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Computer Project – Quantum Engineering

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CHALMERS UNIVERSITY OF TECHNOLOGY
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Summary

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Introduction

The energy associated to alpha particles emitted out of its atom's nucleus is clearly smaller than the one necessary to pass through the barrier generated by the attractive effect of the nuclear forces. That particle, in quantum mechanics, have a small probability of being outside of the nucleus, where the coulomb repulsion will push it further away, due to the uncertainty associated to its trajectory. Classical physics is not capable of explaining such behavior, that is why, the alpha particle decay is the perfect example of the quantum mechanical tunneling effect that will be seen in this report. Moreover, the barrier generated near the nucleus can be roughly modeled by a rectangular potential step, the latter which will be treated in the beginning of this report. When studying the transmission through a rectangular potential we will use the propagation matrix approach. In a second part, by slightly modifying the model used in the first section, we will use a potential well to study the bound states energies associated with it.

Finally, we will use the model in the first section to study the transmission through an array of a random number of barriers, with the same width, length and barrier-to-barrier separation.

1. Transmission through a rectangular potential

As briefly explained in the introduction, in this first section we will use the propagation matrix approach (see1.3 The Propagation Matrix Approach) to calculate the transmission coefficient of a rectangular potential step with, initially, a constant width and height .During the discussion of the obtained results we will analyze what would happen if those values would be modified. Moreover, in order to verify the MatLab code and the values obtained with it, the transmission coefficient will be calculated manually.

1.1 The Time-Independent Schrödinger equation

In Quantum mechanics, the propagation of a wave function $\psi(t)$ in time is given by a wave equation called Schrödinger equation. That equation contains the Hamiltonian (H) associated to the system.

$$i\hbar \frac{\partial \psi(t)}{\partial t} = H\psi(t) \leftrightarrow i\hbar \frac{\partial \psi(t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(r,t)\psi$$

If we consider a time-independent potential we can write the wave function as a multiplication of a spatial function $(\psi(r))$ and a time-dependent function. The spatial wave function can be shown to satisfy the following equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi$$

The last equation is known as the time-independent Schrödinger equation and will be the one used in the remaining of this report.

1.2 The rectangular potential barrier

In this model, we will consider a beam of particles arriving at a rectangular potential barrier of height V_0 and width L. In order to simplify the problem for the manual approach that will be describe later we need to deduce the values for the wave coefficients associated with each region using a few characteristics of this model.

The first thing to do is to impose $A = 1$ in order to simplify the coefficients F and B. Since the particles will be arriving from the left side, we can also assume that the coefficient B is related to the reflected particles. We can therefore say that $B = \ reflection\ amplitude\ r$. Moreover, since the particles will be leaving the region 2 towards the third zone we will not have any reflection coefficient in the third region wave, thus, E is zero. We can also assume that $F = \text{transmission amplitude } t$.

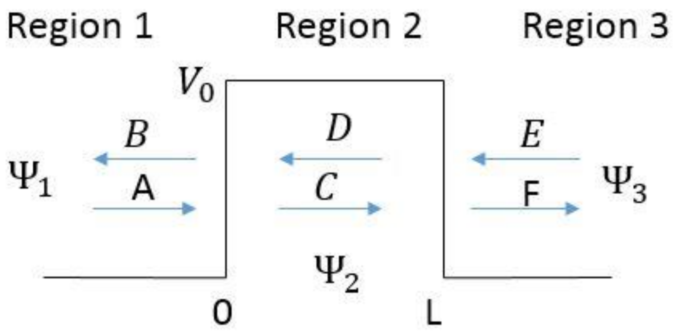


Figure 1 : Rectangular Potential Barrier

1.3 The Propagation Matrix Approach

We are interested in calculating the Transmission coefficient (T), therefore, we must use the solutions of the time-independent Schrödinger equation to deduce it. Considering the Figure 1 : Rectangular Potential Barrier, the general solution to the Schrodinger equation for each region is:

$$\Psi_1 = Ae^{iK_1x} + Be^{-iK_1x}$$

$$\Psi_2 = Ce^{iK_2x} + De^{-iK_2x}$$

$$\Psi_3 = Fe^{iK_1x} + Ee^{-iK_1x}$$

Where we have $K_1 = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}$ and $K_2 = \left(\frac{2m(E-V_0)}{\hbar^2}\right)^{\frac{1}{2}}$

Considering that we will be using MatLab to deduce the value of T it is more convenient to use dimensionless parameters. We know that K_1 and K_2 are both large values, approximately $10^9 m$, and since we also know that the length – scale is about $10^{-9} m$, we can multiply K_1 and K_2 by the typical length to obtain the dimensionless parameter K_1L and K_2L. We would also be interested in not having to provide specific values for E nor for V_0 so we also define the parameter $\beta_1 = \left(\frac{E}{V_0}\right)^{\frac{1}{2}}$ and $\beta_2 = \left(\frac{E}{V_0} - 1\right)^{\frac{1}{2}}$, which are both dimensionless.

The resulting expression for $K_1L$and K_2L will be:

$$K_1L = \left(\frac{2mEL^2}{\hbar^2}\right)^{\frac{1}{2}} = \beta_1\left(\frac{2mV_0L^2}{\hbar^2}\right)^{\frac{1}{2}} = \beta_1\alpha^{\frac{1}{2}}$$

$$K_2L = \beta_2\alpha^{\frac{1}{2}}$$

Using the continuity relations between the boundary of the region 1 with the region 2, which requires that the wave function and its derivative be continuous, we will obtain the following expressions:

$$A + B = C + D$$

$$iK_1A - iK_1B = iK_2C - iK_2D$$

After writing them in a matrix format:

$$\begin{pmatrix} 1 & 1 \\ iK_1 & -iK_1 \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ iK_2 & -iK_2 \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} \leftrightarrow m\begin{pmatrix} A \\ B \end{pmatrix} = n\begin{pmatrix} C \\ D \end{pmatrix}$$

$$\begin{pmatrix} A \\ B \end{pmatrix} = m^{-1}n\begin{pmatrix} C \\ D \end{pmatrix}$$

Which implies that

$$m^{-1}n = \left(\frac{1}{2\sqrt{K_1LK_2L}}\right)\begin{pmatrix} K_1L + K_2L & K_1L - K_2L \\ K_1L - K_2L & K_1L + K_2L \end{pmatrix}$$

$$\left(\frac{1}{2\sqrt{\beta_1\beta_2}}\right)\begin{pmatrix} \beta_1 + \beta_2 & \beta_1 - \beta_2 \\ \beta_1 - \beta_2 & \beta_1 + \beta_2 \end{pmatrix} = d_{12}$$

The matrix resulting from $m^{-1}n$ is be called the discontinuity matrix d_{12}. It will associate the wave function coefficients for the wave from the section 1 with the ones for the wave in the region 2. Moreover, since the continuity condition is also true for the second barrier $2 \rightarrow 1$, we can show (in the same way as we did for the first barrier) that for a coordinate system where the second barrier is in the position $x' = 0$ we have the following equation:

$$\begin{pmatrix} C' \\ D' \end{pmatrix} = d_{21}\begin{pmatrix} F' \\ E' \end{pmatrix}$$

Where the two matrix are composed by the coefficients of the wave functions in the new coordinate system. In order to be able to use this result we need to connect it to the original coordinate system. We will use the following relationship ($x' = x - L$) to deduce the propagation matrix connecting the two different coordinate systems.

$$\Psi_2(x) = \Psi_2'(x - L)$$

$$\Psi_2(x) = \begin{pmatrix} e^{iK_2(x-L)} & e^{-iK_2(x-L)} \end{pmatrix} \begin{pmatrix} C' \\ D' \end{pmatrix} = \begin{pmatrix} e^{iK_2(x)} & e^{-iK_2(x)} \end{pmatrix} \begin{pmatrix} C' e^{-iK_2 L} \\ D' e^{iK_2 L} \end{pmatrix}$$

Therefore, we can deduce that:

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} C' e^{-iK_2 L} \\ D' e^{iK_2 L} \end{pmatrix} = \begin{pmatrix} e^{-iK_2 L} & 0 \\ 0 & e^{iK_2 L} \end{pmatrix} \begin{pmatrix} C' \\ D' \end{pmatrix} = p_2 \begin{pmatrix} C' \\ D' \end{pmatrix}$$

Where p_2 is the propagation matrix. With the same reasoning, we can deduce p_1 for the wave in the third region.

$$\begin{pmatrix} F \\ E \end{pmatrix} = p_1 \begin{pmatrix} F' \\ E' \end{pmatrix} \quad where \quad p_1 = \begin{pmatrix} e^{-iK_1 L} & 0 \\ 0 & e^{iK_1 L} \end{pmatrix}$$

We can, therefore, deduce the transfer matrix (t), which will connect the wave coefficients from the first region to the ones in the third and last region.

$$\begin{pmatrix} A \\ B \end{pmatrix} = d_{12} p_2 d_{21} p_1^{-1} \begin{pmatrix} F \\ E \end{pmatrix} = t \begin{pmatrix} F \\ E \end{pmatrix}$$

As it has already been told, we want to deduce the Transmission coefficient (T). Since we know that the latter is nothing more than the ratio of the flux of particles that are capable of arriving in the third region (penetrating the second barrier) to the flux of particles incident in the first barrier (that arrive in the first region), the T will be :

$$T = \frac{\left|F e^{iK_1 x}\right|^2}{\left|A e^{iK_1 x}\right|^2} \leftrightarrow \frac{1}{|t_{11}|^2}$$

1.4 The Manual Approach

The method presented above is faster to use in the case that you have a program such as MatLab that you can use to retrieve the values for the transmission coefficient. Moreover, as it will be shown in the third section, it is easy to apply it for a random number of barriers. Nevertheless, it is interesting to know how to retrieve the transmission coefficient using another approach so we can, when possible, compare it with the results obtained using the previous method.

As it was explained in 1.2 The rectangular potential barrier, for this type of model we can consider the coefficient E being equal to zero, $A = 1$, B being the reflection amplitude (r) and F the transmission coefficient (t), to simplify the calculations. We will calculate the value of T for two different scenarios.

- When $E < V_0$ and the particles are coming from the left
- When $E > V_0$ and the particles are coming from the left

We will start with the first case. Just as we did for the propagation matrix approach we will use the continuity conditions, but first we will redefine the second wave equation taking in consideration the imaginary coefficient in the K_2. We will use the following relation:

$$K_2 = \left(\frac{2m(E - V_0)}{\hbar^2}\right)^{\frac{1}{2}} = i\left(\frac{2m(V_0 - E)}{\hbar^2}\right)^{\frac{1}{2}} = ik$$

As for the previous method, we will also use $K_1 L = \beta_1 \alpha^{\frac{1}{2}}$ and $K_2 L = ikL = i\beta_2{}' \alpha^{\frac{1}{2}}$

The wave equations will be written as:

$$\Psi_1 = e^{iK_1 x} + re^{-iK_1 x}$$

$$\Psi_2 = Ce^{i(ik)x} + De^{-i(ik)x} = Ce^{-kx} + De^{kx}$$

$$\Psi_3 = te^{iK_1 x}$$

The continuity conditions will provide us with the following expressions:

$$1 + r = C + D \qquad for\ x = 0$$

$$1 - r = \frac{k}{iK_2}(D - C) \qquad for\ x = 0$$

$$Ce^{-kL} + De^{kL} = te^{iK_1 L} \qquad for\ x = l$$

$$\left(\frac{k}{iK_1}\right)\left(-Ce^{-kL} + De^{kL}\right) = te^{iK_1 L} \qquad for\ x = l$$

We now have four linear equations and four unknowns; therefore, we can solve this system. As we are only interested in the transmission coefficient, we will only solve the system for t. We will obtain the following formula:

$$t = \frac{4ie^{-iK_1 L}(kL)(K_1 L)}{(-(kL)^2 + (K_1 L)^2 + 2i(kL)(K_1 L))e^{kL} + \left((kL)^2 - (K_1 L)^2 + 2i(kL)(K_1 L)\right)e^{-kL}}$$

$$t = \frac{4ie^{-i\beta_1\alpha^{\frac{1}{2}}}(\beta_1)(\beta_{2'})}{(-(\beta_{2'})^2 + (\beta_1)^2 + 2i(\beta_{2'})(\beta_1))e^{\beta_{2'}\alpha^{\frac{1}{2}}} + \left((\beta_{2'})^2 - (K_1L)^2 \ + \ 2i(\beta_{2'})(\beta_1)\right)e^{-\beta_{2'}\alpha^{\frac{1}{2}}}}$$

The last equation is given using dimensionless parameters so we can easily plot the transmission coefficient on MatLab. It is also important to remember that:

$$T = \frac{\left|Fe^{iK_1x}\right|^2}{|Ae^{iK_1x}|^2} \leftrightarrow T = |t|^2$$

Therefore, we will be plotting $|t|^2$ and not t.

