Quantum Materials

Introduction to Quantum Mechanics

- Historical evolution from classical physics to quantum physics.
- Exploration of wave-particle duality and the concept of quantum states. Superposition and entanglement: their significance in quantum systems and potential applications.
- The uncertainty principle and its impact on measurement in quantum systems.
- Quantum wave function, Schrödinger equation (time independent). Energy quantization: Introduction to discrete energy levels in atoms and their effects on material properties.

Evolution of Quantum Mechanics

Dual nature of matter

de Broglie wavelength, $\boldsymbol{\lambda = h/p}$

For a cricket ball

mass = 160 g & velocity = 150 km/h

$\lambda = 0.98 \times 10^{-34}$ m $\rightarrow$ so small, not appreciable

For an electron

accelerated by applied potential of 1 V

$\lambda = 1.23$ nm $\left(\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}}\right)$

Heisenberg Uncertainty Principle

It is impossible to simultaneously describe with absolute accuracy the position and momentum of a particle.

$$\Delta x . \Delta p_x \geq \hbar/2$$

Predictions from uncertainty principle:

- Nonexistence of free electron in nucleus
- Estimate of radius of Bohr's first orbit
- Zero point energy of simple harmonic oscillators

Formulation of Quantum Mechanics

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How do we describe a system in Quantum Mechanics?

- Described by a wave function: $\psi(r,t)$
- All information about the system is contained in this $\psi(r,t)$
- Any variation in property/behaviour of the system will be reflected in $\psi(r,t)$.
- Solving the problem in quantum mechanics is to determine $\psi(r, t)$ considering all parameters.

Requirements for ψ

- ψ can be any function, real or complex, akin to the behavior of the real physical system.
- While ψ itself has no physical interpretation, its square ψ^2 evaluated at a particular place at any time gives the **probability of finding** the particle there at that time.

Mathematical requirements

- ψ and $\frac{d\psi}{dr}$ must be finite, continuous and single valued.
- $\psi \rightarrow 0$ as $r \rightarrow \infty$.
- $\int_{-\infty}^{+\infty} \psi^2 dV = 1$

Quantum physics is probabilistic in nature.

Wave function ψ

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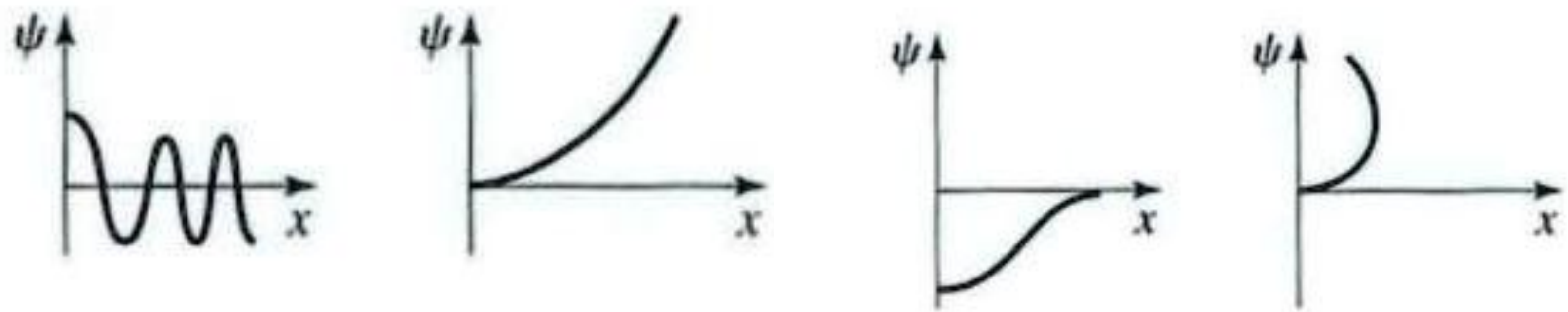
Which is the acceptable wave form?



Is ψ a well behaved wavefunction if

(a) $\psi = A\, sinx$, (b) $\psi = B\, tanx$, (c) $\psi = C\, e^{kx}$, (d) $\psi = De^{ikx}$,

(e) $\psi = A\, sinx + De^{ikx}$

Wave function ψ

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Normalization

The probability that its position *x* will be in the interval $a \leq x \leq b$ is the integral of the density over this interval:

$$P(t) = \int_a^b |\psi(x,t)|^2\, dx$$ where t is the time at which the particle was measured.

