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The quantum tunnelling effect in double barrier structure

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Abstract. The purpose of this paper is to study the quantum tunnelling effect of double barriers. At the beginning, the research background and application of quantum tunnelling effect are described, and then the research purpose is explained. Although the real double barriers are very complex, most of them are composed of double barrier, double triangle barrier and double parabola barrier. The author mainly studies the barrier of double parabola. The reason is that the quantum tunnelling effect proposed by Hund will greatly adjust the internal structure of triangular conical molecules, which has great research significance. In triangular conical molecules, the change of potential energy of a single atom with its position may be very complicated, but the part that can occur with the consequential effect is similar to the potential barrier of a double parabola. In this paper, the wave function, projection and reflection coefficients of the biparabolic barrier tunnelling effect are analysed to determine whether it has a great adjustment effect on triangular conical molecules.

Keywords: quantum tunnelling effect, double parabola barrier, transmission coefficient.

1. Introduction

In the early development of quantum mechanics, de Broglie also proposed the matter wave hypothesis based on the wave-particle duality of light. That is, the micro particles (electrons, protons, neutrons) can also be treated as waves. Because of the volatility of the microscopic particles, when its energy is less than the height of the barrier, they can penetrate the barrier and the particle exhibits volatility which behaves similarly to the wave [1]. This phenomenon is called tunnelling effect. Tunnel effect in quantum mechanics is an important physical phenomenon and has a wide range of applications. The tunnelling effect is entirely due to the fluctuating nature of microscopic particles. Quantum tunnelling effect can very well explain the radioactive element α decay, thermonuclear fusion, metal electron cold emission, semiconductor p-n junction, tunnel diode, etc [2].

In recent years, the research on mesoscale tunnelling effect and photon tunnelling effect has become the focus. For example, the application development in superconducting technology and nanotechnology is more obvious. The tunnelling properties of magnetic tunnelling materials and their spin-related electrons in double barrier tunnelling effect have aroused extensive research interest among experimental and theoretical scholars. At the same time, the tunnelling effect also has quite important application value in the field of microscopic technology, which leads to the birth of scanning tunnel electron microscope [3]. These research work not only rapidly promoted the formation and rapid development of magneto-electronics and spintronics, the emerging disciplines of condensed matter physics in the past decade, but also greatly promoted the development and application of magnetoresistive materials and new spintronic devices in the information industry [4]. In 2011, Wang *et al* studied the transmission probability of a single layer of graphene with a square barrier by means of transmission matrix, and revealed the relationship between the transmission probability and the fermi energy of the incident particle, the width and height of the barrier. These results provide a theoretical reference for the design of graphene-based nanodevices [5]. In 2021, Luo compared the transmittance of the electrons in the tunnelling unilateral barrier with the external magnetic field, so as to obtain the influence of the magnetic field on the transmittance of the electron tunnelling unilateral barrier [6]. In the same year, Li and Dong proposed to simulate the dipolar potential energy of the superGaussian light with large blue detuning and the dynamic dynamical potential energy of the superGaussian light and electrons. By comparing the numerical solution of the super Gaussian barrier to the incident plane wave scattering and the analytical solution to the matter wave scattering, it is found that the problem of the scattering of the matter wave can be effectively simulated when the super Gaussian optical field order is greater than 20 [7].

In recent years, people have paid much attention to the study of the tunnel effect of double barrier in molecular and semiconductor quantum. Ammonia molecule is a classical triangular cone model. Hund proposed as early as 1927 that quantum tunnel effect would greatly adjust the internal structure of triangular cone molecules. The stability of molecular structure can be controlled to varying degrees by selecting the appropriate external conditions. The fundamental goal of this paper is to study the wave functions, transmission coefficient and reflection coefficient of different double barriers. The two sides potential barrier, double parabola potential barrier, double triangle potential barrier as the main research object, the other is too complicated, these three are more representative, can be derived from these three potential barriers of other models. In terms of research significance, this topic wants to study the adjustment effect of quantum tunnelling effect in the double barrier on the internal structure of triangular conical molecules (in triangular conical molecules, there are one heavy atom and three light atoms (or three heavy atoms and one light atom). The image that analyses the change of potential energy composed of three light atoms with position is a double parabola diagram. Therefore, this paper takes the double parabolic barrier as the main research object, and analyses whether the quantum tunnelling effect can occur in heavy atoms.