If we calculate for the second case, when $E > V_0$ the method used will be the same. Nevertheless, there will be one difference when rewriting the wave functions for each region since we will not have an imaginary value for K_2L.

$$\Psi_1 = e^{iK_1x} + \ re^{-iK_1x}$$

$$\Psi_2 = Ce^{\,K_2x} + \ De^{-\,K_2x}$$

$$\Psi_3 = t'e^{iK_1x}$$

The function that we will obtain for $|t'|^2$ will be:

$$|t'|^2 = \frac{4(K_1L)^2(K_2L)^2}{4(K_1L)^2(K_2L)^2 + ((K_1L)^2 - (K_2L)^2)^2\sin^2(K_2L)}$$

$$= \frac{4(\beta_1^2\alpha)\,(\beta_2^2\alpha)}{4(\beta_1^2\alpha)\,(\beta_2^2\alpha) \ + ((\beta_1^2\alpha) \ - (\beta_2^2\alpha)\,)^2\sin^2\left(\beta_2\alpha^{\frac{1}{2}}\right)}$$

Before plotting, the curves associated to $|t'|^2$ and $|t|^2$ we can already deduce their behavior in function of the Energy E. We can see that the latter will increase exponentially when E increases, which is verified by the theory behind this model (tunneling effect) and for the former, we can see that the plot will show oscillations due to the $\sin^2\left(\beta_2\alpha^{\frac{1}{2}}\right)$ term.

1.5 Results and Discussion

After having programmed the MatLab code responsible to calculate the transfer matrix using the propagation matrix method, the first thing that we should do is verify if the graphic that we obtain for a fixed value of width (L) and height (V_0) is correct. In order to do that, as it was told in the beginning of this section, we will compare that graph with the one plotted using directly the formula deduced with the manual approach.

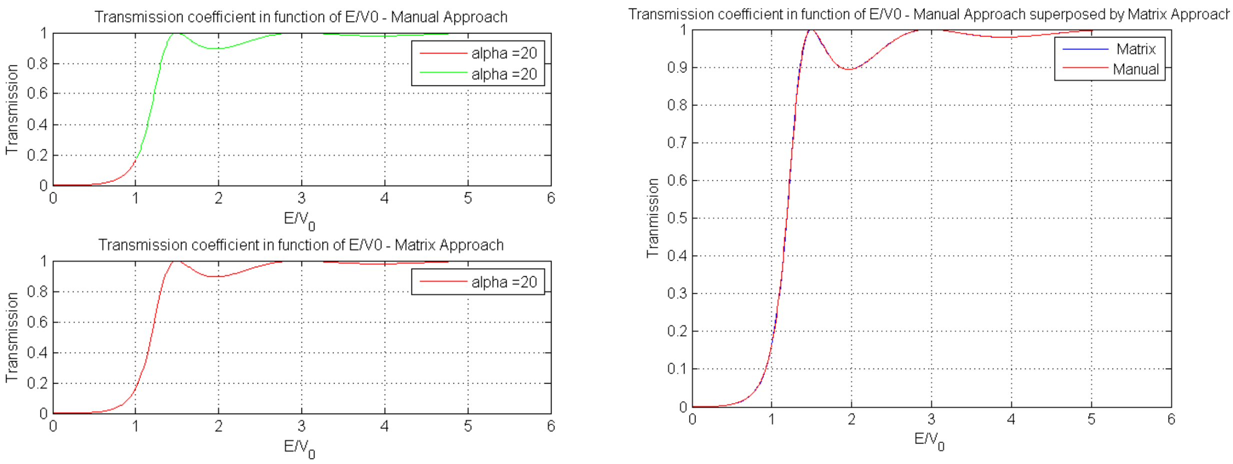


Figure 2 : Graphics comparing the Manual Approach with the Matrix Approach. The alpha is constant, thus, there is no length variation.

We can see that the plots superpose each other perfectly, thus the MatLab code is correct. Moreover, we can see the exponential increase in the Transmission as E/V_0 increases and, when it reach values bigger than one, we can observe the effect of the sinus on the $|t'|^2$ formula. The effect see in the beginning, as told before, can be explained by the tunneling effect, where, even though the energy of the particle is smaller than the width of the step, there still a small probability that the particle will overcome such obstacle. The second effect is the oscillation of the transmission in the zone $\frac{E}{V_0} > 1$. It can be explained by the existence of a small probability of reflection when particle has more energy than the barrier. That small probability comes from the destructive interferences of the wave functions. We will use graph of the Transmission versus the width (L) to better describe that phenomenon. With a second plot, we will increase the value of alpha so we can discuss the effect of increasing length of the barrier (V_0 is kept constant).

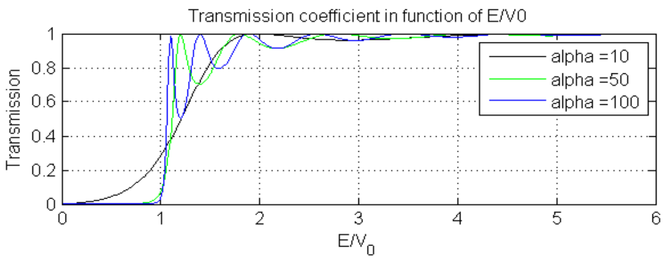


Figure 3 the transmission coefficient in function of E/V0 for three different values of alpha.

As expected we can see that by increasing the width L, thus the alpha value, we decrease the Transmission coefficient for a constant value of $\frac{E}{V_0} < 1$. Moreover, we can see that the frequency of the oscillation increases with the increase of the length of the barrier. We will now plot the transmission in function of the length to discuss about that consequence. We will plot in two different figures for when the $\frac{E}{V_0} < 1$and for when$\frac{E}{V_0} > 1$.

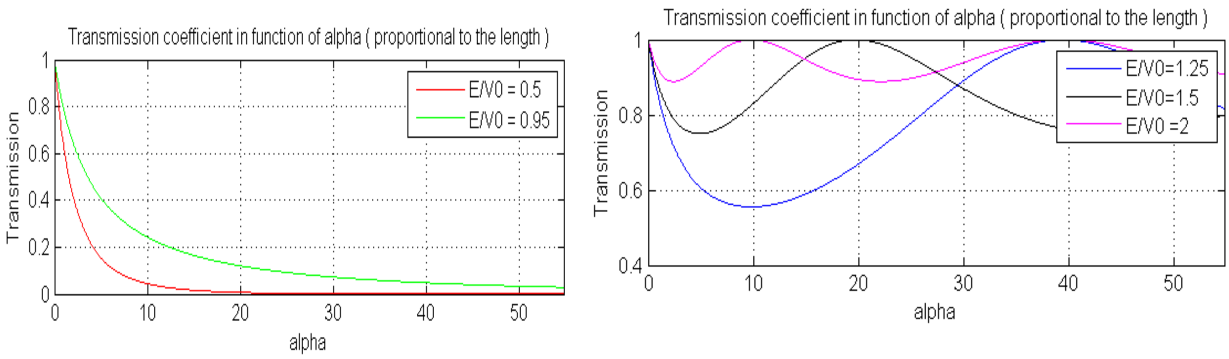


Figure 4 : The transmission coefficient in function of alpha for E/V0 values smaller than one in the left and bigger than on in the right

We can see that the transmission decreases exponentially with increasing the length of the barrier for $\frac{E}{V_0} < 1$, which is logical, if we consider the manual equation that we deduce for the transmission coefficient. Moreover, the longer the barrier the harder it is for a particle to tunnel through it.

If now we look at the picture in the right we can see that there are several pics for the Transmission coefficient, points where there is no reflection whatsoever.

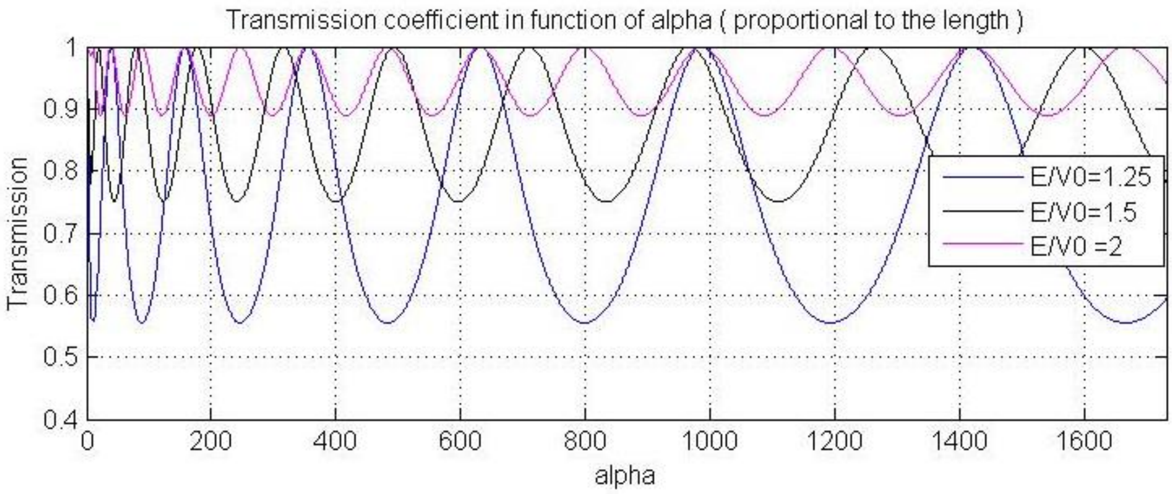


Figure 5

If we look at the formula of the transmission coefficient for $\frac{E}{V_0} > 1$:

$$|t'|^2 = \frac{4(\beta_1^2\alpha)\,(\beta_2^2\alpha)}{4(\beta_1^2\alpha)\,(\beta_2^2\alpha)\ + ((\beta_1^2\alpha)\ - (\beta_2^2\alpha)\,)^2 \sin^2\left(\beta_2\alpha^{\frac{1}{2}}\right)}$$

We can see that if $\sin^2\left(\beta_2\alpha^{\frac{1}{2}}\right)$ goes to zero, we will find $|t'|^2 = 1$. We can therefore predict for which lengths we will find a maximum or minimum transmission.

$$T = 1 \leftrightarrow \sin^2\left(\beta_2\alpha^{\frac{1}{2}}\right) = 0 \leftrightarrow \beta_2\alpha^{\frac{1}{2}} = n\pi \ \ for\ n = 0,1,2,3\ldots$$

$$\beta_2\alpha^{\frac{1}{2}} = n\pi \leftrightarrow L = \frac{n\pi}{K_2} \leftrightarrow L = \frac{n\pi}{\frac{2\pi}{\lambda}} \leftrightarrow L = \frac{n\lambda}{2}$$

We can also do the same thing for when the length is kept constant but the E changes. In that case, we should find the maximum and minimum of the Transmission by changing the wavelength associated with the Energy of the particle.

If we increase the height of the barrier, thus the value of V_0, we will, for a constant Energy, reduce the transmission coefficient if $\frac{E}{V_0} < 1$. If that ratio is still bigger than one, we will increase the wavelength associated with the resulting value of K_2 and thus, by now maintaining K_2 constant and plotting the Transmission in function of length L (alpha but with V_0 constant), we will increase the distance between the pics in the Transition coefficient. By maintaining L constant and only changing the ratio by increasing or decreasing V_0 we will find $T = 1$ for the wavelengths that respect the following condition:

$$\lambda = \frac{2L}{n}$$

This means that, for a certain particle energy (i.e. wavelength) we will obtain the resonant transmission as the increasing barrier width L matches an integer number of ½ wavelength. The same reasoning can be applied when we have a fixed width L, where we will have resonant transmission for a wavelength respecting the condition above.

