Analysis of Electron Double Barrier Tunneling Based on Python

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Abstract. Tunneling is a common phenomenon in microphysics, and resonant tunneling is a tunneling phenomenon under special conditions. Double barrier tunneling is an important quantum mechanical phenomenon, which has important application and research value in condensed matter physics, semiconductor devices, quantum mechanics, and nanotechnology. This study takes the double barrier as an example to observe electron tunneling and find out the influence of different parameters on the tunneling effect. In this study, the wave function is calculated by using the method of Schrodinger equation and transpose matrix, and the image is drawn by Python and numerical operation. In this study, it is found that the barrier width is inversely proportional to the transmittance, and the transmittance and reflectance will change periodically with the distance between the two barriers, and the electrons will reach full transmission at a certain incident energy value. Studying the characteristics and mechanisms of double barrier tunneling helps develop new quantum technologies and devices and promotes technological innovation in related fields.

Keywords: Double barrier tunneling, resonant tunneling, transmittance, reflectance.

1. Introduction

The tunneling effect is a quantum mechanical phenomenon first proposed by Fowler and Nordheim in 1928, known as the Fowler-Nordheim tunneling theory. Shama Parveen et al used the Fowler-Nordheim theory to explain Field emission (FE) phenomena [1]. Experimental observations of tunneling began in the 1930s when research focused on metal-oxide-semiconductor field-effect transistors (MOSFETs). Until now, studies about MOSFETs have not stopped, and nanoscale MOSFETs such as SiO2/6H-SiC MOSFETs [2].

In the mid-20th century, the tunneling effect attracted widespread interest in semiconductor devices and quantum mechanics. In semiconductor devices, the tunneling effect is important for the design and manufacture of tunneling diodes, quantum tunneling devices such as GaAs/AlAs diodes [3], RF power sensors [4], etc. With the development of nanotechnology, research on electron transport at the nanoscale [5] has become increasingly important. The tunneling effect plays a key role in quantum communication at the nanoscale [6]. In quantum computing, the tunneling effect is used to design qubits [7], which is of great significance for the realization of quantum computing. The tunneling effect has also been used to design various sensors and thermoelectric devices [8], using the sensitivity of the tunneling current to achieve highly sensitive sensors and high-efficiency thermoelectric devices.

To sum up, the research motivation of double barrier tunneling involves many fields such as semiconductor device application, theoretical physics research, nanotechnology application, and material science research, and its research is of great significance to promote the development and application of related fields. To understand the basic principles of the various applications mentioned above, this study calculates the wave function through the transition matrix and plots it using Python. The relationships between transmittance and parameters are observed by changing different parameters.
2. Methodology

An asymmetric double barrier model is constructed, which is close to the Quantum resonant tunneling diode (QRTD) of GaAs [9]. In the double barrier model, as shown in Fig.1, it is equal to zero in regions I, III, and V, and V1 and V2 in regions II and IV, respectively. Here, only symmetric double barrier structures are considered, that is, V1 equals V2. As shown in the Fig. 1, when an electron beam is shot into the double barrier from the left side, it is assumed that the energy of the electron beam is sufficient for it to transmit through the double barrier. Nevertheless, during transmission, reflections also occur. Every time an electron enters the next region, a reflection occurs, that is, the wave function in the I to IV region is the superposition of the incident wave and the reflected wave. According to the Schrodinger equation in one-dimensional space, the wave functions of electrons in five regions can be written.

\[
E \cdot \psi = -\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} + V \cdot \psi
\]  

The Schrödinger equation in one-dimensional space is derived from Eq. (1):

\[
\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} \cdot [v - E] \cdot \psi
\]  

According to the formula (2), the e-exponential form of the wave function in five regions can be written as following formulae:

\[
\psi_1 = A_1 e^{ik_1x} + B_1 e^{-ik_1x}, x < a, \ k_1 = \frac{2m_eE}{\hbar^2}
\]  

\[
\psi_2 = A_2 e^{-k_2x} + B_2 e^{k_2x}, a \leq x < b, \ k_2 = \sqrt{\frac{2m_e(V_1-E)}{\hbar^2}}
\]  

\[
\psi_3 = A_3 e^{ik_3x} + B_3 e^{-ik_3x}, b \leq x < c, \ k_3 = \sqrt{\frac{2m_eE}{\hbar^2}}
\]  

\[
\psi_4 = A_4 e^{-k_4x} + B_4 e^{k_4x}, c \leq x < d, \ k_4 = \sqrt{\frac{2m_e(V_2-E)}{\hbar^2}}
\]  

\[
\psi_5 = A_5 e^{ik_5x}, x \geq d, \ k_5 = \frac{2m_eE}{\hbar^2}
\]  

