ELEC4705 – Fall 2009

Tom Smy

LECTURE 6
Tunneling

Contents

6.1. Introduction to Tunneling

Tunneling is a distinct phenomenon in QM. Suppose we have an electron in a voltage barrier as shown in figure 1. Classically the electrons traveling with kinetic energy $E < V_0$ will be reflected when they hit the barrier but they will pass the barrier if $E > V_0$. In QM we deal with this problem by solving the Schrodinger equation, as is explained in the following sections.

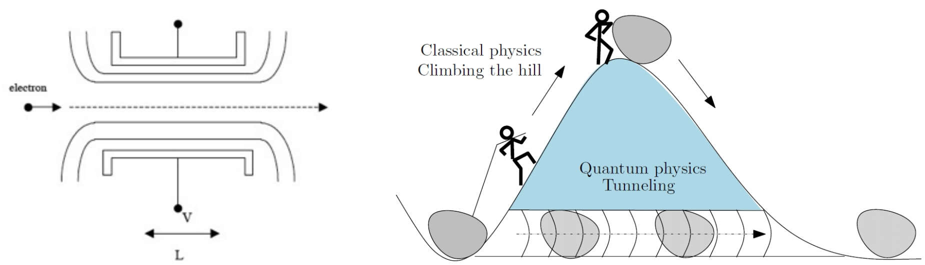
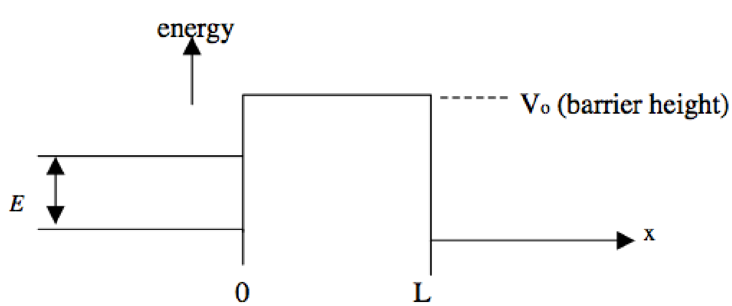


Figure 1. a) Electron movement in a voltage barrier. b) Potential hill and classical and QM transmission.

6.2. Simple Approach

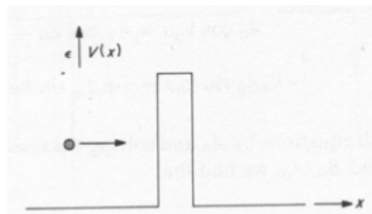


The SE equation for this is described by:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \qquad \text{outside barrier } (V = 0)$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_o)\psi = 0 \qquad \text{inside barrier } (V = V_o)$$

Suppose E < V_o classical physics predicts that the electron can not penetrate the barrier.



The electron (particle) would be described to be entirely reflected back from the barrier (at *x=0*) if its kinetic energy is smaller than V_o.

What does quantum mechanics predict?

1) For x < 0, V(x) = 0 and the solution is same as for free electrons:

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

We can view this solution as sum of two travelling waves:

Incident $\psi_{inc}(x,t) = Ae^{j(kx-\omega t)}$

Reflected $\psi_{ref}(x,t) = Be^{-j(kx+\omega t)}$

2) for 0 < x < L, $\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi}{dx^2} + V_o\psi = E\psi$

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

Since $E < V_o$ we rearrange the previous equation as

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V_o - E)\psi = 0 \quad \text{and define} \quad \alpha = \frac{\sqrt{2m(V_o - E)}}{\hbar}$$

so that

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0$$

Solution:

$$\psi(x) = Ce^{\alpha x} + De^{-\alpha x} \tag{26}$$

$$\psi(x,t) = Ce^{\alpha x}e^{-jwt} + De^{-\alpha x}e^{-j\omega t} \tag{27}$$

Exponential damped solution!