2. Bound States

In this section, we will be interested in studying the bound state energies associated with a potential well. The method that will be used is the same as the one applied in the first section, the propagation matrix approach. We will later compare our values with the bound states associated to the particle in a box.

2.1 Rectangular Potential Well

The rectangular potential well is an extension of the particle in a box model, but where the potential does not goes to infinity. Moreover, in this case we can have a small probability of a particle being outside of the second region.

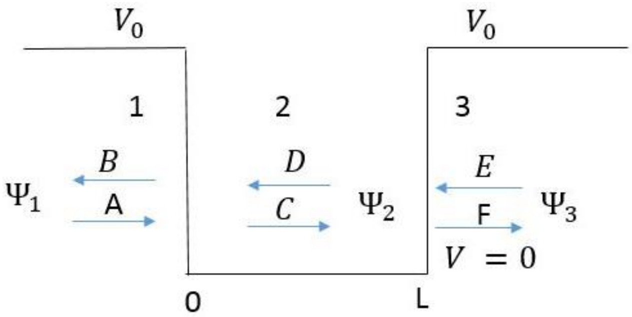


Figure 6

The wave functions associated with each region are:

$$\Psi_1 = Ae^{iK_1x} + Be^{-iK_1x}$$

$$\Psi_2 = Ce^{iK_2x} + De^{-iK_2x}$$

$$\Psi_3 = Fe^{iK_1x} + Ee^{-iK_1x}$$

Since we are considering a potential well $V = V_0$ in the first and third region, K_1 will have an imaginary value and can be written as $K_1 = ik$. Therefore, we will rewrite the equations for the wave functions as:

$$\Psi_1 = Ae^{-kx} + Be^{kx}$$

$$\Psi_2 = Ce^{iK_2x} + De^{-iK_2x}$$

$$\Psi_3 = Fe^{-kx} + Ee^{kx}$$

Thus, if we do not want $\lim_{\mathrm{n}\to\pm\infty} \Psi(\mathrm{n}) = \infty$ we need to assume $A = E = 0$.

Therefore, if we consider the coefficient t_{11}

$$\begin{pmatrix} A \\ B \end{pmatrix} = t \begin{pmatrix} F \\ E \end{pmatrix} \leftrightarrow A = t_{11}F$$

$$A = 0 \leftrightarrow t_{11} = 0 \leftrightarrow \frac{1}{|t_{11}|^2} = T \sim \infty$$

2.2 The Propagation Matrix Approach for a Potential Well

As explained above, one can consider, in a potential well, the regions 1 and 3 being under the influence of a potential V_0 and the zone in the middle of them as not being under the influence of a potential, thus $V = 0$ for the second region . We can, therefore, say that the $K_1$for a potential barrier is equivalent to the $K_2$for the potential well and vice versa. This will be described by the following values of K:

$$K_1 = \left(\frac{2m(E - V_0)}{\hbar^2}\right)^{\frac{1}{2}} \leftrightarrow K_1 L = \left(\frac{2m(E - V_0)L^2}{\hbar^2}\right)^{\frac{1}{2}} = \beta_1 \left(\frac{2mV_0L^2}{\hbar^2}\right)^{\frac{1}{2}} = \beta_1 \alpha^{\frac{1}{2}}$$

$$K_2 = \left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} \leftrightarrow K_2 L = \left(\frac{2mEL^2}{\hbar^2}\right)^{\frac{1}{2}} = \beta_2 \left(\frac{2mV_0L^2}{\hbar^2}\right)^{\frac{1}{2}} = \beta_2 \alpha^{\frac{1}{2}}$$

Where $\beta_1 = (\frac{E}{V_0} - 1)$ and $\beta_2 = \frac{E}{V_0}$

The wave equations associated with the regions will remain:

$$\Psi_1 = Ae^{iK_1x} + Be^{-iK_1x}$$

$$\Psi_2 = Ce^{iK_2x} + De^{-iK_2x}$$

$$\Psi_3 = Fe^{iK_1x} + Ee^{-iK_1x}$$

And, as the last time we will plot:

$$T = \frac{|Fe^{iK_1x}|^2}{|Ae^{iK_1x}|^2} \leftrightarrow \frac{1}{|t_{11}|^2}$$

As it was explained above, the main difference here is that the Transmission coefficient (T) in this case, when plotted, should have, for the bound energy values, an extremely high value. We will also plot the t_{11} coefficient, which, as shown in before, should be zero for when we have a bound state energy.

2.4 Particle in a Box

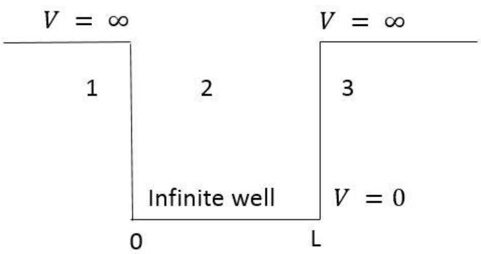


Figure 7: Schema showing the infinite well that will be use to describe the Particle in a Box model.

The particle in a box model consists of a particle moving in an infinitely deep well from which it cannot escape. Therefore, we can say that the probability of finding the particle at $x = 0 \; or \; x = L$ is zero, since we need to respect the continuity condition.

$$\Psi_2(x) = Asin(Kx)$$

By differentiating $\Psi_2(x)$ twice with respect to x and putting that result in the Time – independent Schrodinger equation and solving the resulting equation for k we will obtain:

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

Since for $x = L$, $\Psi_2(x) = 0$ we will find that:

$$KL = \left(\frac{2mEL^2}{\hbar^2}\right)^{\frac{1}{2}} = n\pi$$

Thus, we can say that the allowed energies are (α is the same as used before):

$$E_n = \frac{n^2\hbar^2\pi^2}{2mL^2} \leftrightarrow \frac{E_n}{V_0} = \frac{\pi^2 n^2}{\alpha}$$

In this last equation we use $\frac{E_n}{V_0}$ instead of E_n. In this case the V_0 is the same as the one used in the rectangular potential well. We need to use the ratio because, since the width (L) of the barrier was never explicitly determined (we use the α which contains both $L^2 \; and \; V_0$), it would be impossible to calculate the E_n values (it depends on $\frac{1}{L^2}$). We need to, therefore, introduce the α coefficient. Moreover, when using the rectangular potential well we will obtain the $\frac{E}{V_0}$ values for which we will have bound states. Since we do not explicitly define a V_0, we can only compare the rectangular potential well values with the $\frac{E_n}{V_0}$ ratios.

2.4 Results and Discussion

There are two different methods that we can use (Appendix B for MatLab code) in order to deduce the bound state energy values. They are the:

- Plotting the Transmission coefficient (T) in function of the $\frac{E}{V_0}$

- Plotting the coefficient t_{11} as a function of $\frac{E}{V_0}$. We also reduce the Transmission axis range (e.g. to go from -10^{-10} to 10^{-10}

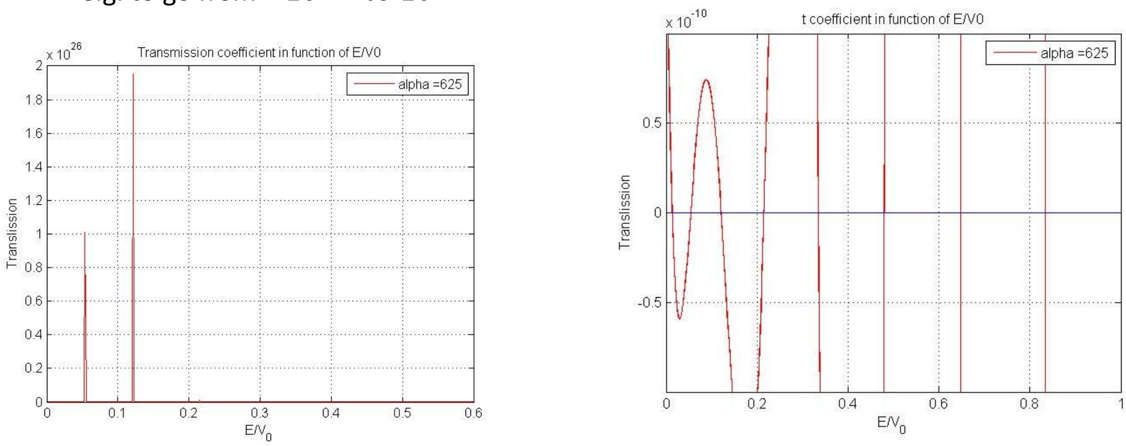


Figure 8 : Two Matlab plots representing the two types of graphics that can be used to recover the bound state energies. The graph in the left corresponds to the first method while the one in the right to the second method.

In the left plot, we used the first method and in the right plot the second method was used. In the first method, we are looking for the maxima points whereas for the second method we search the values for which the curve will pass through zero. By looking to the right plot, we can clearly see that the second method is the most effective when we are trying to identify the Energy values. Moreover, we can also be more precise if we use the values from the t_{11} since the points where the function is zero are easier to identify than the points where the T function has its pics. Therefore, we, from now, will use the second method. It's also important to say that controlling the range of the Transmission axis when plotting the graphic in the second method is fundamental, since we will only be able to properly identify the points for which the curve is crossing zero when we use a small enough range (e.g. -10^{-10} to 10^{-10}, as it was used in the Figure 8). In the table below, we will see the values obtained with the propagation matrix approach and those for the bound state of a particle in a box.

Rectangular Potential well $\alpha = 625$	Particle in a box $\alpha = 625$
0.014	0.015791
0.054	0.0631
0.121	0.142
0.215	0.252
0.3351	0.394
0.48	0.568
0.65	0.773
0.834	1.01*

*Table 1 : Comparison between the Propagation matrix approach and the particle in a box for an alpha = 625. The values are for the $\frac{E}{V_0}$ ratio. *This value theoretically does not correspond to a Bound state energy since E will be bigger than V_0, nevertheless it might explain why we have eight values for the bound state energy when we use the matrix approach.*

If we increase the value of alpha, we will find the following values:

Rectangular Potential well (matrix approach) $\alpha = 6250$		Particle in a box $\alpha = 6250$	
0.0015	0.2525	0.00158	0.26687
0.006	0.293	0.00632	0.30651
0.0135	0.337	0.01421	0.35531
0.024	0.383	0.02527	0.40426
0.0367	0.432	0.03948	0.45637
0.054	0.484	0.05685	0.51164
0.0727	0.0.539	0.07738	0.57007
0.096	0.597	0.10106	0.63165
0.1215	0.657	0.12791	0.6964
0.15	0.72	0.15791	0.7643
0.1815	0.786	0.19108	0.83536
0.216	0.923	0.2274	0.90958

Table 2 : Ratio E/V_0 obtained for the Rectangular potential well using MatLab and manually for the particle in a box. We can see that since the value for alpha is big, we have similar values for both cases.

As we can see if we compare the Table 2 with Table 1, the values for the E/V_0 ratio for the rectangular potential well gets closer to the ones found in a particle in a box when we increase the value of alpha. This is confirmed by the theory, since for the particle in a box the $V_0 \to \infty$ and, by increasing alpha we increase the V_0 associated with the potential well ($\alpha \propto V_0$). We can say that the comparison is relevant for big values of alpha. If we take, for example,$\alpha = 20$, we will find 0.23 and 0.81 for the rectangular potential well while for the particle in a box we will only have 0.49.

Finally, if we now look the values for which the $\frac{E}{V_0} > 1$ we will find the following plot (we will now use the Transmission coefficient (T)).