This leads to the **normalization condition:**

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2\, dx = 1$$

because if the particle is measured, there is 100% probability that it will be *somewhere*..

A particle limited to the x axis has the wave function

$\psi = Ax$ for $0 \leq x \leq 1$;

$\psi = 0$ elsewhere.

(a) Normalize the wave function (find the normalization constant *A*).

(b) Probability to find the particle between *x* =0.45 and *x*=0.55.

(c) Expectation value *x* of the particle's position.

Extraction of information

- Applying certain operations/instruction on wave function ψ, information/ observable can be extracted.
- These information specific operations are called operator for a given observable.

For example momentum operator, $\hat{p}_x \equiv \left(-i\hbar\frac{\partial}{\partial x}\right)$,

Energy operator $\hat{E} \equiv \left(i\hbar\frac{\partial}{\partial t}\right)$

How to use an operator?

$$\hat{A}\,\psi(r,t) = \lambda\psi(r,t)$$

Operator Â operates on the wave function ψ to give the Eigen value λ.

Expectation value (classically, average value)

$$\int_{-\infty}^{+\infty} \psi^* \hat{A}\psi dV = \langle \hat{A} \rangle$$

Extraction of information

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- Is the function e^{3x+5} an Eigen-function of the operator $\frac{d^2}{dx^2}$? If so, what is the corresponding Eigen-value?
- Obtain expressions for the following operator $\left(\frac{d}{dx} + x\right)^2$ and $\left(x\frac{d}{dx}\right)^2$

Postulates of quantum mechanics

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1. State of a physical system: Wave function
2. Operator corresponding to a classical observable
3. Measurement of physical quantity: eigen value equation
4. Probabilistic measurement: expectation value
5. Evolution of wave function (The Schrodinger equation)

Schrodinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\right)\psi(x)=E\psi(x)$$

$$\Rightarrow \frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m(E-V)}{\hbar^2}\psi(x)=0$$

Whole of quantum mechanics is based on finding solution to this equation.

Schrodinger equation

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m(E-V)}{\hbar^2}\psi(x)=0$$

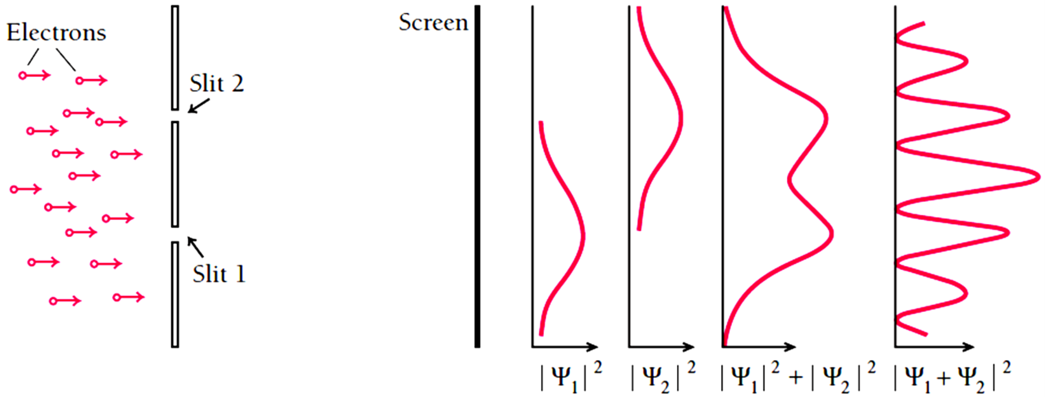
This equation may have multiple solutions!

Which solution is of our use?

