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Quantum tunneling: transmission coefficient calculation and application

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Abstract. Quantum tunneling is one of the most important phenomena in quantum mechanics, showing that microscopic particles can pass through potential barriers even when their energy is lower than the barrier height. This paper focuses on the calculation of the tunneling transmission coefficient and its physical applications. First, the transmission coefficient of a single rectangular barrier is introduced through the one-dimensional time-independent Schrödinger equation and boundary conditions. Then, more realistic barrier shapes, including triangular, parabolic, exponential and Gaussian barriers, are discussed. For some idealized potentials, analytical solutions can be expressed using special functions such as Airy functions, parabolic cylinder functions and Bessel functions, while for smoother and more complicated potentials, the WKB approximation provides an effective method to estimate the transmission probability. The paper also extends the discussion from single barriers to double and multiple potential barriers, where interference effects and resonant tunneling can strongly enhance transmission under specific phase conditions. Finally, the applications of tunneling are considered, especially resonant tunneling diodes and scanning tunneling microscopy. These examples show that the transmission coefficient is not only a theoretical quantity, but also plays an important role in semiconductor devices and atomic-scale surface measurement. Overall, this paper demonstrates how different potential barrier models help connect the mathematical description of quantum tunneling with real physical systems.

Keywords: Quantum tunneling; transmission coefficient; WKB approximation; scanning tunneling microscope.

1. Introduction

Quantum tunneling is an important phenomenon in quantum mechanics. In classical physics, a particle cannot pass through a potential barrier if its energy is lower than the barrier height. However, in quantum mechanics, particles are described by wave functions, and the wave function can extend into the classically forbidden region. Therefore, there is still a non-zero probability that the particle appears on the other side of the barrier. This process is called quantum tunneling [1]. The transmission coefficient is used to describe the probability of tunneling. It depends on the energy of the particle and the shape, height, and width of the potential barrier. For a simple rectangular barrier, the transmission coefficient can be calculated by solving the one-dimensional time-independent Schrödinger equation with boundary conditions. However, realistic potential barriers are usually more complicated and may have triangular, parabolic, exponential, or Gaussian shapes. Therefore, different analytical and approximate methods are needed [2].

Quantum tunneling is commonly introduced through the one-dimensional rectangular barrier. Griffiths and Schroeter show that a particle can still have a finite transmission probability when its energy is lower than the barrier height [3], while Merzbacher defines the transmission coefficient as the ratio between transmitted and incident waves [4]. For more realistic barriers, exact solutions are often difficult to obtain, so approximation methods such as Wentzel–Kramers–Brillouin (WKB) are widely used. Razavy [5], Wen et al. [6], and others discuss tunneling and WKB-type methods in different quantum systems. Tunneling theory has also been extended to double-barrier and multiple-barrier structures, where resonant tunneling can strongly enhance transmission under suitable phase conditions [7]. Recent studies further connect resonant tunneling with semiconductor devices and STM applications [8,9,10].

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This paper focuses on the calculation and application of quantum tunneling transmission coefficients. Section 2 first discusses the single rectangular barrier and then extends the discussion to triangular, parabolic, exponential and Gaussian barriers. The WKB approximation is introduced as a useful method for smooth barriers. After that, double-barrier and multiple-barrier systems are discussed, especially resonant tunneling caused by interference. Finally, Section 3 introduces applications such as resonant tunneling diodes and scanning tunneling microscopy.

2. Quantum tunneling transmission coefficient

2.1. Single rectangular barrier

For a particle in one-dimension single potential barrier, one can directly solve the Schrödinger equation with boundary condition. Particle satisfy Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

in which the potential

$$V(x) = \begin{cases} o \\ V_o \end{cases} \tag{2}$$

Through the general solution, one can find out the wave function in transmitted region, and it is exponentially decay [3]

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, x < 0 \\ Ce^{\kappa x} + De^{-\kappa x}, 0 < x < a \\ Fe^{ikx}, x > a \end{cases} \tag{3}$$

The transmission coefficient is $T = \frac{j_{\text{trans}}}{j_{\text{inc}}}$, which is the ratio between transmitted wave and incident wave. And as wave function is normalized, it can be written as ratio of amplitude, so it is equal to

$$T = \frac{|F|^2}{|A|^2} \tag{4}$$

where A is the incident amplitude and F is the transmitted amplitude [4].