Assume forward transmission (single travelling wave past barrier)

3) <u>For x > L,</u> $\psi(x) = Fe^{jkx}$ $\quad \psi_{trans} = Fe^{j(kx-\omega t)}$

We now need to find A, B, C, D, F. We assume that $\psi(x)$ and $\frac{d\psi}{dx}$ are continuous at x = 0 and x = L. (Assumption of conservation of matter)

We have at x = 0: $A + B = C + D$ and $jkA - jkB = \alpha C - \alpha D$

and at x = L: $Ce^{\alpha L} + De^{-\alpha L} = Fe^{jkL}$ and $jkFe^{jkL} = \alpha Ce^{\alpha L} - \alpha De^{-\alpha L}$

which gives a set of linear equations in A, B, C, D, F

solution: $$\frac{F}{A} = \left[\frac{4jk\alpha Ae^{-jkL}}{\left[(\alpha + jk)^2 e^{-\alpha L} - (\alpha - jk)^2 e^{\alpha L}\right]}\right] \tag{29}$$

Define a transmission coefficient = $\left|\frac{F}{A}\right|^2$ (30)

and we find there is a non- zero probability of an electron penetrating barrier!

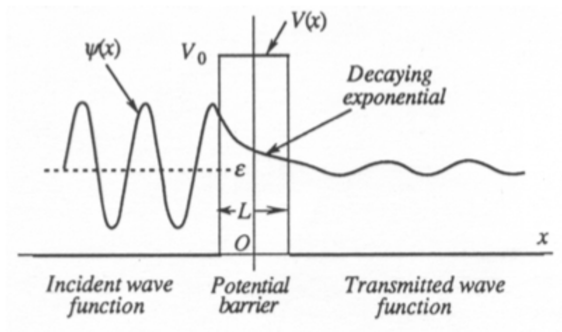
Suppose L is large (this is frequently the case)

Consider solution inside barrier $\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$

where $Ce^{\alpha x}$ is the part of the solution that blows up as x increases. ∴ not physically possible, so C=0.

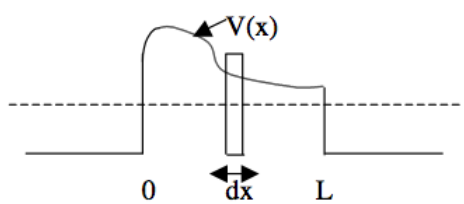
∴ $\psi(x) = De^{-\alpha x}$

∴ probability of electrons penetrating barrier ~ $e^{-2\alpha L}$ (31)



From this analysis we can conclude that a particle approaching a potential barrier of finite thickness and height has a certain probability of penetrating the barrier and appearing on the other side, even though this may be energetically forbidden on a classical basis. The wave function is attenuated within the barrier, and if the barrier is very high or quite thick, the attenuation becomes very strong and the probability of penetration becomes extremely small.

What if barrier is not constant in height? (i.e. not a "square" barrier)



We can imagine complete barriers subdivided into many small sections of length *dx*

probability of getting through section = $e^{-2\alpha(x)dx}$ where $\alpha(x) = \frac{\sqrt{2m(V(x)-E)}}{\hbar}$

probability of getting through entire barrier ~ = $e^{-2\alpha(x_1)dx_1} \cdot e^{-2\alpha(x_2)dx_2} \cdot \ldots$

$$\sim e^{\frac{-2\sqrt{2m}L\int_0^L (V(x)-E)^{1/2}dx}{\hbar}} \quad (32)$$

6.3. Transmission using Potential step and T matrices

A powerful way of modeling tunneling is using T matrices. The easiest analysis is a simple step in the potential. In this case we have a constant potential in both regions. Suppose that we have an upward potential step at $z = 0$ where potential jumps to V_0 at $z = 0$, as shown in figure 2. Classically the electrons traveling with energy $E < V_0$ will be reflected

