QUANTUM MECHANICS A (SPA-5319)

The Finite Potential Barrier

Let us consider a beam of particles of energy E < V_0 incident upon a rectangular potential barrier of height V_0 and width L (see figure 1).

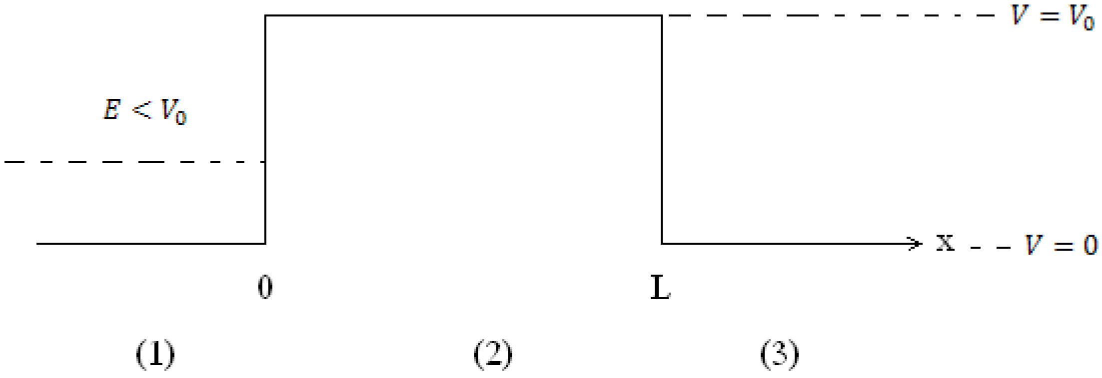

Figure 1: *A beam of particles meets a potential barrier that it has insufficient energy to overcome classically.*

The classical view of this arrangement is that as the particles are incident from the left, and as they have insufficient energy to overcome the barrier, there will be no particles found to the right of the barrier (ever). The quantum mechanical view is completely different. We have already encountered examples where in Quantum Mechanics there is a finite, non-zero probability of detecting a particle or system in a clasically forbidden region (e.g. the finite square well or the QHO). What we will derive in this section is an exact result for the *tunneling transmission* through a rectangular barrier. Quantum Mechanical tunnelling is a real, observed phenomenon, and there exist many devices (such as the scanning tunnelling microscope or organic light emitting diode) that rely on this phenomenon to function.

We can begin the analysis of this set-up by solving the time-independent Schrödinger equation in the three regions indicated in figure 1.

In region 1: V = 0, $\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$, $k = \sqrt{\frac{2mE}{\hbar^2}}$, $\psi_1(x) = Ae^{ikx} + Be^{-ikx}$

Here we can identify the two matter waves found in the solution as an incident (right travelling) and reflected (left travelling) wave.

In region 2: V = V_0 $\frac{\partial^2\psi}{\partial x^2} = \kappa^2\psi$, $\kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$, $\psi_2(x) = Ce^{\kappa x} + De^{-\kappa x}$

We note that, as this region is finite in space, we don't have to eliminate the growing exponential.

In region 3: V = 0 $\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$, $\psi_1(x) = Fe^{ikx}$

We note that, as there is no source of particles to the right of the barrier, we can neglect the left travelling wave (i.e. there is no Ge^{-ikx} term).

As the solutions are plane waves, we can easily write the incident, reflected and transmitted fluxes in regions 1 and 3 as

Region 1: $j_{INC} = |A|^2 \frac{\hbar k}{m}$, $|j_{REF}| = |B^2| \frac{\hbar k}{m}$

Region 3: $j_{TRANS} = |F|^2 \frac{\hbar k}{m}$.

And we recall the definitions of the reflection and transmission coefficients in such a case are:

$$T = \left|\frac{j_{TRANS}}{j_{INC}}\right| = \left|\frac{F}{A}\right|^2$$

$$R = \left|\frac{j_{REF}}{j_{INC}}\right| = \left|\frac{B}{A}\right|^2$$

Now we will apply continuity for both the wavefunction and its spatial derivative at the two boundaries, namely at $x = 0$ and at $x = L$:

ψ continuous $\rightarrow$ $A + B = C + D$ (1) $Ce^{\kappa L} + De^{-\kappa L} = Fe^{ikL}$ (3)