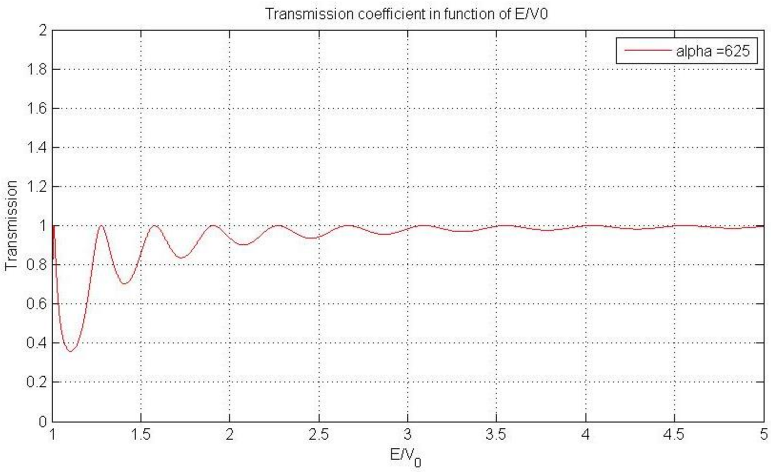


Figure 9 : Plot of the function associated with the Transmission coefficient T for. $\frac{E}{V_0} > 1$ We can observe an oscillation in values for T.

In the figure above we can see oscillation in the value of T even though the Energy of the particle is bigger than V_0. This is explained by the fact that usually there is still some probability of reflection, which, as we can see in some points (especially the ones between $\frac{E}{V_0} = 1$ and $\frac{E}{V_0} = 2$), can be quite big. The points where we have high T(Transmission peaks) are called resonances (can also be called Transmission maxima).

3. Transmission through an array of barriers

In this section, we will study the transmission through an array of barriers. We will adapt the propagation matrix method so it can be used for a random number n of barriers. Moreover, we will also compare our results with the Kronig-Penney potential model.

3.1 Propagation Matrix Approach

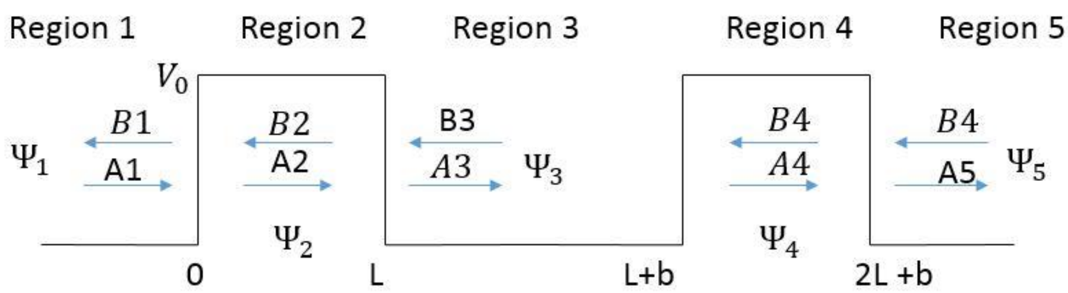


Figure 10 : Schema representing two rectangular barriers.

We will first adapt the method used in the first section for a two rectangular potential array and then deduce the equation for a random number n of arrays. The constants and matrix used are the same as the ones in the first section, any modification will be indicated.

If we begin from where we stopped In the first section we would find the following equation:

$$\begin{pmatrix} A1 \\ B1 \end{pmatrix} = d_{12}p_2d_{21}p_1^{-1}\begin{pmatrix} A3 \\ B3 \end{pmatrix}$$

Obs: in this part, the matrix $p_1$will be slightly modified. We will redefine it as being:

$$p_1 = \begin{pmatrix} e^{-iK_1b} & 0 \\ 0 & e^{iK_1b} \end{pmatrix}$$

As you can see, I replaced L by b. In the case of multiple barriers, we will need to shift the coordinates systems of the value b each time that we want to go from the end of one barrier to the beginning of the other.

For one barrier, we have the term p_1^{-1} that is used to come back to the original coordinate system. When considering multiple barriers, we only want to do that for the last barrier, which will imply that when passing from one barrier to another we will use p_1. We can therefore deduce the following equation for two barriers:

$$\begin{pmatrix} A1 \\ B1 \end{pmatrix} = d_{12}p_2d_{21}p_1d_{12}p_2d_{21}p_5^{-1}\begin{pmatrix} A5 \\ B5 \end{pmatrix}$$

As you can see, the only new matrix introduced here is p_5^{-1}, which will be used to come back to the original coordinate system. We can also use d_{12} when passing from region 3 to 4 because the K values do not change (e.g. $K_2 = K_4$). The same explanation is applied to d_{21}.

To deduce the p_5^{-1} we need to take in account that the coordinate system has been shifted by a value of $2L + b$ in relation to the original one, thus, $x_5 = x + 2L + b$.

$$p_5 = \begin{pmatrix} \exp(-iK_1(2L+b) & 0 \\ 0 & \exp(iK_1(2L+b)) \end{pmatrix}$$

In order to facilitate the writing of the matrix for n barriers we will define:

$$tbarrier = d_{12}p_2d_{21}p_1 \quad \text{and} \quad tboundary = d_{12}p_2$$

Therefore, for a number n of barriers we will have:

$$\begin{pmatrix} A1 \\ B1 \end{pmatrix} = (tbarrier)^{(n-1)}tboundaryd_{21}p_n^{-1}\begin{pmatrix} An \\ Bn \end{pmatrix}$$

The coordinate system will be shifted by a value of $\left(\frac{n-3}{2}+1\right)L + \left(\frac{n-3}{2}\right)b$. Therefore, we will obtain:

$$p_n = \begin{pmatrix} \exp(-iK_1(\left(\frac{n-3}{2}+1\right)L + \left(\frac{n-3}{2}\right)b) & 0 \\ 0 & \exp(iK_1(\left(\frac{n-3}{2}+1\right)L + \left(\frac{n-3}{2}\right)b) \end{pmatrix}$$

Finally, it is important to create another dimensionless value (as we did before, e.g. α). In this case, we will define γ as:

$$\gamma = \frac{2mV_0b^2}{\hbar^2}$$

$$K_1b = \beta_1\gamma^{\frac{1}{2}} \ and \ \ K_2b = \beta_2\gamma^{\frac{1}{2}} \ \ where\ \beta_1 = \left(\frac{E}{V_0} - 1\right) and\ \beta_2 = \frac{E}{V_0}$$

This variable will be used in the Matlab program in order to represent the distance between two rectangular barriers.

3.2 Kronig – Penney potential model

The delta function Kronig- Penney model is a simple, 1D model that consists of an infinite periodic array of delta function potential barriers. It illustrates the formation of energy bands and band gaps in that structure. Its importance is because (beyond being a simple model) it can be used, for example, to provide a model of a 1D crystalline lattice potential, where the potential created by the ions is considered an infinite array of potential wells.

In a first moment, we will consider a Kronig-Penney model where the potential $V(x)$ is defined as a periodic rectangular wave as shown it the picture bellow. Later we will take its limits in order to use the delta function Kronig-Penney model.

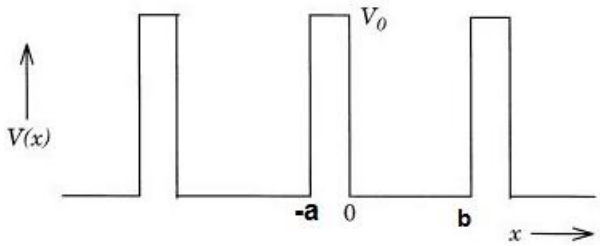


Figure 11 : Rectangular periodic potential barrier.

This model requires the use of the Bloch's functions, which are wave functions for a particle in a periodic environment. A Bloch wave is composed by wave solutions multiplied with a periodic function. In our case, that periodic function has the periodicity as the array of potential barriers.

$$\psi(x) = e^{iKx}u(x) \;\; where\; u(x) \text{ is a periodic function}$$

The solution of the Schrödinger equation for the Kronig-Penney model is found by assuming the solution to be a Bloch function, where $u(x) = u(x+c)$, $c = a + b$ and K is the wave number. This allows the simplification of the Schrödinger equation.

We can say that the mathematical form of the repeating potential is:

$$V(x) = V_0 \quad for - a < x < 0$$

$$V(x) = 0 \quad for\; 0 < x < b$$

In addition, the Schrödinger equation for this model is:

$$\frac{d^2\psi}{dx^2}+\frac{2mE}{\hbar^2}\psi=0 \qquad 0<x<b$$

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

The solutions are in the form:

$$\Psi_1 = Ae^{iK_1x}+\ Be^{-iK_1x} \qquad for-a<x<0$$

$$\Psi_2 = Ce^{iK_2x}+\ De^{-iK_2x} \quad for\ 0<x<b$$

Where $K_2=\left(\frac{2m(E-V_0)}{\hbar^2}\right)^{\frac{1}{2}}$ and $K_1=\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}$ (The same value as the one used in the section 3.1)

Since, we have four unknowns; we need four conditions to determine them, they are:

- Two deduced from the boundary conditions :

$$\Psi_1(0)=\Psi_2(0) \quad \Psi_1'(0)=\ \Psi_2{}'(0)$$

- Two deduced from the Block theorem, where $u(x)=\ u(x+c)$:

$$u(-a)=u(b) \qquad u'(-a)=u'(b)$$

Where the prime denotes the first derivative.

Therefore, by applying the conditions written above we obtain four equations, which will have a nontrivial solution for A, B, C and D if the determinant equation bellow is respected:

$$\begin{vmatrix} 1 & 1 & -1 & -1 \\ K_1 & -K_1 & -K_2 & K_2 \\ e^{i(K_1-K)b} & e^{-i(K_1+K)b} & -e^{ia(K_2-K)} & -e^{i(K_2+K)a} \\ (K_1-k)e^{bi(K_1-K)} & -(K_1+k)e^{-ib(K_1+K)} & -(K_2-k)e^{-i(K_2-K)a} & (K_2+k)e^{i(K_2+K)a} \end{vmatrix}=0$$

The equation above is equivalent to:

$$\mathrm{Cos}(K(a+b))=f=\cos(K_1b)\cos(K_2a)-(\frac{(K_1)\text{^}2\ +(K_2)\text{^}2)}{2(K_1K_2)})\sin(K_1b)sin(K_2a) \quad (1)$$

The Dirac delta function being defined as:

$$\delta(x) = \begin{cases} +\infty, x = 0 \\ 0, \quad x \neq 0 \end{cases}$$

Therefore, we can assume that $V_0 \to \infty$ and $b \to 0$ for the delta function Kronig – Penney model, which will imply that:

$$K_2 a \to 0; \cos(K_2 a) \to 1\,; \sin(K_2 a) \to K_2 a \;\; and\; V_0 a = remains\ constant$$

$$\mathrm{Cos}(Kb) = f = \cos(K_1 b) - \frac{mV_0}{\hbar^2 K_1} asin(K_1 b) = \cos(K_1 b) + \frac{mV_0 ab}{\hbar^2}\frac{sin(K_1 b)}{K_1 b} \qquad (2)$$

Since, as defined before, $K_1 a = \beta_1 \alpha^{\frac{1}{2}}$, $K_2 a = \beta_2 \alpha^{\frac{1}{2}}$ and $K_1 b = \beta_1 \gamma^{\frac{1}{2}}$ we can rewrite 3 and 4 as (In the code the equations will be written in this format):

$$\mathrm{Cos}(K(a+b)) = f = \cos\left(\beta_1 \gamma^{\frac{1}{2}}\right)\cos\left(\beta_2 \alpha^{\frac{1}{2}}\right) - \left(\frac{{\beta_1}^2 + {\beta_2}^2}{2(\beta_1 \beta_2)}\right)\sin(\beta_1 \gamma^{\frac{1}{2}})\sin(\beta_2 \alpha^{\frac{1}{2}}) \quad (5)$$

$$\mathrm{Cos}(K(b) = f = \cos\left(\beta_1 \gamma^{\frac{1}{2}}\right) + \frac{mV_0 ab}{\hbar^2}\frac{sin\left(\beta_1 \gamma^{\frac{1}{2}}\right)}{\beta_1 \gamma^{\frac{1}{2}}} \quad (6)$$

In here, we can also put set the constant value $\frac{mV_0 ab}{\hbar^2} = P$ as $P = (\alpha\gamma)^{\frac{1}{2}}$ obtaining equation (7) for the Delta Kronig Penney model

$$\mathrm{Cos}(Kb) = f = \cos\left(\beta_1 \gamma^{\frac{1}{2}}\right) + (\alpha\gamma)^{\frac{1}{2}} \frac{sin\left(\beta_1 \gamma^{\frac{1}{2}}\right)}{\beta_1 \gamma^{\frac{1}{2}}} \quad (7)$$

With the Kronig- Penney model, the solutions for E are deduced when solving equations 5 and 7. Solutions for both equations are only obtained if $|f| < 1$ since the function $|\cos(kl)| < 1$. The K in $\mathrm{Cos}(Kb)$ is the same as the one in the Bloch wave described above.