Superposition

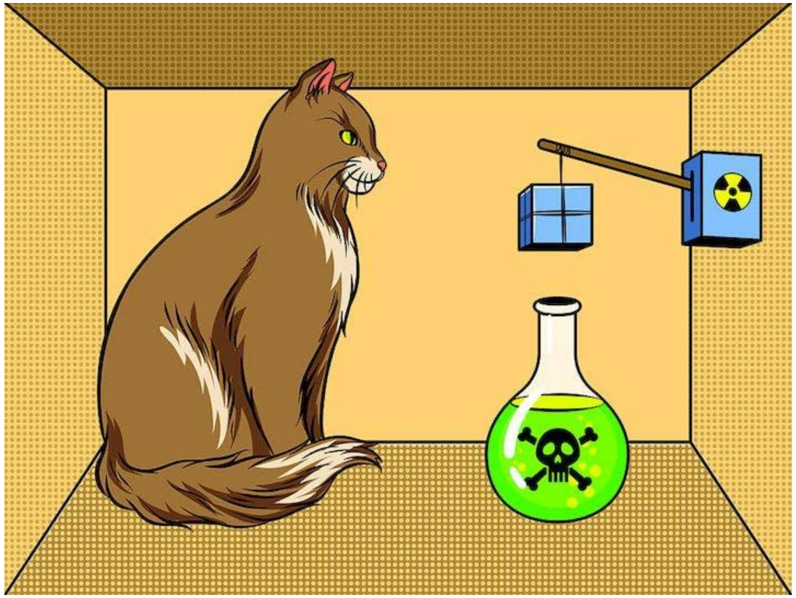
- It is the characteristic property of the waves.
- A linear combination of solutions of Schrödinger's equation is also a solution!

$$\psi = a\psi_1 + b\psi_2$$



It is wave function, not the probability, which are added.

Schrodinger equation



$$\psi_{cat} = a\psi_{cat}^{alive} + b\psi_{cat}^{dead}$$

On opening the box ψ_{cat} will collapse to either ψ_{cat}^{alive} or ψ_{cat}^{dead}.

Superposition & Entanglement

For an electron, there are two quantum states, i.e., spin-up and spin-down states represented by $\psi^{\downarrow}$ and $\psi^{\uparrow}$.

For electron A, Quantum states are: $\psi_A^{\uparrow}$ and $\psi_A^{\downarrow}$

For electron B, Quantum states are: $\psi_B^{\uparrow}$ and $\psi_B^{\downarrow}$

For the combination the quantum state will be the linear combination:

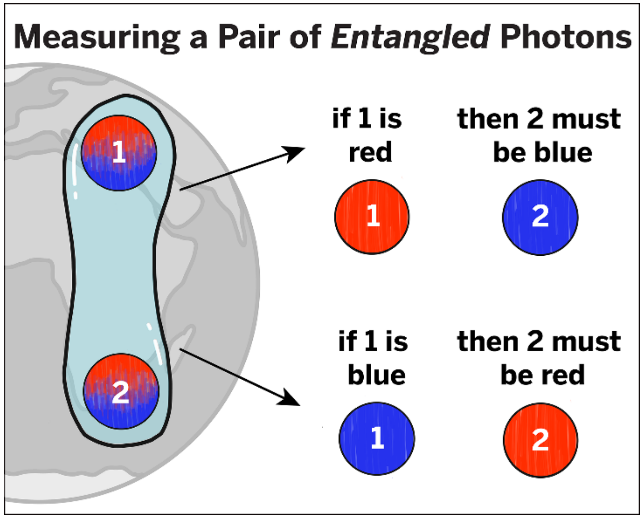
$$\psi = \frac{1}{\sqrt{2}}\left(\psi_A^{\uparrow}\psi_B^{\downarrow} \pm \psi_A^{\downarrow}\psi_B^{\uparrow}\right)$$

$\rightarrow$ requirement of Pauli exclusion principle.

Entangled-state of two quantum particles

These two electrons are related with each other with some condition, they are entangled

Quantum Entanglement



Quantum entanglement

Phenomenon of a group of particles being generated, interacting, or sharing spatial proximity in such a way that the quantum state of each particle of the group cannot be described independently, even when the particles are separated by a large distance.

Key Characteristics:

Non-locality: Particles seem to be "connected" over large distances.

Quantum Correlation: Measurement of one particle affects the state of the other.

Examples

- **Superconductors:** Cooper pair.
- **Superconducting qubits:** IBM's or Google's quantum computers.
- **Trapped ions/atoms:** Ions or atoms can be entangled by controlled laser interactions.
- **Beam Splitters:** Entangled photon pairs can be generated using beam splitters and polarizers.

Particle inside a box – application of Schrödinger's equation

Free particle (No restriction – no force – no potential !)

Particle is free to move on x-axis.

