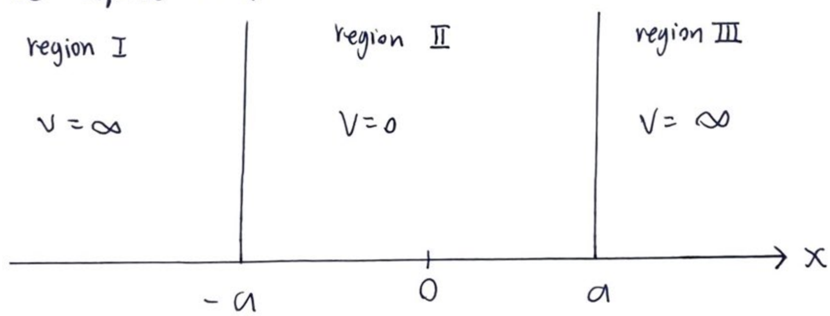
$$\Psi(x) = C_1 e^{i\frac{p}{\hbar}x} + C_2 e^{-i\frac{p}{\hbar}x}$$

or

$$= C_1' \sin\left(\frac{p}{\hbar}x\right) + C_2' \cos\left(\frac{p}{\hbar}x\right)$$

- no constraints on p & E in free space (continuous)
- quantisation will come from boundry conditions

13.2 Infinite Square Well



- $V=\infty$, a particle of finite energy cannot penetrate into this region $\rightarrow \Psi_{I,III}(x) = 0$
- $V(x)=0$, solutions $\Psi_{II}(x)$ as for 13.1

$$\Psi(x) = A\cos kx + B\cos kx$$

where $k = \frac{p}{\hbar} = \frac{\sqrt{2me}}{\hbar} = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}$

Boundary Conditions:

(i) $\Psi(x)$ should be continuous and single valued

(ii) $\Psi(x) \rightarrow 0$ lim $x \rightarrow \infty$ to ensure normalisation

(iii) $\frac{d}{dx}\Psi(x)$ should be continuous for finite $V(x)$

Here $\psi(a) = \psi(-a) = 0$

$$\left.\begin{array}{ll} x = a & A\cos ka + B\sin ka = 0 \\ x = -a & A\cos ka - B\sin ka = 0 \end{array}\right\}$$

Two ways to satisfy:

case 1: $B = 0 \quad \therefore \cos ka = 0$

$$ka = \frac{n\pi}{2} \qquad n \text{ is odd integer}$$

case 2: $A = 0 \quad \therefore \sin ka = 0$

$$ka = \frac{n\pi}{2} \qquad n \text{ is even integer}$$

- As before, energy quantised with quantum number n
- Two families of solutions

$$\left.\begin{array}{ll} \sin\left(\frac{n\pi}{2a}x\right) & n \text{ even} \\ \cos\left(\frac{n\pi}{2a}x\right) & n \text{ odd} \end{array}\right\}$$

$P = \hbar k$,

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{8ma^2} = \frac{h^2 n^2}{8 \cdot 4ma^2} = \frac{n^2 h^2}{8md^2} \qquad \text{(as before)}$$

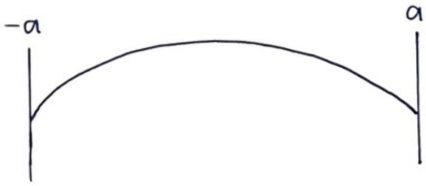
$$\psi(x) = C \begin{bmatrix} \cos \\ \sin \end{bmatrix} \left(\frac{n\pi}{2a}x\right)$$

C is for normalisation

$$C^2 \int_{-a}^{a} \sin^2\left(\frac{n\pi}{2a}\right) dx = 1 \rightarrow C = \frac{1}{\sqrt{a}}$$

$\psi_1(x)$

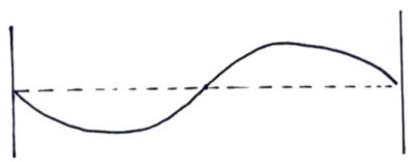
$n = 1$



$\frac{1}{\sqrt{a}} \cos\left(\frac{\pi}{2a}x\right)$

$\psi_2(x)$

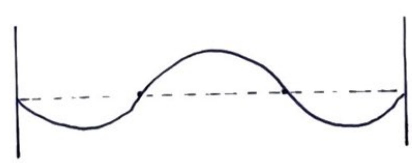
$n = 2$



$\frac{1}{\sqrt{a}} \sin\left(\frac{\pi}{a}x\right)$

$\psi_3(x)$

$n = 3$



$\frac{1}{\sqrt{a}} \cos\left(\frac{3\pi}{2a}x\right)$

13.3 Expectation values and Superpositions

For all states $\psi_n \langle x \rangle = \int_{-a}^{a} \psi_n^* x \psi_n \, dx = 0$

