Particle seeing a barrier

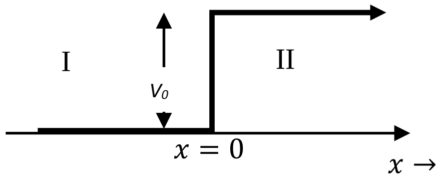

Figure 4.1: Particle incident on a barrier

$$V(x) = 0 \qquad x < 0$$

$$V(x) = V_0 \qquad x > 0$$

What happens when $E > V_0$?

Region I:

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

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

(The first term is for the particle moving to the right with the probability $|A|^2$ and momentum $+\hbar k$; the second term for the particle moving towards left.)

Region II:

$$\psi(x) = Ce^{ik_2x} + De^{-ik_2x}$$

$$k_2 = \left(\frac{2m(E - V_0)}{\hbar^2}\right)^{\frac{1}{2}}$$

We could exclude particles moving to the left in this region and so put $D = 0$ since the problem is that of a particle incident on the barrier from the left.

Wave function and first derivative is continuous

$$A + B = C$$

$$k_1(A - B) = k_2 C$$

A way to think. Consider N_0 particles. So $|A|^2 N_0$ is the number of particles moving to the right. The rate of particles passing through a given point is $v|A|^2 N_0$ where the velocity $v = \hbar k_1/m$.

Reflection

$$R = \frac{v_1 |B|^2 N_0}{v_1 |A|^2 N_0} = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

Transmission

$$T = \frac{k_2 |C|^2}{k_1 |A|^2} = \frac{4 k_1 k_2}{(k_1 + k_2)^2}$$

Particle gets reflected even though the energy E is greater than the barrier height!!!

What if $E < V_0$? $R = 1$

Square well potential

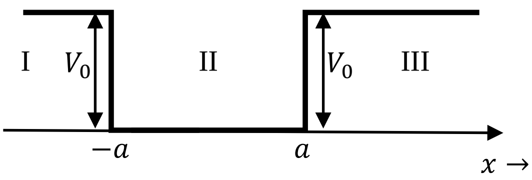

Figure 4.2: Square well - finite potential well

The height of the walls is finite,

$$V(x) = V_0 \qquad x < -a$$

$$V(x) = 0 \qquad -a \leq x \leq a$$

$$V(x) = V_0 \qquad\qquad x > a$$

First let us consider $E < V_0$

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

Solving this (remember the solutions for $K > 0$ are a special case of $K < 0$),

$$\psi_I = Ce^{kx}$$

$$\psi_{II} = A'e^{ik_1x} + B'e^{-ik_1x} = A\cos k_1x + B\sin k_1x$$

$$\psi_{III} = De^{-kx}$$

$$k = \left(\frac{2m(V_0 - E)}{\hbar^2}\right)^{\frac{1}{2}} \qquad k_1 = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}$$

which gives exponential decay/rise for the functions ψ_I and ψ_{III} and oscillating solutions for ψ_{II}.

Boundary conditions: Wavefunction and first derivative should be continuous. This gives two conditions

$$k_1 \tan k_1a = k$$

$$k_1 \cot k_1a = -k$$

or write it like,

$$\epsilon^{1/2}\tan\epsilon^{1/2} = (v_0 - \epsilon)^{1/2}$$

where,

$$\epsilon = a^2k_1^2 = \frac{2ma^2E}{\hbar^2}$$

$$v_0 = a^2(k_1^2 + k^2) = \frac{2ma^2V_0}{\hbar^2}$$

This can be solved graphically.

Fix v_0 and then plot $\epsilon^{1/2}\tan\epsilon^{1/2}$ and $(v_0 - \epsilon)^{1/2}$ as a function of ϵ on the same graph. The points of intersection give the solutions.

Similarly do it for the other equation $\epsilon^{1/2}\cot\epsilon^{1/2} = -(v_0 - \epsilon)^{1/2}$

The interesting result one obtains here is that there are only a limited number of bound states, i.e. energy levels below the potential energy V_0.

For example, putting $v_0 = 12$ yields $\epsilon = 1.47\ and\ 11.37$ from the tan equation plot and $\epsilon = 5.68$ from the cot plot.

