Analysis of One-dimensional Double-potential Barrier Structures Resonant Tunnelling Based on Transmission Matrices

Zihan Zhang *

Department of Physics, University of Toronto, Ontario, Canada

* Corresponding author: zihanandy.zhang@mail.utoronto.ca

Abstract. The comprehension of the tunnel effect, the passage of matter waves and particles across a high potential barrier, was the most astounding of all discoveries in quantum mechanics. Research on tunnelling in semiconductors and superconductors, as well as the development of scanning tunnelling microscopy, garnered five Nobel prizes in physics. In this study, the resonant tunnelling effect of electron tunnelling through a one-dimensional double-potential barrier was found and verified by solving the time-independent Schrödinger equation and calculating the transmittance rate of the electron tunnelling through the two potential barriers by using the transmission matrix technique performed by MATLAB. According to the analysis, the transmittance rate was one under certain specific conditions (under some specific incident energy values or some specific distance between two potential barriers), which was called as resonant tunnelling. However, in this study, square potential wells were analyzed, which can be considered merely as ideal models in real life, and therefore all results are idealized. For further investigations, researchers can use more realistic parameters to set up potential wells and analyze real-life problems.

Keywords: Quantum tunnelling, Resonant tunnelling, Transmission matrix.

1. Introduction

The theory of quantum mechanics appeared in 1900 and one of some of the first phenomena and experiments that scholar discovered, conducted, and explained was the photoelectric effect [1-3]. An important concept introduced and realized in the photoelectric effect is the binding energy. Since the energy of the electrons in a metal sheet is naturally lower than the binding energy, they cannot leave the sheet. To visualize this behavior, one introduces the concept of a potential well, where the top of the potential well is the binding energy, and since the electrons do not have enough energy to exceed the binding energy, they tend to stay at the bottom of the potential well. The reason why electrons become free electrons in the photoelectric effect is the same as explained by classical mechanics. According to classical mechanics, particles or objects can escape the potential well only if their energy is greater than the potential energy.

In the photoelectric effect, electrons gain energy greater than the potential energy by absorbing photons and are therefore able to escape the potential well. However, if there are two potential wells nearby, according to classical mechanics, a particle cannot move from one potential well to the other if there is not enough energy for the particle to cross the barrier between the two potential wells, the area under the potential curve is called classically forbidden region since it’s impossible to happen based on the classical mechanical theory. According to quantum mechanics, a particle can move from one to the other without having to overcome the potential well [4]. It was known that the electron could be described as a wave function and by calculating the wave function of the electron in different regions, one found that the wave function was not zero on both sides of the potential barrier, meaning that the complex square of the wave function was not zero, indicating that the electron could be found on either side of the barrier as the electron has tunneled through the potential barrier.

Nowadays, with the development of quantum physics, it has been applied to more and more fields with many application scenarios, e.g., semiconductors, optics, optoelectronics, and optoelectronic devices [5-8]. In addition, the invention of superconductors and scanning tunnelling microscopes is also based on quantum tunnelling [9, 10]. Therefore, the study of quantum tunnelling is crucial to understanding the mechanisms behind these technologies and innovating new quantum-based technologies. The motivation for this article was to discover the tunnelling effect under double potential barriers and to observe the resonant tunnelling effect. Below will state the method, result, analysis, and the discussion for this study.

2. Methdology

For this study, the transmission matrix technique was used and the calculation and plotting were proceeded via MATLAB. For the electron tunnelling through one potential barrier, assume the square barrier with its left edge located at x=0 with its width as a and the height as V0. The zero potential was defined at the bottom of the barrier and the energy (E) for the incident electron was less than V0. There were three distinct regions 1, 2 (classically forbidden region), and 3 defined as x>a, 0<x<a, and x<0. The schematic sketch is shown in Fig. 1.