3.3 Reports and Discussion

In a first moment, we are going to plot (Appendix C for the Matlab code) the Transmission coefficient for a constant width, height and barrier –to-barrier separation and for three different numbers of barriers (N).

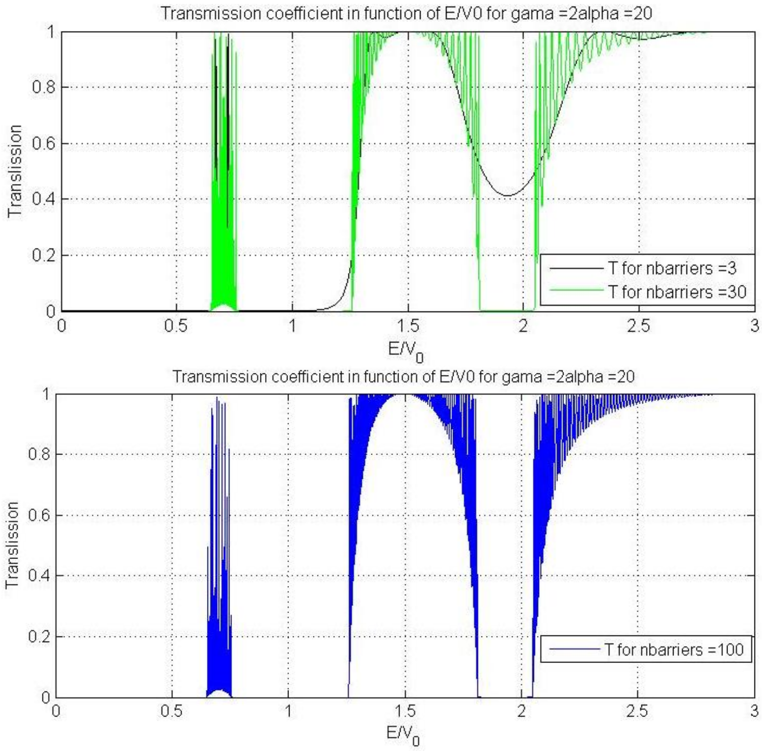


Figure 12 : Transmission Coefficient in function of E/V_0 for three different numbers of barriers (N). In black we see for three barriers, green for N = 30 and blue for N = 100. We can see that by increasing the value of N we delay the value of E/V_0 for which the Transmission will stop reaching zero.

As we can see in Figure 12, we can observe an oscillating behavior for the Transmission, which becomes stronger as the value of the number of barriers (N) increases. We can also observe, when $N = 3$, two intervals for which the T value goes to zero and a third one where it is reduced by slightly more than half. Therefore, we can see that the T for the regions in between of those where the Transmission coefficient has its pics is less reduced for a biggerE/V_0 . For a sufficiently big E/V_0 we almost have a continuous Transmission coefficient of one, just as we would have for an $N = 1$. We can see that by increasing the value of N we will increase the value of E/V_0 for which the Transmission will stop reaching zero.

We can distinguish two different zones: one where the transmission has its biggest values, the allowed region, and a second, called forbidden region, where the transmission coefficient is heavily reduced. The forbidden region corresponds to destructive wave interferences between the reflected and transmitted waves in the front and back of the potential barriers, while the allowed region corresponds to constructive wave interferences. Moreover, we can see that as N value increases, the value for the Transmission coefficient (T) in the forbidden regions is reduced. That consequence is expected, since, for bigger values of N, the effect of the destructive and constructive interferences in the Transmission increases.

We will now compare the T (E) function with the function (see section 3.2) describing the rectangular Kronnig-Penney (KP) model and the Dirac Kronnig Penney (DKP) model.

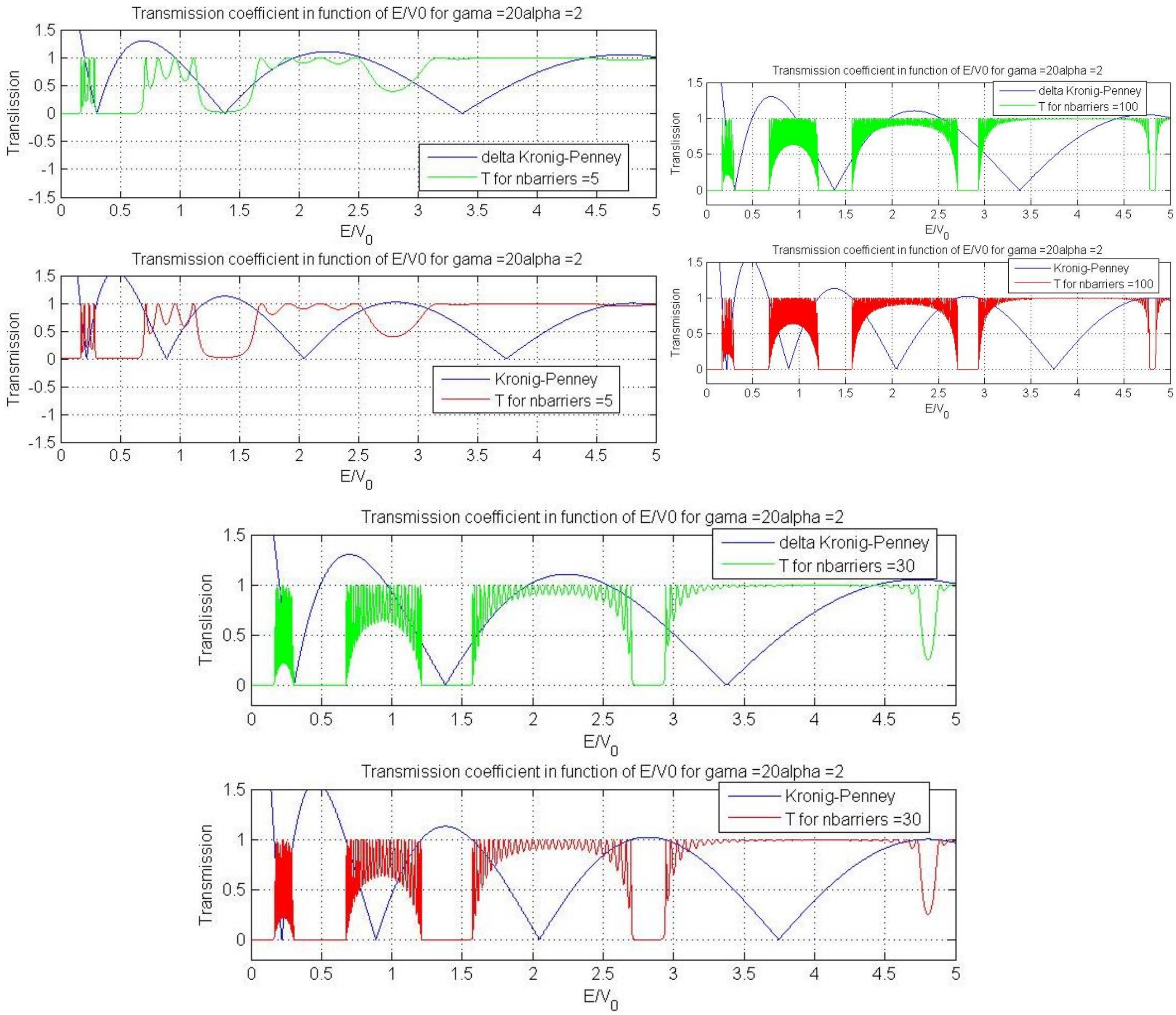


Figure 13 : As we can see in the three images above, we compare the Kronnig – Penney to the matrix approach for a constant value of alpha and gamma while changing the number of barriers.

As we can see in the Figure 13 , the KP model considering and infinite number of rectangular barriers and the DKP is not a good approximation to the Transmission in a finite array of barriers for a low number of barriers, e.g. 5. In addition, we can see that by increasing the number of barriers we can rapidly increase the validity of the KP and DKP models. Indeed, due to the nature of both models, the bigger the number of the barriers used to calculate the transmission with the matrix approach, the better the agreement with the KP and DKP model we will obtain. From now on, we will use a number of 30 barriers and evaluate the KP model agreement alone. This value for the number of barriers will be used for reasons of visual clarity of the plot (although a higher value would present a better agreement).

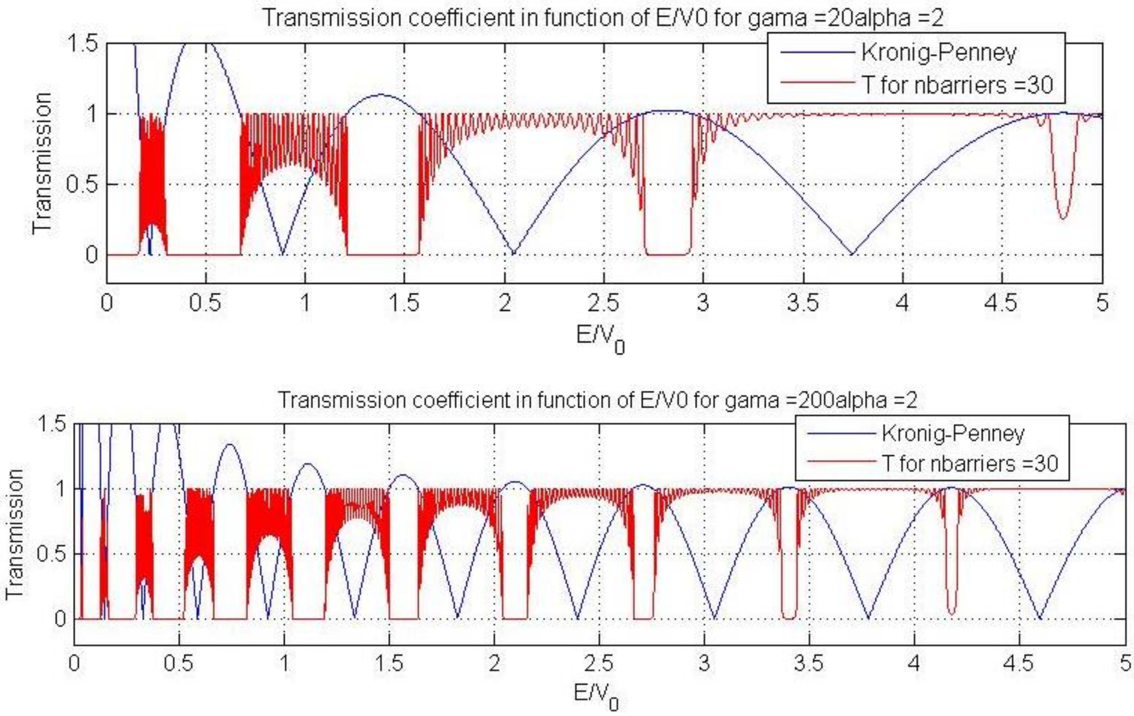
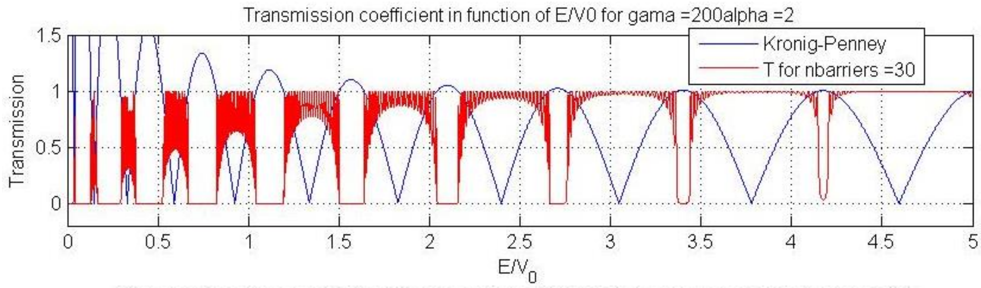


Figure 14 : As we can see in the images above, we compare the Kronnig – Penney to the matrix approach for a constant value of alpha and number of barriers for two different gamma values. The bigger the gamma, the better the result

As we can observe in the figure above, by increasing gamma we can considerably increase the agreement between KP and the matrix approach. Therefore, this means that by increasing the distance between barriers, i.e. the gamma, we decrease the discrepancy between the two models. Moreover, we can obtain a good agreement for both intervals, i.e. when the Energy of the particle is smaller than height of the barrier and when the opposite is true. One can see that a good result is obtained with gamma equals to 200, we will keep it at this value for future comparisons.