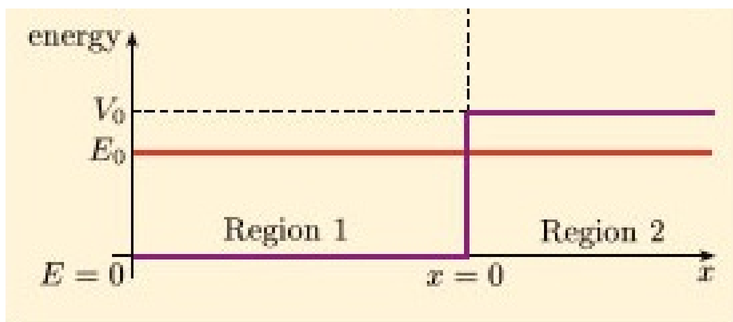


Figure 2. Step Barrier

when they hit the barrier but they will pass the barrier if $E > V_0$.

The QM description of electrons in a region of constant potential is a simple plane wave (at least if the energy of the electron is greater then the potential). We can identify three expected waves . An incoming wave in region 1 moving towards the barrier. A reflected wave moving in region 1 to the left and transmitted wave moving to the right in region 2. The incoming wave in $z < 0$ is $\exp(ik_1z)$ where $k_1 = \sqrt{2mE}/\hbar$. The outgoing waves are

- the reflected wave: $r\exp(-ik_1z)$ where $k_1 = \sqrt{2mE}/\hbar$
- the transmitted wave: $t\exp(ik_2z)$ where $k_2 = \sqrt{2m(E - V_0)}/\hbar$

Note that r and t are called *reflection* and *transmission amplitudes* and in general can be complex. Initally we assume that $E > V_0$ and so k_2 is real (we will relax this condition later) and all the waves propagate (to be general we included a 4th which is moving in region 2 from right to left).

$$\psi(z) = \left\{ \begin{array}{ll} A\exp(ik_1z) + B\exp(-ik_1z), & z < 0 \\ C\exp(ik_2z) + D\exp(-ik_2z), & z > 0 \end{array} \right\} \quad (6.1)$$

The wave function and its derivative must be continues at $z = 0$ so we have

$$\begin{aligned} A + B &= C + D \\ k_1(A - B) &= k_2(C - D) \end{aligned} \tag{6.2}$$

We can find the waves in right in terms of the waves in left as below:

$$\begin{aligned} C &= \frac{1}{2}(1 + k_1/k_2)A + \frac{1}{2}(1 - k_1/k_2)B \\ D &= \frac{1}{2}(1 - k_1/k_2)A + \frac{1}{2}(1 + k_1/k_2)B \end{aligned} \tag{6.3}$$

By substituting $A = 1$ (arbitrary assignment of the incident electron flux), $B = r$, $C = t$ and $D = 0$ (as we expect no electrons traveling to the left in region 2) we have:

$$\begin{aligned} t &= \frac{2k_1}{k_1 + k_2} \\ r &= \frac{k_1 - k_2}{k_1 + k_2} \end{aligned} \tag{6.4}$$

6.3.1. Density of currents

As we are interested in the flow of electrons i.e. the current we need an expression for the current density. Quantum Mechanics tells us that the current density is calculated for a given wave $\psi(x) = F \exp(ikx)$ by

$$J = \frac{1}{2}[\psi^*(\frac{\widehat{p}}{m}\psi) + (\frac{\widehat{p}}{m}\psi)^*\psi] \tag{6.5}$$

where $\widehat{p} = -i\hbar\frac{d}{dx}$ and $E = \frac{\hbar^2 k^2}{2m}$. So we have

$$\begin{aligned} J &= \frac{1}{2}[Fe^{ikx}(\frac{-i\hbar}{m}\frac{d(Fe^{ikx})}{dx}) + (\frac{-i\hbar}{m}\frac{d(Fe^{ikx})}{dx})^* Fe^{ikx}] \\ &= \frac{1}{2}[\frac{|F|^2\,\hbar k}{m} + \frac{|F|^2\,\hbar k}{m}] \\ &= |F|^2\frac{\hbar k}{m} \end{aligned} \tag{6.6}$$