$\frac{d\psi}{dx}$ continuous $\rightarrow$ $ik(A - B) = \kappa(C - D)$ (2) $\kappa(Ce^{\kappa L} - De^{-\kappa L}) = ikFe^{ikL}$ (4)

We have obtained a set of four simultaneous equations. Note that we have five unknowns (A, B, C, D, and F), but we are <u>not</u> interested in solving for all of the unknowns simultaneously. If we remind ourselves of the transmission coefficient, we see that it is the ratio F/A that we are actually seeking. After some manipulation, we obtain this ratio:

$$\frac{F}{A} = \frac{4ik\kappa\, e^{-ikL}}{(\kappa + ik)^2\, e^{-\kappa L} - (\kappa - ik)^2\, e^{\kappa L}}$$

This can be rewritten in terms of the convenient quantity α and its complex conjugate as

$$\frac{F}{A} = \frac{4ik\kappa e^{ikL}}{\alpha^2 e^{-\kappa L} - \alpha^{*2} e^{\kappa L}}$$

where $\alpha = \kappa + ik$ and $\alpha^* = \kappa - ik$.

This gives the transmission coefficient as

$$T = \left|\frac{F}{A}\right|^2 = \left(\frac{4ik\kappa e^{ikL}}{\alpha^2 e^{-\kappa L} - \alpha^{*2} e^{\kappa L}}\right)^* \left(\frac{4ik\kappa e^{ikL}}{\alpha^2 e^{-\kappa L} - \alpha^{*2} e^{\kappa L}}\right) = \frac{16\kappa^2 k^2}{(\kappa^2+k^2)^2 (e^{\kappa L}+e^{-\kappa L})^2 + 16\kappa^2 k^2}$$

Eliminated α and α*, this can also be written as

$$T = \frac{4\kappa^2 k^2}{(\kappa^2 + k^2)^2 sinh^2(\kappa L) + 4\kappa^2 k^2}$$

where we have used the hyperbolic function $sinh(\theta) = (e^{\theta} + e^{-\theta})/2$.

We could repeat this whole process for the case $E > V_o$, and obtain the relevant transmission coefficient, but it would be tedious. If we inspect the solutions in region 2, however, we note that rather than obtaining the sum of simple growing and decaying exponentials, we would obtain a similar sum of complex exponentials (plane waves) and that these would be characterised by a wavenumber, *q*, given by

$$q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

So we can simply replace κ by iq in the previously obtained transmission coefficient, yielding

$$T = \frac{4q^2 k^2}{(k^2 - q^2)^2 sin^2(qL) + 4q^2 k^2}$$

It is worth noting that the hyperbolic function has been replaced by the trigonometric function.

The classically strongly forbidden case: There exist a family of realistic situations where the analysis of Quantum Mechanical tunneling can be simplified significantly by considering the *classically strongly forbidden* case. What is meant by "classically strongly forbidden" is that the particle or particles encounter a tall or thick barrier, where classically we really, really would not expect any transmission at all (hence strongly forbidden). One obvious condition that would give rise to this would be $E \ll V_o$, shown in figure 2.

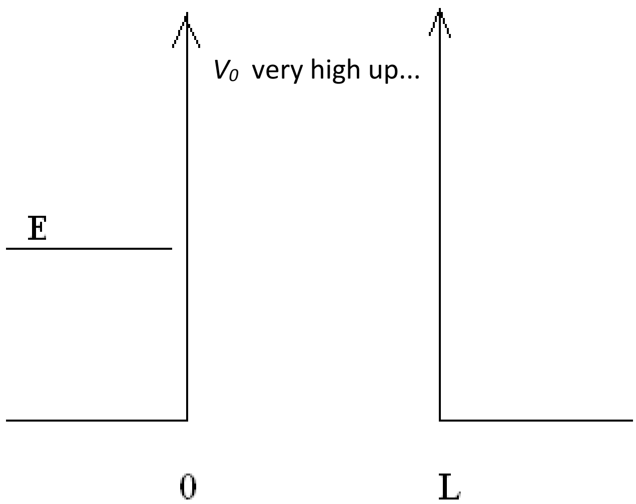

Figure 2: *A classically strongly forbidden tunneling situation, where the height of the barrier is very much greater than the energy of the particle or particles.*

