Advanced Quantum Mechanics Lab

Study of the Transmission Coefficient of a General Double Barrier

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Contents

1. Objectives

The aim of this experiment is to study numerically the transmission coefficient, T, of the following double barrier potentials which are traversed by an electron:

- Symmetric double barrier.
- Asymmetric double barrier.
- Asymmetric double barrier with external bias.

2. Overview and Theory

2.1 Simple double barrier problem

When an electron's energy matches that of the quantum states in a double barrier potential well, its transmission probability becomes unity, a phenomenon known as resonant tunnelling. This was predicted in the 1960s and later observed in GaAlAs-GaAs-GaAlAs hetero-structures.

The simplest of all one-dimensional problems are square barriers and square wells in one dimension. For those problems, in each region of constant potential V the Schrodinger equation has the simple form:

$$\left(\frac{p^2}{2m} + V\right)\psi = E\psi, \tag{2.1}$$

This equation can be solved for each of the regions of constant potential, and appropriate boundary conditions[1] can be imposed at the potential discontinuities to obtain the complete wave-function. The well-known solution to **Equation 2.1** is:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \tag{2.2}$$

where k, the wave number[2], is defined as:

$$k(x) = \sqrt{\frac{2m(E - V(x))}{\hbar^2}} \tag{2.3}$$

Thus, when the energy of the particle is larger than the potential ($E - V > 0$), k is real and the wave-functions are plane waves. However, when the energy of the particle is smaller than the potential ($E - V < 0$), k is imaginary and the wave-function takes the form:

$$\psi(x) = Ae^{-\chi x} + Be^{\chi x}, \tag{2.4}$$

[1] Continuity of both the wave-function and its derivative.

[2] We make explicit the dependence of k and V on x to make this definition general.

where:

$$\chi(x) = \sqrt{\frac{2m(V(x) - E)}{\hbar^2}} \tag{2.5}$$

This method is used to compute the transmission coefficient for a double barrier. In general, the tunnelling attenuation factor for two barriers is approximately the product of the attenuation factors for each barrier. However, under resonating conditions in the intermediate well, the electron can pass through both barriers without attenuation, resulting in a transmission coefficient of 1. Assuming a left-to-right incident wave, an exact analytical expression can be obtained for the transmission coefficient T:

$$T = \frac{\frac{2^8 k_1 \chi_2 k_3 \chi_4 k_5}{|K|^2}}{(k_1^2 + \chi_2^2)(\chi_2^2 + k_3^2)(k_3^2 + \chi_4^2)(\chi_4^2 + k_5^2)}, \tag{2.6}$$

where K is defined as:

$$\begin{aligned}
K = {} & \exp(\chi_2 w_2 + \chi_4 w_4) \times \\
& \times (\exp i(-\varphi_1 + \varphi_2 + \varphi_3 + \varphi_4 + \varphi_5) - \exp i(\varphi_1 + \varphi_2 - \varphi_3 - \varphi_4 + \varphi_5)) + \\
& + \exp(\chi_2 w_2 - \chi_4 w_4) \times \\
& \times (-\exp i(-\varphi_1 + \varphi_2 + \varphi_3 - \varphi_4 - \varphi_5) + \exp i(\varphi_1 + \varphi_2 - \varphi_3 + \varphi_4 - \varphi_5)) + \\
& + \exp(-\chi_2 w_2 + \chi_4 w_4) \times \\
& \times (-\exp i(-\varphi_1 - \varphi_2 - \varphi_3 + \varphi_4 + \varphi_5) + \exp i(\varphi_1 - \varphi_2 + \varphi_3 - \varphi_4 + \varphi_5)) + \\
& + \exp(-\chi_2 w_2 - \chi_4 w_4) \times \\
& \times (\exp i(-\varphi_1 - \varphi_2 - \varphi_3 - \varphi_4 - \varphi_5) - \exp i(\varphi_1 - \varphi_2 + \varphi_3 + \varphi_4 - \varphi_5)),
\end{aligned} \tag{2.7}$$

and:

$$\begin{aligned}
&\varphi_1 = k_3 w_3; && \varphi_2 = \arctan\frac{\chi_2}{k_1}; && \varphi_3 = \arctan\frac{\chi_2}{k_3}; \\
&\varphi_4 = \arctan\frac{\chi_4}{k_3}; && \varphi_5 = \arctan\frac{\chi_4}{k_5}.
\end{aligned} \tag{2.8}$$

