Proceedings of the 3rd International Conference on Computing Innovation and Applied Physics
DOI: 10.54254/2753-8818/25/20240950

Analysis of tunneling effect in different structures of one-dimensional barriers

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Abstract. Through the construction of mathematical model and the derivation of quantum mechanics formula, transmission coefficients of different one-dimensional barrier are explored. The difference of transmission coefficient and other properties under different materials was studied by controlling the change amount in the experiment. This study focuses on the analysis of one-dimensional barrier transmission coefficients of triangles and trapezoids, and ensures the accuracy of the experimental process through a large number of literature analysis. On this basis, the study of quantum tunneling effect should be easier, and it will be applied to more fields, which will play a crucial role for further research in the future. The special point of this experiment is to analyze and compare the transmission coefficient of different forms of one-dimensional barrier, compare the theoretical value with the actual value, and correct.The purpose of this experiment is to re-examine the original inherent conclusions and add new ones, so as to keep pace with the time.

Keywords: One-Dimensional Barrier, Quantum Tunneling Effect, Transmission Coefficients, Schrödinger Equation, Airy Functions.

1. Introduction

The intriguing phenomenon of quantum tunneling has long captivated the minds of physicists. Unlike classical physics, which precludes the possibility of a particle crossing an energy barrier without sufficient kinetic energy, quantum mechanics allows for this baffling event. Thanks to the wave-like nature of particles in quantum mechanics, their existence is defined not by specific locations but by wave functions that distribute probabilities over a range of positions. This wave function introduces a non-zero probability that a particle, such as an electron, can 'tunnel' through an energy barrier, even when it appears energetically impossible [1].

Quantum tunneling is not a newly observed phenomenon but is deeply rooted in the origins of quantum mechanics. When Erwin Schrödinger laid down his wave equation in 1926, it provided a robust mathematical framework that could describe the dynamics of particles in various types of potential fields, including energy barriers. This equation was groundbreaking, opening doors for a comprehensive academic investigation into the realm of quantum tunneling. Experimental validations over the years

DOI: 10.54254/2753-8818/25/20240950

have often supported the theoretical calculations based on the Schrödinger equation, solidifying its standing in the scientific community [2].

Schrödinger's equation has played a pivotal role in quantum physics. Introduced in a series of papers in 1926, the equation stands as a monumental contribution to science. It has a deterministic nature that incorporates the wave mechanics of quantum systems, and it is often interpreted using a probabilistic lens [2]. The versatility of the Schrödinger equation is truly remarkable. Whether it's employed in the study of electrons within potential wells or in the complex configurations of molecules, it serves as an essential mathematical tool for understanding quantum systems. It's not just confined to non-relativistic quantum mechanics but extends its reach to quantum field theory as well [3]. The practical implications of the Schrödinger equation are vast. For instance, it can calculate the energy eigenvalues and corresponding eigenfunctions or wave functions for quantum systems. This probabilistic interpretation allows for the computation of expectation values for physical observables like position, momentum, and energy [4]. One of the most important applications of the equation lies in its utility for studying quantum tunneling. By solving the equation, one can determine the probability amplitude of a particle crossing an energy barrier [4].

For a one-dimensional energy barrier, solving the Schrödinger equation leads people to find out the tunneling probability. This equation reveals that the tunneling probability decreases exponentially as the width of the barrier and the energy difference between the barrier and the particle increase [1]. The implications of this are substantial, showing how even infinitesimal changes in these parameters can dramatically affect the likelihood of tunneling. The notion of quantum tunneling also finds applications in modern technologies like tunneling microscopes and quantum computing. Recent research focuses on the transmission coefficient of particles in various barrier structures, particularly ladder and triangular barriers, which have been less explored but hold promise for new applications [1,5].

2. Formulas and derivations

In the following, the indispensable values for solving the problem of calculating one-dimensional barrier structures will be explained and analyzed, and the different shapes of barrier structures will be analyzed and discussed in an exemplary manner.