Let us consider $E \ll V_o$, another way of saying this is that $\kappa L \gg 1$, as $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$. If we recall the transmission coefficient for a rectangular barrier is given by the equation T= $\frac{16\kappa^2 k^2}{(\kappa^2+k^2)^2(e^{\kappa L}+e^{-\kappa L})^2+16\kappa^2 k^2}$, and apply the condition $\kappa L \gg 1$, we can easily derive the result for the transmission in the classically strongly forbidden case:

$$T = \frac{16E(V_o-E)e^{-2\kappa L}}{{V_o}^2} = A(E)\, e^{-2\kappa L}$$

We find that (mathematically) the transmission coefficient can be split into a slowly varying function of energy, $A(E)$, and a single decaying exponential, $e^{-2\kappa L}$. This is an important result which is used widely and encountered frequently in the research literature. It is very useful. In summary, we have is a tunnelling probability that is:

a) exponentially decaying with distance

b) characterised by the extinction coefficient $\kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$.

An overview of the results so far for the rectangular barrier: The transmission coefficients in the two cases of $E < V_0$ and $E > V_0$ can be rewritten in terms of the energy and barrier height as:

$$E < V_0\,, \qquad T_{(E)} = \frac{1}{1+\frac{\sinh^2(\kappa l)}{4\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)}}, \qquad \kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$E > V_0, \qquad T_{(E)} = \frac{1}{1+\frac{\sin^2(ql)}{4\left(\frac{E}{V_0}\right)\left(\frac{E}{V_0}-1\right)}}, \qquad q = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

In figure 3 I have sketched the transmission coefficient as a function of the ratio of the particle energy to the barrier height (so when this ratio is 1 when $E = V_0$). Please note that the transmission is not-zero within the classically forbidden region. Also note the oscillations in the classically allowed region.

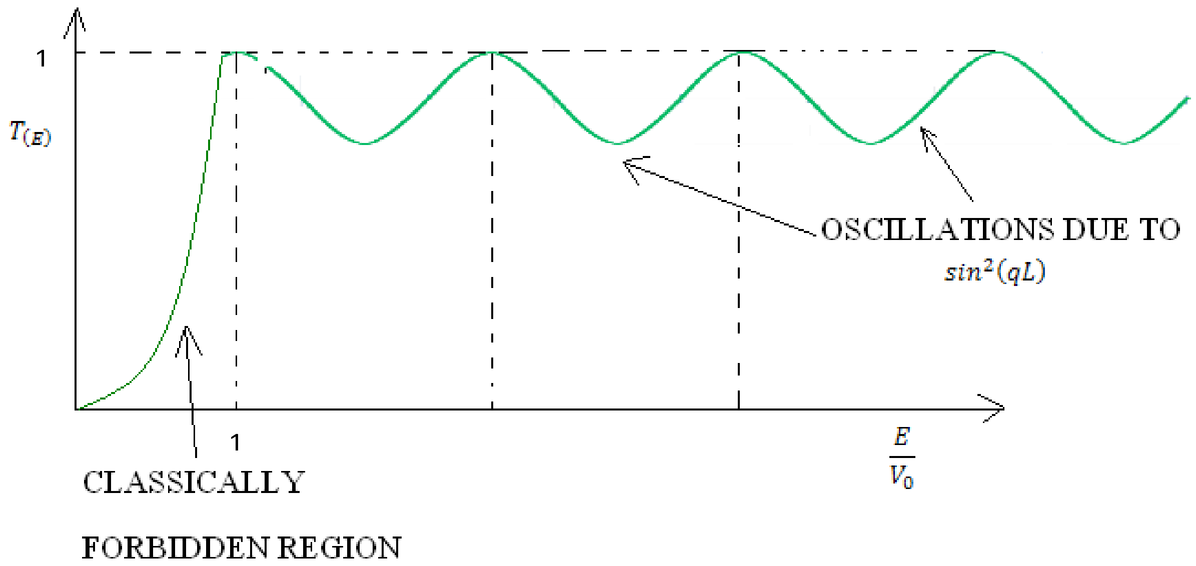

Figure 3: *the transmission coefficient versus thet ratio of particle energy to barrier height, for a rectangular potential barrier.*

If we take the classically strongly forbidden case (e.g. $E << V_0$) we can sketch the transmission coefficient variation with barrier thickness (or tunneling distance). This is a simple exponential decay, as shown in figure 4, which is characterised by the extinction coefficient, κ. Since the extinction coefficient itself is determined by the difference between the particle energy and the barrier height, it follows that the higher the particle energy the smaller the extinction coefficient and the more pronounced the tunneling (the transmission coefficient drops off slower with distance).