2.2 Solving for an arbitrary potential

The method described in the previous section is useful for determining the transmission coefficient T when the potential is built up of a discrete number of sections of constant potential. However, when we have a double potential barrier in the presence of an external bias, this method is only useful for making a rough approximation (by averaging the potential in each region). If we want to be more precise in determining T, we need to resort to the **propagation matrix method**, which we will describe here.

Suppose an electron of energy E and mass m encounters an arbitrary one-dimensional potential energy profile $V(x)$ from the left. We can divide the potential into a number of potential energy steps, as shown in **Figure 1**, and then we can apply the propagation matrix method, that we will describe in the following section.

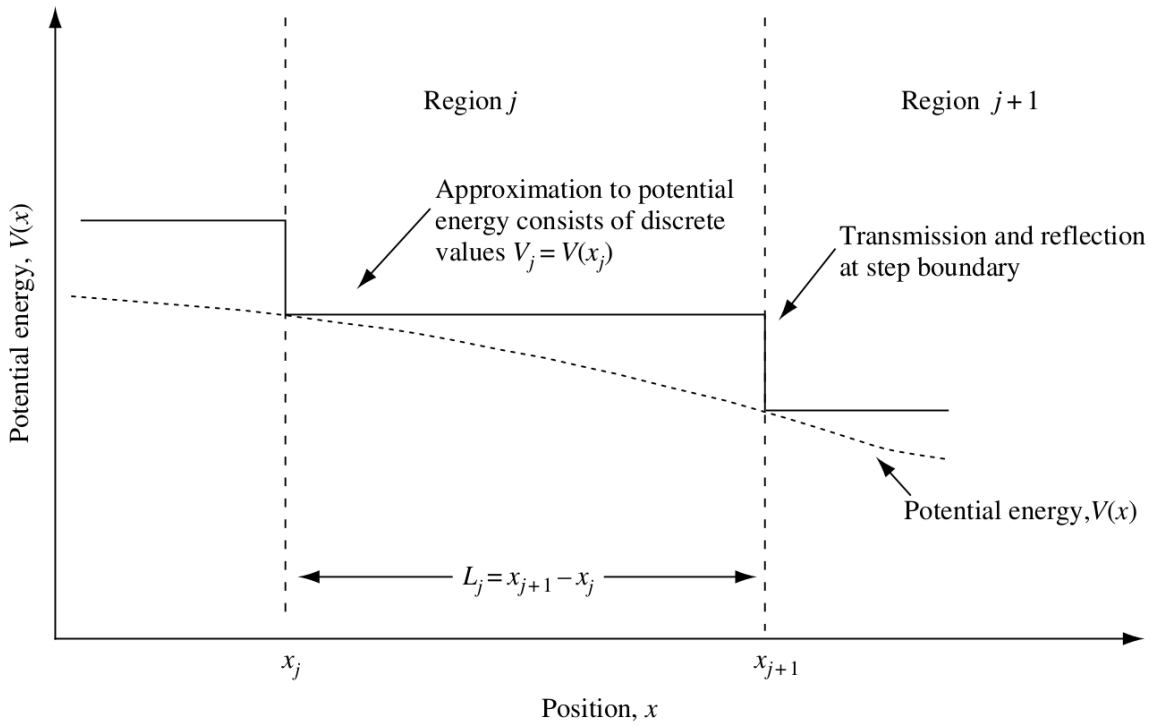

Figure 1: Diagram illustrating approximation of a smoothly varying one-dimensional potential energy profile $V(x)$ with a series of potential energy steps [1].