So we can conclude

- for the incident wave $\exp(ik_1 z)$ the current density is $\hbar k_1|1|^2/m$.
- for the reflected wave $r\exp(-ik_1 z)$ the current density is $\hbar k_1|r|^2/m$
- for the transmitted wave $t\exp(ik_2 z)$ the current density is $\hbar k_2|t|^2/m$

From here from can obtain the *transmission* and *reflection coefficients* which are defined as the the ratio of currents as below:

$$T = \frac{\hbar k_2|t|^2/m}{\hbar k_1|/m} = \frac{k_2}{k_1}|t|^2 = \frac{4k_1k_2}{k_1+k_2}$$

$$R = \frac{\hbar k_1|r|^2/m}{\hbar k_1/m} = |r|^2 = (\frac{k_1-k_2}{k_1+k_2})^2 \tag{6.7}$$

An important check is that T and R must satisfy $T+R=1$, because every incident particle must be reflected or transmitted (conservation of particles).

For the other case where $E < V_0$, k_2 will be imaginary so the waves in right hand side are real (typically decaying) exponentials with wave number $\kappa_2 = \sqrt{2m(V_0-E)}/\hbar$ i.e. $k_2 = i\kappa_2$. These decaying (non propagating waves) we call evanescent waves. We know that an evanescent (decaying) wave does not carry current. So in this case we have $T=0$ and $R=1$.

Classically the transmission would be $T=1$ for all energies higher than the step but in quantum mechanics $T \longrightarrow 1$ only for high energies. For $E < V_0$ both the classical and quantum mechanical result in $T=0$.

6.4. T matrix

The above solution was for a single step. It can be written in useful way using a matrix. The T matrix can be used to simply analyse a sequence of step transitions and form more complicated barriers.

The relation we found in 6.3 can be rewritten in matrix from as

$$\begin{pmatrix} C \\ D \end{pmatrix} = T^{(21)} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \tag{6.8}$$

The reflection and transmission coefficients can be obtained from the T matrix.

$$\begin{pmatrix} t \\ 0 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} 1 \\ r \end{pmatrix} \tag{6.9}$$

So we have

$$r = -\frac{T_{21}}{T_{22}} \quad , \quad t = \frac{T_{11}T_{22} - T_{12}T_{21}}{T_{22}} \tag{6.10}$$

The T matrix for the step potential above for $E > V_0$ considering equations 6.3 is given by

$$T^{(21)} = \frac{1}{2k_2} \begin{pmatrix} k_2+k_1 & k_2-k_1 \\ k_2-k_1 & k_2+k_1 \end{pmatrix} \equiv T(k_2,k_1). \tag{6.11}$$

If $E < V_0$ we have $k_2 = i\kappa_2$.

In the above we had assumed that the step is at the origin ($z = 0$). A more flexible formulation is if we apply potential at $z = d$. We then need to fix T matrix as below.

$$T(d) = \begin{pmatrix} e^{-ik_2 d} & 0 \\ 0 & e^{ik_2 d} \end{pmatrix} T(0) \begin{pmatrix} e^{ik_1 d} & 0 \\ 0 & e^{-ik_1 d} \end{pmatrix} \quad (6.12)$$

Note that if in equation 6.12, the wave numbers in both sides are equal then we will have $T(d) = A^{-1}(d)T(0)A(d)$.

The formulation of T matrix in equation 6.8, allows us to simply multiply the T matrices for complex barriers in one dimension as follows (for example see figure 3):

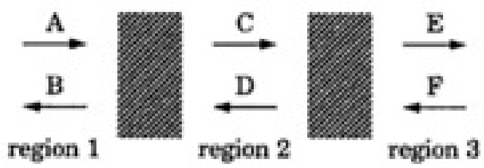


Figure 3. waves in three Region

$$\begin{pmatrix} E \\ F \end{pmatrix} = T^{(32)} \begin{pmatrix} C \\ D \end{pmatrix} = T^{(32)} T^{(21)} \begin{pmatrix} A \\ B \end{pmatrix} = T^{(31)} \begin{pmatrix} A \\ B \end{pmatrix} \quad (6.13)$$

where

$$T^{(31)} = T^{(32)} T^{(21)} \quad (6.14)$$

6.5. Square Barrier

Consider the potential barrier as shown in figure 4.