Tunnelling

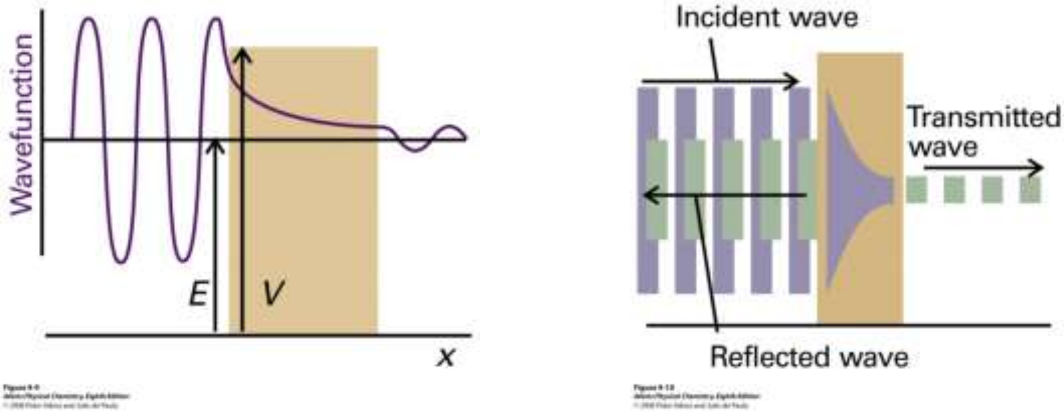

Figure 4.3: A particle tunnelling through a barrier

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < a \\ 0 & x > a \end{cases}$$

Let us worry about the situation when $E < V_0$

$$\psi_I(x) = A\, e^{ik_1 x} + Be^{-ik_1 x} \qquad x < 0 \qquad k_1\hbar = \sqrt{2mE}$$

$$\psi_{II}(x) = C\, e^{k_2 x} + Be^{-k_2 x} \qquad 0 < x < a \qquad k_2\hbar = \sqrt{2m(V_0 - E)}$$

$$\psi_{III}(x) = E\, e^{ik_1 x} + Fe^{-ik_1 x} \qquad x > a \qquad k_1\hbar = \sqrt{2mE}$$

ψ must be continuous, $d\psi/dx$ must be continuous --> gives 4 equations, 6 unknown coefficients

Shoot the particles from the left, so we can put $F = 0$.

Transmission probability

$$T = \left|\frac{E}{A}\right|^2 = \left\{1 + \frac{\left(e^{k_2 a} - e^{-k_2 a}\right)^2}{16\epsilon(1-\epsilon)}\right\}^{-1} \qquad \epsilon = \frac{E}{V_0}$$

What happens when the barrier is high, wide? $T \approx 16\epsilon(1-\epsilon)e^{-2k_2 a}$ exponential decrease

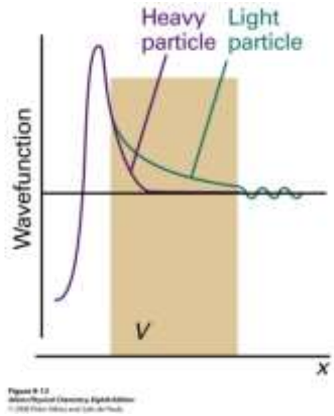

Figure 4.4: Tunnelling of heavy and light particles.

Tunnelling in chemistry

1) NH_3 inversion

2) Tunnelling of protons between acid-base: enzyme catalyzed reactions

3) DNA

4) electron tunnelling determines the rates of electron transfer reactions

Scanning Probe Microscope - STM and AFM

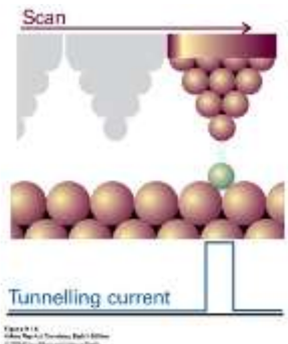

Figure 4.5: STM e- tunnelling

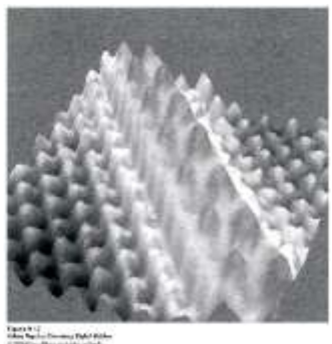

Figure 4.6: STM image of Cs atoms on GaAs surface

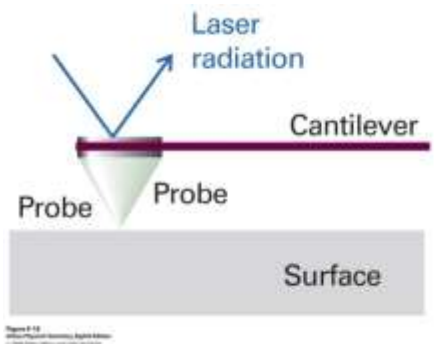

Figure 4.7: AFM principle