$$\langle E \rangle = E_n$$

If we form a superposition state

$$\psi(x) = \sum_n c_n \psi_n(x)$$

$$\langle E \rangle = \sum_n c_n^2 E_n$$

e.g. $\psi(x) = \frac{1}{\sqrt{2}} \psi_1(x) + \frac{1}{\sqrt{2}} \psi_2(x)$

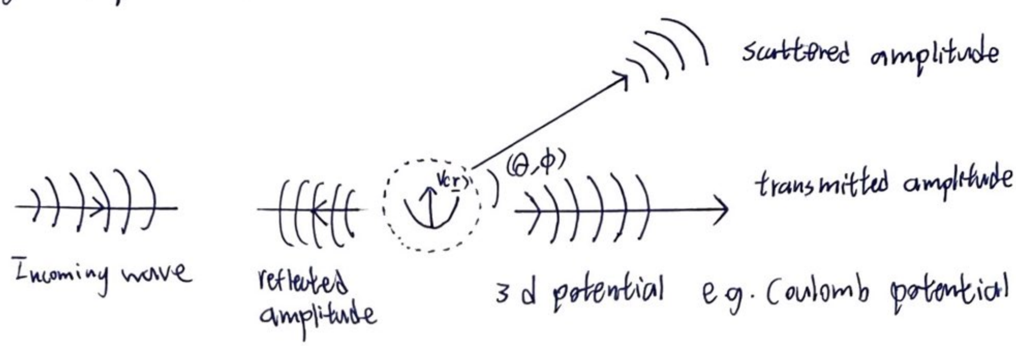
$$\langle E \rangle = \frac{1}{2} E_1 + \frac{1}{2} E_2$$

$\langle x \rangle \neq 0$ (if superposition contains states of opposite parity)

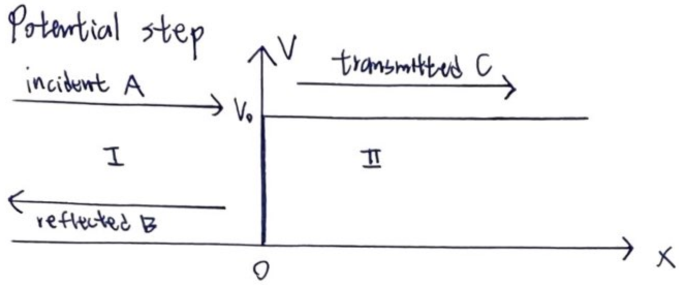
14. Scattering and Potential Steps

14.1 Scattering of a quantum particle from a potential

A general problem in QM is the treatment of this scattering



14.2 Potential step



Plane wave solutions in both regions for $E > V_0$

Define flux: no. of particles crossing unit area per unit time

flux = particle density (m^{-3}) × velocity $(m s^{-1})$

- How to normalise an ∞ plane wave?

In region I:

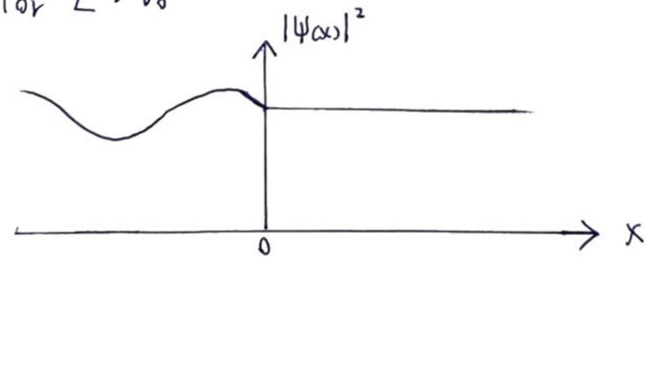
$$\psi_I(x) = A e^{ik_I x} + B e^{-ik_I x}, \quad k_I^2 = \frac{2m}{\hbar^2} E$$

In region II:

$$\psi_{II}(x) = C e^{ik_{II} x}, \quad k_{II}^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$$\text{flux} = \underbrace{|C|^2 |e^{ik_{II}x}|^2}_{\text{particle density}} \times \underbrace{\hbar \frac{k_{II}}{m}}_{\text{velocity}} = \frac{\hbar k_{II}}{m} |C|^2$$

For $E > V_0$



14.3 Reflection and Transmission Probability

In region where $V(x) = 0$

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

$$\frac{d^2}{dx^2}\psi_{I}(x) + \frac{2mE}{\hbar^2}\psi_{I}(x) = 0$$

$$\psi_{I}(x) = Ae^{ik_I x} + Be^{-ik_I x}$$

$$\psi_{II}(x) = Ce^{ik_{II} x}$$

In region where $V(x) = V_0$

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

Impose boundary conditions: $u(x)$ and $u'(x)$ must be continuous.