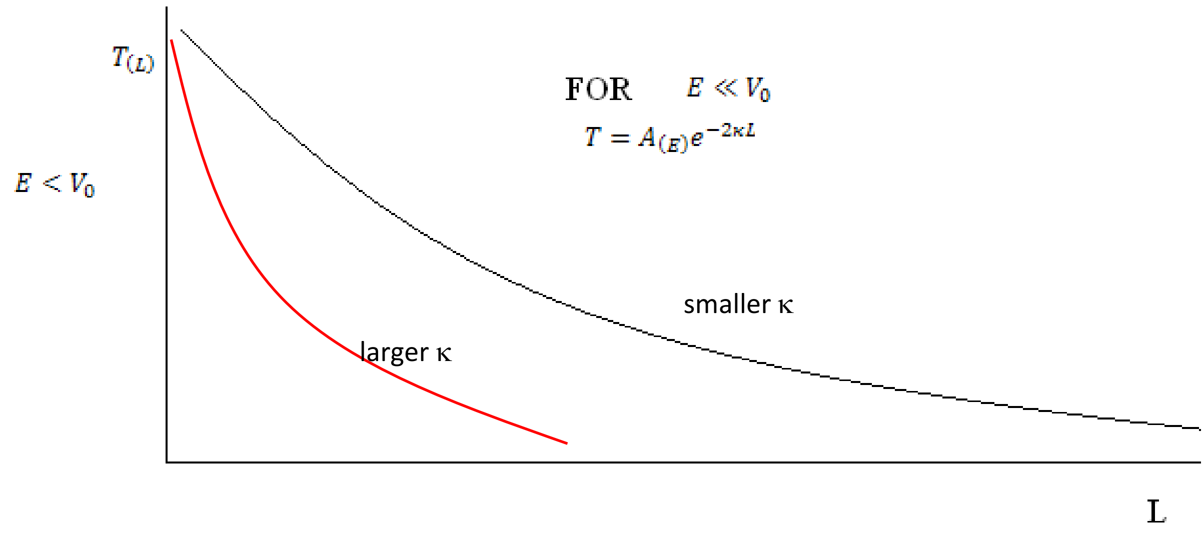

Figure 4: *The transmission coefficient versus barrier width in the classically strongly forbidden case.*

In the classically allowed case of $E \geq V_0$. On the other hand, the plot of transmission coefficient versus barrier width, shown in figure 5, displays some interesting effects.

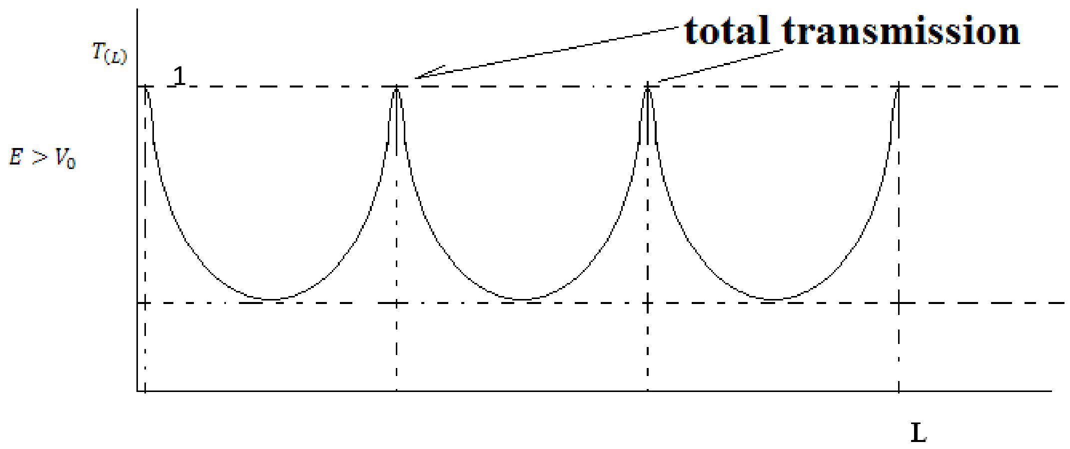

Figure 5: *transmission coefficient versus barrier width in the classically allowed case* $E \geq V_0$.

