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CH101

Class 5; Physical Chemistry

Tunnelling of electrons across a barrier: Consider an electron (particle-wave) located at the left side of the barrier. The barrier is a potential energy barrier. At the left of the barrier, the potential energy of the electron is zero (0). At the right of the barrier the potential energy of the electron is also zero (0). However, the barrier has a height of V (potential energy) which is much larger than the energy of the electron E; i.e. at the barrier E<V. We need to find the wavefunction of the particle before the barrier, at the barrier and after the barrier. Then we will calculate the transmission coefficient (probability). This would be a function of the width of the barrier (L).

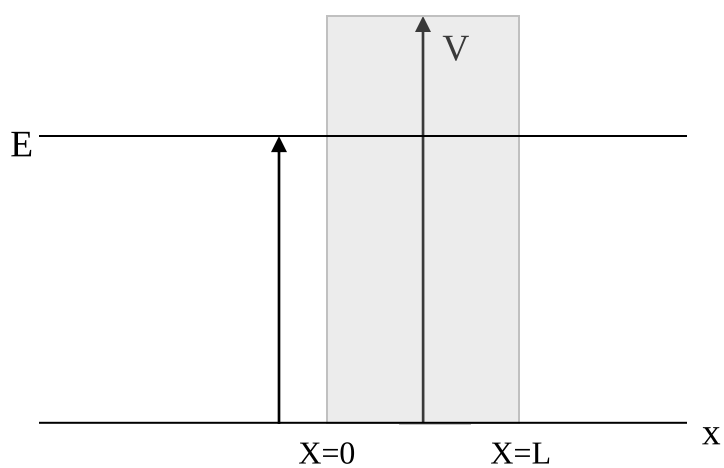

Figure 1 (A schematic of a tunnelling barrier)

Quantum mechanics considers electrons to have both wave and particle like properties. Tunneling is an effect of the wavelike nature of electron.

An important an interesting application of this nature of electron is the design and operation of scanning tunnelling microscope (STM). In STM a tip is scanned across the sample surface and the tunnelling current is related to the separation between the tip and the sample surface. Thus from the current one can measure the distance and surface profile of a conducting surface. Shown below is a typical geometry of the metallic tip and conducting surface that is used in STM. One scans the surface across its length and breadth and thus measures the surface profile from the tunnelling current.

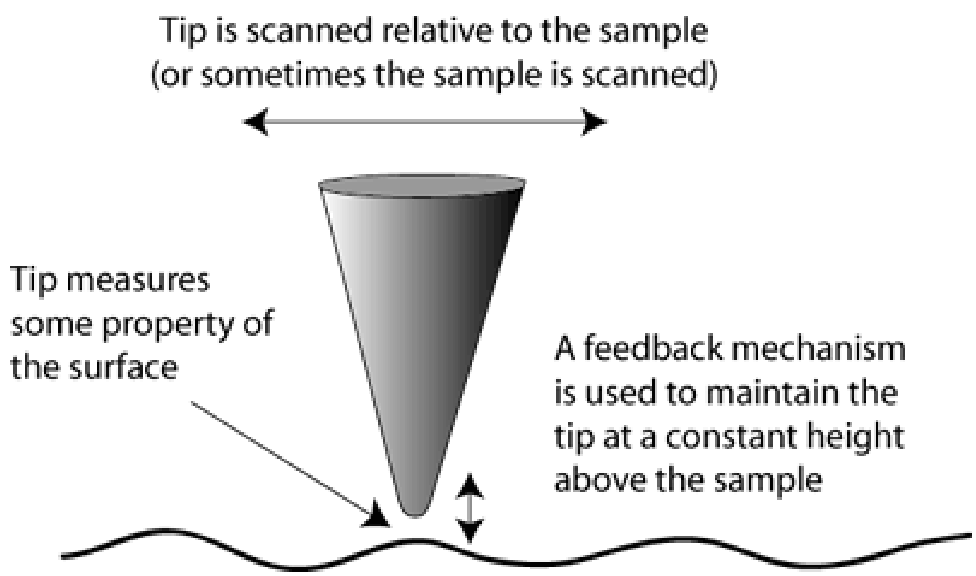

Figure 2. An application of electron tunneling. The Scanning Tunneling Microscope (the basic principle of operation is shown here).

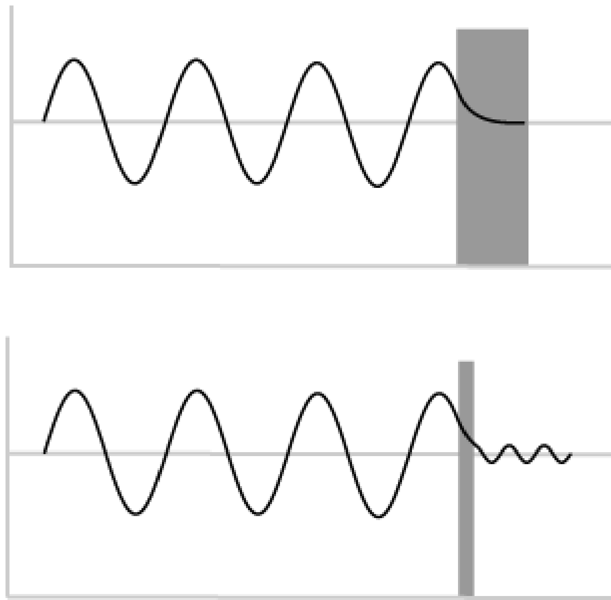

Figure 3.