Time independent Schrodinger Equation:

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2mE}{\hbar^2}\psi(x)=0$$

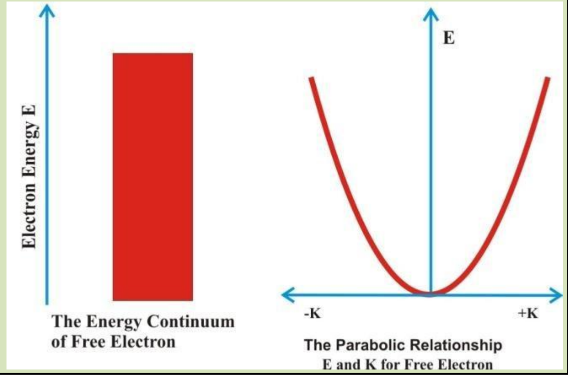
$$\frac{\partial^2\psi(x)}{\partial x^2}+k^2\psi(x)=0 \qquad \text{when } k=\sqrt{\frac{2mE}{\hbar^2}}$$

Solution of this equation can be

$$\boldsymbol{\psi(x)=Ae^{i(kx)}} \textbf{ or } \boldsymbol{Be^{-i(kx)}}$$

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

Since k may have any value, particle may have *any* energy!



Particle inside a box – application of Schrödinger's equation

Bound particle (A restriction is in place!)

Particle is free to move on x-axis only in a permitted region.

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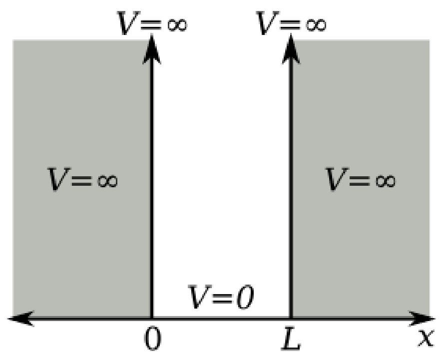


Schrodinger Equation for 0 ≤ x ≤ L

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m(E - \cancel{V}^{\,0})}{\hbar^2}\psi(x) = 0, \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$

$$\int_{-\infty}^{0} \cancel{|\psi(x)|^2 dx}^{\,0} + \int_{0}^{L} |\psi(x)|^2 dx + \int_{L}^{+\infty} \cancel{|\psi(x)|^2 dx}^{\,0} = 1$$

$\psi(x) = A sin(kx) + B cos(kx)$

Boundary conditions: $\psi_{x=0} = 0$ and $\psi_{x=L} = 0$

$\psi_{x=0} = 0 = 0 + B$

$\psi_{x=L} = 0 = A\ sin(kL)$

$$k = \frac{n\pi}{L}, \qquad n = 0, \pm 1, \pm 2, \ldots$$

$$\psi_n(x) = A\sin(k_n x) = A\sin\left(\frac{n\pi}{L}x\right)$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}, \qquad n = 1,2,3 \ldots$$

Particle inside a box – application of Schrödinger's equation

$$\int_{x=0}^{x=L} |\psi(x)|^2 dx = 1$$

$$\psi_n(x) = ASin\left(\frac{n\pi x}{L}\right)$$

$$\int_{x=0}^{x=L} \left|ASin\left(\frac{n\pi x}{L}\right)\right|^2 dx = 1$$

$$\frac{A^2}{2}\int_{x=0}^{x=L} \left[1 - Cos\left(\frac{2n\pi x}{L}\right)\right] dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{L}{2n\pi}Sin\left(\frac{2n\pi x}{L}\right)\right]_0^L = 1$$