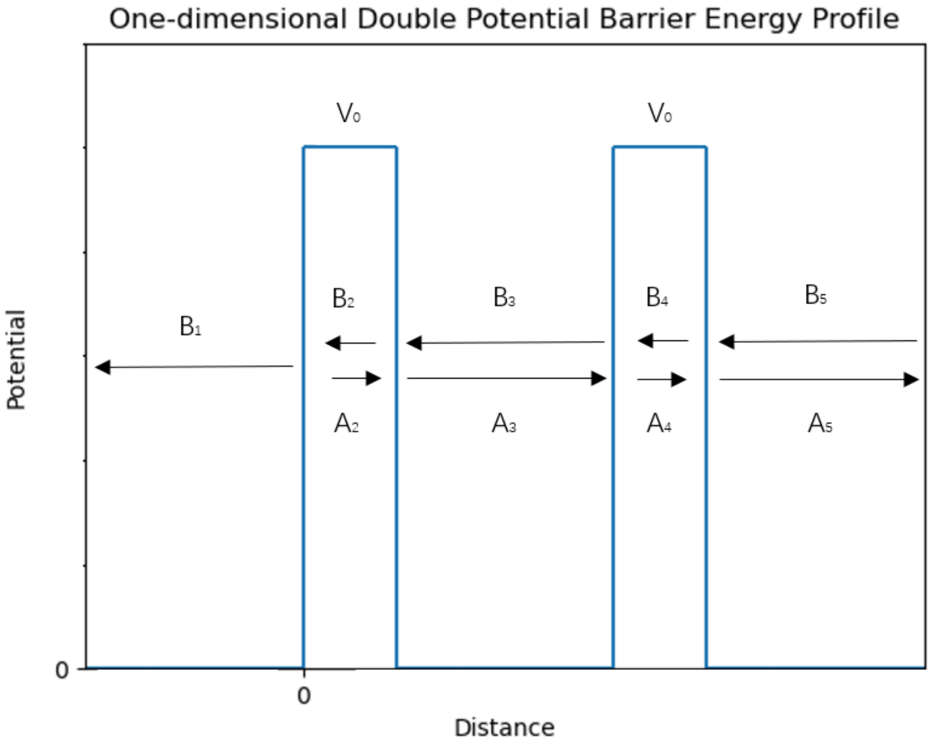

Figure 1. Schematic sketch of the one-dimensional double potential barrier.

Therefore, the potential energy in different regions could be written as:

$$V(x)\begin{cases} 0, & x > a \\ V_0, & 0 < x < a \\ 0, & x < 0 \end{cases} \tag{1}$$

Using the separation of variable technique, one can get the following equations:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\varphi(x) = E\varphi(x) \tag{2}$$

In regions 1 and 3, V=0, the equation (2) is then:

$$-\frac{\hbar^2}{2m}\varphi(x)\frac{d^2}{dx^2} = E\varphi(x) \tag{3}$$

Therefore, k_1 is:

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \tag{4}$$

In region 2, $V=V_0$, $E<V_0$, therefore the equation (2) is then:

$$-\frac{ħ^2}{2m}\varphi(x)\frac{d^2}{dx^2}=(E-V_0)\varphi(x) \tag{5}$$

Therefore, k_2 is:

$$k_2=-\frac{\sqrt{2m(E-V_0)}}{ħ} \tag{6}$$

The solution of the wave function in different regions is:

$$\varphi_E(x)=\begin{cases} Ae^{-ik_1x}+Be^{ik_1x}, & x>a \\ Ce^{k_2x}+De^{-k_2x}, & 0<x<a \\ Fe^{-ik_1x}+Fe^{ik_1x}, & x<0 \end{cases} \tag{7}$$

By changing some variables:

$$\varphi_E(x)=\begin{cases} A_1e^{-ik_1x}+B_1e^{ik_1x}, & x>a \\ A_2e^{k_2x}+B_2e^{-k_2x}, & 0<x<a \\ A_3e^{-ik_1x}+B_3e^{ik_1x}, & x<0 \end{cases} \tag{8}$$

Applying the boundary conditions and assume:

$$k_i=-\frac{\sqrt{2m(E-V_i)}}{ħ} \tag{9}$$

Based on the continuity of the wave function and the continuity of the derivative of the wave function, can obtain:

$$A_1+B_1=A_2+B_2,\ \ at\ x=a \tag{10}$$

$$k_1A_1-k_1B_1=k_2A_2-k_2B_2,\ \ at\ x=a \tag{11}$$

$$A_2e^{k_2a}+B_2e^{-k_2a}=A_3e^{k_3a}+B_3e^{-k_3a},\ \ at\ x=0 \tag{12}$$

$$k_2A_2e^{k_2a}-k_2B_2e^{-k_2a}=k_3A_3e^{k_3a}+k_3B_3e^{-k_3a},\ \ at\ x=0 \tag{13}$$