2.2.1 Propagation matrix method

We will now explain the propagation matrix method, which can be divided into 4 parts.

Propagation at the step

Assuming the discretisation of the potential shown in **Figure 1**, we can define the transmission coefficient of the j-th potential step as:

$$k_j = \sqrt{\frac{2m(E - V_j)}{\hbar^2}}, \tag{2.9}$$

and the wave-functions which are solution to the Schrödinger equation in the regions i and j, respectively, can be defined as:

$$\begin{aligned} \psi_j &= A_j e^{ik_j x} + B_j e^{-ik_j x} \\ \psi_{j+1} &= C_{j+1} e^{ik_{j+1} x} + D_{j+1} e^{-ik_{j+1} x} \end{aligned} \tag{2.10}$$

Note that in each region of the potential there is a wave-function travelling left-to-right (coefficients A and C) and a wave-function travelling right-to-left (coefficients B and D).

As we mentioned before, both wave-functions are constrained by the fact that both ψ and $d\psi/x$ should be continuous at the discontinuities of the potential. We must impose:

$$\psi_j|_{x=x_{j+1}} = \psi_{j+1}|_{x=x_{j+1}}\,, \qquad \left.\frac{d\psi_j}{dx}\right|_{x=x_{j+1}} = \left.\frac{d\psi_{j+1}}{dx}\right|_{x=x_{j+1}} \tag{2.11}$$

Substituting the wave-functions from **Equation 2.10** into these conditions, we obtain[3]:

$$\begin{aligned} A_j e^{ik_j x_{j+1}} + B_j e^{-ik_j x_{j+1}} &= C_{j+1} e^{ik_{j+1} x_{j+1}} + D_{j+1} e^{-ik_{j+1} x_{j+1}} \\ A_j e^{ik_j x_{j+1}} - B_j e^{-ik_j x_{j+1}} &= \frac{k_{j+1}}{k_j} C_{j+1} e^{ik_{j+1} x_{j+1}} - \frac{k_{j+1}}{k_j} D_{j+1} e^{-ik_{j+1} x_{j+1}} \end{aligned} \tag{2.12}$$

By organizing into rows and columns the terms that contain left-to-right traveling waves of the form e^{ikx} and right-to-left traveling waves of the form e^{-ikx} , one may write these equations for a potential step at position $x_{j+1} = 0$ as a matrix equation:

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} A_j \\ B_j \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \frac{k_{j+1}}{k_j} & -\frac{k_{j+1}}{k_j} \end{bmatrix} \begin{bmatrix} C_{j+1} \\ D_{j+1} \end{bmatrix} \tag{2.13}$$

In order to obtain a more useful expression that will enable us to directly obtain the coefficients A_j and B_j from the coefficients C_{j+1} and D_{j+1} of the previous step, we need to get rid of the matrix on the left by taking its inverse. Since:

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}^{-1} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \tag{2.14}$$

we may write:

$$\begin{bmatrix} A_j \\ B_j \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ \frac{k_{j+1}}{k_j} & -\frac{k_{j+1}}{k_j} \end{bmatrix} \begin{bmatrix} C_{j+1} \\ D_{j+1} \end{bmatrix} = P_{j_{\text{step}}} \begin{bmatrix} C_{j+1} \\ D_{j+1} \end{bmatrix}, \tag{2.15}$$

where:

$$P_{j_{\text{step}}} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_{j+1}}{k_j} & 1 - \frac{k_{j+1}}{k_j} \\ 1 - \frac{k_{j+1}}{k_j} & 1 + \frac{k_{j+1}}{k_j} \end{bmatrix}, \tag{2.16}$$

is the matrix that gives us the information about the propagation at the discontinuities of the potential.