$$\frac{A^2}{2}L = 1$$

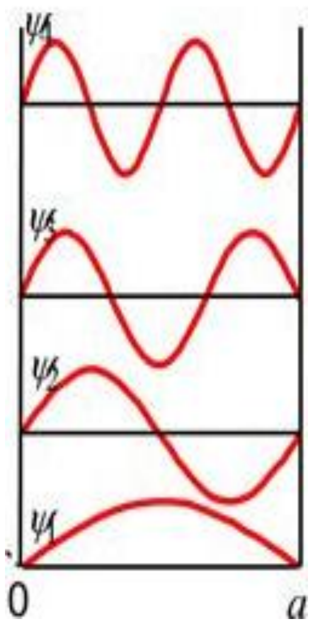
$$A = \sqrt{\frac{2}{L}}$$

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

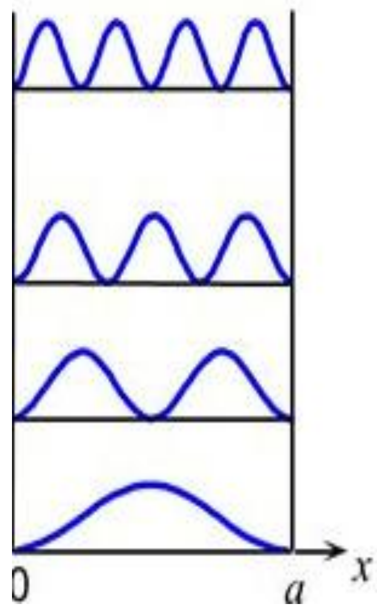
$$\boxed{E = \frac{\hbar^2\pi^2}{2mL^2}n^2}$$

Particle inside a box – application of Schrödinger's equation

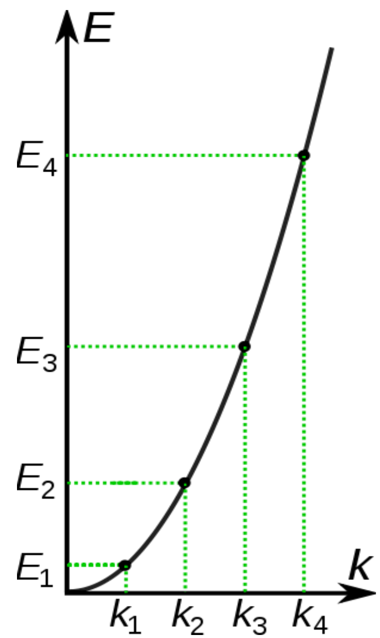
$$\psi_n(x) = ASin\left(\frac{n\pi x}{L}\right) = \sqrt{\frac{2}{L}}Sin\left(\frac{n\pi x}{L}\right) \qquad E = \frac{\hbar^2\pi^2}{2mL^2}n^2$$



Wave functions



Probabilities



Particle inside a box – application of Schrödinger's equation

- What is the probability that a particle, trapped in a box of width L, is found to be between 0.4L and 0.5L in 1^{st} excited state?
- Find the expectation value of position of a particle, trapped in a box of width L in ground state and 1^{st} excited state.

Particle inside a box – application of Schrödinger's equation

A small 0.40-kg cart is moving back and forth along an air track between two bumpers 2.0 m apart. Assuming no friction; collisions with the bumpers are perfectly elastic so that between the bumpers, the cart maintains a constant speed of 0.50 m/s. Treating the cart as a quantum particle, estimate the value of the principal quantum number that corresponds to its classical energy.

$$K = \frac{1}{2}mv^2 = \frac{(0.4)(0.5)^2}{2} = 0.05\,J$$

If the cart as a quantum particle then energy is

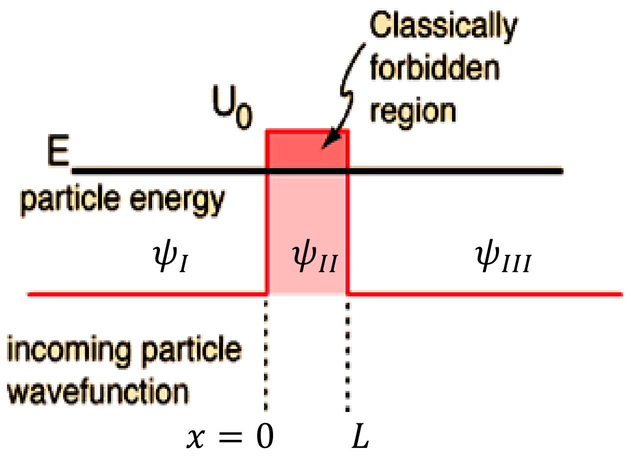
$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}n^2 = \frac{\pi^2(1.05\times10^{-34})^2}{2(0.4)(2)^2} = 1.7\times10^{-68}n^2\ J$$

$$0.05\,J = 1.7\times10^{-68}n^2\ J$$

$$n = (K/E_1)^{1/2} = (0.050/1.700\times10^{-68})^{1/2} = 1.2\times10^{33}$$

In the limit of high quantum numbers, there is no advantage in using quantum formalism because we can obtain the same results using classical mechanics.