The top image indicates that when the electron (wave) reaches the barrier, the wave doesn't abruptly end. On the other hand it decays exponentially in the barrier. When the barrier is thick then the electron cannot cross the barrier.

On the other hand, as shown in the bottom image, if the barrier is quite thin (about a nanometer or so), part of the wave does get through. Therefore, there is a finite probability (however small) of finding the electron on the other side of the barrier.

We need to write the Hamiltonians before, at and after the barrier, solve the equations, find the wavefunctions and then transmission coefficient from them.

The general Hamiltonian: $\hat{H} = \hat{T} + \hat{V}$

Before the barrier (x<0): V=0; hence $\hat{H} = \hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

$\hat{H}\,\Psi = E\,\Psi$ **has the solution,** $\Psi = Ae^{ikx} + Be^{-ikx}$**; where** $k = \frac{(2mE)^{1/2}}{\hbar}$

At the barrier: $0 \le x \le L$

$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + \hat{V}\ \Psi = \mathrm{E}\ \Psi$. **However, E < V; thus according to classical physics the particle has insufficient energy to cross the barrier.**

$\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = (\mathrm{V} - \mathrm{E})\ \Psi$ **;** $(\mathrm{V} - \mathrm{E}) > 0$

The solution is therefore, $\Psi = Ce^{\kappa x} + De^{-\kappa x}$**; where** $\kappa = \frac{\{2m(V-E)\}^{1/2}}{\hbar}$

To the right of the barrier: x > L; V = 0 hence $\hat{H} = \hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$

$\hat{H}\ \Psi = \mathrm{E}\ \Psi$ **has the solution,** $\Psi = A'e^{ikx} + B'e^{-ikx}$**; where** $k = \frac{(2mE)^{1/2}}{\hbar}$

Thus the complete wavefunction for a particle incident from the left side of the barrier consists of (a) an incident wave and a wave reflected from the barrier; (b) a wave whose amplitude changes exponentially inside the barrier; and (c) a wave that is oscillatory and propagates on the right of the barrier after tunnelling through the barrier successfully.

The conditions that the wave must satisfy are

(A) That the wave must be continuous at the barrier positions X=0 and X=L. This means the value of the wavefunction obtained from the left of the barrier and on the barrier must be same at X = 0. Similarly, the value of the wavefunction obtained from after the barrier and at the barrier must be the same at X = L.

(B) That the slope of the wavefunction must be continuous. In other words, the first derivatives of the wavefunctions at X = 0 obtained from before and after the barrier must be the same. Similarly the value of the first derivatives of the wavefunctions obtained form functions at the barrier and after the barrier at X = L must be the same.

Applying the condition of continuity of the wavefunction (at x = 0), we get

$$A + B = C + D \qquad (1)$$

and at x = L

$$Ce^{\kappa L} + De^{-\kappa L} = A'e^{ikL} + B'e^{-ikL} \quad (2)$$

Applying the conditions of the first derivatives being continuous

At x = 0, we get

$$ikA - ikB = \kappa C - \kappa D \qquad (3)$$

And at x = L we get

$$\kappa Ce^{\kappa L} - \kappa De^{-\kappa L} = A'ike^{ikL} - B'ike^{-ikL} \quad (4)$$

We have **four equations and six unknowns**.

We can put one more condition. Since we are considering the tunneling of electrons (particles) to the right of the barrier, we can safely assume that once the particle has crossed the right side of the barrier it does not come back. Hence B’ = 0.

Thus equation (2) can be replaced by

$$Ce^{\kappa L} + De^{-\kappa L} = A'e^{ikL} \qquad (5)$$

And equation (4) can be replaced by

$$\kappa Ce^{\kappa L} - \kappa De^{-\kappa L} = A'ike^{ikL} \qquad (6)$$

The probability that a particle moves towards the right of the left-side of the barrier is proportional to $|A|^2$

And the probability that a particle travels to the right of the right-side of the barrier is proportional to $|A'|^2$

Hence the transmission probability (coefficient) T,

$$T = \frac{|A'|^2}{|A|^2} = \{1 + \frac{(e^{\kappa L} - e^{-\kappa L})^2}{16\varepsilon(1-\varepsilon)}\}^{-1}$$

Where $\varepsilon = \dfrac{E}{V}$**;** $\kappa = \dfrac{\{2m(V-E)\}^{1/2}}{\hbar}$ and $k = \dfrac{(2mE)^{1/2}}{\hbar}$

(Solving this is your homework).