Propagation within the step

Propagation inside a region of equal potential of length L_j carries only phase information so that $A_j e^{ik_j L_j} = C_{j+1}$ and $B_j e^{-ik_j L_j} = D_{j+1}$. In matrix form:

$$\begin{bmatrix} e^{ik_j L_j} & 0 \\ 0 & e^{-ik_j L_j} \end{bmatrix} \begin{bmatrix} A_j \\ B_j \end{bmatrix} = \begin{bmatrix} C_{j+1} \\ D_{j+1} \end{bmatrix} \tag{2.17}$$

As before, we can find a more useful expression:

$$\begin{bmatrix} A_j \\ B_j \end{bmatrix} = \begin{bmatrix} e^{-ik_j L_j} & 0 \\ 0 & e^{ik_j L_j} \end{bmatrix} \begin{bmatrix} C_{j+1} \\ D_{j+1} \end{bmatrix} = P_{j_{\text{free}}} \begin{bmatrix} C_{j+1} \\ D_{j+1} \end{bmatrix} \tag{2.18}$$

where:

$$P_{j_{\text{free}}} = \begin{bmatrix} e^{-ik_j L_j} & 0 \\ 0 & e^{ik_j L_j} \end{bmatrix} \tag{2.19}$$

[3]Note here that, for semiconductor heterostructures with different effective electron mass, current continuity requires that all factors (k_{j+1}/k_j) in be replaced with $(m_j k_{j+1}/m_{j+1} k_j)$. As we are working with the same effective electron mass everywhere, we will omit this consideration.

Combined propagation for the step

Combining the free propagation and the step propagation, we can obtain the propagation matrix P_j for the j-th region:

$$P_j = P_{j_{\text{free}}} P_{j_{\text{step}}} = \frac{1}{2} \begin{bmatrix} \left(1 + \frac{k_{j+1}}{k_j}\right) e^{-ik_j L_j} & \left(1 - \frac{k_{j+1}}{k_j}\right) e^{-ik_j L_j} \\ \left(1 - \frac{k_{j+1}}{k_j}\right) e^{ik_j L_j} & \left(1 + \frac{k_{j+1}}{k_j}\right) e^{ik_j L_j} \end{bmatrix}, \tag{2.20}$$

Propagation through an arbitrary number of step potentials

For the general case of N potential steps, we can write down the propagation matrix for each region and multiply out to obtain the total propagation matrix:

$$P = \prod_{j=1}^{N} P_j = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \tag{2.21}$$

Then, we can write:

$$\begin{bmatrix} A \\ B \end{bmatrix} = P \begin{bmatrix} C \\ D \end{bmatrix} \tag{2.22}$$

Where A and C (B and D) are the coefficients of the right-travelling (left-travelling) wave on the left and right sides of the potential, respectively.

The total propagation matrix P satisfies continuity in ψ and and $d\psi/dx$ between adjacent regions. Since the particle is incident from the left, we know that $A = 1$, and if there is no reflection at the far right then $D = 0$. We may then rewrite:

$$\begin{bmatrix} 1 \\ B \end{bmatrix} = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \begin{bmatrix} C \\ 0 \end{bmatrix} \tag{2.23}$$

From this, we obtain $1 = p_{11}C$, so the transmission probability $|C|^2$ is simply:

$$|C|^2 = \left| \frac{1}{p_{11}} \right|^2 \tag{2.24}$$

3. Methods

In this analysis, we will compute the transmission probability for three different potentials: the symmetric double barrier potential, the asymmetric double barrier potential, and the asymmetric double barrier potential with external bias. We will compute the transmission probability in two different ways: using the *propagation matrix method* and using the analytic expression provided in **Section 2.1**. For the first two potentials, there is no problem in using this expression, as the potential is always constant in each region. However, for the potential with the external bias we will need use the average potential in each region of non-constant potential. The result will, of course, be an approximation.

The core of the *propagation matrix method* implementation, which has been programmed with `python` and uploaded as a GitHub repository, can be found here. On the other hand, the core of the method using the given analytic expression can be found here.