For 1D tunneling problem, in the region before barrier, the wave function can be written as superposition of an incident wave and reflected wave. For $E < V_0$, the transmitted wave is no longer propagation wave but exponentially decrease. This is the solution for most classical rectangular potential barrier. If the paper considers more general conditions, like triangular potential barrier, or even promote to the natural world, with potential barrier in any condition, such as: parabola shape, exponential shape or Gaussian shape [5].

2.2. Single potential barrier with more complex shape

For a triangular potential barrier, it decreases linearly with position and can be written as

$$V(x) = \begin{cases} V_0 - Fx, 0 < x < d \\ 0, x > d \end{cases} \tag{5}$$

where V_θ is the barrier height and F denotes the slope of the potential. And then substitute into Schrödinger equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0 + Fx)\psi = 0 \tag{6}$$

To convert the equation into standard Airy differential equation, whose analytical solution is known, this paper would introduce a transformed variable $\xi = \left(\frac{2mF}{\hbar^2}\right)^{1/3}\left(x - \frac{V_0 - E}{F}\right)$, and then the equation becomes

$$\frac{d^2\psi}{d\xi^2} - \xi\psi = 0 \tag{7}$$

Therefore, the general equation is

$$\psi(x) = A\,Ai(\xi) + B\,Bi(\xi) \tag{8}$$

where (Ai) and (Bi) denote the Airy functions. And the transmission coefficient is still $T = \frac{|F|^2}{|A|^2}$.

For a parabola potential barrier, $V(x) = V_\sigma - \frac{1}{2}m\omega^2x^2$, where V_σ is the maximum potential. Substitute it into time-independent Schrödinger Equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V_0 + \frac{1}{2}m\omega^2x^2\right)\psi = 0 \tag{9}$$

To solve this equation, the paper introduces the transformed variable z. This would turn the equation into a standard parabolic cylinder equation, whose analytical solution is given by parabolic cylinder function. Then the author can find the general solution

$$\psi(x) = AD_\nu(z) + BD_\nu(-z) \tag{10}$$

with

$$z = \sqrt{\frac{2m\omega}{\hbar}}e^{-i\pi/4}x, \nu = -\frac{1}{2} + i\frac{E - V_0}{\hbar\omega} \tag{11}$$

For an exponential potential barrier in which a potential that exponentially depends on position, it could be written as:

$$V(x) = V_0e^{-\frac{x}{a}} \tag{12}$$

where V_θ is the barrier height and a represents the barrier decay length. And then substitute it into time-independent Schrödinger Equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V_0e^{-x/a}\right)\psi = 0 \tag{13}$$

To find the general solution, again, the paper uses transformer variable. This time, define: $u = \frac{2a}{\hbar}\sqrt{2mV_0}e^{-x/(2a)}$. Then the author can turn the Schrödinger equation into a standard Bessel differential equation. Therefore, the general solution can be expressed as

$$\psi(x) = AJ_{i\mu}(u) + BJ_{-i\mu}(u) \tag{14}$$

where J represent Bessel function of the first kind, and $\mu = \frac{2a}{\hbar}\sqrt{2mE}$ is the dimensionless energy parameter. The exponential potential barrier is closer to realistic than the rectangular and triangular barriers because it has a smoother transition of energy.