Several formulae for easy computation and programming will be listed, these are the long formulas that are selected when calculating the wave function:

\[
x_1 = \left(\frac{ik_4-k_3}{2ik_3}\right)\left(\frac{k_4-ik_3}{2k_4}\right)e^{-k_4c-ik_3c+ik_4d+k_4d} + \left(\frac{ik_3+k_4}{2k_3}\right)\left(\frac{ik_5+k_4}{2k_4}\right)e^{k_4c-ik_3c+ik_5d-k_4d}
\]
\[ y_1 = \left( \frac{ik_3 + k_4}{2ik_3} \right) \left( \frac{k_4 - ik_5}{2k_4} \right) e^{-k_4c+ik_3c+ik_4d+k_4d} + \left( \frac{ik_3 - k_4}{2ik_3} \right) \left( \frac{ik_5 + k_4}{2k_4} \right) e^{k_4c+ik_3c+ik_5d-k_4d} \] (9)

\[ x_2 = \left( \frac{k_2 - ik_3}{2k_2} \right) e^{ik_2b + k_2b} x_1 + \left( \frac{k_2 + ik_3}{2k_2} \right) e^{-ik_2b + k_2b} y_1 \] (10)

\[ y_2 = \left( \frac{k_2 + ik_3}{2k_2} \right) e^{ik_2b - k_2b} x_1 + \left( \frac{k_2 - ik_3}{2k_2} \right) e^{-ik_2b - k_2b} y_1 \] (11)

\[ x_3 = \left( \frac{ik_1 - k_2}{2ik_1} \right) e^{-k_2a - ik_1a} x_2 + \left( \frac{k_2 + ik_1}{2ik_1} \right) e^{k_2a - ik_1a} y_2 \] (12)

\[ y_3 = \left( \frac{ik_1 + k_2}{2ik_1} \right) e^{-k_2a + ik_1a} x_2 + \left( \frac{ik_1 - k_2}{2ik_1} \right) e^{k_2a + ik_1a} y_2 \] (13)

According to the boundary conditions and the properties of the quantum wave function, the following relationship can be obtained by combining Eqs. (3) to (7):

\[ A_5 = \frac{A_1}{x_3} \] (14)

\[ A_4 = \left( \frac{k_4 - ik_5}{2k_4} \right) e^{ik_5d + k_4b} A_5 \] (15)

\[ A_3 = \left( \frac{ik_3 - k_4}{2ik_3} \right) e^{-k_4c - ik_3c} A_4 + \left( \frac{ik_3 + k_4}{2ik_3} \right) e^{k_4c - ik_3c} B_4 \] (16)

\[ A_2 = \left( \frac{k_2 - ik_3}{2k_2} \right) e^{ik_2b + k_2b} A_3 + \left( \frac{k_2 + ik_3}{2k_2} \right) e^{-ik_2b + k_2b} B_3 \] (17)

\[ B_1 = \frac{A_2 y_3}{x_3} \] (18)

\[ B_4 = \left( \frac{ik_5 + k_4}{2k_4} \right) e^{ik_5d - k_4b} A_5 \] (19)

\[ B_3 = \left( \frac{k_4 + ik_1}{2ik_1} \right) e^{-k_4c + ik_1c} A_4 + \left( \frac{ik_3 - k_4}{2ik_3} \right) e^{k_4c + ik_3c} B_4 \] (20)

\[ B_2 = \left( \frac{ik_3 + k_2}{2k_2} \right) e^{ik_3b - k_2b} A_3 + \left( \frac{k_2 - ik_3}{2k_2} \right) e^{-ik_3b - k_2b} B_3 \] (21)

### 3. Results and Discussion

Through numerical simulation, after setting it to a certain number, the remaining value can be obtained. In this study, 1 will be set for ease of calculation. After the above values are obtained, assuming the incident energy E and the height of the barrier V (i.e., the energy of the barrier), E is 2eV, and V1 and V2 are both 4eV. In addition to these, positions a, b, c, and d need to be proposed, which are 0nm, 0.4nm, 2.4nm, and 2.8nm respectively. Bring the Eq. (8) to (13) into the relations (14) to (21), and bring the resulting relationship from the last step into the wave function (3) to (7). Brining the simulated values into the wave function, one obtains Fig. 2. The red line is the constructed double barrier model, and the blue line is the wave function. In regions I, III, and V, the wave function presents the form of the standing wave, while in regions II and IV, the wave function presents an exponential decline.
The known formula for calculating transmittance is:

\[ T = \frac{|A_5|^2}{|A_1|^2} = \frac{A_5^* A_5}{A_1^* A_1} \]  \hspace{1cm} (22)

Here, \( A^* \) represents the conjugate of \( A \). In Python calculation, one can use the conjugate in the numpy library to convert \( A \) directly to conjugate. When the wave function is plotted numerically, \( A \) is assumed to be 1. Therefore, the transmittance formula in this study can be written as:

\[ T = A_5^* A_5 \]  \hspace{1cm} (23)