In summary, the following simulations are presented:

Type of Potential	Simulation Method
Symmetric double barrier	Analytic solution from **Section 2.1**
Symmetric double barrier	Propagation matrix method
Asymmetric double barrier	Analytic solution from **Section 2.1**
Asymmetric double barrier	Propagation matrix method
Asymmetric double barrier with external bias	Analytic solution from **Section 2.1**
Asymmetric double barrier with external bias	Propagation matrix method

Table 1: Simulations that are presented.

The parameters that have been used for the simulations are shown in **Table 2**.

Parameter	Value
Effective mass of the electron everywhere	$0.067m_e$

Table 2: Simulation parameters.

4. Results

4.1 Symmetric double barrier potential

The symmetric double barrier potential we have simulated is shown in **Figure 2**. The transmission coefficient as a function of the electron energy that we have obtained with each of the two methods is shown in **Figure 3**. As you can see, both methods give exactly the same results.

4.2 Asymmetric double barrier potential

The asymmetric double barrier potential we have simulated is shown in **Figure 4**. The transmission coefficient as a function of the electron energy that we have obtained with each of the two methods is shown in **Figure 5**. Note that, again both solutions coincide exactly.

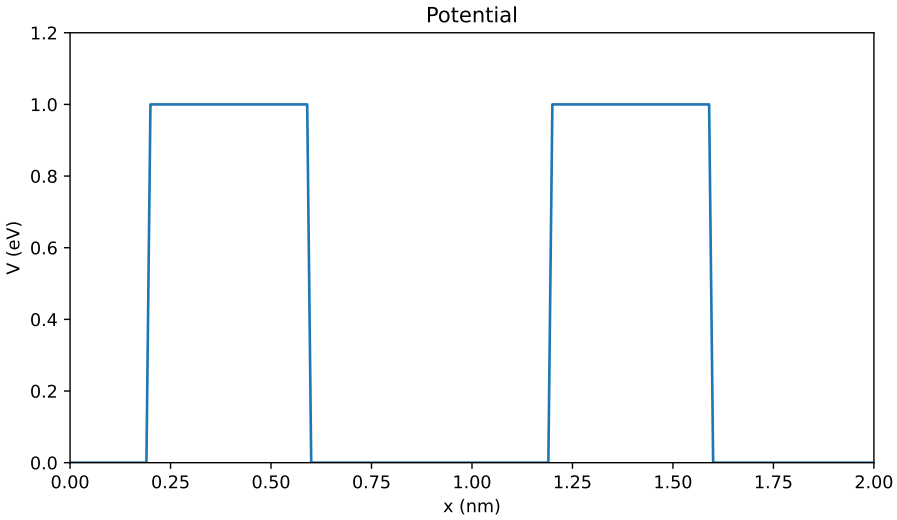

Figure 2: Symmetric double barrier potential.