For a Gaussian potential barrier, the barrier is slightly different. Unlike the previous barrier, Gaussian barrier does not have general equation because it does not transform into standard differential equation. Therefore, method of approximation such as WKB are adopted. The potential can be written as

$$V(x) = V_0 e^{-\frac{x^2}{a^2}} \tag{15}$$

where V_θ is the height and a is width of barrier. Substituting into time-independent Schrödinger Equation gives

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V_0 e^{-x^2/a^2}\right)\psi = 0 \tag{16}$$

This cannot be transformed into a standard differential equation with a simple analytical solution. Therefore, the WKB approximation can be applied. The wave function inside classical forbidden region is [5]

$$\psi(x) \approx \frac{C}{\sqrt{\kappa(x)}}\exp\left(-\int^x \kappa\,(x')dx'\right) + \frac{D}{\sqrt{\kappa(x)}}\exp\left(+\int^x \kappa\,(x')dx'\right) \tag{17}$$

where $\kappa(x) = \frac{\sqrt{2m[V(x)-E]}}{\hbar}$. By substituting Gaussian potential, it is calculated that the transmission probability is

$$T \approx \exp\left[-2\int_{x_1}^{x_2} \kappa\,(x), dx\right] \tag{18}$$

and the turning point satisfies $V_0 e^{-x^2/a^2} = E$, thus $x_{1,2} = \pm a\sqrt{\ln\left(\frac{V_0}{E}\right)}$. The author could notice that: even though for most idealized potential barriers, the analytic solution does exist. Realistic tunneling problems usually involve smoothly varying potentials, and the differential equation cannot be transformed to a standard equation. Therefore, exact analytic solutions are difficult or unavailable. In this case, the WKB approximation is an efficient way to estimate the transmission probability of this kind of wave function [5].

For the one-dimensional time-independent Schrödinger Equation,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi = 0 \tag{19}$$

the wave number is defined as $k(x) = \frac{\sqrt{2m(E-V(x))}}{\hbar}$ inside the forbidden region where $E < V(x)$. Defining $\kappa(x) = \frac{\sqrt{2m(V(x)-E)}}{\hbar}$, the WKB approximation gives

$$\psi(x) \approx \frac{C}{\sqrt{\kappa(x)}}\exp\left(-\int^x \kappa\,(x')dx'\right) + \frac{D}{\sqrt{\kappa(x)}}\exp\left(+\int^x \kappa\,(x')dx'\right) \tag{20}$$

Thus, transmission probability becomes

$$T \approx \exp\left[-2\int_{x_1}^{x_2} \kappa\,(x)dx\right] \tag{21}$$

where x_1 and x_2 are classical turning points determined by $V(x) = E$.

Thus, the paper could find that the WKB method to find an approximate solution is more accurate for smoother potential barriers. The physical meaning of the WKB exponent is: the accumulated decay of the wave function inside the forbidden region. As the forbidden region is higher or larger, the region for integer is larger, so that the transmission coefficient is smaller, and decreases exponentially [7].

Also, with the WKB method, this paper can simplify the analytic solution for the triangular and other potential barriers the author mentioned in the previous part. For example, in a triangular potential barrier, the author can solve the Schrödinger Equation and find the analytic solution depends on the Airy function, which means it is complex if the author use it for calculating the T value. But if the author uses WKB approximation for tunneling probability, it can simplify the solution

$$T \approx \exp\left[-\frac{2}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V_0 - Fx - E)}\;dx\right] \tag{22}$$

Different potential barriers' shapes represent different physics modules of the tunneling system. The rectangular system is the simplest idealize module. Because the potential in the region is constant everywhere, and the Schrödinger equation can be solved directly with boundary conditions.

However, the sharp edge of potential is different from most real situations. The triangular barrier improved this limit, because the potential varies linearly with the position, and this is a good imitation for electric field exert electric potential on a particle. For exponential barriers and Gaussian barriers, they are smooth, and the trend also satisfies realistic interactions. Potential usually changes continuously but not suddenly, Also, Gaussian barrier usually useful for localized barrier, because it is concentrated in a finite spatial and decays rapidly away from the center. For $V(x) = V_0 e^{-x^2/a^2}$, the maximum potential is V_0 and potential quickly close to 0 as $|x|$ increases. But Gaussian barrier usually doesn't lead to a simple transmitted coefficient [11].

So far, the tunneling process has been discussed for a single potential barrier. However, in realistic quantum world, there would usually be multiple potential barriers, which would lead to more complex behavior.