From the above calculation, the transmittance is a function of (b-a), (d-c), and (c-d) on the exponential term. According to Fig.1, the two barrier widths are (b-a) and (d-c) respectively. In order to obtain the relationship between barrier width and transmittance, only the barrier width is changed without changing the rest of the above conditions. In a python drawing, a value is taken every 0.001nm in the range from 0nm to 10nm and taken as the value of (b-a) and (d-c), that is, the width of the two barriers. As shown in Fig. 3, the obtained image shows an exponential decline in transmittance, which decreases rapidly and drops to 0 at a position less than 1nm. As can be seen from Fig. 3, the relationship between transmittance and barrier width is as follows: the larger the barrier width is, the smaller the transmittance is. This phenomenon explains the skin effect. Taking Permalloy films as an example, the greater the thickness, the less permeability. And permeability changes with thickness very quickly [10].

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**Figure 2.** Wave function image of the electron under the double barrier

**Figure 3.** The relation between the width of barriers and transmissivity.
When the wave function is plotted numerically, $A$ is assumed to be 1. Therefore, the reflectivity formula in this study can be written as:

$$ R = \frac{|B_1|^2 B_1^* B_1}{|A_1|^2 A_1^* A_1} \quad (24) $$

The distance between the two barriers can be expressed as $(c-b)$. In order to obtain the relationship between the barrier distance and transmittance and reflectivity, only the distance between the barriers $(c-b)$ is changed without changing the rest of the above conditions. In the Python drawing image, take a value every $0.001\text{nm}$ in the range from $0\text{nm}$ to $10\text{nm}$ and act as a numerical value, that is, the width of the two barriers. According to the Fig. 4 transmittance and reflectance change periodically with the distance between the two barriers, and the sum of transmittance and reflectance is 1.

![Figure 4. The relation between transmissivity and reflectivity with distance of two barriers](image)

**Figure 4.** The relation between transmissivity and reflectivity with distance of two barriers

In double barrier tunneling, the electron is described as a wave function and its behavior is affected by the wave properties. When the distance between the two barriers changes, the wave function will have interference and diffraction phenomena, resulting in periodic changes in transmittance and reflectivity.

All the above analysis changes the characteristic observed transmittance of the barrier without changing the incident electron beam. In this analysis, the incident energy will be changed. Since the above calculations are all cases where the incident energy is less than the barrier height (barrier energy), the incident energy cannot exceed the barrier height in this numerical analysis. When drawing an image using Python, a value is taken every $0.001\text{eV}$ in the range from $0\text{eV}$ to $4\text{eV}$ and is taken as the value of the incident energy of the electron. As shown in Fig. 5, with the increase of incident energy, the electron will reach full transmission at a certain incident energy value. This particular incident energy value is called the resonance energy, at which point the electron will be completely transmitted unhindered.
Fig. 5. The relation between incident energy and transmittance

Seen from Fig. 4 and Fig. 5, when the distance between the two barriers or the incident energy reaches a certain value, the transmission rate will increase to one, which is called resonance transmission. When a particle passes through the first barrier, it is possible to reflect back and forth between the two barriers. Since particles also have the property of fluctuation, if the energy of the particles makes these waves which are reflected back and forth reinforce each other after superposition, the amplitude of the wave function between the two barriers will become large, resulting in an increase in the probability of tunneling. Conversely, if the waves cancel each other out, the tunneling probability is reduced. According to Fig. 5, there are three different resonance energies in the incident energies from 0eV to 4eV, which are about 0.4eV, 1.5eV, and 3.25eV respectively. As illustrated in Fig. 6, the incident energy of the selected electron is 1.495eV, and the amplitude of the wave function of the incident electron is basically the same as that of the outgoing electron.

Fig. 6. The distance as a function of energy for barrier and wave function.

4. Conclusion

To sum up, in this study, qualitative variables are studied for the double barrier tunneling of electrons. When the wave function is plotted, it can be seen that the wave function of the electron in the barrier decreases exponentially and rapidly. Therefore, when the barrier width increases, the transmittance quickly drops to 0, which reflects the skin effect. When the barrier spacing is changed, it is found that the perspective and reflectance change periodically with the barrier spacing. When the incident energy is equal to the resonance energy, complete transmission is formed. Symmetric two-side barrier tunneling in this study is a phenomenon in quantum mechanics that describes the tunneling of a microscopic particle through barriers. Although this phenomenon is feasible in theory,
there are some limitations in practical application. In practical applications, different temperatures, different materials, noise, etc. will have an impact on the tunneling effect. Moreover, it is difficult to find a two-sided situation that strictly conforms to symmetry. The tunneling effect has important application prospects in quantum mechanics and nanoscience (nanoscale electronic devices, quantum tunneling microscopy, etc.). In energy science, the nanoscale energy conversion devices made by using the tunneling effect can effectively improve the energy conversion rate. This study is only a basic theoretical explanation of some phenomena in quantum tunneling, providing some clear-proof processes and methods for beginners.

References