2. Theory and method

2.1. Research theory

In quantum mechanics, the motion state of the microscopic system is described by a wave function, and the differential equation reflecting the motion law of the microscopic particles is the first order differential equation with diameter (r, t) for time. That is,

$$ih\frac{\partial\Phi}{\partial t} = -\frac{\partial\Phi}{\partial t}\nabla^2\Phi + U(r)\Phi. \tag{1}$$

It is called the time-dependent Schrodinger equation, where $U(r)$ is a function of the force field. If the force field acting on the particle does not change with time, that is, the force field is represented by the potential energy $U(r)$, and it does not contain time, then the equation satisfied by the stationary wave function is

$$-\frac{\mathrm{h}^2}{2\mu}\nabla^2\Phi + \mathrm{U(r)}\Phi = \mathrm{E}\Phi. \tag{2}$$

It is called the Schrodinger equation of stationary state, where E represents the energy of a microscopic particle in the state described by this wave function, and its energy has a definite value.

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2.2. Research methods

The following is an introduction to the Wenzel-Kramers-Brillouin (WKB) law, which was proposed in 1926. In elementary quantum mechanics, this paper describes the evolution of the mechanical system using the Schrodinger equation as the fundamental equation.

Regarding the propagator in the Feynman path integral theory, it is obtaining a formal wave function that depends on the action amount of each path itself, i.e.,

$$\Phi = \mathrm{e}^{\mathrm{i}S/\mathrm{h}}. \tag{3}$$

In fact, the Schrodinger equation in terms of partial differential equation can also be given such a formal solution. Take this wave function into the Schrodinger equation and one can get that

$$\frac{1}{2\mathrm{m}}\left(\frac{\mathrm{dS}}{\mathrm{dx}}\right)^2 - \frac{\mathrm{ih}}{2\mathrm{m}}\frac{\mathrm{d}^2\mathrm{S}}{\mathrm{dx}^2} = E - V. \tag{4}$$

Then it has known that this action quantity depends on the specific propagation path, and the final physical result should be the wave function weighted average of all paths, which is the connotation of Feynman path integral theory [8]. Thus, one can, in turn, expand this action in accordance of the reduced Planck constant as

$$\mathrm{S} = \mathrm{S}_0 + (-\mathrm{ih})\mathrm{S}_1 + (-\mathrm{ih})^2\mathrm{S}_2 + \cdots + (-\mathrm{ih})^{\mathrm{n}}\mathrm{S}_{\mathrm{n}} + \cdots. \tag{5}$$

When $\hbar$ =0, it is found that $\mathrm{S} = \mathrm{S}_0$ in the classical case, and it satisfies the corresponding principle. In this sense, the Eq. (2) will change to $\frac{1}{2\mathrm{m}}(\frac{\mathrm{dS}}{\mathrm{dx}})^2 = E - V$, or equivalently,

$$\frac{dS}{dx} = \sqrt{2m(E-V)} \tag{6}$$

The basic equations of the comparative Hamilton-Jacobi theory ($\nabla\mathrm{S} = \mathrm{p}$) also agree. By using WKB approximation, the above method can be used to decompose wave function, and then expand the action to any order to calculate and solve the Schrodinger equation technology. Of course, this idea can be extended to a wider place, not only to the Schrodinger equation, or even to quantum mechanics.