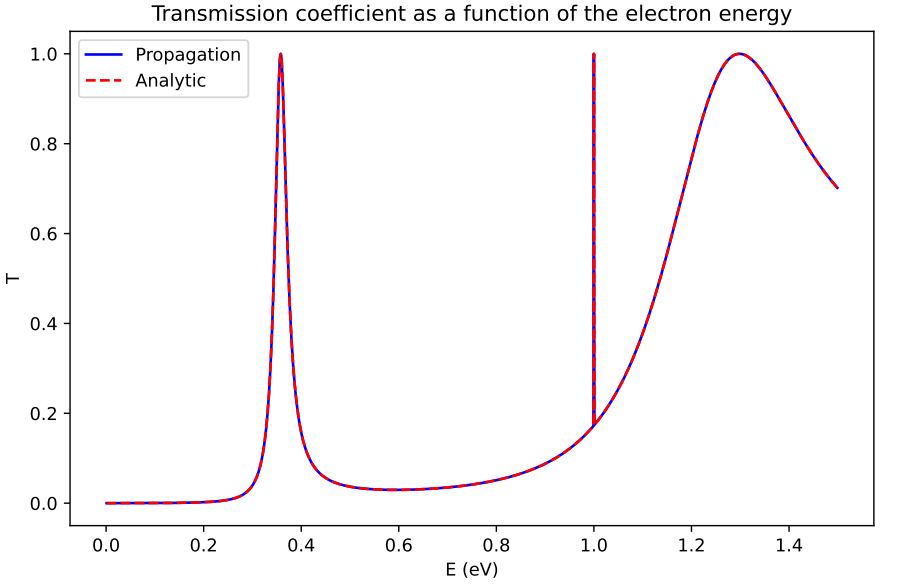

Figure 3: Plot of the transmission coefficient as a function of the electron energy for the symmetric double barrier potential.

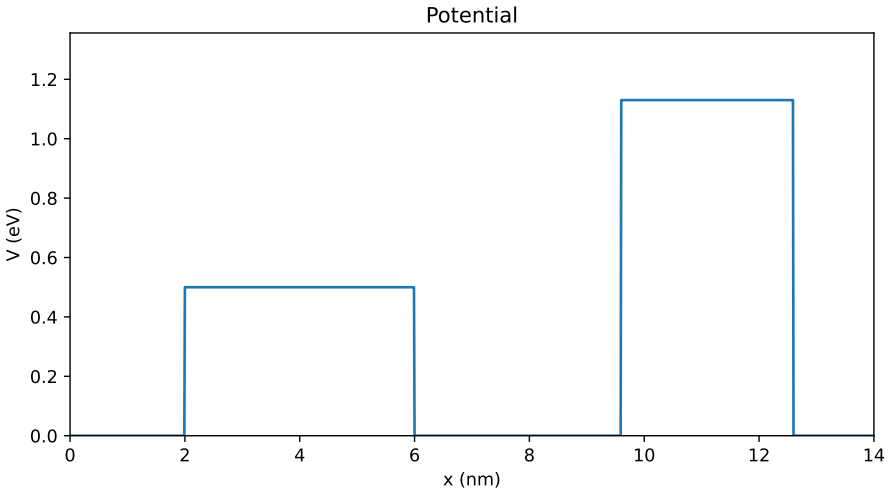

Figure 4: Asymmetric double barrier potential.

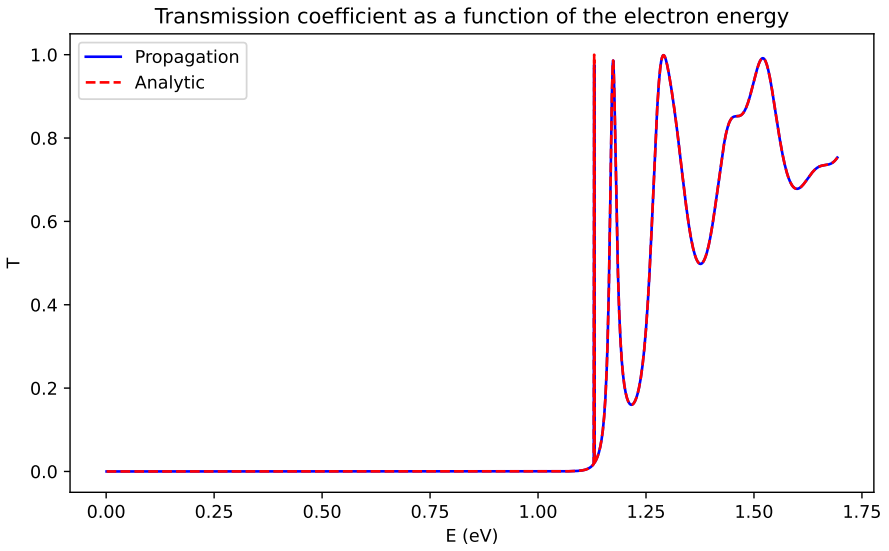

Figure 5: Plot of the transmission coefficient as a function of the electron energy for the asymmetric double barrier potential.

