Lecture 18

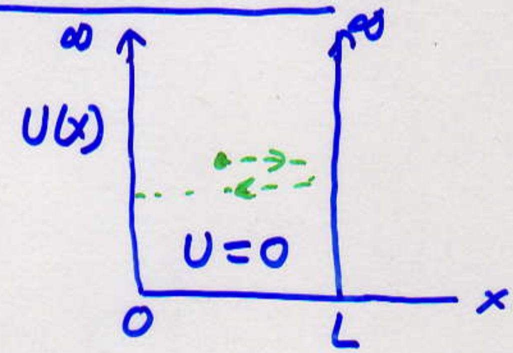
Chapter 40

Quantum Mechanics

Here we solve Schroedinger eqn for realistic physical systems with appropriate boundary conditions. This gives allowed energy values (eigenvalues) and wave functions (eigenfunctions). These can be used to calculate expectation values or average values of physical properties.

Particle in a Box or Particle in Infinite Square Well potential

$$U(x) = 0 \quad \text{for } 0<x<L$$
$$= \infty \quad \text{for } x \le 0 \text{ or } x \ge L$$



$\Rightarrow \quad \psi(x) = 0 \quad$ at $x \le 0$ or $x \ge L$

In region $0<x<L$, Schroedinger eqn

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

where $k^2 = \dfrac{2mE}{\hbar^2}$

Two independent soln : $\sin kx$ and $\cos kx$

$\Rightarrow$ Energies of [illegible]

[illegible] are quantized.

Eigenfunctions

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

Normalization:

$$\int_0^L |\psi_n(x)|^2 dx = A^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = A^2 \frac{L}{2} = 1$$

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

General Solution

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

Boundary conditions at $x=0$ + L and normalization condition give A, B and k.

$$\psi(0) = 0 + B = 0 \Rightarrow B = 0$$

$$\boxed{\psi(x) = A \sin kx}$$

$$\psi(L) = A \sin kL = 0$$

$$\Rightarrow \boxed{kL = n\pi}, \quad n = 1, 2, \cdots$$

Allowed energy levels

$$kL = \sqrt{\frac{2mE}{\hbar^2}}\, L = n\pi$$

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

$\Rightarrow$ Energies of particles in a box are quantized.

Eigenfunctions

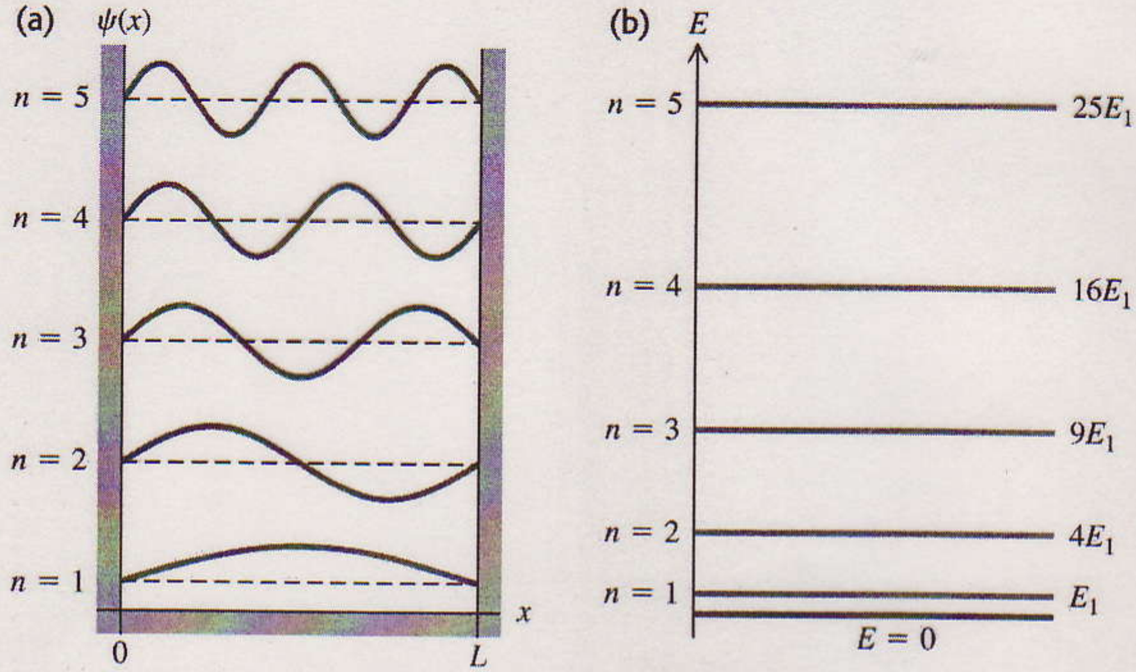
$$\psi_n(x) = A \sin \frac{n\pi x}{L}$$

Normalization:

$$\int_0^L |\psi_n(x)|^2 dx = A^2 \int_0^L \sin^2 \frac{n\pi x}{L}\, dx = A^2 \frac{L}{2} = 1$$

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

The wave functions and energy levels



The wavefunctions are

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}}, \quad n = 1, 2 \ldots \qquad E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

The lowest energy or ground state energy

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2} = \frac{h^2}{8mL^2} \qquad \hbar = \frac{h}{2\pi}$$

Excited state energies

$$\boxed{E_n = n^2 E_1} \qquad n = 1, 2, 3 \ldots$$

Energy of a particle in a box is quantized, similar to energy quantization in hydrogen atom

Since $n=0$ is not allowed, particle is never at rest

Classically all E including $E=0$ are possible

Particle can be excited from one state to another by em-wave of right frequency:

$$hf = E_f - E_i$$
$$= E_3 - E_1 = 9E_1 - E_1 = 8E_1 \quad \text{for } f=3,\ i=1$$

Particle can emit em-wave by transition from higher energy level to a lower one. Here

$$hf = E_i - E_f = 8E_1 \quad \text{if } i=3 \text{ and } f=1$$

Example

Electron confined to a one-dimensional infinitely deep energy well with $L = 10^{-10}\,\text{m} = 0.1\,\text{nm}$ (size of an atom)

a) Ground state energy of electron

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} = \frac{h^2}{8mL^2} = \frac{(6.63\times10^{-34})^2}{8(9.11\times10^{-31})(1\times10^{-10})^2}$$
$$= 6.031\times10^{-18}\,\text{J} = 37.7\,\text{eV}$$

b) Electron makes a transition from $n=1$ to $n=3$ by an incident electromagnetic wave. How much energy transferred?

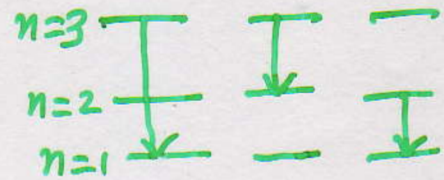
$$\Delta E_{31} = E_3 - E_1 = 8E_1 = 4.83\times10^{-17}\,\text{J} = 302\,\text{eV}.$$

c) Wavelength of em-wave

$$hf = \frac{hc}{\lambda} = \Delta E_{31} \Rightarrow$$
$$\lambda = \frac{hc}{\Delta E_{31}} = \frac{1240\,\text{eV-nm}}{302\,\text{eV}} = 4.11\,\text{nm}$$

(d) Electron has been excited to 2nd excited state ($n=3$). What wavelengths of em-wave can it emit by deexcitation?

Three ways of deexcitation



$n_3 \to n_1$ transition

$$h f_{31} = \frac{hc}{\lambda_{31}} = \Delta E_{13}$$

$$\lambda_{31} = \frac{hc}{\Delta E_{13}} = 4.11 \text{ nm (as in part c)}$$

$n_3 - n_2$ transition

$$\lambda_{32} = \frac{hc}{\Delta E_{23}}, \quad \Delta E_{23} = E_3 - E_2 = 9E_1 - 4E_1$$
$$= 5E_1 = 188.5 \text{ eV}$$

$$\lambda_{32} = \frac{1240}{188.5} = 6.57 \text{ nm}$$

$n_2 - n_1$ transition

$$\lambda_{21} = \frac{hc}{\Delta E_{12}}, \quad \Delta E_{12} = E_2 - E_1 = 4E_1 - E_1$$
$$= 3E_1 = 113.1 \text{ eV}$$

$$\lambda_{21} = \frac{1240}{113.1} = 10.96 \text{ nm}$$

Coment on Quantization

Boundary condition at $x = L \Rightarrow kL = n\pi$, $\frac{2\pi}{\lambda} L = n\pi$

$\Rightarrow \boxed{\lambda_n = \frac{2L}{n}} \Rightarrow$ only certain wavelengths are allowed, corresponding to a quantum state.