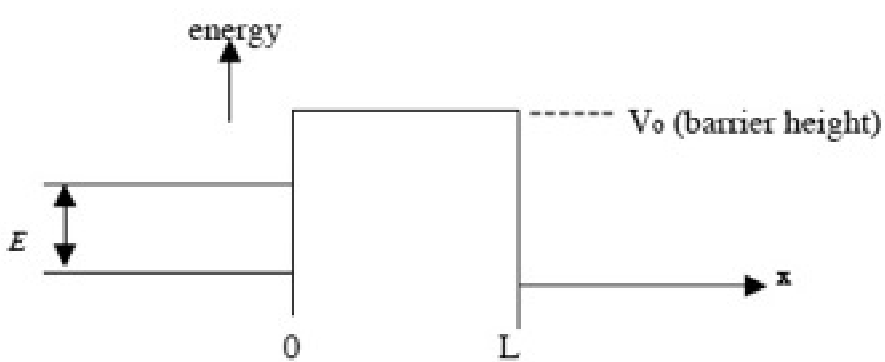


Figure 4. Potential Energy Barrier

(a) Shift the barrier so it is centered at the origin with $a = L/2$ and we have,

$$V(z) = \left\{ \begin{array}{ll} V_0 & -a/2 < z < a/2 \\ 0 & elsewhere \end{array} \right\} \tag{6.15}$$

(b) $E < V_0$
(c) the potentials at regions 1 and 3 are zero so $k_1 = k_3$
(d) for the upward step (region 1 to 2) we need a translation of $d = -a/2$ and for the downward step (region 2 to 3) we need as translation of $d = a/2$.
(e) The expect solution would have the form shown in Fig. 5 with incoming, reflected and transmitted waves and a evanescent wave in the barrier. We could get the exact solution by solving the SCE.

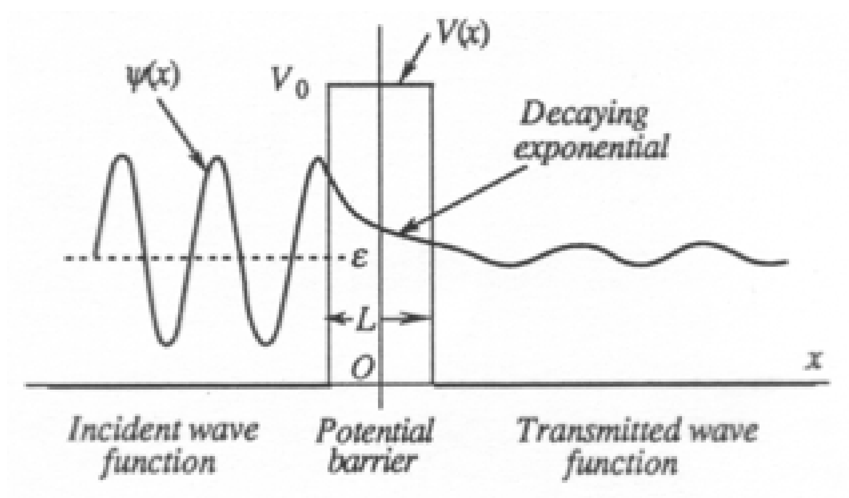


Figure 5. Square Barrier Solution

However, if we are interested in the reflection/transmission behaviour of the barrier we can simply use the T matrix. Considering the mentioned points we have the T matrix as follows

$$T = \begin{pmatrix} e^{-ik_1a/2} & 0 \\ 0 & e^{ik_1a/2} \end{pmatrix} T(k_1, k_2) \begin{pmatrix} e^{ik_2a/2} & 0 \\ 0 & e^{-ik_2a/2} \end{pmatrix}$$
$$\times \begin{pmatrix} e^{ik_2a/2} & 0 \\ 0 & e^{-ik_2a/2} \end{pmatrix} T(k_2, k_1) \begin{pmatrix} e^{-ik_1a/2} & 0 \\ 0 & e^{ik_1a/2} \end{pmatrix} \tag{6.16}$$