We note that the transmission coefficient periodically peaks at 1. That is, there is no reflection whatsoever. The explanation is simple: T = 1 for $E > V_0$ if $sin(ql) = 0$ as the denominator will go to one in the expression for T. This is the case if $qL = n\pi$, and as q is the wavenumber of the matter wave, $q = 2\pi/\lambda$, this gives $L = \frac{n\lambda}{2}$ (i.e. the well width is must be an integer number of ½ wavelengths to have T=1).

For a given particle energy, and thus wavelength, the resonant transmission will occur as the increasing barrier width in figure 5 matches exactly an integer number of half wavelengths, as shown in figure 6.

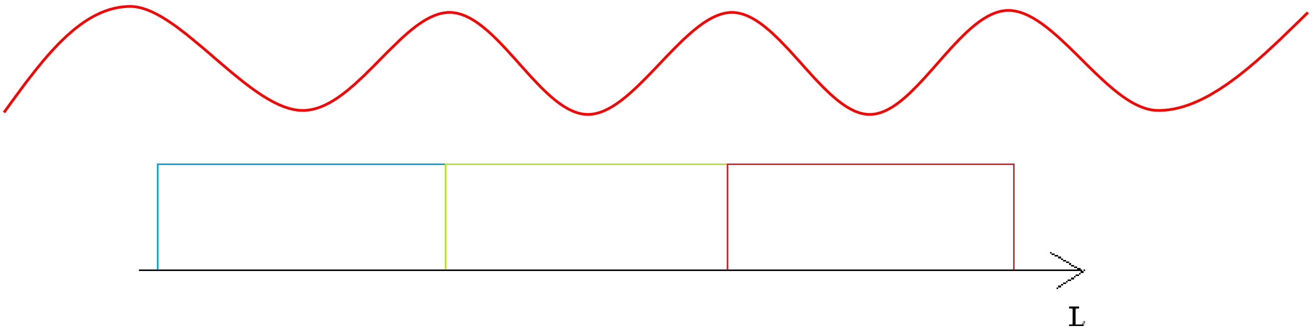

Figure 6: *resonant transmission occurs when the barrier width is an integer number of ½ wavelengths.*

The same resonant transmission condition applies if we consider a fixed barrier width and a varying particle energy (and therefore wavelength). This case is shown in figure 7.

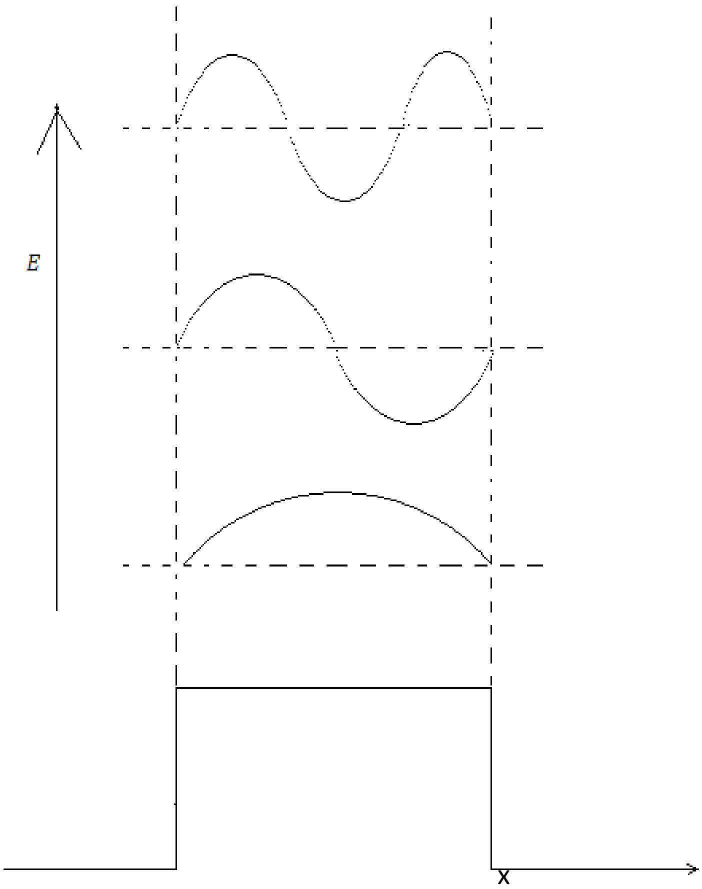

Figure 7: *for a fixed barrier width, resonant transmission occurs as particle energy increases*

It is worth noting that the case $E > V_0$, for matter waves encountering a barrier of width L and height V_0 , is mathematically equivalent to particles encountering a *well* of width L and *depth* V_0. This situation is shown in figure 8.