It is necessary to introduce the transmissivity coefficient before analyzing the various barriers later. In the context of quantum mechanics, the transmissivity coefficient refers to a quantity that characterizes the probability of a quantum particle, such as electrons, tunneling through a potential energy barrier. This coefficient is a fundamental concept in quantum mechanics and plays a crucial role in understanding the tunneling phenomena. and value of the transmissivity coefficient can range from 0 to 1, where $T = 1$ indicates the particle complete transmission and $T = 0$ indicates there only exist reflection. In this part, different barriers will be compared, including the square barrier, triangle barrier, and trapezoid barrier. This article will introduce the basic condition of these three barriers and analysis the distinction of transmissivity [6].

2.1. Square barrier

This basic barriers of the one-dimensional square barrier can be expressed as

$$V(x) = \begin{cases} 0 \ , x < 0, x > a \\ V_0 \quad ,0 \le x \le a \end{cases}. \tag{1}$$

When the $0 \le x \le$ a, the potential energy is a limited value, while the potential energy is zero when x outside. Sketch of this barrier is shown in Figure 1.

The tunneling in the single one-dimensional can embody the wave property of particle. It means that even if the energy of the particles are smeller than the barriers, they have probabilities to pass through the barriers. The probabilities are increasing with the decrease of the height and the width of the barriers. However, the pass through coefficient will sharply decrease when the $U_0 - \mathrm{E} = 5\mathrm{eV}$, and the width of the barrier surpass 50nm, the quantum concept will become classical macroscopic theory.

One can get the solution of the one-dimensional by solving the stationary Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}+V(x)\right]\Psi(x)=E\Psi(x). \tag{2}$$

Thus, the three individual equations for different regions are given by

$$\begin{cases}\frac{d^2\Psi_1}{dx^2}+k_1^2\Psi_1=0\\ \frac{d^2\Psi_2}{dx^2}+k_2^2\Psi_2=0\\ \frac{d^2\Psi_3}{dx^2}+k_3^2\Psi_3=0\end{cases} \tag{3}$$

where $k_1=\frac{\sqrt{2mE}}{\hbar}$, $k_2=\frac{\sqrt{2m(E-V_0)}}{\hbar}$, and $k_3=\frac{\sqrt{2mE}}{\hbar}$.

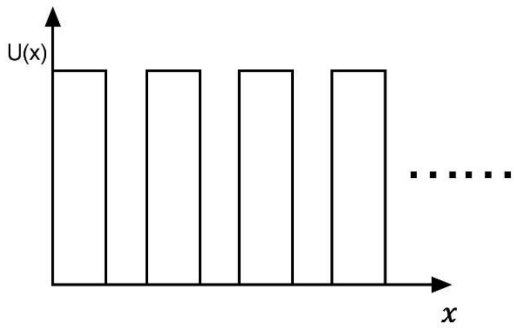

Figure 1. This picture shows the structure of one-dimension square barrier.

When $E>U_0$, one can get the wave function by solving these equations

$$\begin{cases}\Psi_1=A_1e^{ik_1x}+B_1e^{-ik_1x}\\ \Psi_2=A_2e^{ik_2x}+B_2\,e^{-ik_2x}\\ \Psi_3=A_3e^{ik_1x}+B_3e^{-ik_1x}\end{cases} \tag{4}$$

where Ψ_1,Ψ_2,Ψ_3 are the wave functions of the parts I, II, III. The authors define the first item and the positive index as right spread, the second item and negative index as left spread. The III part does not exist left wave function so the $B_3=0$. According to the continuity and differentiability condition, it is found that

$$\begin{cases}A_1+B_1=A_2+B_2\\ A_1-B_1=\frac{k_2}{k_1}(A_2-B_2)\end{cases} \tag{5}$$

when $x=0$, and they are

$$\begin{cases}A_2e^{(ik_2a)}+B_2e^{-ik_2a}=A_3e^{ik_1a}\\ A_2e^{(ik_2a)}-B_2e^{-ik_2a}=\frac{k_1}{k_2}A_3e^{ik_1a}\end{cases} \tag{6}$$

when $x=a$. Solving these simultaneous equations and it is arrived that

$$A_3=\frac{4k_1k_2e^{-ik_1a}}{(k_1+k_2)^2e^{-ik_2a}-(k_1-k_2)^2e^{ik_2a}}A_1. \tag{7}$$

