Simulation Analysis of Factors Affecting the Quantum Tunneling Effect in 1D Double Potential Barriers Structures

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Abstract. The working principle of a large number of modern scientific equipment has been applied to the quantum tunneling effect. Although the explanations for the relevant principles of this effect are clarified, the calculation process is very complex and difficult to understand. Previous studies combine specific applications without theoretical model references. This study adopts the method of using the time-independent Schrodinger equation to solve the wave function, which is more convenient to obtain the expression of transmission probability. Then, one discusses the relationship between transmission probability and potential barrier width, potential barrier spacing, and incident particle energy. The experimental results show that the transmission probability decreases exponentially from 1 to 0 as the potential barrier width gradually increases. As the potential barrier width increases, the transmission probability exhibits a clear periodic oscillation relationship, the oscillation period remains unchanged, and this paper derives the relationship between the oscillation period and the potential barrier width. As the incident energy of particles gradually increases, the transmission probability exhibits periodic changes, and the minimum value of transmission probability increases with the periodic changes. Based on the analysis, the smaller the potential barrier width, the greater the incident energy, and the more likely quantum tunneling occurs.

Keywords: Quantum tunneling, resonant tunneling, double potential barriers.

1. Introduction

Quantum tunneling effect is one of the most important parts in modern physics, which explains that quantum objects can tunnel through potential barriers (energy barriers) in a way that is impossible for particles in classical physics. In classical physics, if the incident energy of a particle is greater than the height of the potential barrier, the particles will all cross the potential barrier without reflection; If the incident energy of a particle is less than the height of the potential barrier, then all particles should be reflected by the potential barrier and cannot pass through it [1]. However, in the system of quantum mechanics, any particle passing through a finite width potential barrier, regardless of the magnitude of the incident energy, has a certain probability of passing through or being reflected by the potential barrier.

A large number of modern devices have utilized quantum tunneling effects, such as scanning tunneling microscopes, plasma resonators, and nanoelectronic circuit designs [2]. Meanwhile, the practical application of quantum tunneling effect is also very specific. Scanning tunneling microscope is a device that utilizes quantum tunneling effect to accurately image at the atomic level. By detecting changes in micro current on the probe, the arrangement of atoms can be accurately scanned. This has been one of the main methods used by scientists in recent years to study material surfaces [3]. Some research teams have also applied this effect to quantum plasmas to accurately obtain the current density voltage (J-V) in nano scale metal insulator metal (MIM) junctions, and have constructed corresponding self consistent models [2]. Resonant tunneling diode is the earliest semiconductor device developed by humans that utilizes the quantum tunneling effect. Although the application scenarios of this semiconductor device have become diverse with the development of the times, its application in optoelectronics and logic circuits still requires in-depth research. Some research teams have demonstrated the magnitude and position of current in the resonance peak by reviewing the GaAs/AlGaAs double barrier resonant tunneling diode system and adopting new calculation methods [4]. Due to the special structure of the double potential barrier, a potential well is also formed between the two barriers, resulting in resonance tunneling effects in the double potential barrier structure. At present, many research teams have conducted theoretical research on the resonance tunneling effect under this structure, constructed many specific barrier models, and adopted different calculation methods [5-8].

In order to demonstrate the basic principle of quantum tunneling effect, this study will construct a one-dimensional symmetric double potential barrier structure model, strictly solve the time-independent Schrodinger equation in different regions according to the relevant theories of quantum mechanics, and use the properties of the wave function at the boundary to obtain the expression of the transmission probability of particles passing through the one-dimensional double-sided potential barrier, and analyze the relationship between the transmission probability and which variables. Discuss the change in effective mass of incident particles and their impact on transmission probability when passing through non square potential barriers (semiconductor heterojunction). Drawing the graph about relationship between transmission probability and related variables was and summarizing the physical meaning expressed in the results.

2. Methodology

As shown in the fig. 1, the same height of the one-dimensional double potential barrier, $U_1 = U_2 = U_0$. Its potential energy function $U(x)$ is

$$U(x) = \begin{cases} U_0, a < x < b, c < x < d \\ 0, others \end{cases} \quad (1)$$

The potential barrier widths are $L_1 = b - a$, $L_2 = d - c$. The distance between two potential barriers is$\Delta = c - b$. The first, third, and fourth regions are generally superconductors, conductors, metals, semiconductor materials. Electrons can move freely with zero potential energy, while the second and fourth regions are generally insulating layers, making it difficult for electrons to pass through and can be considered as potential barriers.