4.3 Asymmetric double barrier potential with external bias

The asymmetric double barrier potential with external bias that we have simulated is shown in **Figure 6**. Furthermore, the transmission coefficient as a function of the electron energy that we have obtained with each of the two methods is shown in **Figure 7**.

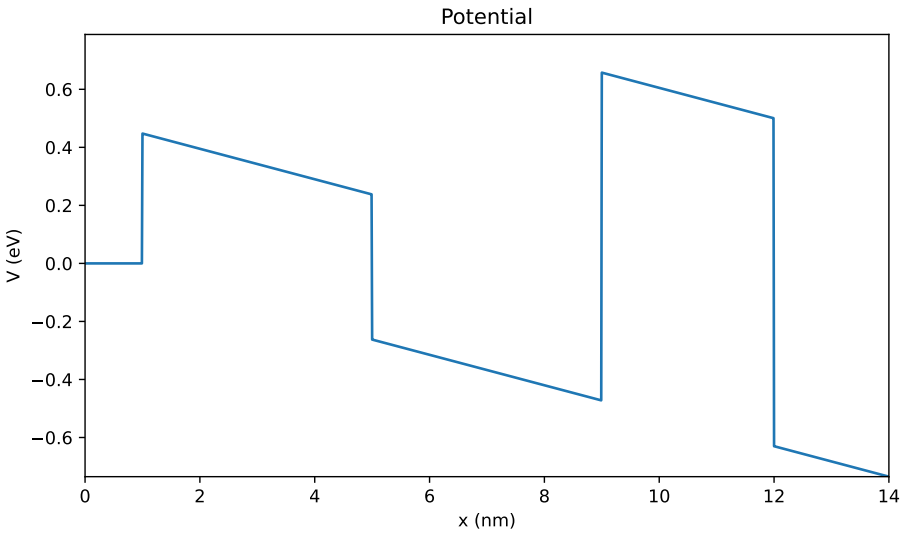

Figure 6: Asymmetric double barrier potential with external bias.

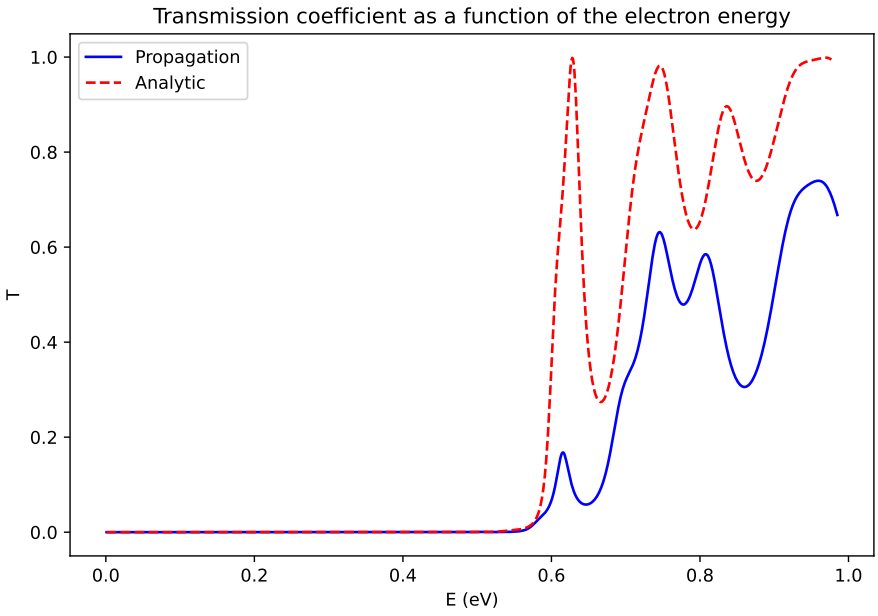

Figure 7: Plot of the transmission coefficient as a function of the electron energy for the asymmetric double barrier potential with external bias.