This gives $A + B = C$ and $ik_I(A-B) = ik_{II}C$

rearranging:
$$A = \left(1 + \frac{k_{II}}{k_I}\right)\frac{C}{2}$$

$$B = \left(1 - \frac{k_{II}}{k_I}\right)\frac{C}{2}$$

Reflection coefficient R

$$R = \frac{\text{reflected flux}}{\text{incident flux}} = \frac{|B|^2 \frac{\hbar k_I}{m}}{|A|^2 \frac{\hbar k_{II}}{m}} = \frac{|B|^2}{|A|^2} = \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)^2$$

Transmission coefficient

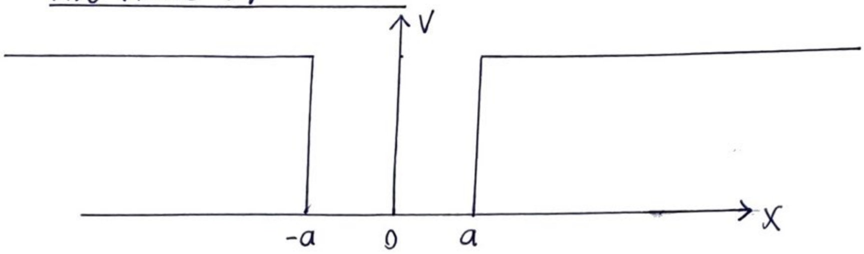
$$T = \frac{|Ce^{ik_{II}x}|^2 \times \frac{\hbar k_{II}}{m}}{|Ae^{ik_I x}|^2 \times \frac{hk_I}{m}} = \frac{4k_I k_{II}}{(k_I + k_{II})^2}$$

$$R + T = 1$$

15. Barriers and Quantum tunneling and the Finite Squre Well

Quantum Mechanics
6th edition
Alastair I.M. Rae
Jim Napolitano

The finite square well



The potential is given by :

$$V = 0 \qquad -a \le x \le a$$

$$V = V_0 \qquad |x| > a$$

We only consider bound states where the total energy E is less than V_0. The general solution to the Schrödinger equation in the first region is identical to the corresponding result in the infinite case. In the region $|x| > a$, the Schrödinger equation becomes

$$\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} - (V_0 - E)u = 0$$

*u is the wavefunction Ψ
$\Psi(x,t) = u(x)\,T(t)$

which has general solution :

$$u = Ce^{\kappa x} + De^{-\kappa x}$$

where C and D are constants and $\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$.

If $x > 0$, C must equal zero, otherwise the wave function would tend to infinity as x tends to infinity, in breach of the boundary conditions. Thus we have

$$u = De^{-\kappa x} \qquad x > a$$

A similar argument leads to

$$u = Ce^{\kappa x} \qquad x < -a$$

As the discontinuities in the potential at $x = \pm a$ are now finite rather than infinite, the boundary conditions require that both u and $\frac{du}{dx}$ be continuous at these points. From the infite square well (13.2) and the above two equations, we have :

$$A\cos ka + B\sin ka = De^{-\kappa a}$$

$$-kA\sin ka + kB\cos ka = -\kappa De^{-\kappa a}$$

$$A\cos ka - B\sin ka = Ce^{-\kappa a}$$

$$kA\sin ka + kB\cos ka = \kappa Ce^{-\kappa a}$$

These equations lead to:

$$2A\cos ka = (C+D)e^{-Ka} \quad 5.38$$

$$2kA\sin ka = K(C+D)e^{-Ka} \quad 5.39$$

$$2B\sin ka = (D-C)e^{-Ka} \quad 5.40$$

$$2kB\cos ka = -K(D-C)e^{-Ka} \quad 5.41$$

If we divide 5.39 by 5.38 and 5.41 by 5.40:

$$\left.\begin{array}{ll} k\tan ka = K & \text{unless } C=-D \text{ and } A=0 \\ k\cot ka = -K & \text{unless } C=D \text{ and } B=0 \end{array}\right\} \quad 5.42$$