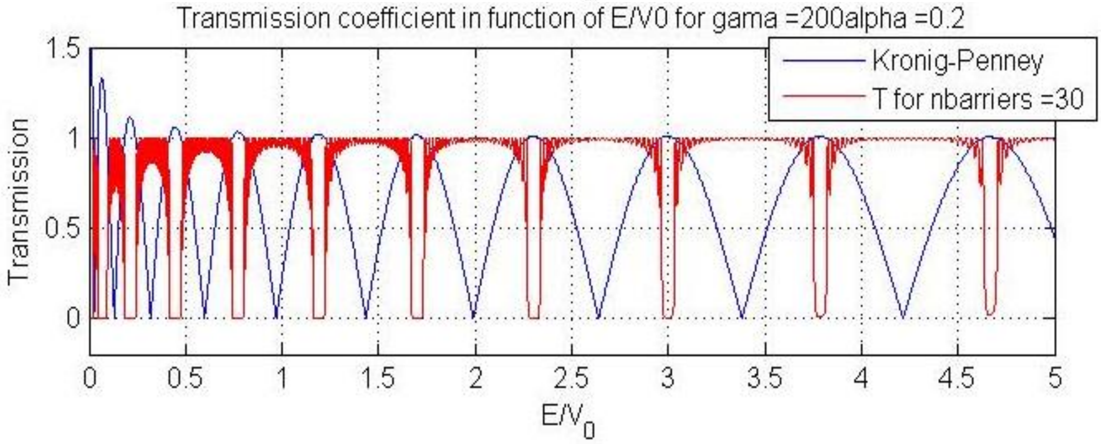


Figure 15 : As we can see in the images above, we compare the Kronnig – Penney to the matrix approach for a constant gamma and number of barriers and for two different alpha values. The smaller the alpha, the better the agreement

We can observe that the plot where we have the lowest alpha presents the best agreement. This shows that by decreasing the width of the barrier we decrease the discrepancy between the two plots. This might be explained by the fact that by decreasing the width, we increase the transmission in each barrier, i.e. decrease the effect of each barrier on the KP plot. Thus, decreasing the effect of having a infinite number of barriers on the Transmission vs E/V_0 curve for the KP model, making it more similar to the one obtained with the matrix approach (with a finite number of barriers).

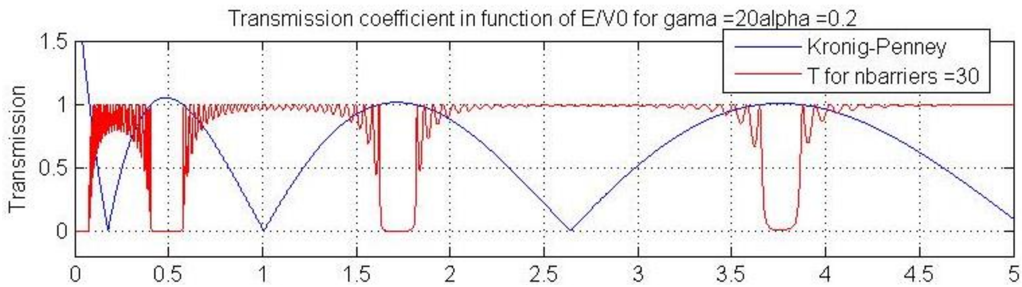
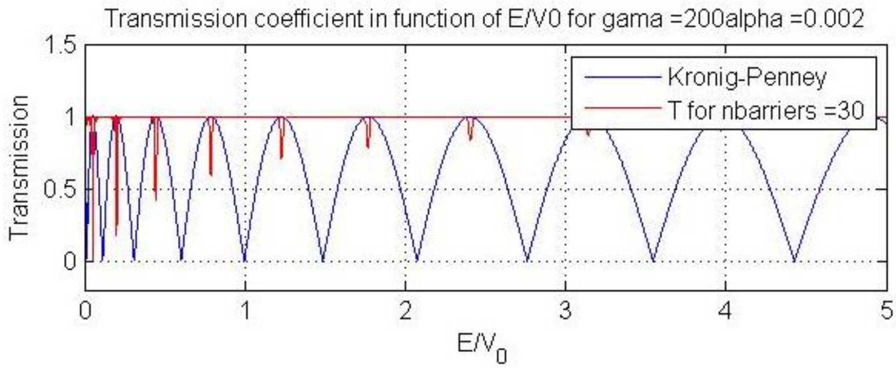


Figure 16 : We compare the Kronnig – Penney model to the matrix approach for a smaller value of gamma than the one in Figure 15. Although the result is not as good as for a higher gamma, it does present a certain agreement.

Above one can see that even for a smaller values of gamma the effect of reducing alpha is considerable and can present a certain agreement when looking at the allowed / forbidden zones, i.e. where for the KP curve we have a value bigger than 1.

Bellow it can be seen that if the value of alpha is reduced too much, the Trasmission no longers reaches zero after $\frac{E}{V_0} > \sim 0.2$ when looking at the plot made with the matrix approach. This is related to the fact that by reducing alpha we reduce the width of each barrier and, therefore, increase the trasmission through each barrier. This, in turn , reduced the number of compltly forbidden zones and we can no longer consider the KP model a good approximation. If we go further in the $\frac{E}{V_0}$ domain , i.e. higher values than 5, the red curve will remain nearly constant (with the value of one) , making the KP model not agree with the matrix approach. By increasing the number of barriers we can improve this agreement.



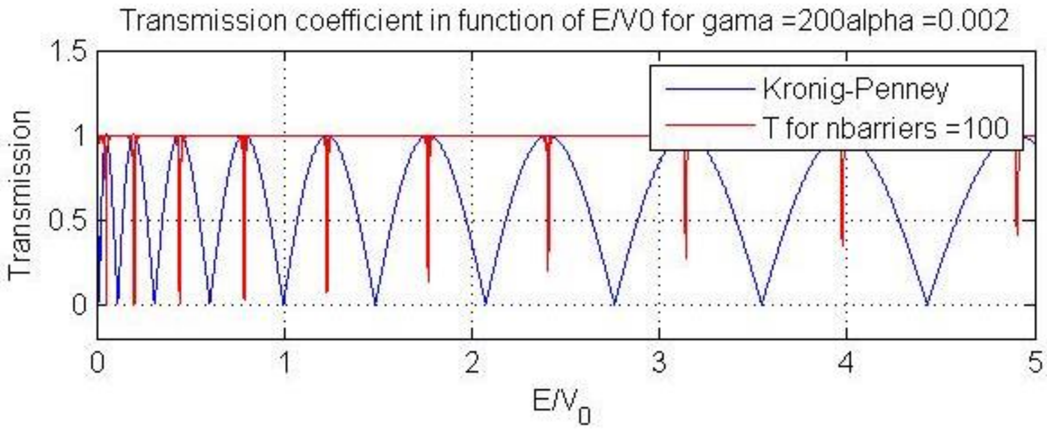


Figure 17: We compare the Kronnig – Penney model to the matrix approach for the same value of gamma as Figure 15 but an even smaller alpha. We do not obtain a good result.

The statement above is not only valid for a small value of alpha, but also for higher values of alpha and gamma. Indeed, for any finite number of barriers we will reach an E/V_0 value where the matrix approach curve will become nearly constant and no longer agrees with the KP model. One can state that this agreement decays with increasing E/V_0 value when using a finite number of barriers.

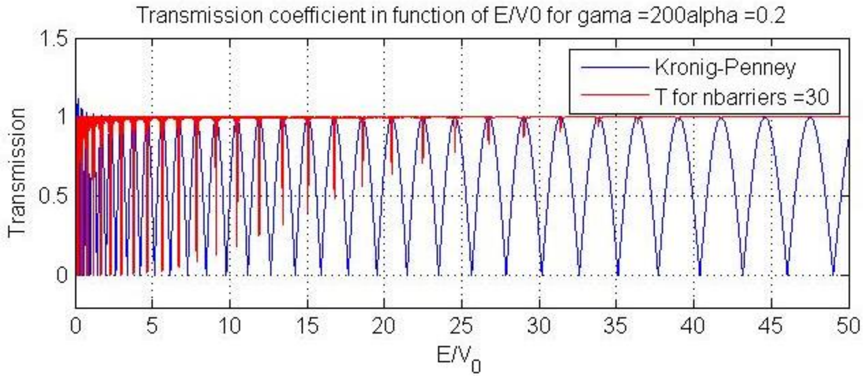


Figure 18 : We compare the Kronnig – Penney model to the matrix approach for the same value of gamma and alpha as Figure 15, but for a larger domain of E/V_0. We can see here how the red curve behaves at higher E/V_0 values.

We will know discuss the agreement between the DKP model and the matrix approach. Just as before, we will start by increasing the gamma value.

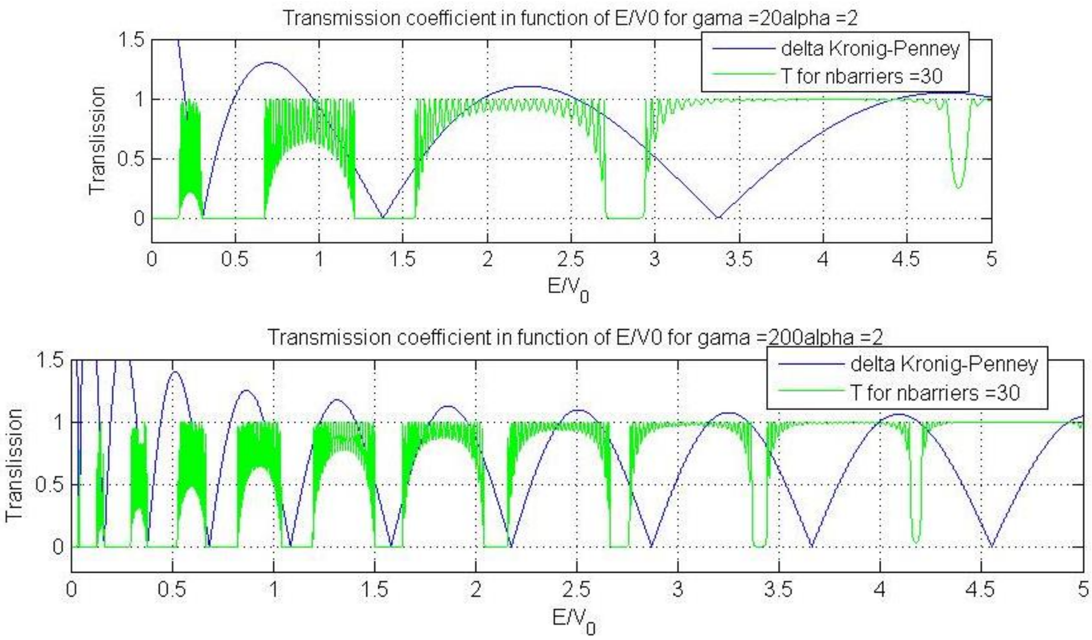


Figure 19 : We compare the Delta Kronnig – Penney model to the matrix approach for a constant value of barriers and alpha. We can see that although improving the agreement, it is not enough to be considered a good result.

As it is possible to observe above, we obtain a drastic improvement by increasing the gamma value, nevertheless, it is not sufficient to be able to say that we have a good agreement. Indeed, the KP model is much better for this value of alpha and gamma. This is mostly because of the biggest difference between the KP and DKP model, which is considering delta functions for the latter. Therefore, although the distance between barriers will affect the validity of the model, there is still the big discrepancy between the barrier width, i.e. alpha, used in the matrix approach (and KP model) and the one considered for the DKP. Until this is factor is taken in consideration one will most likely not be able to obtain a good agreement with the KDP model.