Using definition 6.11 we have:

$$T = \frac{1}{2k_1k_2}\begin{pmatrix} e^{-ik_1a/2} & 0 \\ 0 & e^{ik_1a/2} \end{pmatrix} \times$$
$$\begin{pmatrix} 2k_1k_2\cos k_2a + i(k_1^2+k_2^2)\sin k_2a & -i(k_1^2-k_2^2)\sin k_2a \\ i(k_1^2-k_2^2)\sin k_2a & 2k_1k_2\cos k_2a - i(k_1^2+k_2^2)\sin k_2a \end{pmatrix} \times$$
$$\begin{pmatrix} e^{-ik_1a/2} & 0 \\ 0 & e^{ik_1a/2} \end{pmatrix} \quad (6.17)$$

We see that the middle part is a function of the width of the barrier and is does not depend on the location of origin. However the phase factors on the sides are dependent on the location of the origin.
Using definition in 6.10 and some mathematical operations we will have:

$$t = \frac{2k_1k_2\, e^{-ik_1a}}{2k_1k_2\cos k_2a - i(k_1^2+k_2^2)\sin k_2a} \quad (6.18)$$

where as we know, $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(E-V_0)}/\hbar$, so the flux coefficient is as follows (illustrated in figure next page (Fig 5.6 p157)).

$$T = |t|^2 = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 - (k_1^2-k_2^2)\sin^2 k_2a} = [1+\frac{V_0^2}{4E(E-V_0)}\sin^2 k_2a]^{-1} \qquad for\ E > V_0 \quad (6.19)$$

for $E < V_0$ then we do $k_2 = i\kappa_2$

$$T = |t|^2 = \frac{4k_1^2\kappa_2^2}{4k_1^2\kappa_2^2 - (k_1^2-\kappa_2^2)\sin^2 \kappa_2a} = [1+\frac{V_0^2}{4E(V_0-E)}\sin^2 \kappa_2a]^{-1} \qquad for\ E < V_0 \quad (6.20)$$

for $E = V_0$ we have

$$T(E=V_0) = |t|^2 = [1+\frac{ma^2V_0}{2\hbar^2}]^{-1} \qquad for\ E = V_0 \quad (6.21)$$

Notes:

- Classically for $E < V_0$ we have no transmission ($T = 0$). But in quantum mechanics approach the particles can tunnel through the barrie however the probability of transmission may be small, figure6
- Classical for $E > V_0$ we have $T = 1$. But in quantum mechanics transmission coefficient has a peak of 1 when we have $\sin k_2a = 0$, figure 6.