3. Applications

The following is a small segment of the hypothetical barrier of a single atom in a triangular conical molecule. The wave function of the particle in the double parabola potential field is calculated below. The six regions separated by vertical lines in the Figure 1 are regions A, B, C, D, E, F.

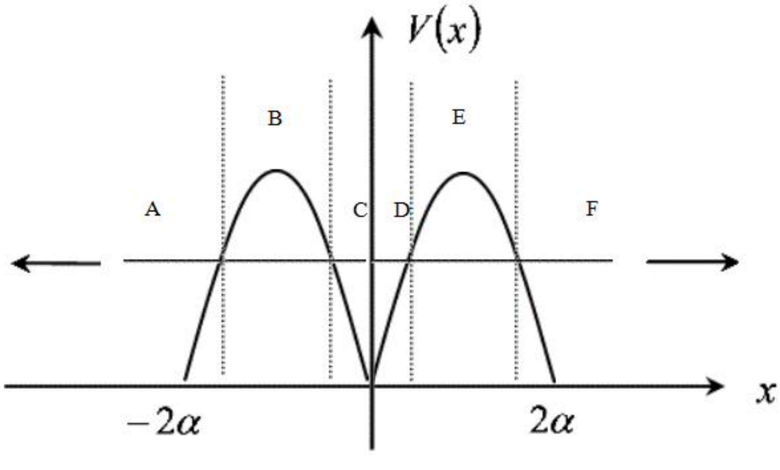

Figure 1. Sketch of the double parabola barrier.

For this double parabola barrier, the potential is given by

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$$V(x)=\begin{cases} -\dfrac{\mathrm{V_0}}{\mathrm{a^2}}(\mathrm{x}+\mathrm{a})^2+\mathrm{V_0}, -2a\le x\le 0 \\ -\dfrac{\mathrm{V_0}}{\mathrm{a^2}}(\mathrm{x}-\mathrm{a})^2+\mathrm{V_0}, \qquad 0\le x\le 2a \end{cases} \tag{7}$$

The Schrodinger equation for each region can be obtained according to Eq. (2), and the wave function satisfy the relation

$$\begin{cases} \dfrac{\mathrm{d^2\Phi}}{\mathrm{dx^2}}+\dfrac{2\mu}{\mathrm{h^2}}E\Phi=0 \qquad x\le -2a \\ \dfrac{\mathrm{d^2\Phi}}{\mathrm{dx^2}}+\dfrac{2\mu}{\mathrm{h^2}}E\Phi=0 \qquad 2a\le x \end{cases} \tag{8}$$

and

$$\begin{cases} \dfrac{\mathrm{d^2\Phi}}{\mathrm{dx^2}}+m(x+a)^2+n\Phi=0 \quad -2a< x\le 0 \\ \dfrac{\mathrm{d^2\Phi}}{\mathrm{dx^2}}+m(x-a)^2+n\Phi=0 \qquad 0< x\le 2a \end{cases}. \tag{9}$$

Here, the constants are $\frac{2\mu U_0}{h^2a^2}=\mathrm{m}$ and $\frac{2\mu}{h^2}(\mathrm{E}-\mathrm{U_0})=\mathrm{n}$. In addition, $\mathrm{k_1}=\sqrt{2\mu\big(\mathrm{E}-\mathrm{V_1(x)}\big)}/\mathrm{h}$ and $\mathrm{k_2}=\sqrt{2\mu\big(\mathrm{E}-\mathrm{V_2(x)}\big)}/\mathrm{h}$ are also fixed.

If the particle is incident from the left with a certain energy and hits the barrier and if the wave function changes slowly and the energy of the incident particle is not too close to the peak of the wave function, WKB approximation can be used to deal with the phenomenon of particles penetrating the barrier [9]. According to classical mechanics, the particle is knocked back at $x=a$, but according to quantum mechanics, the particle has a certain chance of penetrating the barrier given the volatility of the particle. Of course, in many cases, the odds are small. Now the author aims to calculate the magnitude of the penetration probability T of the double barrier.