Write the equation above using matrix as:

$$\begin{bmatrix} e^{k_1x_1} & e^{-k_1x_1} \\ k_1e^{k_1x_1} & -k_1e^{-k_1x_1} \end{bmatrix}\begin{bmatrix} A_1 \\ B_1 \end{bmatrix}=\begin{bmatrix} e^{k_2x_1} & e^{-k_2x_1} \\ k_2e^{k_2x_1} & -k_2e^{-k_2x_1} \end{bmatrix}\begin{bmatrix} A_2 \\ B_2 \end{bmatrix} \tag{14}$$

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix}=\begin{bmatrix} -k_1e^{-k_1x_1} & e^{-k_1x_1} \\ -k_1e^{k_1x_1} & e^{k_1x_1} \end{bmatrix}\begin{bmatrix} e^{k_2x_1} & e^{-k_2x_1} \\ k_2e^{k_2x_1} & -k_2e^{-k_2x_1} \end{bmatrix}\begin{bmatrix} A_2 \\ B_2 \end{bmatrix} \tag{15}$$

Therefore, the transmission matrix (T_mat) is:

$$\begin{bmatrix} -k_1e^{-k_1x_1} & e^{-k_1x_1} \\ -k_1e^{k_1x_1} & e^{k_1x_1} \end{bmatrix}\begin{bmatrix} e^{k_2x_1} & e^{-k_2x_1} \\ k_2e^{k_2x_1} & -k_2e^{-k_2x_1} \end{bmatrix} \tag{16}$$

Since the quantum tunnelling effect is a Markov chain, meaning the process that is happening only depends on the previous process [11] and each tunnelling event could be represented by a link between neighboring Markov Chain [12], the electron tunnelling through two potential barriers in one dimension could be described as:

$$\begin{bmatrix} A_5 \\ B_5 \end{bmatrix}=T\_mat(4)\times T\_mat(3)\times T\_mat(2)\times T\_mat(1)\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} \tag{17}$$

where A1 and B1 are the resultant wave functions and A2, and B2 are the wave function of the incident electron. Therefore, the transmission rate could be calculated as:

$$\frac{|B_1|^2}{|B_5|^2} \tag{18}$$

And the reflection rate could be calculated as:

$$\frac{|A_5|^2}{|B_5|^2} \tag{19}$$

The transmission matrix (16) and the equation for electron tunnelling through two potential barriers in one dimension (17) were then imported into MATLAB for calculation and plotting. In the first simulation, the potential V0 was set to 10eV and the width of the potential barrier was 0.05nm, the distance between two potential barriers was 10nm. Besides, in the second simulation, the potential V0 was set to 10eV and the width of the potential barrier was 0.02nm, the incident electron energy was 1eV. For both simulation, the parameter A_1 was set as 0 and B_1 was set as 1 for simplicity.

3. Results and Discussion

Based on the calculation of the transmission rate and the reflection rate of an electron, the relationship between the transmission rate and reflection rate with respect to the incident energy and the distance between the potential barrier is shown in the Fig. 2 and Fig. 3.