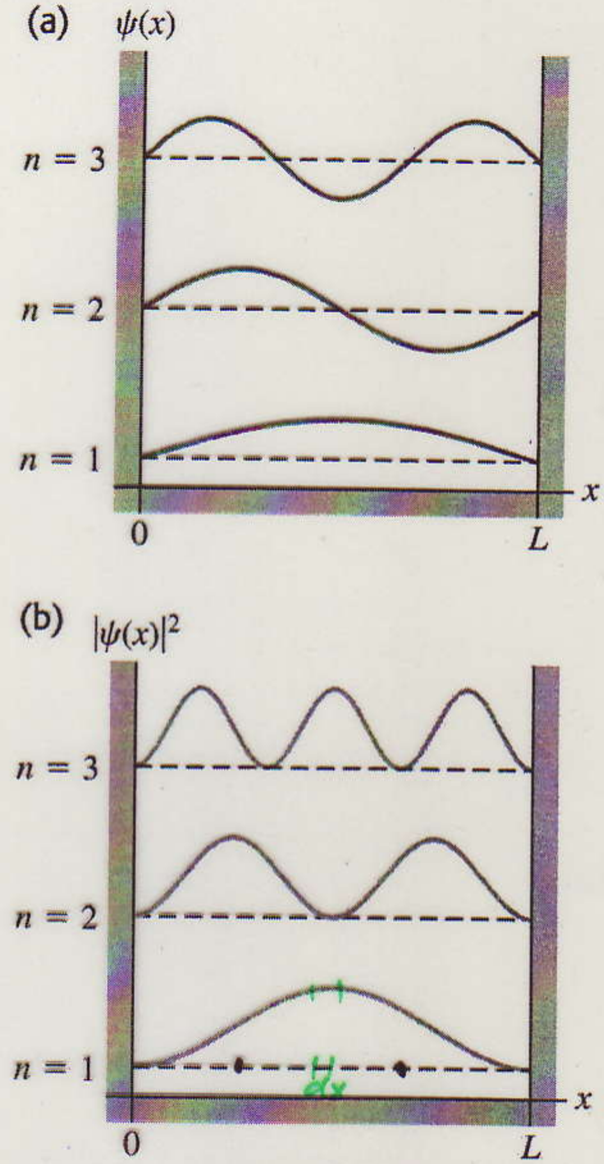
Note wavelengths allowed in box are identical to allowed wavelengths in a string fixed at both ends. Boundary conditions determine these in both cases.

Because particles behave like waves, the allowed quantum states are those in which the b.c.'s on the wave functions of the system are satisfied.

Probability and normalization

Here ψ_n and corresponding probability density $P(x) = |\psi(x)|^2$ have been plotted.

Note ψ_n can be positive or negative, but $|\psi_n|^2$ is positive or zero, since it represents prob. density. $|\psi_n|^2$ is zero at the nodes of the wave function, also at the walls.



Example: Ground-state Electron confined in 10^{-10} m = 0.1 nm wide infinite potential well.

a) Find probability of electron being in the left one-third of well

$$P(0<x<\tfrac{L}{3}) = \int_0^{L/3} P(x)\,dx$$

$$= \int_0^{L/3} |\psi(x)|^2 dx = \frac{2}{L}\int_0^{L/3} \sin^2 \frac{\pi x}{L}\, dx = \frac{1}{2\pi}\left[\frac{2\pi}{3} - \sin\frac{2\pi}{3}\right]$$

$$= 0.20$$

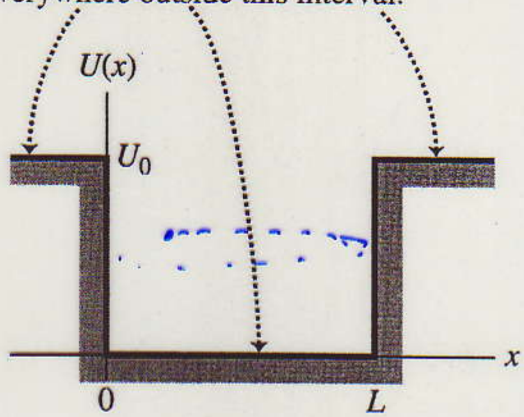
Similarly $P(\tfrac{2L}{3} < x < L) = 0.20$