Therefore, the transmissivity coefficient of this barrier can be expressed as

$$T = \frac{|A_3|^2}{|A_1|^2} = \frac{4k_1^2k_2^2}{\left(k_1^2 - k_2^2\right)^2 sin^2k_2a + 4k_1^2k_2^2}. \quad (8)$$

When $E < U_0,\ k_2$ is an imaginary number. So one should make the $k_2 = ik_3, k_3 = \sqrt{\left(\frac{2\mu(U_0 - E)}{\hbar}\right)}$. Thus, it is arrived that

$$A_2 = \frac{2ik_1k_3e^{-ik_1a}}{\left(k_1^2 - k_3^2\right)shk_3a + 4k_1^2k_3^2}A_1 \quad (9)$$

In this case, the transmissivity of this barrier can be expressed

$$\mathrm{D} = \frac{\left(4\mathrm{k}_1^2\,\mathrm{k}_3^2\right)}{\left(\left(\mathrm{k}_1^2 + \mathrm{k3}^2\right)^2 \mathrm{sh}^2\,\mathrm{k}_3\,\mathrm{a} + 4\mathrm{k}_1^2\,\mathrm{k}_3^2\right)}. \quad (10)$$

Figure 2 shows the transmissivity coefficient as a function of energy E.

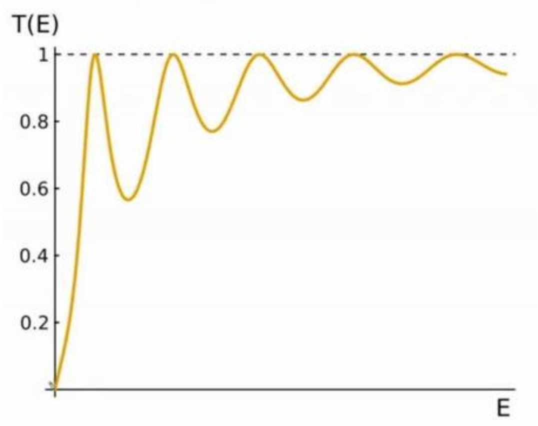

Figure 2. Diagram of the transmission coefficient of the square barrier.

2.2. Triangle barrier

Actually, there does not exists an essential difference between a square barrier and a trianglar barrier. The basic form is familiar, and it can be expressed in Figure 3. Triangle barriers are often used as idealized models for various physical systems. They can represent situations such as the behavior of electrons in semiconductor devices, the behavior of particles in quantum wells, or the potential energy profile in tunneling phenomena. So it is important to calculate the transmissivity coefficient to know about the system [7].

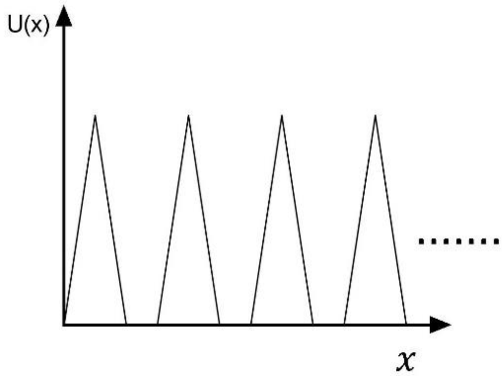

Figure 3. this picture shows one-dimension triangular barrier structure.