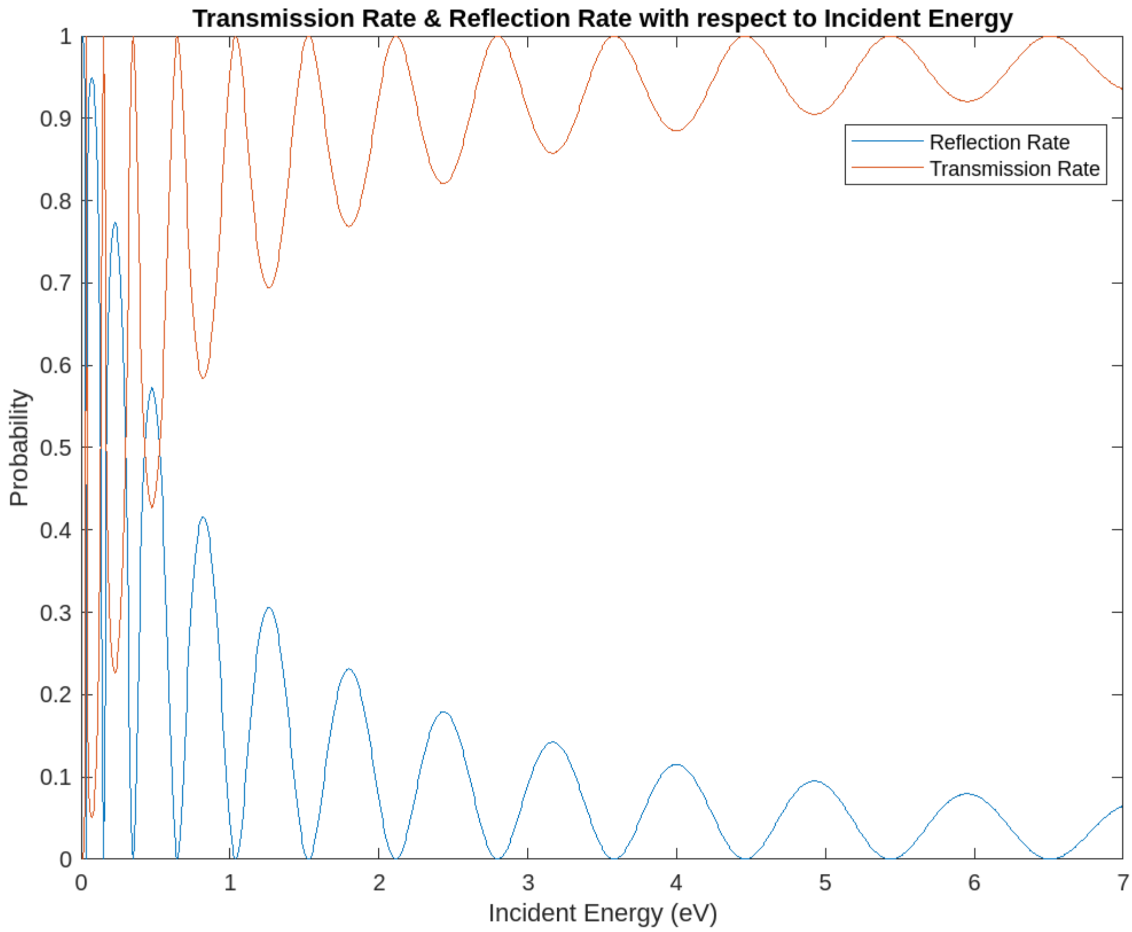

Figure 2. The transmission rate and reflection rate with respect to incident energy

In both simulations, it was observed that the probability of the electron found behind the potential barrier was not zero. In the first simulation, by varying the energy of the incident electron while holding other variables constant, the transmission rate was 1 at some specific energies. Also, in the second simulation, by varying the distance between two potential barriers while holding other variables constant, the transmission rate was 1 at some specific distances. This phenomenon was called as resonant tunnelling. The max transmission rate with respect to the energy, appeared to be proportional to the square root of the energy. Also, for the max transmission rate with respect to the distance between the potential barrier, it appeared to be equally distanced and the distance between two max transmissions was half of the de Broglie wavelength of the electron.