Thus $P(\tfrac{L}{3} < x < \tfrac{2L}{3}) = 1 - 0.20 - 0.20 = 0.6$

$P(x=\tfrac{1}{2}L)\,dx = |\psi(x=\tfrac{L}{2})|^2 dx, \quad dx = 0.01L$

Finite Potential Well

The potential energy U is zero in the interval $0 \le x \le L$ and has the constant value U_0 everywhere outside this interval.



If $E < U_0$

If a particle is trapped in a finite potential well of height U_0 and if particle energy $E < U_0$, classically particle will remain trapped. Quantum mechanically, particle has finite prob. of being outside the well.

For $0 < x < L$, Schroedinger eqn

$$\frac{d^2\psi}{dx^2} + k^2\psi(x) = 0 \quad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

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

For $x < 0$ and $x > L$, Schroedinger Eqn.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E\psi$$

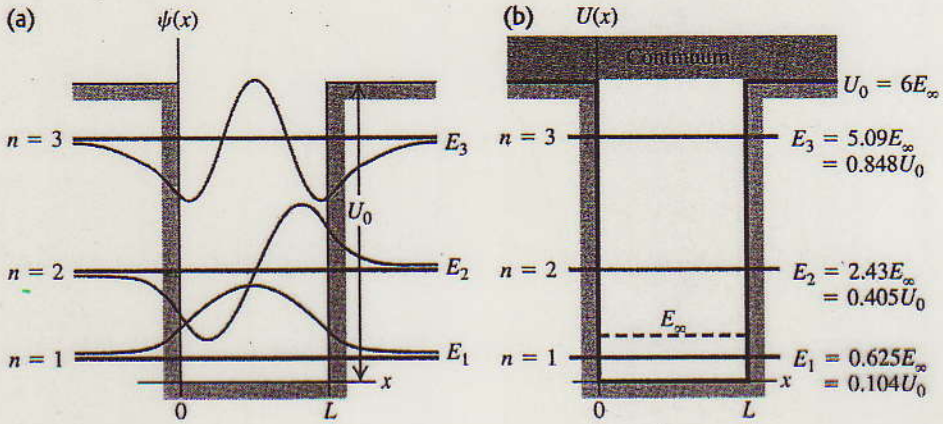
$$\Rightarrow \quad \frac{d^2\psi}{dx^2} - \frac{2m(U_0 - E)}{\hbar^2}\psi(x) = 0 \Rightarrow \boxed{\frac{d^2\psi}{dx^2} - K^2\psi(x) = 0}$$

Soln. for $U_0 > E$

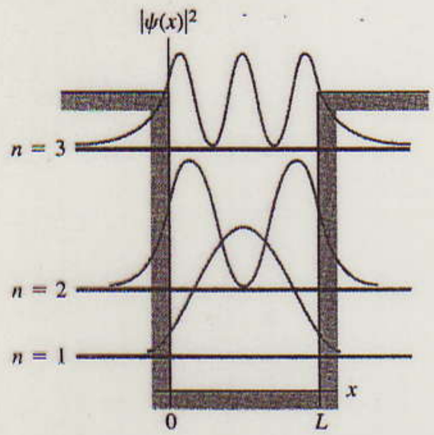
$$\psi(x) = Ce^{Kx} + De^{-Kx}, \quad \text{where } K^2 = \frac{2m(U_0 - E)}{\hbar^2}$$

[illegible], ~~continuous at x = 0 and x = L~~, + ~~normalization~~ + ~~ψ = 0 at x → ∞~~ condition determine 5 unknowns

Wave Functions, energy levels and probability density for finite U_0.