Considering the effect of the distance between barriers on DKP model, we can predict it by using the formula deduced in section 3.2.

$$\mathrm{Cos}(Kb) = f = \cos\left(\beta_1 \gamma^{\frac{1}{2}}\right) + (\alpha\gamma)^{\frac{1}{2}} \frac{sin\left(\beta_1 \gamma^{\frac{1}{2}}\right)}{\beta_1 \gamma^{\frac{1}{2}}} \quad (7)$$

We can see here that by increasing gamma we increase the frequency of oscillation of the function f, allowing the model to improve the agreement. Nevertheless, the gamma in the term $(\alpha\gamma)^{\frac{1}{2}}$ is cancelled by gamma in $\beta_1 \gamma^{\frac{1}{2}}$. This shows that gamma will only affect the w (as in $\cos(wx)$ and $\sin(wx)$ where $x = \frac{E}{V_0}$). Therefore, we need to modify the value of alpha if we want only to modify the position of the DKP peaks, i.e. without changing the number of oscillations.

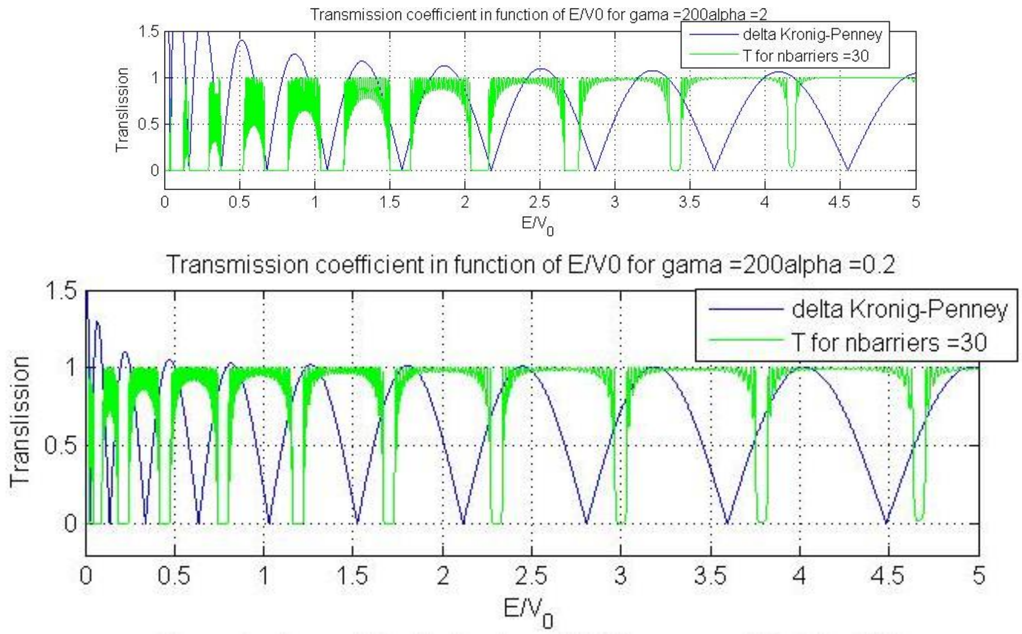


Figure 20: We compare the Delta Kronnig – Penney model to the matrix approach for a constant value of barriers and gamma. We can see that we know obtain good agreement for smaller values of E/V_0, i.e. smaller than one.

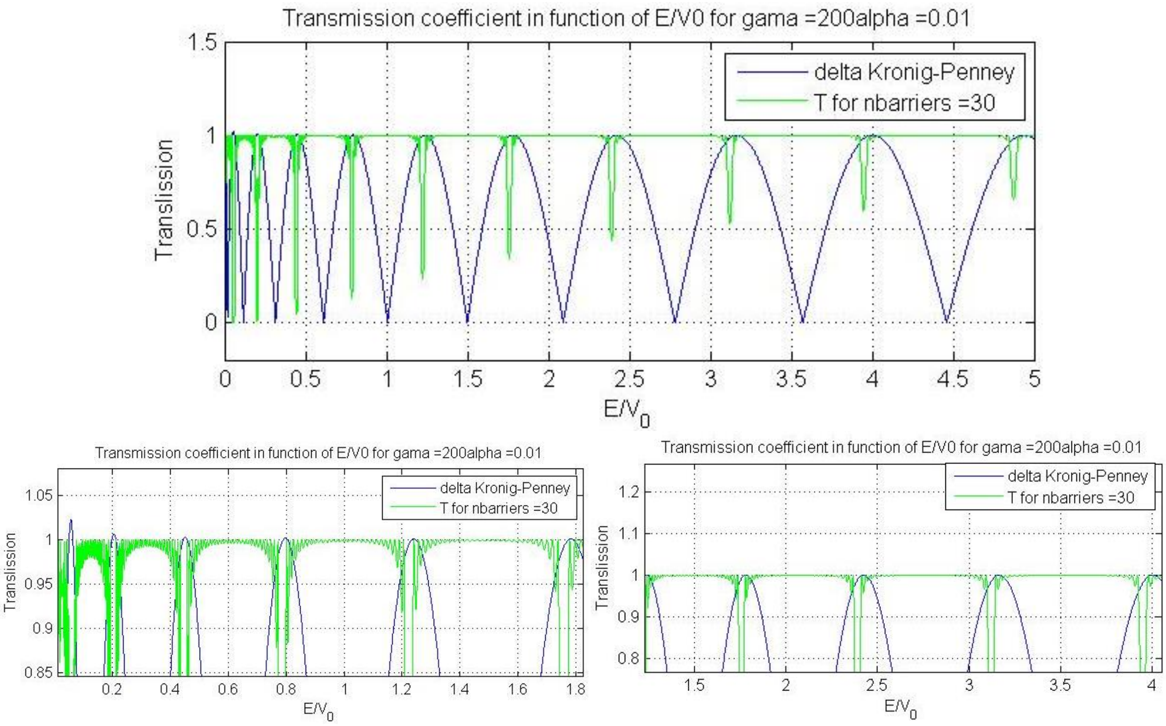


Figure 21 : We compare the Delta Kronnig – Penney model to the matrix approach for a constant value of barriers and gamma. We can see here that we obtain better agreement when looking at the peaks of the green and blued functions.

By looking at the images above, we can clearly see that by reducing the value of alpha the agreement with the matrix approach will be improved. This is expected as; by reducing alpha, we will be considering a smaller width for the barrier, which will become closer to the one used in the DKP model. Nevertheless, decreasing too much alpha will make the matrix approach related function stop reaching zero at smaller E/V_0 values. This will in turn decrease the validity of the model. Just as for the KP model, we will always have this issue when comparing the matrix approach for a finite number of barriers with the DKP model. Nevertheless, we can improve the result by increasing the number of barriers (obtaining a good agreement), as we can see below. The latter is plausible, since in DKP we have an infinite number of barriers.

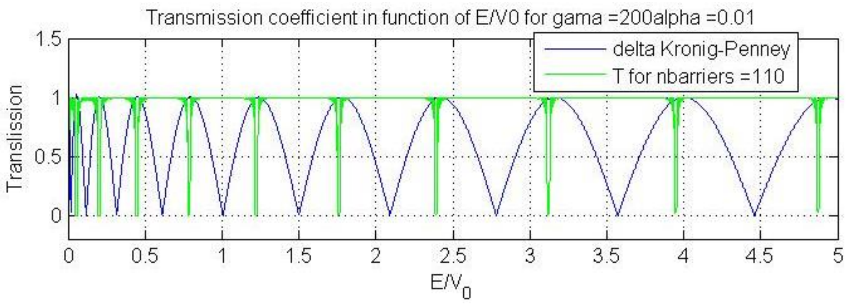


Figure 22 : We compare the DKP model to the matrix approach. We can see here that we obtain a good agreement.

As it has been shown in this section, it is possible to obtain a good agreement between DKP / KP model and the matrix approach. Moreover, one can also say that it is easier, i.e. the conditions do not need to be extreme (huge values of gamma and number of barriers while extremely small alpha), for us to obtain a good agreement using the KP model. With a gamma of 200, alpha of 2 and 30 barriers, the result was acceptable for the KP model, while the same cannot be told for the DKP model.

Finally, if we plot the Damping, defined as $-ln(T)$ we will be able to easily detect which regions correspond to the forbidden zones, since, the higher the damping, the higher the decrease in the amplitude of T. We can see that for values of $\frac{E}{V_0}$ higher than two the damping is nearly always zero. This effect of this can be seen in the Transmission curve, where it is mostly equal to one for values of $\frac{E}{V_0}$ higher than two. Lastly, just before $\frac{E}{V_0} = 3.5$ we can see a small increase in the Damping, which we could associate to the decrease in the Transmission near that value.

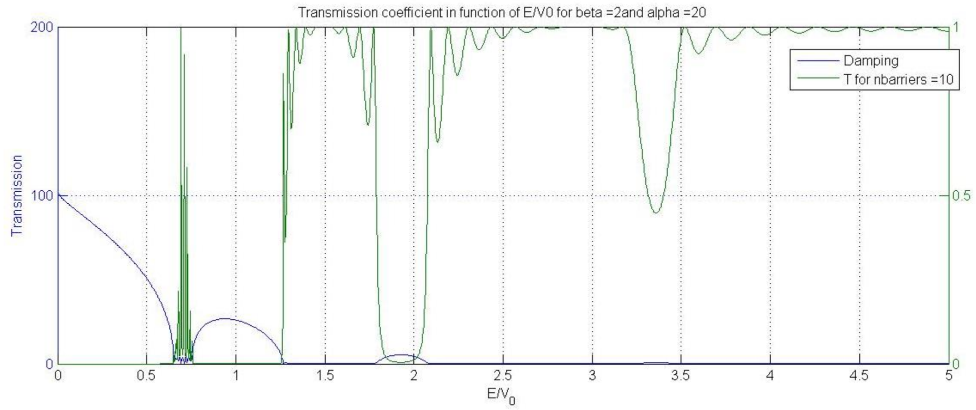


Figure 23: Plot of the Damping and the T function. We can see that for each forbidden zone we see an increase in the Damping value. For the allowed zones, the Damping is equal to zero.