As you can see, in this case there is quite a large discrepancy between the transmission coefficient approximated with the analytical expression and the one obtained by the

propagation matrix method.

5. Discussion

5.1 Symmetric double barrier

If we look at the plot on **Figure 3**, we can identify a single transmission resonance corresponding to a single bound state of the electron in the potential well, where the transmission probability becomes unity. It corresponds to an energy of $E = 0.358\ eV$. Furthermore, in the range of energies we have worked with, there is yet another transmission resonance corresponding to a state of higher energy than the potential, at around $E = 1.2985\ eV$, which does not correspond to a bound state.

Comparing the two methods used to compute the transmission coefficient, we can see that the results obtained are completely identical. This was expected, as there is no approximation involved in any of the two methods, so the fact that they give us the same results gives us confidence that we have programmed things correctly.

5.2 Asymmetric double barrier

In this case, if we look at the plot in **Figure 5**, we can see that there aren't any bound states of the electron in the potential well, as there are no peaks in the transmission coefficient below the energy of the potential barriers. The lack of symmetry causes the probability of transmission for any electron with an energy below that of the barriers to go to zero. It is only for energies higher than $E = 1.13\ eV$ (the height of the highest barrier of the two) that the transmission probability starts to increase, eventually reaching ~ 1 for $1.174\ eV$, $1.2904\ eV$ and $1.52\ eV$.

Here, again, we see that the results obtained using both methods are exactly the same, as expected.

5.3 Asymmetric double barrier with external bias

In the presence of an external bias, the transmission coefficient drops considerably, with a maximum just under 0.8 (for the propagation matrix method). An interesting thing here is the difference between the results obtained using the analytic formula given in **Section 2.1** (which in this case is an approximation) and those given by the propagation matrix method. There is a clear similarity in the general shape of the transmission curve in both cases (the maxima and minima are around the same energy values), but the analytic approximation overestimates the transmission coefficient by a considerable amount. In fact for an energy of $\sim 0.6\ eV$, it estimates a transmission coefficient of 1, whereas the propagation matrix

method gives a transmission coefficient just under 0.2. If we compute the approximate relative error in this point, which is the point of maximum discrepancy between the two methods, we obtain:

$$\varepsilon_{\text{rel}} = \frac{1 - 0.2}{1} \cdot 100\% = 80\% \tag{5.1}$$

Therefore, with the approximation used with the analytical expression from **Section 2.1**, we are introducing errors of up to 80%. This is huge!

6. Conclusions

With these simulations, we have been able to compute the transmission coefficient for three different kinds of one-dimensional potentials, using two different methods: the first an analytical expression used for computing the transmission coefficient in a double potential barrier and the second a numerical *propagation matrix method* used to compute the transmission coefficient of an arbitrary potential by splitting it into a succession of potential steps.

We have found that, in the symmetric double barrier potential, a transmission resonance occurs at an energy of $E = 0.358\ eV$, which corresponded to a bound state of the potential well generated between the two barriers. We have also found that neither the asymmetric double barrier potential nor the asymmetric double barrier potential with external bias have any resonant bound states in their potential wells. In the asymmetric double barrier potential without external bias, there are several resonances at energies higher than that of the barriers, although none inside the well itself. However, in the presence of an external bias, the transmission coefficient was much lower, with a maximum just under 0.8, even for high energies.

In terms of the methods employed for the calculation of the transmission coefficient, we have seen that, for simple potentials consisting of defined regions of constant potential, the analytical expression is much faster. However, when the potential is more complex in shape, the approximations that are required in order to be able to apply this method give very large errors that can reach values of $\sim 80\%$. In those cases, it is much more better to use the more reliable propagation matrix method, even if it is a little slower.

Bibliography

[1] A F J Levi. *Applied Quantum Mechanics*. Cambridge University Press, 2006. ISBN: 9780521860963 (cit. on p. 3).