$E_\infty \equiv E_1$ of infinite square well potential



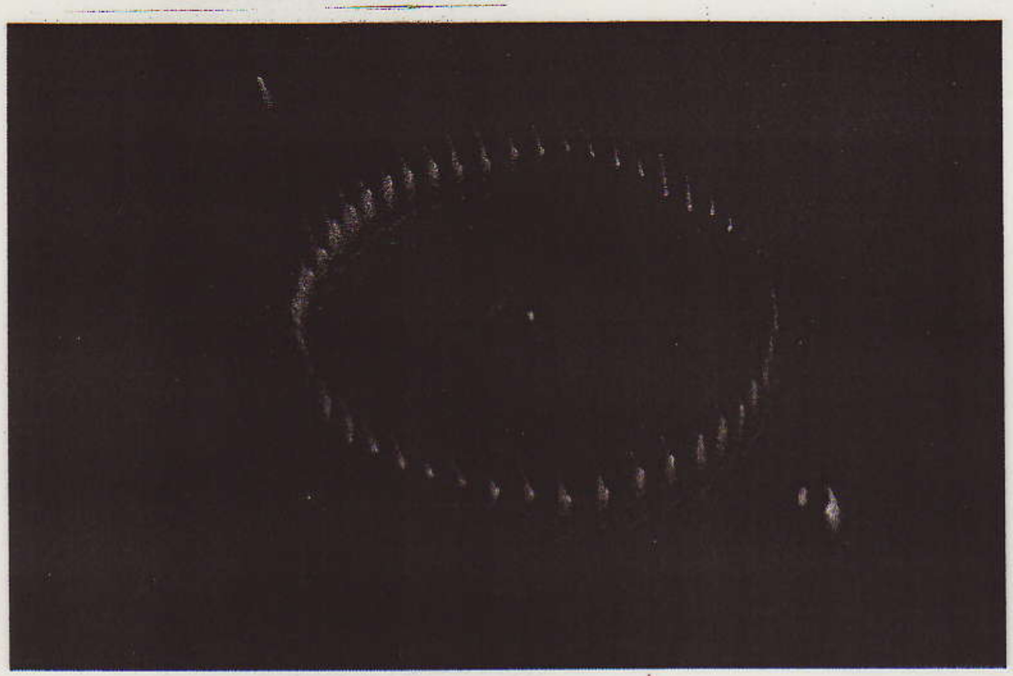
Solns. of these two eqns. with proper boundary conditions, give finite number of bound states inside the well and continuum of states when $E > U_0$.

If $U_0 = 6E_\infty$ (where E_∞ = grd. state energy of infinite potential problem), there are three bound states inside the well, ~~with~~ whose wavefunctions, energy levels and probability density are shown above.

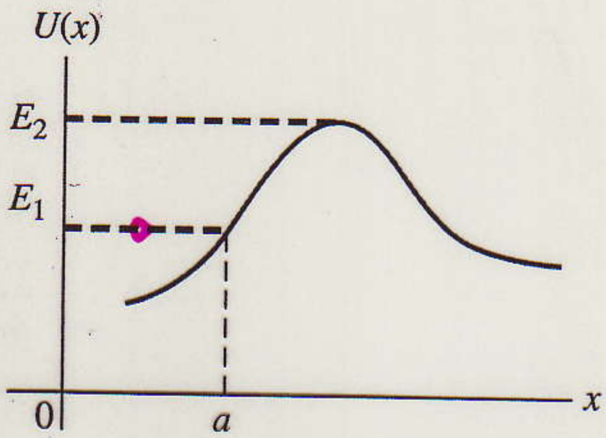
(Detailed calulation beyond the scope of this course)

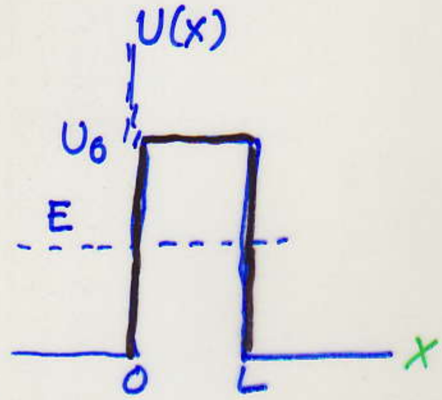
Note probability density and wave functions nonzero outside the well.