2.3. Double and multiple potential barriers

Now, the paper considers a double-barrier

$$V(x) = \begin{cases} V_0, 0 < x < a \\ 0, a < x < a + b \\ V_0, a + b < x < 2a + b \end{cases} \tag{23}$$

where a is the barrier width and b is the separation between the two barriers.

Since there are two barriers, there would be transmission and reflection in the space of them, so the paper needs to consider the interference. And the total transmission probability for two identical barriers becomes

$$T = \frac{1}{1 + \frac{4R}{(1-R)^2}\sin^2(kb)} \tag{24}$$

where $k = \frac{\sqrt{2mE}}{\hbar}$ and R is the reflection coefficient of each barrier. When the phase condition $kb = n\pi$ is satisfied, constructive interference occurs, and transmission coefficient is close to 1. This phenomenon is known as resonant tunneling.

The expression of T shows that transmission probability not only depends on width and height of barrier, but also on phase accumulated between them. The numerical simulation shows that after particle incident, wave is reflected and transmitted at the first barrier. The reflected wave interference with the incident wave, and the transmitted component enter the gap between the two barriers. At start, the amplitude of the wave is high and relatively concentrated in space. As time goes by, the wave separates in space and amplitude drop, trend to become uniform [7]. The double barrier system therefore demonstrated that there is an important difference between the classical and quantum worlds. In classical conditions, adding a barrier would simply make transmission more difficult. However, in quantum mechanics, a new barrier can provide resonance and therefore even enhance transmitted particle energy. That is why multi-barrier structure are useful in semi-conductor physics.

A very important feature of a double-barrier system is resonance tunneling. In a single barrier, wider and higher potential barrier only decreases the transmission coefficient. But within two barriers, the region inside them acts like a potential well. The wave that is transmitted through the first barrier would travel in the well and be partially reflected by the second barrier, therefore moving back and forth inside the region. As the phase accumulates in the region and satisfies the resonance condition, constructive interference would occur. Therefore, the transmission coefficient could be large, even close to 1 [2]. Physically speaking, the particle is temporarily trapped in the quasi-bound state between the barriers, and then escape through the barriers. The wave leaks through both sides of the barrier. On the incident side, the reflected wave would undergo destructive interference because of resonance. On the transmitted side, the transmitted wave undergoes constructive interference. So, the effect of a double barrier is: adding another barrier does not always reduce transmission; it can enhance transmission in certain energy conditions [8]. The double-barrier model can be further extended to a system containing N potential barriers. In this structure, the wave function is transmitted and reflected in each space that is divided by potential barriers. So, the transmission coefficient is determined by interference of a large number of regions in propagation path. For a region with constant potential, the wave function can be written as

$$\psi_j(x) = A_j e^{ik_j x} + B_j e^{-ik_j x} \tag{25}$$

where A_j and B_j represent right-moving and left-moving amplitudes respectively. As the number of barriers increases, directly evaluating the equation for each boundary becomes complex. So, the transform matrix method is commonly used: $M_{\text{total}}(A_R\ B_R)$. The total transfer matrix is obtained by all matrices barriers and the free propagation region for wave

$$M_1 P_1 M_2 P_2 \cdots M_N \tag{26}$$

For N identical periodically arranged barriers, it can be written as $(M_{cell})^N$, where M_{cell} represents one barrier together with one separation region [6].

The physical behavior of a multi-barrier system is more complex than a single barrier. Each region between two barriers can be estimated as a potential well. The wave function can be temporarily confined within these wells, producing quasi-bound states. Since the wells are coupled through finite barriers, the quasi-bound energy levels of individual wells interact and split into several closely spaced resonant levels.

3. Application

The calculation of tunneling transmission coefficient is important in many quantum devices. One typical application is the resonant tunneling diode, which is based on a double-barrier or multiple-barrier semiconductor structure. In this device, electrons can pass through the barriers efficiently only when their energy matches the resonant energy level inside the quantum well. Therefore, the current does not simply increase with voltage, but can show a peak when resonance occurs. This property makes resonant tunneling useful for high-speed electronic devices and energy-selective electron transport.