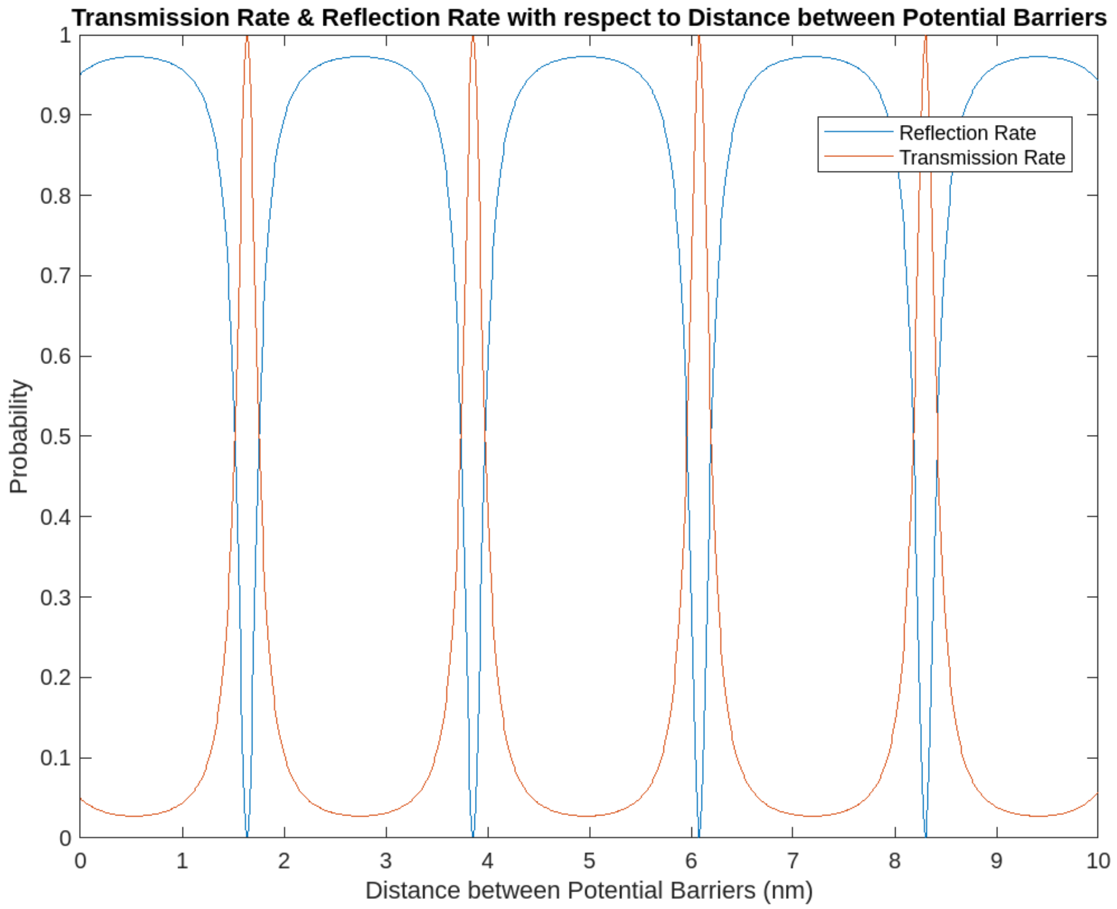

Figure 3. The transmission rate and reflection rate with respect to the distance between potential barriers.

Based on solving the time-independent Schrödinger equation and using the transmission matrix technique, the transmission probability for an electron to tunnel through double potential barriers in one dimension could be calculated and plotted. The width of the potential barrier should be small because if electrons were incident at the barrier, then the transmitted wave function in the classical forbidden region will be decayed exponentially [13], to ensure the tunnelling effect happens, a thin energy barrier allows the wave function not decayed to zero in classical forbidden region is crucial. The resonant tunnelling phenomenon was observed as a result, which was at some specific situation, the transmission rate was 100%. The resonant tunnelling effect and transmission matrix technique used for this study could also be implemented to the periodic potential barriers in one dimension and that was related to the material science and the energy band phenomenon. Also, the tunnelling effect and similar calculations used for this study could be used to solve the infinite potential barriers in higher dimensions, such as in three dimensions, which was related to the quantum dot theory. Resonant tunnelling could also be used to build resonant tunneling diodes, magnetic field sensors, transistors and electron flow switch [14]. Since there is no perfect square potential barrier in the real world, the result of this study could be treated as a close approximation of the real-world situation. The potential of the barrier, the interval between barriers, and particle energy in this study could be modified in the future to fit and approximate in the specific real-world research situation and be implemented in more fields.

4. Conclusion

To sum up, the focus of this study was to observe and verify the quantum tunneling effect and one-dimensional resonance tunneling effect of an electron in MATLAB simulation using the transmission matrix technique. According to the MATLAB calculation of electron transmission rate, it can be observed that the probability of an electron being found behind the potential barrier was not zero, which provides strong evidence for the quantum tunneling effect. In addition, the transmission rate was one for some specific incident energy conditions or for some specific distance conditions between the potential barriers. Strong evidence was provided for the resonant tunneling effect of electrons tunnelling through a one-dimensional double potential barrier under specific conditions. The quantum tunneling effect and the one-dimensional resonant tunneling effect provide a theoretical basis for future research and industry, and are expected to have applications in semiconductors, optoelectronics, optics, and other fields.

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