Real atoms in a 2-D well



Potential barriers and tunneling



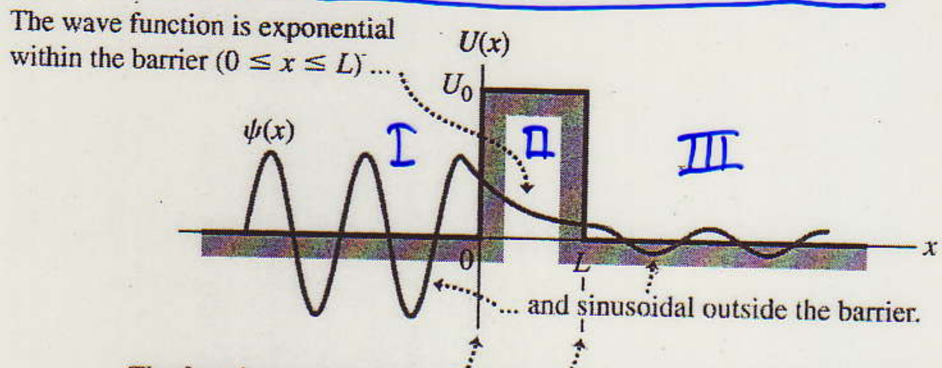


Potential barrier is a potential energy function with a maximum as shown above.

Classically a particle of energy $E < U_0$, will remain to the left of the barrier. If $E \geq U_0$ the particle may be found on the right of the barrier.

Quantum mechanically there is a probability that the particle will be found on the right side of the barrier. This penetration of the barrier ~~of~~ by a particle is called <u>tunneling</u>.

Tunneling through a square potential barrier



The function and its derivative (slope) are continuous at $x = 0$ and $x = L$ so that the sinusoidal and exponential functions join smoothly.

Classically particle of energy $E < U_0$ incident on the barrier will get reflected.

Quantum mechanically all regions are accessible to particle.

Wave functions in 3 regions are shown.

Since probability density $P(x) = |\psi(x)|^2$, probability of finding particle in region III is nonzero.

Quantum calulation of transmission coefficient gives

$$\boxed{T \simeq G e^{-2KL}}$$

Reflection coeff $R = 1 - T$

where $K = \dfrac{\sqrt{2m(U_0-E)}}{\hbar}$ and

$$G = 16 \frac{E}{U_0}\left(1 - \frac{E}{U_0}\right) \quad \text{for } E \ll U_0$$

Example: 30 eV electron incident on 40 eV square barrier

a) Tunneling prob. when $L = 1\,nm$

$G = 16\left(\frac{30}{40}\right)\left(1 - \frac{30}{40}\right) \boxed{= 3}$, $2KL = 2\dfrac{\sqrt{2(9.11\times10^{-31})\,10\times1.6\times10^{-19}}}{1.054\times10^{-34}}(1\times10^{-9}) \boxed{= 32.4}$

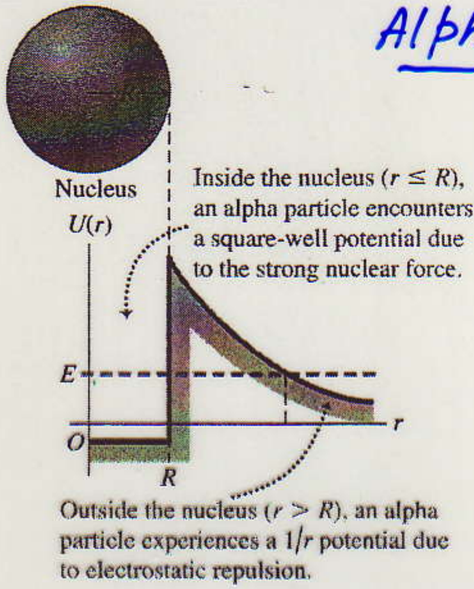
$$\boxed{T \simeq 3 \times e^{-32.4} = 2.55\times10^{-14}}$$

b) $T = ?$ when $L = 0.1\,nm$. $\boxed{2KL = 3.24}$

$T = 3 \times e^{-3.24} = \boxed{0.117}$ $\Rightarrow$ Prob. of transmission 13 orders of magnitude ~~lower~~ higher.

Applications of Tunneling

Alpha Decay by Heavy Nuclei



Heavy unstable nuclei decay by emitting α - particles (nuclei of He atoms).

To escape the nucleus, α - particle penetrates the barrier created by the combination of attractive nuclear force and Coulomb repulsion, which is several times higher than the energy of the α - particle.