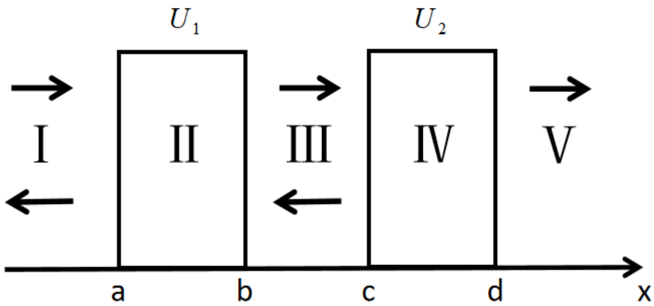

Figure 1. Structure diagram of the double potential barriers structures

By dividing 5 different regions and solving the time-independent Schrodinger equation for each region, the wave function equation for each region can be obtained [9]. The wave function equation system is as follows:

$$\begin{cases} \psi_I(x) = Ae^{ik_1x} + A'e^{-ik_1x} \\ \psi_{II}(x) = Be^{ik_2x} + B'e^{-ik_2x} \\ \psi_{III}(x) = Ce^{ik_1x} + C'e^{-ik_1x} \\ \psi_{IV}(x) = De^{ik_3x} + D'e^{-ik_3x} \\ \psi_V(x) = Fe^{ik_1x} \end{cases} \quad (2)$$

Assuming that the incident energy of microscopic particles is less than the height of the potential barrier, $E < U_0$, so in the function (2) that $k_1 = \sqrt{2mE}/\hbar$, $k_2 = k_3 = \sqrt{2m(U_0 - E)}/\hbar$, using the properties of wave functions at the boundaries of each region, obtain

$$\frac{F}{A} = 4k_1^2 k_2^2 e^{-ik_1(L_1+L_2)} / \{4k_1^2 k_2^2 \cosh(k_2 L_1)\cosh(k_2 L_2) + \sinh(k_2 L_1)\sinh(k_2 L_2)(k_1^2 + k_2^2)^2 e^{i2k_1\Delta} - 2ik_1 k_2 (k_1^2 - k_2^2)\sinh[k_2(L_1 + L_2)] - \sinh(k_2 L_1)\sinh(k_2 L_2)(k_1^2 - k_2^2)^2\} \tag{3}$$

Squaring the modulus of Eq. (3), one sets

$$\beta = k_1/k_2 = \sqrt{E/(U_0 - E)} \tag{4}$$

The transmission probability satisfies the following expression

$$T = 4\beta^4 / \{\beta^2(\beta^2 - 1)^2 \sinh(2k_2 L) + (\beta^2 + 1)^4 \sinh^4(k_2 L)\sin^2(k_1\Delta) + 4\beta^4 \cosh^2(2k_2 L) - 2(\beta^2 + 1)^2 \sin(k_1\Delta)\sinh^2(k_2 L) \cdot [(\beta^3 - \beta)\cos(k_1\Delta)\sinh(2k_2 L) + 2\beta^2 \cosh(2k_2 L)\sin(k_1\Delta)]\} \tag{5}$$

When an incident particle passes through a non-square potential barrier, due to the different periodic potentials of different potential barriers, the effective mass of the incident particle will change, and the wave number of the wave function in different regions will also change accordingly [10-12]. Therefore, the equation for transmission probability should satisfy the following function

$$T' = \frac{m_0}{m_{N+1}} \frac{k_{N+1}}{k_0} T \tag{6}$$

Here, m_0 is the mass of incident particles, m_{N+1} is the effective mass of particles in the right region of the rightmost potential barrier, k_0 is the wave number of the wave function in the left region of the leftmost potential barrier, k_{N+1} is the wave number of the wave function in the right region of the rightmost potential barrier. However, when calculating a symmetric square potential barrier, the incident particle passes through a potential barrier with the same periodic potential, and its effective mass does not change, therefore

$$\frac{m_0}{m_{N+1}} \frac{k_{N+1}}{k_0} = 1 \tag{7}$$

And the transmission probability can still be numerically simulated using Eq. (5).

3. Results and Discussion

As shown in the Fig. 2 is the relationship between the transmission probability and potential barrier width of one-dimensional double potential barriers. The incident particle is an electron, and the incident energy of the particle is $E = 5eV$, the potential barrier height is $U_0 = 10eV$, the distance between two potential barriers is $\Delta = 1nm$. From the figure, it can be noticed that when the potential barrier width is 0, there is nonexistent potential barrier in the structural model, so the transmission probability is 1. As the width of the potential barrier gradually increases, the transmission probability decreases exponentially, and reduce to 0 when the potential barrier width is about $L = 4nm$. It illustrates that the smaller the potential barrier width, the more likely the incident particles are to occur quantum tunneling effects.