This article uses successive conditions to calculate the transmissivity coefficient before. Using transfer matrix algorithm to calculate transmissivity coefficient can also be useful. So transfer matrix algorithm will be used to calculate the trianglar barrier transmissivity coefficient. To get the transmission coefficient of triangular barriers, it is useful to list the time-independent Schrödinger equation as shown in Eq. (2). Assume a triangular barrier that is given by

$$\begin{cases} U(x) = s_1 x, 0 \leq x \leq \frac{1}{2}a \\ U(x) = U_m - s_1 x, \frac{1}{2} \leq x \leq a \\ U(x) = 0, x < 0 \text{ or } x > a \end{cases} \quad (11)$$

with $s_1 = \frac{2U_m}{a}$. For convenience the notation $A_{k\lambda} \equiv A_i(-\rho_k U_\lambda)$, $B_{k\lambda} \equiv B_i(-\rho_k U_\lambda)$, $A'_{k\lambda} \equiv A'_i(-\rho_k U_\lambda)$, $B'_{k\lambda} \equiv B'_i(-\rho_k U_\lambda)$ are adopted, where the A'_i and B'_i are the derivatives of the Airy functions respecting to the argument and $\rho_1 = \left(\frac{2m}{\hbar^2 s_1^2}\right)^{\frac{1}{3}}$. Assume $S = \frac{2i\mu_1 k_1}{\pi^2} \frac{e^{-ik_2 a}}{(\alpha\beta - \gamma\delta)}$, where the constants are given by

$$\alpha = \left[A_{22}B'_{23} - A'_{23}B_{22}\right] + i\mu_2 k_2 [A_{22}B_{23} - A_{23}B_{22}] \quad (12)$$

$$\beta = \left[A'_{11}B'_{12} - A'_{12}B'_{11}\right] + i\mu_1 k_1 \left[A_{11}B'_{12} - A'_{12}B_{11}\right] \quad (13)$$

$$\gamma = \left[A'_{11}B_{12} - A_{12}B'_{11}\right] + i\mu_1 k_1 [A_{11}B_{12} - A_{12}B_{11}] \quad (14)$$

$$\delta = \left[A'_{23}B'_{22} - A'_{22}B'_{23}\right] + i\mu_1 k_2 \left[A_{23}B'_{22} - A'_{22}B_{23}\right] \quad (15)$$

in which $\mu_1 = \frac{1}{\rho_1 s_1}$ and $\mu_2 = -\frac{1}{\rho_1 s_1}$. So, the transmission coefficient can be written as

$$T = \frac{k_2}{k_1}|S|^2 = \frac{4\mu_1^2 k_1 k_2}{\pi^4} \frac{1}{|\alpha\beta - \gamma\delta|^2}. \quad (16)$$

2.3. *Trapezoidal barrier*

The trapezoidal barrier can be described as below:

$$V(x) = \begin{cases} v_0 + Fx, 0 \leq x \leq a \\ 0, \quad x < 0, x > a \end{cases}. \quad (17)$$

Consider the real condition, the trapezoidal barriers can be expressed in Figure 4.

DOI: 10.54254/2753-8818/25/20240950

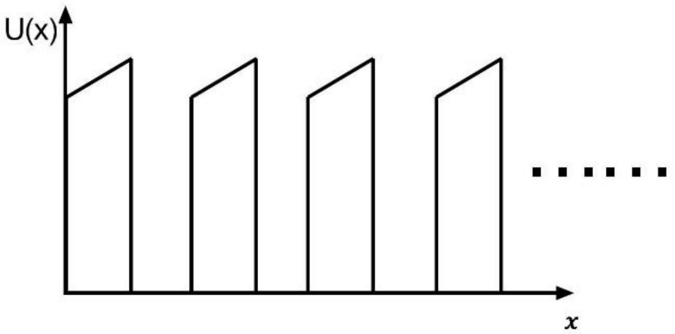

Figure 4. this picture shows one-dimension trapezoidal barrier structure.