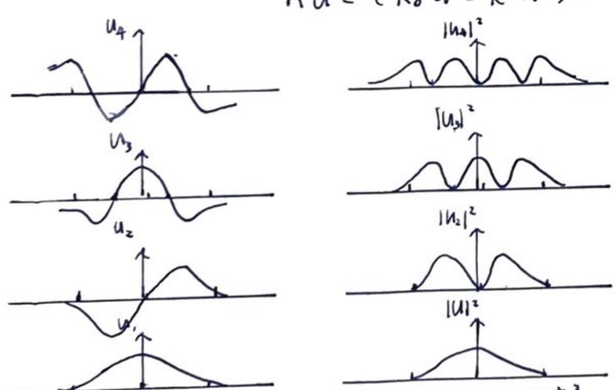
Both conditions 5.42 must be satisfied simultaneously, so we have two sets of solutions subject to the following conditions:

$$\left.\begin{array}{ll} k\tan ka = K & C=D \text{ and } B=0 \\ -k\cot ka = K & C=-D \text{ and } A=0 \end{array}\right\} \quad 5.43$$

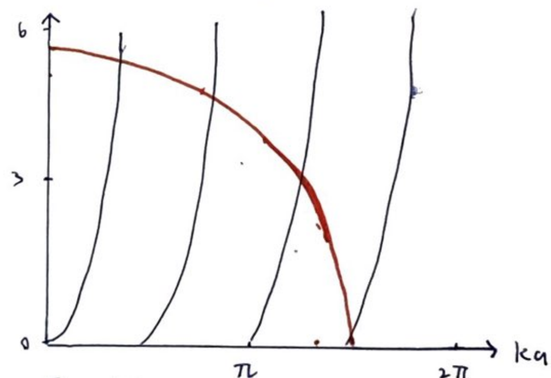
Remembering that $k = \frac{\sqrt{2mE}}{\hbar}$ and $K = \frac{\sqrt{2m(V_0-E)}}{\hbar}$, we see that equations 5.43 determine the allowed values of the energy. The solutions to the equations cannot be expressed algebraicly and needs to be done graphicaly or by [illegible]. To obtain solution graphically, we first define k_0 so that $k_0^2 = \frac{2mV_0}{\hbar^2}$ and use the definitions of k and K to rewrite equations 5.43 as

$$\left.\begin{array}{l} ka\tan ka = (k_0^2a^2 - k^2a^2)^{\frac{1}{2}} \\ -ka\cot ka = (k_0^2a^2 - k^2a^2)^{\frac{1}{2}} \end{array}\right\} \quad 5.44$$

$$Ka = (k_0^2a^2 - k^2a^2)^{\frac{1}{2}}$$



Position probability distributions, $V_0 = \frac{25\hbar^2}{2ma^2}$



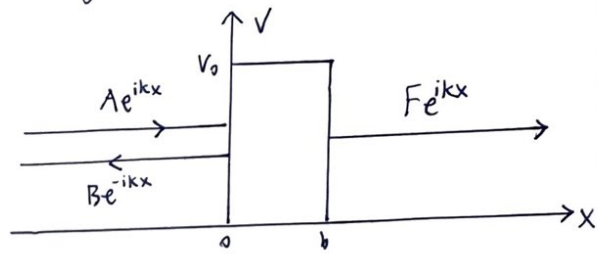
The circular quadrant represents Ka and the other lines are graphs of $\tan ka$ and $\cot ka$. $k_0 a = 5$ for this graph and intersections are solutions.

For finite square well in the later case the wavefunctions decay exponentially in the region $|x| > a$ instead of going to zero at $x = \pm a$. The wave function penetrates a region where the total energy is less than V_0. There is a probability of finding a particle where it could not be classically as it would then have negative kinetic energy.

Quantum mechanics implies that a particle is able to pass through a potential energy barrier which is impenetrable according to classical mechanics. This phenomenon is known as quantum-mechanical tunnelling or the tunnel effect.

Quantum Mechanical Tunnelling

We consider the case of a beam of particles of momentum $\hbar k$ and energy $E = \frac{\hbar^2 k^2}{2m}$ approaching a barrier of height V_0 ($V_0 > E$) and width b.