Problem of finite potential barrier



$$\boldsymbol{V} = \begin{cases} 0 & x \le 0 \\ U_0 & 0 < x < L \\ 0 & x \ge L \end{cases}$$

$$\frac{\partial^2 \boldsymbol{\psi}(\boldsymbol{x})}{\partial \boldsymbol{x}^2} + \frac{2\boldsymbol{m}(\boldsymbol{E}-\boldsymbol{V})}{\hbar^2}\boldsymbol{\psi}(\boldsymbol{x}) = \mathbf{0}$$

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi_I(x) = 0$$

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} + \frac{2m(E-U_0)}{\hbar^2}\psi_{II}(x) = 0$$

$$\frac{\partial^2 \psi_{III}(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi_{III}(x) = 0$$

$$k_1^2 = \frac{2mE}{\hbar^2}, \qquad k_2^2 = \frac{2m(U_0-E)}{\hbar^2}$$

Problem of finite potential barrier

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} + k_1^2 \psi_I(x) = \mathbf{0}$$

$$\boldsymbol{\psi_I = Ae^{ik_1x} + Be^{-ik_1x}}$$

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} - k_2^2 \psi_{II}(x) = \mathbf{0}$$

$$\boldsymbol{\psi_{II} = Ce^{k_2x} + De^{-k_2x}}$$

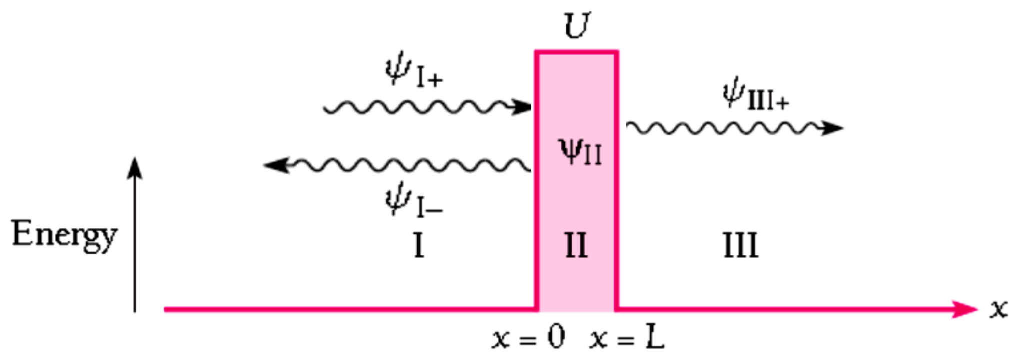
$$\frac{\partial^2 \psi_{III}(x)}{\partial x^2} + k_1^2 \psi_{III}(x) = \mathbf{0}$$

$$\boldsymbol{\psi_{III} = Fe^{ik_1x} + Ge^{-ik_1x}}$$

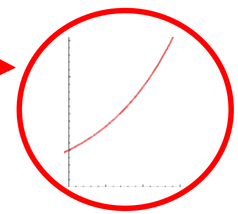
Problem of finite potential barrier

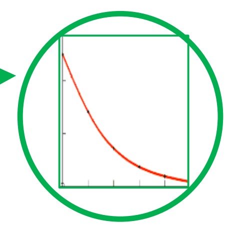
$$\psi_I = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_{I+} \qquad \psi_{I-}$$