In zone A away from a, the wave function is

$$\Phi_1=A\mathrm{k_1}^{-\frac{1}{2}}\mathrm{e}^{i(\int_x^a \mathrm{k_1dx}-\frac{\pi}{4})}+A'\mathrm{k_1}^{-\frac{1}{2}}\mathrm{e}^{-i(\int_x^a \mathrm{k_1dx}-\frac{\pi}{4})}. \tag{10}$$

In zone C away from b, the wave function is

$$\Phi_3=B\mathrm{k_1}^{-\frac{1}{2}}\mathrm{e}^{i(\int_b^x \mathrm{k_1dx}-\frac{\pi}{4})}+B'\mathrm{k_1}^{-\frac{1}{2}}\mathrm{e}^{-i(\int_b^x \mathrm{k_1dx}-\frac{\pi}{4})}. \tag{11}$$

As the WKB theory applies, the approximate solution shall be

$$\Phi_2=\frac{1}{2}B\mathrm{K_1}^{-\frac{1}{2}}\tau_1^{-1}\mathrm{e}^{\int_a^x \mathrm{K_1dx}}-iB\mathrm{K_1}^{-\frac{1}{2}}\mathrm{e}^{\int_a^x \mathrm{K_1dx}}+\frac{1}{2}B'\mathrm{K_1}^{-\frac{1}{2}}\tau_1^{-1}\mathrm{e}^{-\int_a^x \mathrm{K_1dx}}+iB'\mathrm{K_1}^{-\frac{1}{2}}\mathrm{e}^{-\int_a^x \mathrm{K_1dx}} \tag{12}$$

where $\tau_1=\mathrm{e}^{\int_a^b \mathrm{K_1dx}}$. The WKB in region A is applied by using the connection formula at A. Similarly, the wavefunction in the D region is

$$\Phi_4=C\mathrm{k_1}^{-\frac{1}{2}}\mathrm{e}^{i(\int_x^c \mathrm{k_1dx}-\frac{\pi}{4})}+C'\mathrm{k_1}^{-\frac{1}{2}}\mathrm{e}^{-i(\int_x^c \mathrm{k_1dx}-\frac{\pi}{4})} \tag{13}$$

In the F region away from d, with only projected waves and no reflected waves. The W.K.B approximately solves as

$$\Phi_6=D\mathrm{k_2}^{-\frac{1}{2}}\mathrm{e}^{i(\int_d^x \mathrm{k_2dx}-\frac{\pi}{4})}=D\mathrm{k_2}^{-\frac{1}{2}}\cos(\int_a^x \mathrm{k_2dx}-\frac{\pi}{4})+iD\mathrm{k_2}^{-\frac{1}{2}}\sin(\int_d^x \mathrm{k_2dx}-\frac{\pi}{4}) \tag{14}$$

Then the W.K.B is applied in region E. The approximate solution shall be

$$\Phi_5 = \frac{1}{2} D K_2^{-\frac{1}{2}} \tau_2^{-1} e^{\int_c^x K_2 dx} - iD K_2^{-\frac{1}{2}} \tau_2 e^{\int_c^x K_2 dx} \tag{15}$$

Where $\tau_2 = e^{\int_c^d K_2 dx}$. The equations are obtained and solved by using the continuity of the wave function Φ_3, Φ_4 and its derivative at x=0. Namely,

$$B = -\frac{iD}{2}\left(\frac{1}{2\tau_2} - 2\tau_2\right) e^{i\alpha}, B' = -\frac{iD}{2}\left(\frac{1}{2\tau_2} + 2\tau_2\right) e^{-i\alpha}. \tag{16}$$

where $\alpha = i\left(\int_0^c k_2 dx - \int_b^0 k_1 dx\right)$.