In fact, trapezoidal barriers provide a simplified yet meaningful model to study the behavior of quantum particles encountering potential energy barriers in various systems. They are valuable tools for understanding quantum phenomena in different contexts, from electron transport in semiconductors to particle behavior in quantum wells. One can also get transmissivity coefficient of this system. Suppose a signal trapezoidal and the particles will conform to the Schrödinger equation

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E, (x < 0, x > a) \\ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (V_0 + Fx)\psi = E\psi, (0 \le x \le a) \end{cases} \quad (18)$$

The author makes $k = \frac{\sqrt{2mE}}{\hbar}$, and $\xi = \kappa\left(\frac{\epsilon}{F} - x\right)$, where $\epsilon = E - V_0$, $\kappa = \left(\frac{2mF}{\hbar^2}\right)^{\frac{1}{3}}$, so the original equation set can be rewritten:

$$\frac{d^2\psi}{d\xi^2} - \xi\psi = 0. \quad (19)$$

This is Airy functions, the solution can be expressed the linear combination with $Ai(\xi)$ and $Bi(\xi)$. When the $x < 0$ and $x > a$, wave functions can be described as:

$$\begin{cases} \psi_l = A_l e^{ikx} + B_l e^{-ikx} \\ \psi_r = A_r e^{ikx} + B_r e^{-ikx} \end{cases} \quad (20)$$

When $0 \le x \le a$, the wave function can be described as:

$$\psi_c = A_c Ai(\xi) + B_c Bi(\xi). \quad (21)$$

According to real situation, there are not particles passing into the barrier, so $B_r = 0$. Due to the continuity condition in $x = 0$ and $x = a$, then one can get the following solutions. When $x = 0$,

$$\begin{cases} A_l + B_l = A_c Ai\left(\xi_{max} + B_c Bi(\xi_{max})\right) \\ ik(A_l - B_l) = \kappa\left(A_c Ai'(\xi_{max}) + B_c Bi'(\xi_{max})\right) \end{cases} \quad (22)$$

where $\xi_{max} = -\frac{\kappa\epsilon}{F}$, and when $x = a$,

$$\begin{cases} A_r e^{ika} = A_c Ai\left(\xi_{min} + B_c Bi(\xi_{min})\right) \\ ikA_r e^{ika} = \kappa\left(A_c Ai'(\xi_{min}) + B_c Bi'(\xi_{min})\right) \end{cases} \quad (23)$$

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where $\xi_{min} = \kappa\left(a - \frac{\epsilon}{F}\right)$. Next, solve these functions set simultaneously, it is found that

$$\begin{cases} A_c = \pi e^{ika}\left(Bi'(\xi_{max}) - \frac{ik}{\kappa}Bi(\xi_{min})\right)A_r \\ B_c = -\pi e^{ika}\left(Ai'(\xi_{min}) - \frac{ik}{\kappa}Ai(\xi_{min})\right)A_r \end{cases} \tag{24}$$

Overall, one can get the transmission coefficient of trapezoidal barriers [8]

$$T = \begin{cases} \frac{4\theta^2 k^2}{\left(k^2 - \theta^2\right)^2 sin^2(\theta a) + 4\theta^2 k^2}, E > V_0 \\ \frac{4}{4 + k^2 a^2} \qquad , E = V_0 \\ \frac{4\Theta^2 k^2}{\left(k^2 + \Theta^2\right)^2 sinh^2(\Theta a) + 4\Theta^2 k^2}, E < V_0 \end{cases} \tag{25}$$

where $\theta = \frac{\sqrt{2m(E - V_0)}}{\hbar}$, $\Theta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$.

3. Applications

The authors begin by exploring the importance of one-dimensional barriers in the realm of quantum mechanics, where these systems manifest in various unique configurations. Each of these structures has its own set of characteristics and consequential applications. One such captivating structure is the one-dimensional periodic barrier, which is composed of recurring potential barriers and wells aligned along a single spatial axis. This regimented form of energy landscape is remarkably different from systems with random or irregular barriers where the potential energy varies without a pattern. The periodic nature of these barriers allows for phenomena like band formation and resonant tunneling, and they have been foundational to advanced research in quantum mechanics and solid-state physics [1].

Moving beyond academic interest, periodic barriers have also found practical applications. In real-world scenarios, these barriers are usually constructed in artificially engineered materials, particularly semiconductors. In such materials, what's known as superlattices are engineered by stacking alternating layers of different semiconductor materials. The result is a predictable, periodic potential energy landscape, offering a perfect real-world representation of a one-dimensional periodic barrier. The vast range of applications for these superlattices extends from optoelectronic devices to thermoelectric modules that are adept at converting heat into electricity. These modules serve as both a testimony and a playground for exploring and utilizing the unique properties of periodic barriers [9].