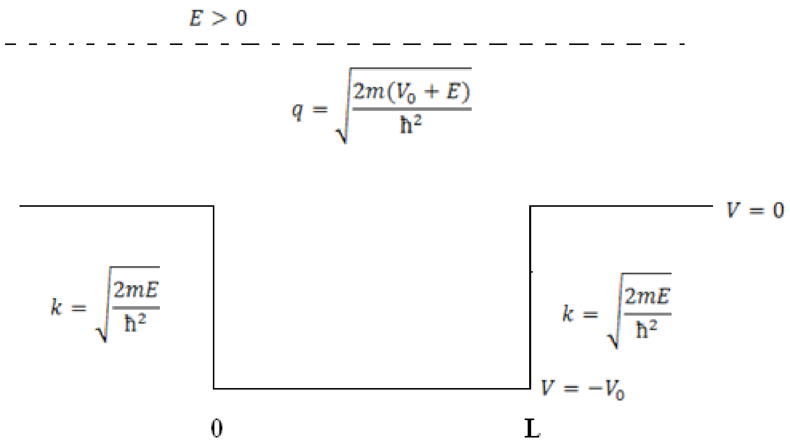

Figure 8: *a beam of particles encountering a well of width L and depth V_0.*

The only difference between the mathematics derived in the classically allowed situation for the barrier and this situation is that the wavenumber, q, for the matter wave above the well is given by $q = \sqrt{2m(V_0 + E)/\hbar^2}$ (exercise).

The equivalent of figure 3 for the example of particles encountering a well is sketched in figure 9. We note that the potential strength parameter, ζ_0 , determines whether resonant transmission is more or less prominent.

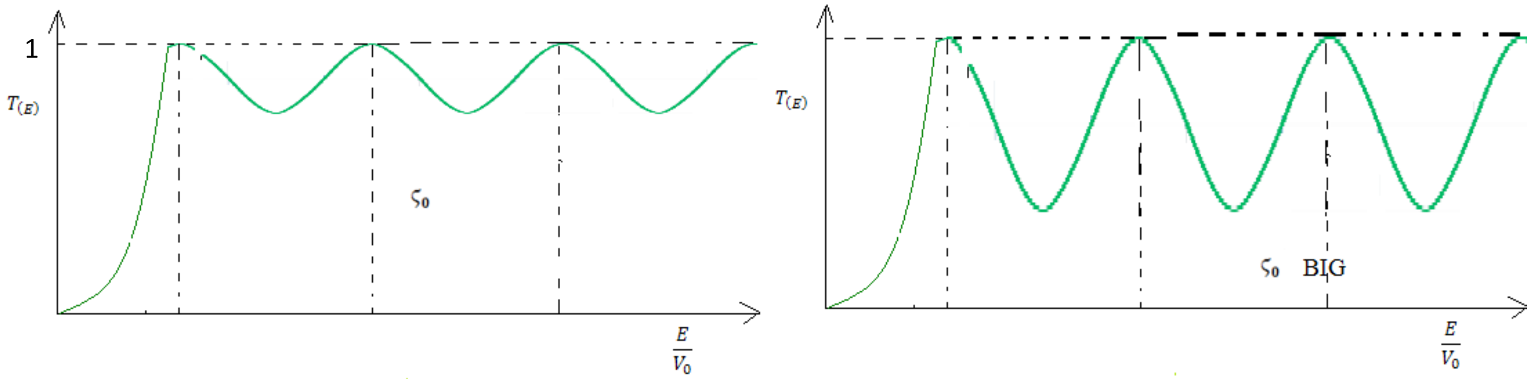

Figure 9: *the transmission coefficient for a beam of particles of energy E, encountering a well of width L and depth V_0, plotted versus the energy to well depth ratio for large and small values of the potential strength parameter.*