$$\psi_{II} = \cancel{Ce^{k_2x}} + De^{-k_2x}$$





$$\psi_{III} = Fe^{ik_1x} + \cancel{Ge^{-k_1x}}$$

$$\psi_{III+} \qquad \psi_{III-}$$

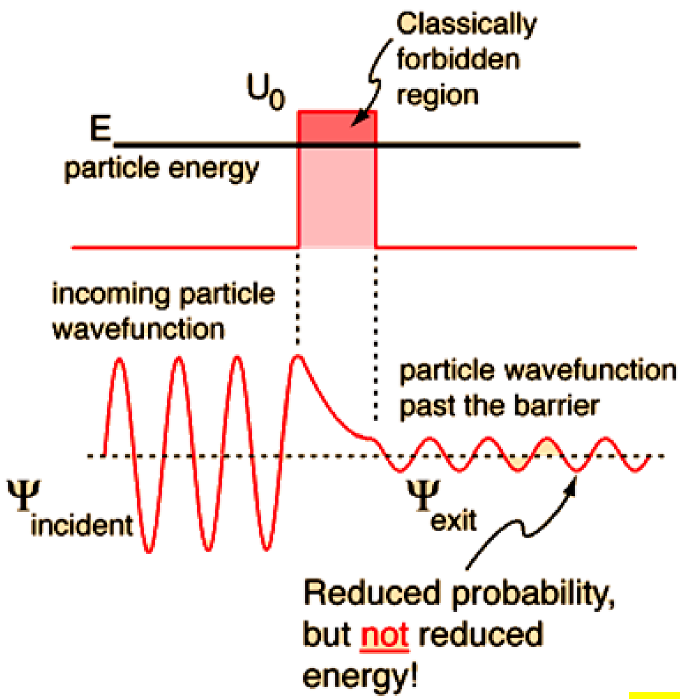
Problem of finite potential barrier

$$\psi_i = Ae^{ik_1x} + Be^{-ik_1x}$$
$$\psi_b = De^{-k_2x}$$
$$\psi_o = Fe^{ik_1x}$$

$$k_1^2 = \frac{2mE}{\hbar^2},$$

$$k_2^2 = \frac{2m(U_0 - E)}{\hbar^2}$$

Quantum mechanical tunneling



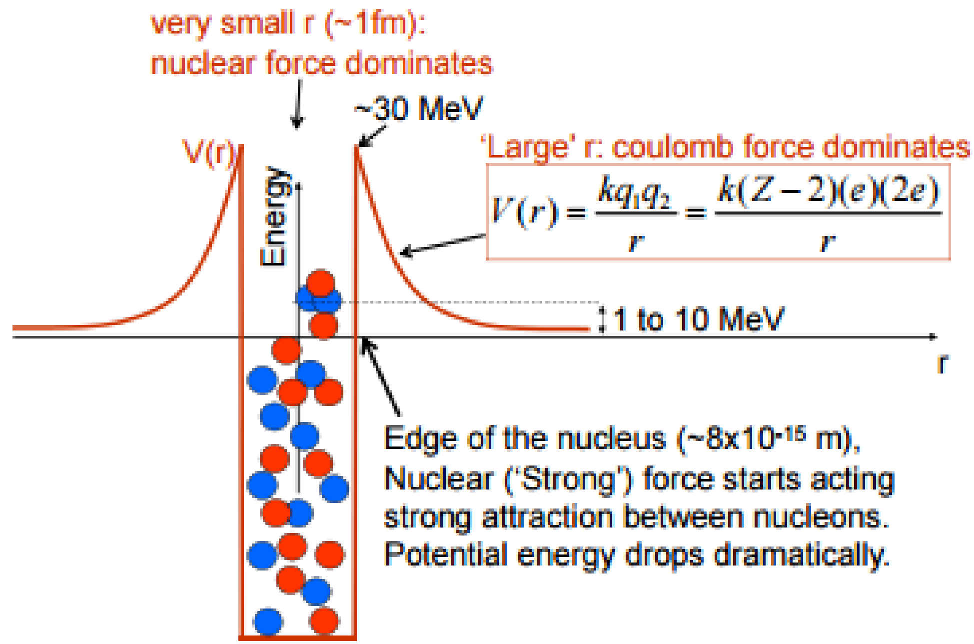
Transmission probability

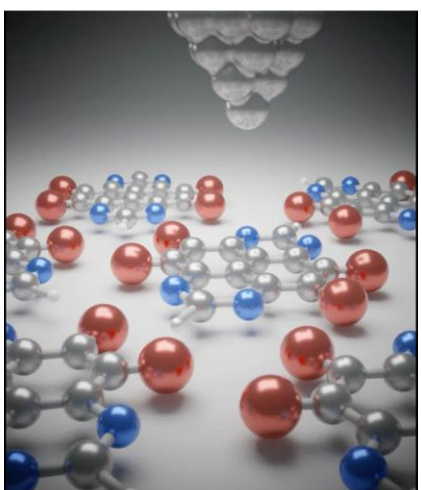
$$\mathrm{T} = \left|\frac{F}{A}\right|^2$$

$$T \approx 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right)e^{-2k_2L}$$

Applications - Particle encountering a potential barrier

Radioactive decay:
Probability of nucleons coming outside the nucleus energy well.





- **Semiconductors:** Tunnelling is essential in tunnel diodes and transistors.
- **Nuclear Fusion:** Tunnelling allows particles to overcome repulsive forces in nuclear reactions.
- **Scanning Tunneling Microscopy (STM):** Utilizes tunnelling to image surfaces at the atomic level.