Nuclear Fusion : The Sun is powered by fusion of protons.

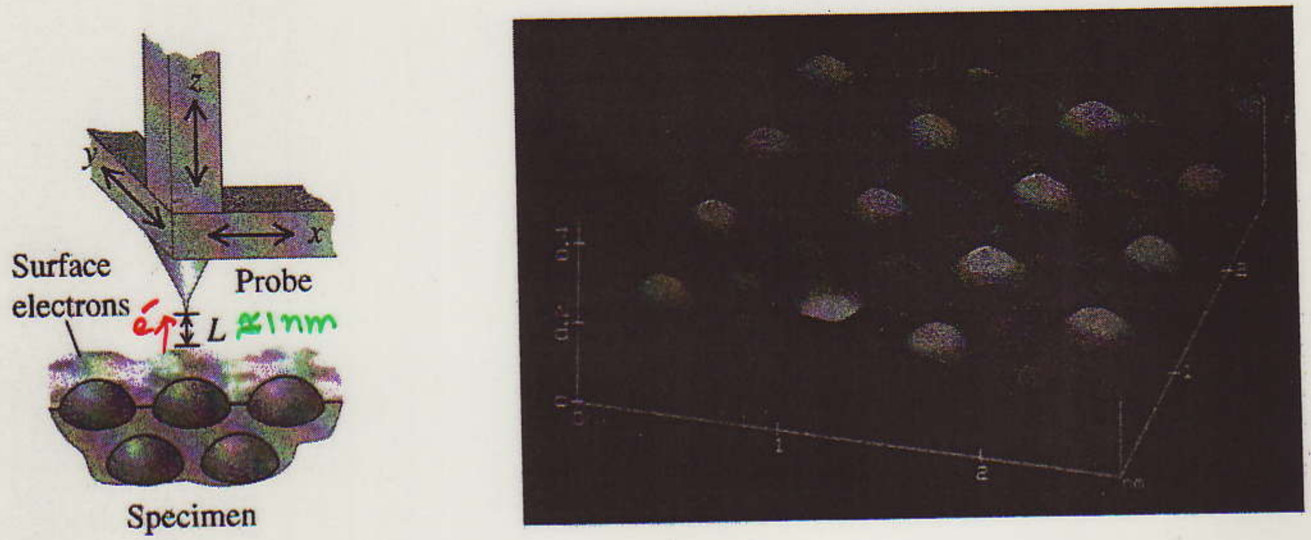
Protons must overcome tremendous Coulomb repulsion barrier to come together.

Classically it would not be possible.

Quantum mechanically protons can overcome Coulomb barrier by tunneling and fuse together.

Scanning Tunneling Microscope (STM)

(a) (b)



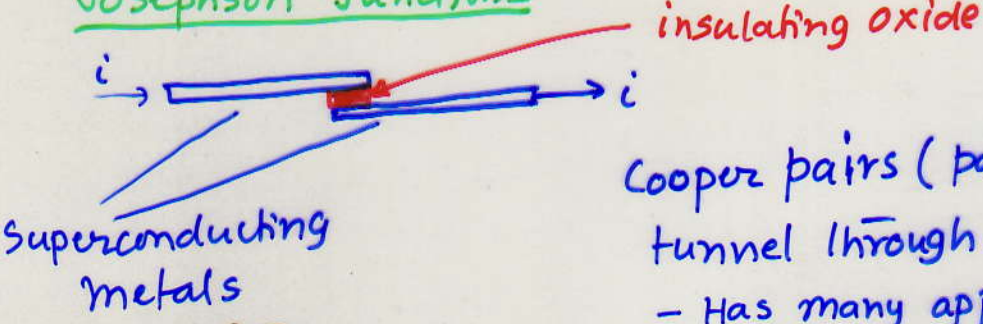
STM uses electron tunneling to create images of surfaces down to scale of individual atoms.

Figure (a) shows the needle that probes the surface of specimen.

Figure (b) is an image of sodium atoms on the surface of platinum crystal.

(Read text for details)

Josephson Junctions



$T < T_c$

Cooper pairs (pairs of electrons) tunnel through oxide layer.

- Has many applications
- detection of tiny magnetic fields