OBS: In the title, beta is equals to the gamma used in the previous plots

Appendix A

In this Appendix, you can see the code that was used to calculate the transmission coefficient using the propagation matrix coefficient for the first model.

```
function [] =Problem1()

% Use the propagation matrix approach to calculate the transmission coefficient T of a
% rectangular potential step with width L and Height V0.
%           k_1                         k_2                      k_1
%
%                                        2
%               1           |----------------------|  V_0       3
%                           |                      |
%           A1---->         |            A2---->   |
%           B1 <----        |         B2 <----     |             A3---->
%                           |                      |        B3 <----
%     ----------------------|                      |-------------------  0          | energy
%                           0                      L
%*******************************************************************
% number of E/V0 values
n=50000;

% number of L values
nl = 50000;

% vector of values of E/V0
EoverV0vect = linspace(0,6,n);
EoverV0vect3 = linspace(1,6,n);
EoverV0vect2 = linspace(0,1,n);

% to store the calculated value for T
Tvect = zeros(8,n);
transmissiontest = zeros(8,n);
transmissiontestprime = zeros(8,n);

% values for alpha
alfasquare = linspace(0,3000,nl);

% under a constant L of 10^-9, we will calculate for three diferent L points
alfa = [10,50,100];

for z=1:3
```

```
    for o=1:n

        b = sqrt(EoverV0vect(1,o));
        c = sqrt(EoverV0vect(1,o)-1);

        k_1L=b*((alfa(z))^(1/2));
        k_2L=c*((alfa(z))^(1/2));

        % the discontinuity Matrix
        D12 = (1/(2*((b*c)^(1/2)))).*[b+c,b-c;b-c,b+c];
        D21 = (1/(2*((b*c)^(1/2)))).*[b+c,c-b;c-b,b+c];

        % the propagation Matrix
        P2 = [exp(-1i*k_2L),0;0,exp(1i*k_2L)];
        P1 = [exp(-1i*k_1L),0;0,exp(1i*k_1L)];

        % the transfer Matrix
        t = D12*P2*D21/P1;

        % the Trasmission coefficient
       Tvect(z,o) = 1/(abs(t(1))^2);

        % In order to plot the function that will verify the propagation
        % matrix method
        cprime = sqrt(1-EoverV0vect2(1,o));
        bprime = sqrt(EoverV0vect2(1,o));

       k_1Lprime=bprime*((alfa(z))^(1/2));
        k_2Lprime=cprime*((alfa(z))^(1/2));

        cprimeprime = sqrt(EoverV0vect3(1,o)-1);
        bprimeprime = sqrt(EoverV0vect3(1,o));

        k_1Lprimeprime=bprimeprime*((alfa(z))^(1/2));
        k_2Lprimeprime=cprimeprime*((alfa(z))^(1/2));

        transmissiontest(z,o) = abs(((4*1i*bprime*cprime)/((-(cprime^2)+(bprime^2) +
2*1i*cprime*bprime)*exp(k_2Lprime)+((cprime^2)-(bprime^2)+2*1i*bprime*cprime)*exp(-
k_2Lprime)))*exp(-1i*k_1Lprime))^2;

        transmissiontestprime(z,o) =
(4*(k_1Lprimeprime^2)*(k_2Lprimeprime^2))/(4*(k_1Lprimeprime^2)*(k_2Lprimeprime^2)+(((k_1Lprim
eprime^2-k_2Lprimeprime^2)^2)*((sin(k_2Lprimeprime))^2)));

    end
```

```
end

% for a fixed E/V0 value we will plot the transmition, we will now change the distance L, so
the value of Alfa from 0 to 3 and for 3 different E/V0 points

alfa2 = alfasquare.^(1/2);
Eoverv0 = [0.5,0.95,1.25,1.5,2];
for z=1:5
    for o=1:n

        b = sqrt(Eoverv0(z));
        c = sqrt(Eoverv0(z)-1);

        k_1L=b*((alfa2(1,o))^(1/2));
        k_2L=c*((alfa2(1,o))^(1/2));

        % the discontinuity Matrix
        D12 = (1/(2*((b*c)^(1/2)))).*[b+c,b-c;b-c,b+c];
        D21 = (1/(2*((b*c)^(1/2)))).*[b+c,c-b;c-b,b+c];

        % the propagation Matrix
        P2 = [exp(-1i*k_2L),0;0,exp(1i*k_2L)];
        P1 = [exp(-1i*k_1L),0;0,exp(1i*k_1L)];

       % the transfer Matrix
        t = D12*P2*D21/P1;
        % the Trasmission coefficient
        Tvect(z+3,o) = 1/(abs(t(1))^2);


    end

end
       % After this there was still the code to plot the images, but, otherwise, the code
finishes here.
```

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Appendix B

In this Appendix, you can see the code that was used to calculate Transmission coefficient T and the coefficient t used to deduce the bound states in the second section.

```
function [] =Problem2()
```

```
%           k_1                         k_2                       k_1
%                                         2
%               1                   3
%
%           A1---->                   A2---->
%           B1 <----                B2 <----                 A3---->
%                                                        B3 <----
%     ----------------------|V_0                    |-------------------
%                           |                       |
%                           |                       |
%                           |                       |
%                           |                       |
%                           |                       |
%                           |-----------------------|  | energy  0
%                           0                       a
%********************************************************************
%% eV% number of E/V0 values
n=500;

% number of L values
nl = 500;

% vector of values of E/V0
EoverV0vect = linspace(0,1,n);

% to store the calculated value for T
Tvect = zeros(8,n);
tvect = zeros(8,n);

% We will calculate for three diferent alpha points
alfa = [625,50,6250];
for z=1:3
    for o=1:n
```

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```
        c = sqrt(EoverV0vect(1,o));
        b = sqrt(EoverV0vect(1,o)-1);

        k_1L=b*((alfa(z))^(1/2));
        k_2L=c*((alfa(z))^(1/2));

        D12 = (1/(2*((b*c)^(1/2)))).*[b+c,b-c;b-c,b+c];
        D21 = (1/(2*((b*c)^(1/2)))).*[b+c,c-b;c-b,b+c];

        P2 = [exp(-1i*k_2L),0;0,exp(1i*k_2L)];
        P1 = [exp(-1i*k_1L),0;0,exp(1i*k_1L)];

        t = D12*P2*D21/P1;

        T = 1/(abs(t(1))^2);

        Tvect(z,o)= T;
        tvect(z,o)= t(1);
    end

end


After this there was still the code to plot the images, but, otherwise, the code finishes here
```

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Appendix C

The code used to calculate the Transmission coefficient for the finite array of potential barriers is the one bellow:


```
function [] =Problem3F()
```

```
% % Use the propagation matrix to calculate the transmission coefficient T for
% % an array of N rectangular potential barriers, each habing width a height
% % V_0 and a barrier to barrier separation b.Calculate and plot how T depends
% % on the energy for an increasing number of barriers. Do you see any
% % oscillations in the transmission? Any regions where the transmision is
% % heavily reduced? What is the underlying physical explanation? Play with
% % the parameters( potential width, heigth, separation), and compare your
% % results wiwth those of theory. When / in what limits is the theoretical
% % model valid? Can you predict where the regions of high transmission (
% % bands) will apear? Also plot the damping -ln (T) and T.
% % we have a width a, distance between the barriers b and a hegth V_0
```

Initialazing terms and vectors

```
% number of E/V0 values
n=5000;

% number of barriers

nbarrier = 110;

% we'll use the transfer matrix methode
% vector of values of E/V0

EoverV0vect = linspace(0,5,n);

% to store the calculated value for T

Tvect = zeros(1,n);
minuslnTvect = zeros(1,n);
kronigpennyvect = zeros(1,n);
deltakronigpennyvect = zeros(1,n);
abskronigpenneyvect = zeros(1,n);
deltaabskronigpennyvect = zeros(1,n);
```

```
% alfa = (V0*(a^2)*2*m)/(h^2); - a the length of the barriers
% We considere alfa dimensioneles and since k_1 is in the order of ~ 10^9
% and a ~ 10^-9 m  we consider alfa^2 to vary betwen 0-3 as for the E/V0
% gama = (V0*(b^2)*2*m)/(h^2); - b the distance between barriers
% Just as for alfa we consider gama dimensionelles since b will be in the order of 10^(-9) m.
% thus we will have Kb and Ka where we'll have respectivilly b or c multiplied by gama or
alfa ^1/2

% Alfa related to the length of the barriers
% Beta related to the distance between barriers

alfa = 0.01;
gama = 200;
```

Here we will calculate the transmition using the - Matrix Approach - Kronig - Penney model - Delta - Kronnig - Penney model

```
for o=1:n
    % b = E/V0 and c = E/V0 - 1

    b = sqrt(EoverV0vect(1,o));
    c = sqrt(EoverV0vect(1,o)-1);

    % (((E/V0)*V0*(b^2)*2*m)^(1/2))/(h^2)

    k_1gama = b*((gama)^(1/2)); % Related to E/V0 and to the distance between barriers

    % (((E/V0)*V0*(a^2)*2*m)^(1/2))/(h^2)

    k_1a=b*((alfa)^(1/2)); % Related to E/V0 and the length of the barrier
    k_2a=c*((alfa)^(1/2)); % Related to E/V0 -1 and the length of the barrier

    % We know that [A1;B1] = (1/(2*((b*c)^(1/2))))*D12*[A2;B2]

    D12 = (1/(2*((b*c)^(1/2)))).*[b+c,b-c;b-c,b+c];
    D21 = (1/(2*((b*c)^(1/2)))).*[b+c,c-b;c-b,b+c];


    % for x=a we can use the x' = 0 using the relation psi2(x)=psi2'(x-a)
    % in that way we find [A2;B2] = P2 * [A2';B2']

    P2 = [exp(-1i*k_2a),0;0,exp(1i*k_2a)];

    % Same thing as before but for the third part [A3;B3] = P1 * [A3';B3'], we will consider
```

```
where to pass from psi2'(x')=psi2''(x'-b)

    P1 = [exp(-1i*k_1gama),0;0,exp(1i*k_1gama)];

    % we'll define a variable responsable for representing the
    % passage of the particle by one barrier

    trasnfer1 = D12*P2*D21*P1;

    % we'll also define a matrix responsible for the passage
    % througth the last boundary

    transferbdr = D12*P2;

    % the matrix responsible to shift the wave function back to
    % it's original corrdinate system

    Pnbarrier = [exp(-1i*(k_1a*(1+(((nbarrier)-3)/2))+k_1gama*...
        (((nbarrier)-3)/2))),0;0,exp(1i*(k_1a*(1+(((nbarrier)-3)/2))+k_1gama*...
        (((nbarrier)-3)/2)))];



    % for  a nbarrier number of barriers we'll obtain a trasfer
    % matrix

    transfertot = (trasnfer1^(nbarrier-1))*transferbdr*D21*(Pnbarrier^(-1));

    % Trasmission

    T = 1/(abs(transfertot(1))^2);

    Tvect(1,o)= T;

    % Damping

    minuslnTvect(1,o) = -log(T)/log(exp(1));
```

Here I use the Kronig Penney model and the Delta Kronig Penney model

```
    % Kronig penney

    kronigpennyvect(1,o) = cos(k_1gama)*cos(k_2a) -(((k_1a^2)+(k_2a^2))/(2*...
        k_1a*k_2a))*sin(k_1gama)*sin(k_2a);
```

```
    % Dirac Kronig penney

    deltakronigpennyvect(1,o) = cos(k_1gama) + ((gama*alfa)^(1/2)/(2*k_1gama))*...
        sin(k_1gama);


    % Use if want to plot the absolut value of the Kronigpenneyvect
    % or the absolut value of the Dirac Kronig penney

    abskronigpennyvect(1,o) = abs(kronigpennyvect(1,o));
    deltaabskronigpennyvect(1,o) = abs(deltakronigpennyvect(1,o));

end
```

Plotting

```
% Open a figure canvas

figure(1);

subplot(2,1,1)

hold on;

% Plot transmission probability as a function of energy
% Simply replace deltakronigpenneyvect by the deltaabskronigpenneyvect or
% the deltaallowedforbiddenvect and it will plot the desidered functions

plot(EoverV0vect,deltaabskronigpennyvect(1,:),'b-',EoverV0vect,  Tvect(1,:),'g-');

% Add labels to axes

xlabel('E/V_0');
ylabel('Translission');

% Add figure title

title(strcat('Transmission coefficient in function of E/V0 for gama = ',num2str(gama),'alpha =
',num2str(alfa)));
legend('delta Kronig-Penney ' ,strcat('T for nbarriers = ',num2str(nbarrier)));

% Scale axes

xlim([0 max(EoverV0vect)]);
```

```
ylim([-0.2 1.5]);

% Turn on bounding box and background grid

box on;
grid on;

hold off
subplot(2,1,2)

hold on;

% Plot transmission probability as a function of energy

plot(EoverV0vect, abskronigpennyvect(1,:),'b-',EoverV0vect, Tvect(1,:),'r-');

% Add labels to axes

xlabel('E/V_0');
ylabel('Transmission');

% Add figure title

title(strcat('Transmission coefficient in function of E/V0 for gama = ',num2str(gama),'alpha =
',num2str(alfa)));
legend('Kronig-Penney' ,strcat('T for nbarriers = ',num2str(nbarrier)));

% Scale axes

xlim([0 max(EoverV0vect)]);
ylim([-0.2 1.5]);

% turn on bounding box and background grid

box on;
grid on

figure(2);

hold on;

% Plot transmission probability as a function of energy

plot(EoverV0vect, minuslnTvect(1,:));

% Add labels to axes
```

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```
xlabel('E/V_0');
ylabel('Transmission');

% Add figure title

title(strcat('Transmission coefficient in function of E/V0 for gama = ',num2str(gama),'and
alpha = ',num2str(alfa)));
legend(strcat('Damping') );

% Scale axes

xlim([0 max(EoverV0vect)]);
ylim([0 70]);

% Turn on bounding box and background grid

box on;
grid on

hold off

end
```

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