With these wave functions in mind, one can compute the transmission coefficient of the particle in the bielectric parabolic potential field below. It is found that $T = \frac{D}{\frac{1}{2}B\left(\frac{1}{2\tau_1} - 2\tau_1\right) + B'\left(\frac{1}{2\tau_1} + 2\tau_1\right)}$ and thus

$$T = \frac{8}{\frac{1}{16}\tau_1^{-2}\tau_2^{-2} + 4\tau_1^2\tau_2^2 + 4 + \left(\frac{1}{4\tau_1^2} - 4\tau_1^2\right)\left(\frac{1}{4\tau_2^2} - 4\tau_2^2\right)\cos 2\alpha + \frac{\tau_1^2}{\tau_2^2} + \frac{\tau_2^2}{\tau_1^2}}. \tag{17}$$

The reflection coefficient $R = \frac{\left[B\left(\frac{1}{2\tau_1} + 2\tau_1\right) + B'\left(\frac{1}{2\tau_1} - 2\tau_1\right)\right]^2}{\left[B\left(\frac{1}{2\tau_1} - 2\tau_1\right) + B'\left(\frac{1}{2\tau_1} + 2\tau_1\right)\right]^2}$, and can be simplified as

$$R = \frac{\frac{1}{16}\tau_1^{-2}\tau_2^{-2} + 4\tau_1^2\tau_2^2 - 4 + \left(\frac{1}{4\tau_1^2} - 4\tau_1^2\right)\left(\frac{1}{4\tau_2^2} - 4\tau_2^2\right)\cos 2\alpha + \frac{\tau_1^2}{\tau_2^2} + \frac{\tau_2^2}{\tau_1^2}}{\frac{1}{16}\tau_1^{-2}\tau_2^{-2} + 4\tau_1^2\tau_2^2 + 4 + \left(\frac{1}{4\tau_1^2} - 4\tau_1^2\right)\left(\frac{1}{4\tau_2^2} - 4\tau_2^2\right)\cos 2\alpha + \frac{\tau_1^2}{\tau_2^2} + \frac{\tau_2^2}{\tau_1^2}}. \tag{18}$$

Thus, the relation that $R + T = 1$ is satisfied. This formula represents the sum of the particle transmission probability and the reflected probability equal to 1, and is a reasonable result that should be obtained. For the one-dimensional barrier scattering problem, the sum of the reflection coefficient and the transmission coefficient is equal to one. Specifically, when $V_2(x) = 0$, it is found that [10]

$$T = \frac{D}{\frac{1}{2}B\left(\frac{1}{2\tau_1} - 2\tau_1\right)}, R = \frac{B\left(\frac{1}{2\tau_1} + 2\tau_1\right)^2}{B\left(\frac{1}{2\tau_1} - 2\tau_1\right)^2}. \tag{19}$$

It can be seen that the scattering of microscopic particles by a tight set of double parabolic barriers cannot be regarded as a simple combination of independent scattering by each parabolic barrier, and their reflections at their respective left and right interfaces are coherent.

4. Conclusion

The above calculation results are mainly theoretical calculation process, the software can be more intuitive results, such as the above four images, and the analysis of transmission calculation needs to solve a series of one-dimensional Schrodinger equations, the core of which is to solve the linear equations. The linear equation system is expressed as a matrix equation. With the help of MATLAB, the solving process of transmission coefficient can be greatly simplified. According to the above calculation results, the heavy atoms in the triangular conical molecule can indeed have quantum tunnelling effect. For heavy atoms, its potential energy is provided by the plane of three light atoms, heavy atoms in classical mechanics will force in three light atoms outside the centre of the plane, and in quantum mechanics may because quantum tunnel through the high potential energy to another position, but also because the force to the original equilibrium position, so there is a slight simple harmonic movement.

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According to the above results can be obtained again, the conditions for the quantum tunnelling effect can be roughly judged. At the same time, the quantitative analysis of the double parabolic barrier is also conducted, various problems such as the expression of the tunnelling projection reflection of the double parabolic barrier are solved by WKB method.

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