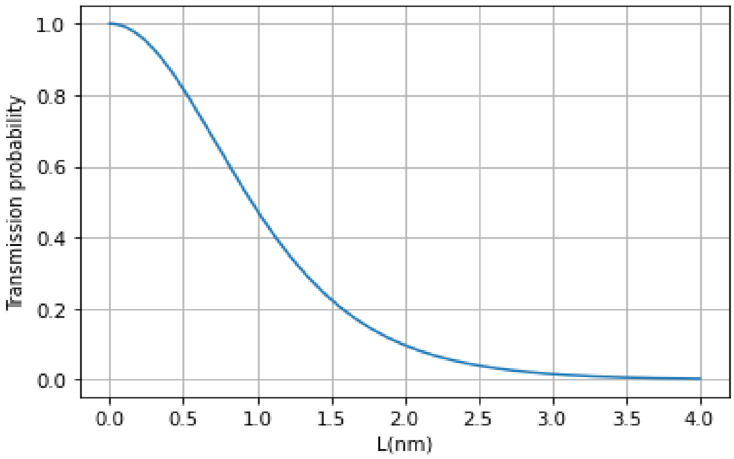

Figure 2. The relationship between the transmission probability and potential barrier width of one-dimensional double potential barriers

As shown in Fig. 3 is the relationship between the transmission probability and potential barrier spacing of one-dimensional double potential barriers. The incident particle is an electron, and the incident energy of the particle is $E = 5eV$, the potential barrier height is $U_0 = 10eV$,the potential barrier width $L = 1nm$. When the potential barrier spacing is 0, there is only one potential barrier in the structural model, which conforms to the single potential barrier structural model, and the transmission probability is less than 1. As the distance between potential barriers increases, the transmission probability gradually increases to 1 and then decreases again, showing a clear periodic oscillation relationship, and the oscillation period remains unchanged. The Fig. 4 shows when the potential barrier width increases to $L = 2nm$, the transmission probability still exhibits a clear periodic oscillation, with no change in the oscillation period, but the minimum transmission probability decreases and the peak width narrows.

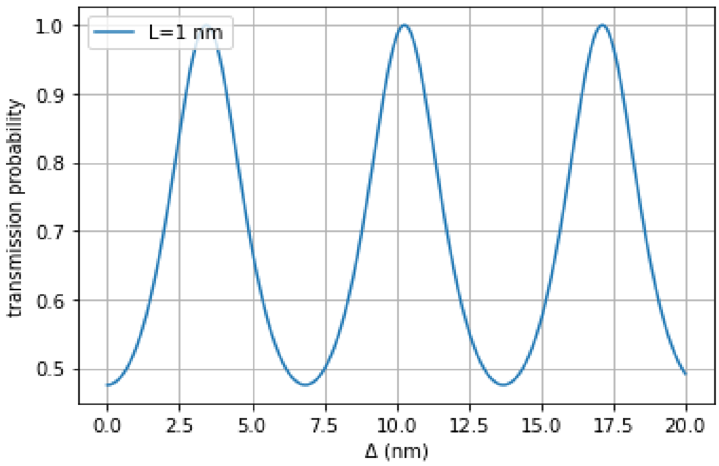

Figure 3. The relationship between the transmission probability and potential barrier spacing of one-dimensional double potential barriers when $L = 1nm$

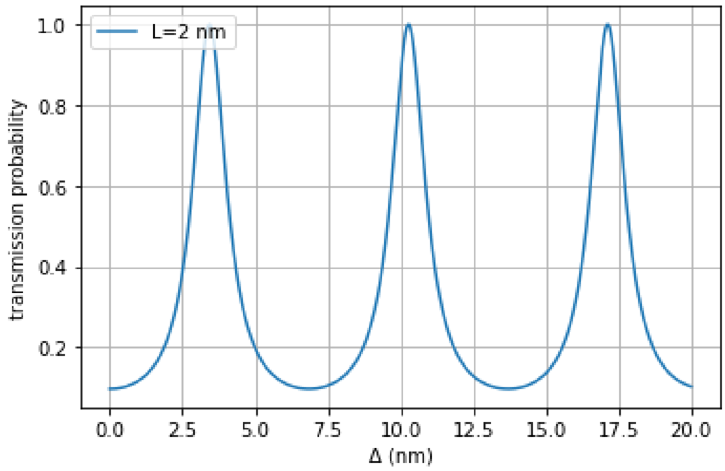

Figure 4. The relationship between the transmission probability and potential barrier spacing of one-dimensional double potential barriers when $L = 2nm$