Within the intriguing domain of one-dimensional periodic barriers, the authors encounter a specialized structure known as the square barrier. In this structure, regions of constant potential energy are punctuated by abrupt changes, either rising or falling to a different constant value. This structured energy profile makes square barriers particularly common in semiconductor heterostructures, especially in Gallium Arsenide/Aluminum Gallium Arsenide (GaAs/AlGaAs) systems. Their well-defined structural nature renders them amenable to mathematical modeling [10]. This, in turn, allows square barriers to serve as an ideal testbed for analytical solutions and computational simulations, enriching the body of literature in both quantum mechanics and engineering.

As the authors delve deeper into computational simulations, it's worth noting that tools like MATLAB offer robust platforms for modeling these complex quantum structures. MATLAB provides functionalities for numerically solving the Schrödinger equation, thereby enabling simulations that capture not just basic tunneling but also intricate phenomena like resonant tunneling and energy band formation. Such simulations offer compelling graphical outputs that deepen people's understanding of particle behavior under varying barrier parameters, contributing to both academic research and practical applications.

One of the most remarkable aspects of periodic barriers is their role in quantum tunneling. These structures enable a phenomenon known as resonant tunneling, which occurs under specific conditions and at particular energy levels. This quantum form of resonance is a result of the constructive interference between the wave functions of tunneling particles, leading to significantly increased tunneling probabilities. This is a unique quantum behavior that has potentially transformative applications in ultrafast electronic devices where high-speed data transmission is critical.

Further broadening people's perspective, the paper turns to band theory to explore the electronic properties of materials. Unlike isolated atoms, which have discrete energy levels, electrons in solids reside in continuous bands of energies separated by gaps known as band gaps. In the context of tunneling, these band gaps serve as zones where the tunneling probability is incredibly low. However, the quantum mechanical phenomenon of tunneling allows particles to circumvent these high-energy barriers under certain conditions. Such a feat has far-reaching implications, especially in semiconductor technology where controlled tunneling phenomena are harnessed in various cutting-edge electronic components like tunnel diodes [11].

In summary, one-dimensional barriers in their various forms offer a fertile ground for both theoretical exploration and practical applications. Understanding the transmission coefficients in these barriers, especially in configurations like ladder and triangular barriers, can provide keen insights into the manipulative potential of quantum tunneling effects. Whether in academic research or in the fabrication of advanced electronic devices, these insights prove invaluable.

4. Conclusion

Quantum tunneling has far-reaching implications across multiple disciplines.The results show that when the width of the potential well is constant, the width of the potential barrier increases with the width of the potential well .The width of the microstrip decreases, and the beam between each adjacent quantum well decreases.The coupling between the bound energy levels is used to decrease and gradually change the microband.When the barrier width is fixed, it increases with the potential well widthLarge, resonance transmitted resonance energy gradually to the direction of low energyWhile moving, the resonant transmission peaks gradually become more and more sharp, both the distance between microstrips also gradually decreases. In electronics, it forms the basis of operation for tunnel diodes, devices that take advantage of the tunneling effect to allow current to flow even at very low voltages. Through experimental analysis and matlab calculation, tunnel effect can be applied to different conditions. By means of Schrödinger formula, the conclusions drawn from the theory can be further confirmed and finally applied to the practice of real life. Beyond semiconductors, the phenomenon is crucial in enabling the function of Scanning Tunneling Microscopes, which provide atomic-level imaging of materials. Additionally, in astrophysics, tunneling plays an essential role in nuclear fusion processes that fuel stars.Conclusions based on experiments play a vital role in academic research or in the development of cutting-edge scientific and technological equipment. In biochemistry, the concept is applied to explain certain enzymatic reactions that would otherwise be deemed too slow based on classical considerations alone.

Authors Contribution

All the authors contributed equally and their names were listed in alphabetical order.

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