A fraction of the particles will be reflected at the barrier with momentum $-\hbar k$, but some will tunnel through to emerge with momentum $\hbar k$ at the far side of the barrier. The incident, transmitted and reflected beams are all represented by plane waves, so the wave function on the incident side is:

$$u = A\exp(ikx) + B\exp(-ikx) \qquad 5.45$$

Inside the barrier the wave function has the same form as 5.31:

$$u = C\exp(Kx) + D\exp(-Kx) \qquad 5.46$$

and beyond the barrier ($x > b$), the wave function will have the form:

$$u = F\exp(ikx) \qquad 5.47$$

As the barrier does not reach to infinity, we can't drop the first term in 5.46 as we did in finite square well. The boundary conditions requiring both u and $\frac{du}{dx}$ be continuous at $x=0$ and $x=b$ can be applied in much the same way to give:

$$\left.\begin{aligned} &A + B = C + D \\ &A - B = \frac{K}{ik}(C - D) \end{aligned}\right\} x = 0 \qquad\qquad 5.48$$

$$\left.\begin{aligned} &Ce^{Kb} + De^{-Kb} = Fe^{ikb} \\ &Ce^{Kb} - De^{-Kb} = \frac{ik}{K}Fe^{ikb} \end{aligned}\right\} x = b$$

Adding the first two equations and add/subtracting the second two gives:

$$\left.\begin{aligned} &2A = \left(1 + \frac{K}{ik}\right)C + \left(1 - \frac{K}{ik}\right)D \\ &2Ce^{Kb} = \left(1 + \frac{ik}{K}\right)Fe^{ikb} \\ &2De^{-Kb} = \left(1 - \frac{ik}{K}\right)Fe^{ikb} \end{aligned}\right\} \qquad 5.49$$

Recombining:

$$\frac{F}{A} = \frac{4iKk\exp(-ikb)}{(2iKk + K^2 - k^2)\exp(-Kb) + (2iKk - K^2 + k^2)\exp(Kb)} \qquad 5.50$$

In many practical cases, the tunnelling probability is quite small, so we can ignore the term in $\exp(-Kb)$, and transmittance is $|F|^2/|A|^2$, which is:

$$\frac{|F|^2}{|A|^2} = \frac{16K^2k^2}{(K^2+k^2)^2}e^{-2Kb} = \frac{16E(V_0 - E)}{V_0^2}e^{-2Kb} \qquad 5.51$$

We can use this to calculate the rate at which particles pass through the barrier in the case where f particles approach the barrier per second as:

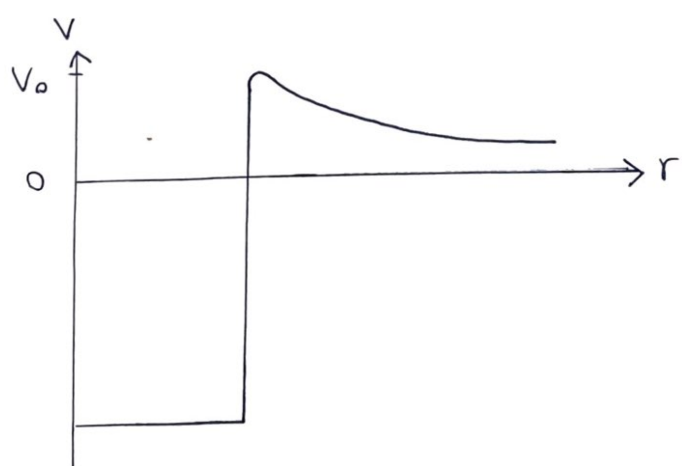
$$\Gamma = f\frac{16E(V_0-E)}{V_0^2}\exp(-2Kb) = \frac{n\hbar k}{m}\frac{16E(V_0-E)}{V_0^2}\exp(-2Kb) \qquad 5.52$$

where n is the number of particles per unit length in the incident beam and the particle speed is $\frac{\hbar k}{m}$.

We see that the tunnelling probability is largely determined by the exponential decay of the wave function within the ~~...~~ barrier: the lower and narrower the barrier is, the greater the likely hood of tunnelling.

Physical example of tunelling – Alpha Decay

The alpha particle consists of two protons and two neutrons bounded so tightly it can be seem as an α particle before emission. The interaction between the α particle and the rest of the nucleus has two components. The first is the strong nuclear force and is attractive. The second is the Coulomb interaction which is repulsive and acts at larger distances. The total interaction potential energy is shown below. If the alpha particle occupies a quantum state whose energy is less than zero, it will remain there and the nucleus will be stable. If the form of the potential ~~energy~~ is such that the lowest energy state of the of the alpha particle is greater than zero, but less than V_0, it will be able to escape by quantum tunnelling.



Potential energy of interaction between an alpha particle and a nucleus against distance from center of nucleus.