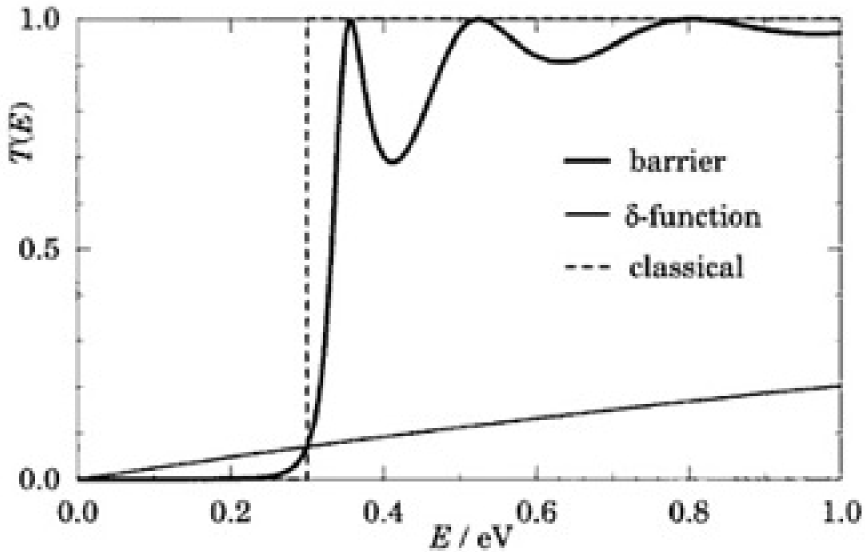


Figure 6. Transmission coefficient; Classical, QM

6.5.1. Not Constant barrier

In case of having a barrier which does not have a constant height as is shown in figure 7, then we can imagine complete barriers subdivided into many small sections of length dx and $k(x) = \sqrt{\frac{2m(V(x)-E)}{\hbar}}$.

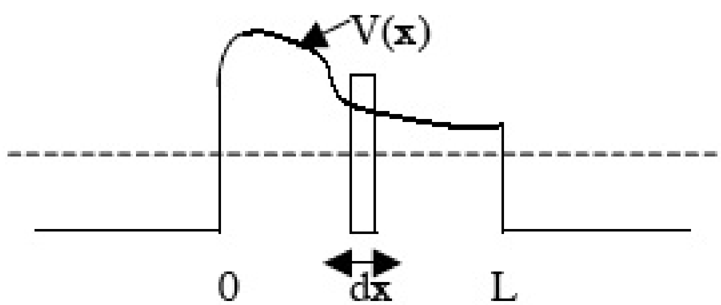


Figure 7. Not a Square barrier

6.6. Practical Examples

6.6.1. Field Emission Displays:

Concider figure 8. The screen can be controlled by controlling the stream of electrons.

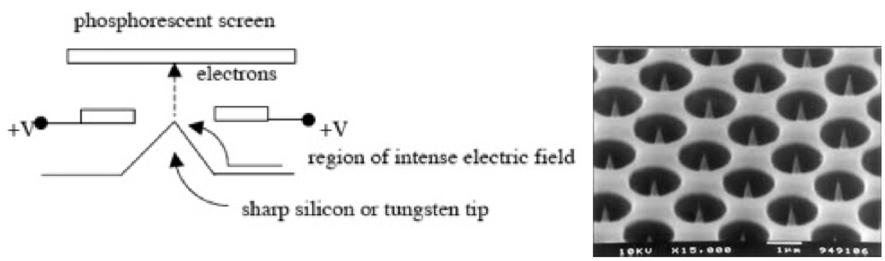


Figure 8. Array of emitting tips for flat panel display

The electric field and potential energy are related by equation 6.22

$$E = \frac{-1}{q}\frac{dV}{dx} \tag{6.22}$$

and electron energy diagram is shown in figure 9

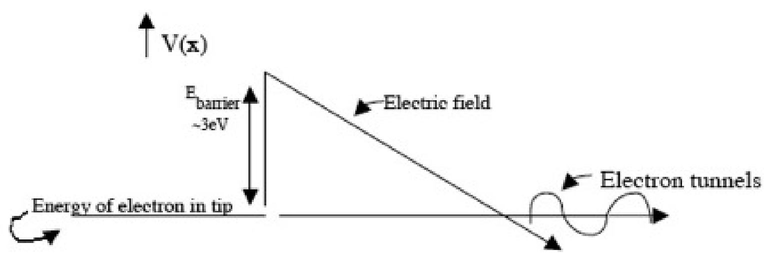


Figure 9. Electron Energy Diagram

6.6.2. Minimum Gate Oxide Thickness in MOSFET

When the gate oxide is very thin, a current can flow from gate to source or drain by electron tunneling through the gate oxide. This effect limits the thickness of the gate oxide as processes are scaled, see figures 10 and 11. The same effect is of great use in electrically programmable logic devices, such as EAROM (Electrically Alterable Read Only Memory). By controlling the control-gate, source, and drain voltages, the very thin tunnel oxide between the floating gate and the drain of the device