This phenomenon of periodic oscillation is called resonance tunneling effect. Given a transmission probability of 1, the expression for the potential barrier spacing can be derived from Eq. (5) as follows:

$$\Delta = \frac{1}{k_1}\left\{arctan\left[\frac{2k_1k_2}{k_1^2-k_2^2}coth(k_2L)\right] + 2n\pi\right\} \tag{8}$$

Where n is an integer, it can be inferred from the expression that when the potential barrier spacing satisfies this equation, the transmission probability reaches its maximum of 1, while when it does not satisfy this equation, the transmission probability rapidly decreases. This is because the area between two potential barriers can be considered as a potential well. If the width of the potential well reaches a specific value which satisfy the equation in Eq. (8), the incident particle will undergo multiple reflections at the potential well interface after entering the potential well. Because the incident particle maintains phase coherence in the transmitted wave, there is a possibility that the transmission probability is close to 1, and making tunneling has resonant characteristic. Therefore, by adjusting the potential barrier spacing, resonance tunneling effects can be artificially induced to increase the transmission probability of particles.

As shown in Fig. 5 is the relationship between the transmission probability and the energy of the incident particle. The incident particle is an electron, the potential barrier height is $U_0 = 10eV$,the potential barrier width $L = 1nm$. When the potential barrier spacing is small ($\Delta = 3nm$), as the incident energy of the particle increases, the transmission probability slowly increases from 0 to 1 and then slowly decreases again, and periodic changes cannot be clearly observed from the curve in the figure. When the potential barrier spacing increases slightly ($\Delta = 7nm$), the growth rate of transmission probability significantly accelerates, and the second point with a transmission probability of 1 can be observed on the curve in the figure. When the potential barrier spacing is large ($\Delta = 15nm$), periodic changes of transmission probability can be clearly observed from the curve in the figure, and as the incident energy increases the oscillation period increases, but the oscillation amplitude is decreases. Therefore, by synthesizing the curves under three different potential barrier spacing, one can conclude that the larger the potential barrier spacing, the easier it is for resonance tunneling to occur.

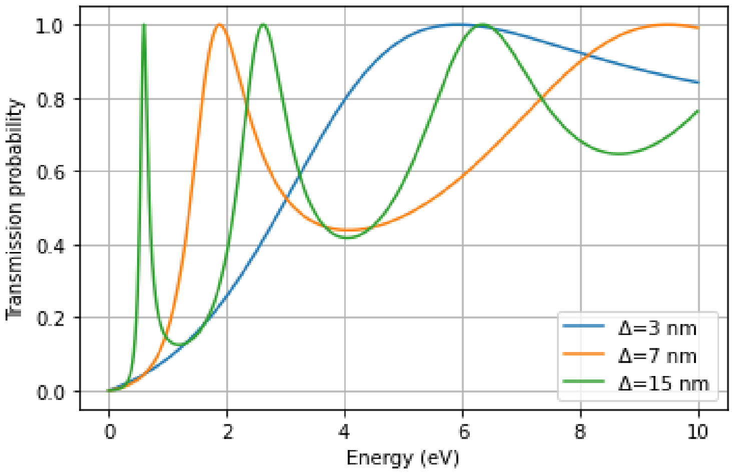

Figure 5. The relationship between the transmission probability and the energy of the incident particle under different potential barrier spacing

4. Conclusion

To sum up, this study uses the method of solving wave functions in different regions to obtain the time-independent Schrodinger equation system, and obtains the expression for the transmission probability of one-dimensional symmetric double potential barriers. The relationship between transmission probability and potential barrier width, potential barrier spacing, and incident energy is numerically simulated, and drawing the corresponding curve graphs. It is clearly concluded that the smaller the potential barrier width, the more likely the incident particle is to undergo tunneling effects. The transmission probability oscillates periodically with the potential barrier spacing, and the transmission probability also increases periodically as the energy of the incident particle gradually increases. Meanwhile, the influence of the incident particle passing through a non square potential barrier was discussed, and the conclusion was drawn that the non square potential barrier will affect the effective mass of the incident particle, thereby changing the transmission probability and calculate the corresponding equation. This research also discusses the relationship and differences between square and non square potential barriers, as well as their impact on transmission probability. It explains to some extent how different potential barriers affect transmission probability, which is beneficial for students in related fields to understand the principles and processes of quantum tunneling. However, it should be noted that the calculation which factors are related to the transmission probability of asymmetric double potential barriers are ignored. In the future, similar computational methods can be used to perform numerical simulations and image analysis on this structural model.

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