Another important application is the scanning tunneling microscope, see Fig. 1. In STM, electrons tunnel between a sharp metallic tip and the surface of a sample. Since the tunneling probability depends exponentially on the distance between the tip and the sample, even a very small change in surface height can cause a large change in tunneling current. Therefore, by measuring this current, STM can obtain surface information at the atomic scale. These examples show that tunneling is not only a theoretical phenomenon, but also a useful mechanism for controlling and detecting microscopic systems [1]. More specifically, the tunneling current in STM depends approximately on the tip-sample separation as $I \propto e^{-2\kappa d}$, where d is the distance between the tip and the sample, and κ is related to the height of potential barrier. This means that a very small change in distance would have a large influence on current within exponential correlation. Therefore, a slight change in height on the surface can be detected.

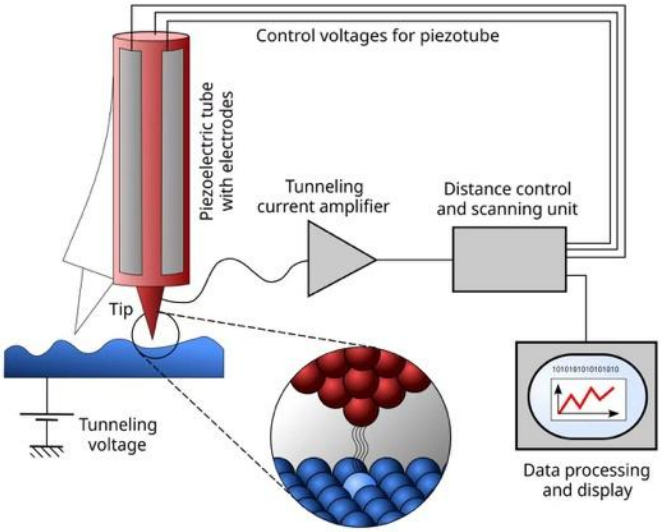

Fig. 1 Schematic diagram of a scanning tunneling microscope [10].

In addition, the STM current can not only detect the geometrical height of material, but also the electronic structure of material. According to the tunneling theory of STM, the tunneling current is related to the local density of electronic states near the Fermi level. Therefore, the image obtained by STM should not be simply understood as a pure “surface height map”. Instead, it reflects both the topographic structure and the electronic properties of the surface. This is important because different atoms, defects, or adsorbed molecules on the surface may produce different tunneling currents even when their physical height difference is very small [1].

The strong distance dependence of tunneling current is the key reason why STM can reach atomic-scale resolution. For example, if the tip-sample separation changes only by a small fraction of a nanometer, the tunneling current can change significantly [10]. This exponential sensitivity allows STM to detect individual atoms, surface defects, and local electronic features. Therefore, STM provides a direct experimental application of the transmission coefficient in quantum tunneling: a small change in barrier width leads to an exponential change in transmission probability and hence tunneling current [9]. This connects the theoretical expression of tunneling probability with a real measurement technique.

4. Conclusion

This paper has discussed the calculation of quantum tunneling transmission coefficients and their applications. Quantum tunneling shows that a particle can pass through a potential barrier even when its energy is lower than the barrier height, which is impossible in classical mechanics. The transmission coefficient is an important quantity because it describes the probability of this tunneling process. This paper first introduced the single rectangular barrier, where the Schrödinger equation can be solved directly using boundary conditions. Then, more complex barriers, including triangular, parabolic, exponential and Gaussian barriers, were discussed. For some barriers, analytical solutions can be expressed using special functions, while for smooth and realistic barriers, the WKB approximation provides an effective method to estimate the transmission probability.

The discussion was then extended to double-barrier and multiple-barrier systems. These systems show that tunneling is not only affected by barrier height and width, but also by interference and phase accumulation. Under resonance conditions, the transmission coefficient can become very large, even close to one. This is important for understanding resonant tunneling diodes and semiconductor devices. Scanning tunneling microscopy also shows the practical value of tunneling, because its current depends exponentially on the distance between the tip and sample. In future studies, more realistic potentials, numerical simulations, and higher-dimensional tunneling systems could be explored. These directions would further connect tunneling theory with modern quantum devices and experimental techniques.

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