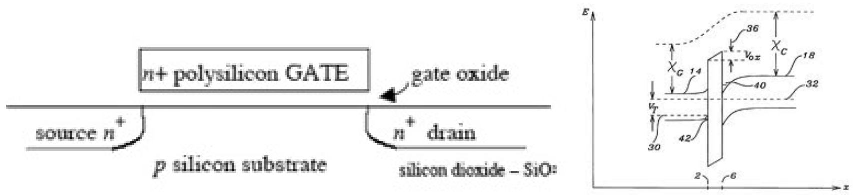


Figure 10. mosfet structure

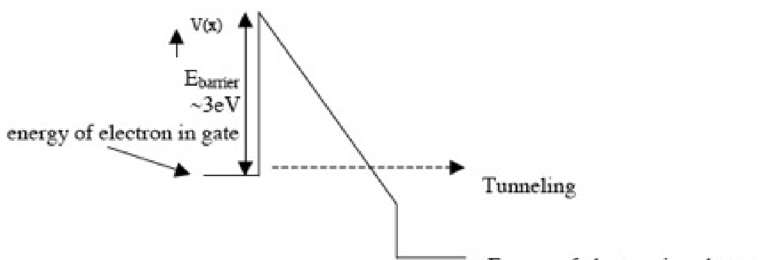


Figure 11. Electron Energy in substrate

is used to allow electrons to "tunnel" to or from the floating gate to turn the cell on or off respectively, see the structure shown in figure 12

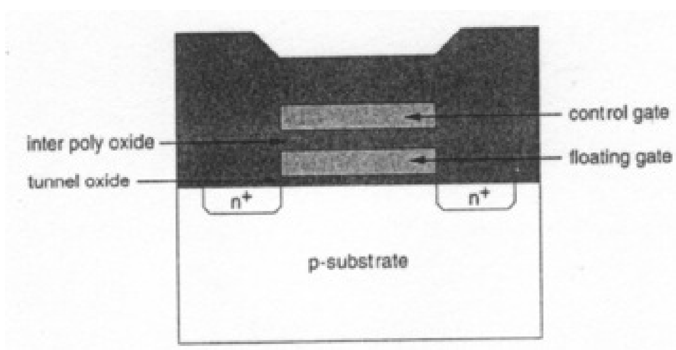


Figure 12. Electron Energy in substrate

6.6.3. Cold fusion

We find that if deuterons can be brought close enough together they will fuse.

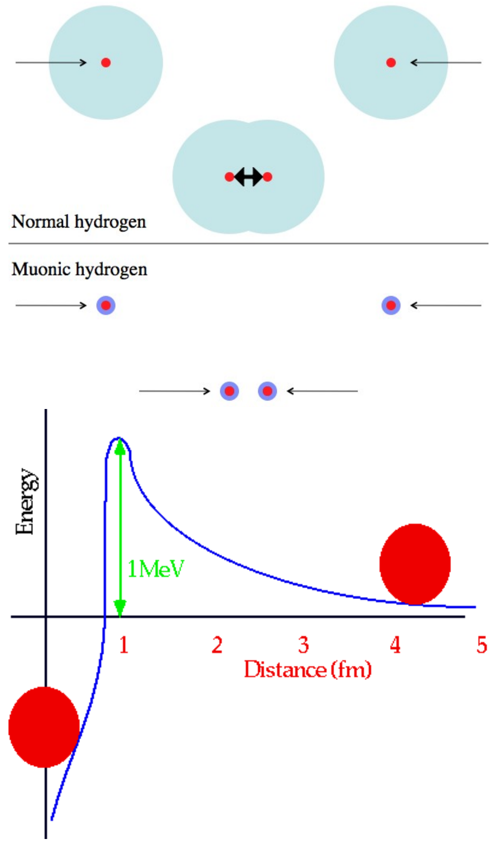


Figure 13. Cold Fusion