

Graphical Approach to Eigenvalue Problems of The One-Dimensional Finite Deep Square Potential Well

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Abstract. The one-dimensional finite-depth potential well problem under certain boundary conditions discussed in this paper is mainly the eigenvalue problem in quantum mechanics. The basis of this article is the solution of Schrodinger equation and the treatment of transcendental equation. In many quantum mechanics textbooks, the one-dimensional infinite potential well problem is regarded as the foundation of quantum mechanics because it is easy to handle and understand. On this basis, this paper discusses the more challenging finite-depth potential well situation. In this paper, the transcendental equation is obtained by analogy between the wave function with time and the continuity of the boundary conditions. In order to solve the problem that transcendental equation is difficult to solve in this process, this paper adopts the method of solving numerical solutions by using images, which includes two different cases of odd and even functions. This paper reveals the possibility of particles appearing outside the well in this problem, and on this basis, some discussions and analysis are made on the one-dimensional asymmetric finite-depth potential well problem.

Keywords: Bound state; Parity; Wave function; Schrodinger equation; Transcendental equation.

1. Introduction

The potential well model, an idealized physical system in the large field of quantum mechanics, offers a special viewpoint to investigate the behavior law of particles in limited space. Among them, the one-dimensional finite depth square potential well has drawn the attention of numerous researchers due to its straightforward mathematical structure and rich physical implications [1,2]. It not only aids in the theoretical development of researchers' comprehension of the fundamentals of quantum mechanics [3], but it also offers theoretical justification for the exact experimental manipulation of microscopic particles.

A straightforward physical situation with a constant potential energy barrier inside a certain interval is well described by a one-dimensional finite deep square potential. The parameters of the potential well have a significant impact on the energy and wave function of a particle that is contained within it [4]. The particle's energy level structure, the wave function's spatial distribution, and the particle's dynamic behavior in the potential well are all indicative of this influence. Consequently, it is crucial to investigate particle behavior in one-dimensional finite deep square potential wells in order to solve the puzzle of quantum mechanics and further the advancement of associated experimental methods [5].

Through theoretical analysis and numerical system simulation, the goal of this research is to examine the energy and wave function properties of a particle in a one-dimensional finite deep square potential well in a bound state. This work analyzes the impact of potential well parameters on particle state and deduces in detail the expression of energy level and wave function of particle in potential well. The author intends to gain a deeper understanding of the behavior law of particles in limited space as well as new insights and approaches for the advancement of experimental physics and quantum mechanic's research.

2. Symmetric square potential well

2.1. Model and Methods

First, the author writes the potential energy equation for a one-dimensional finite deep potential well, which is

$$V(x) = \begin{cases} -V_0, & -a \leq x \leq a \\ 0, & |x| \geq a \end{cases} \quad (1)$$

Where V_0 is a positive constant and a is the width of the well [6]. It is shown in Fig. 1.

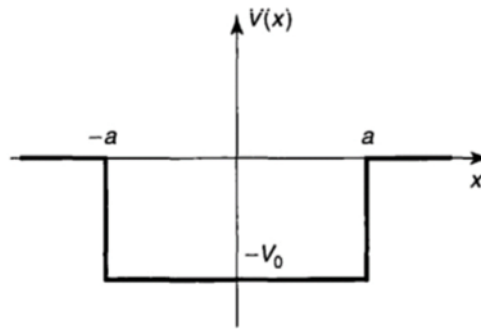


Fig. 1 The finite square well

Second, the continuity of the function is used to write the boundary conditions of a one-dimensional finite deep potential well. Knowing that the wave function satisfies continuity, it is only necessary to consider whether its derivative satisfies continuity. The potential energy is not infinite at all positions and is also finite at the two jump points, so its derivative is also continuous. For the boundary conditions, it is found that ψ and ψ' are continuous. Considering the case of bound state, ψ satisfies the following equation: $\psi(\pm\infty) = 0$. Then the Schrödinger equation for different regions and their corresponding general solutions can be derived [7].

In the region of $|x| > a$ the potential is 0, at which point the Schrödinger equation can be illustrated as $-\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} = E\psi$. Define $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$, then it is found that

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi \quad (2)$$

This equation is much like the wave equation, but it does not include time. The general solution of this equation is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}. \quad (3)$$

Under the condition that $\psi(\pm\infty) = 0$ is satisfied, the general solution can be written as

$$\psi(x) = \begin{cases} C_1 e^{-\kappa x}, & x > a \\ C_2 e^{\kappa x}, & x < -a \end{cases} \quad (4)$$

In the region of $|x| < a$ the potential is $-V_0$, at which point the Schrödinger equation can be illustrated as $-\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} - V_0\psi = E\psi$. Define $l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar}$, then

$$\frac{d^2\psi}{dx^2} = -l^2\psi. \quad (5)$$

Although E is negative in the bound state, it can be seen from that $E > V_{min}$, meaning that its value must be greater than $-V_0$. Thus l is also a positive real number. The general solution of the equation is

$$\psi(x) = C \sin(lx) + D \cos(lx), \quad -a < x < a. \quad (6)$$

Since the potential well has spatial reflection invariance, the wave function in the well has a definite cosmic symmetry, that is, ψ is either an odd function or an even function.

2.2. Even and Odd Parities

For the case of even function, the wave function can be expressed as [8]

$$\psi(x) = \begin{cases} C_1 e^{-\kappa x}, & x < -a \\ D \cos(lx), & -a < x < a \\ C_2 e^{\kappa x}, & x > a \end{cases} \quad (7)$$

It can be deduced under the condition of ψ , ψ' are continuous at $x = a$ that $C_1 e^{-\kappa a} = D \cos(la)$ and $-\kappa C_1 e^{-\kappa a} = -lD \sin(la)$. Combining these two equations, it can be found that

$$\kappa = l \tan(la). \quad (8)$$

Here, Eq. (8) is a transcendent equation. Solve this transcendent equation by finding the intersection of graphs and do the following transformation $\kappa^2 + l^2 = \frac{2mV_0}{\hbar^2}$ and $\varepsilon = la$, $\eta = \kappa a$. Combining these equations, it can be found that

$$(\varepsilon^2 + \eta^2) = \frac{2mV_0^2 a^2}{\hbar^2} \quad (9)$$

and

$$\eta = \varepsilon \tan(\varepsilon). \quad (10)$$

Clearly, the Eq. (10) is a circular equation. In this circular equation, V_0 determines the magnitude of the radius of the circle, which means different V_0 s will cause the image to have different intersections and the equation has different solutions. The intersections of Eq. (9) and Eq. (10) is shown in Fig. 2.

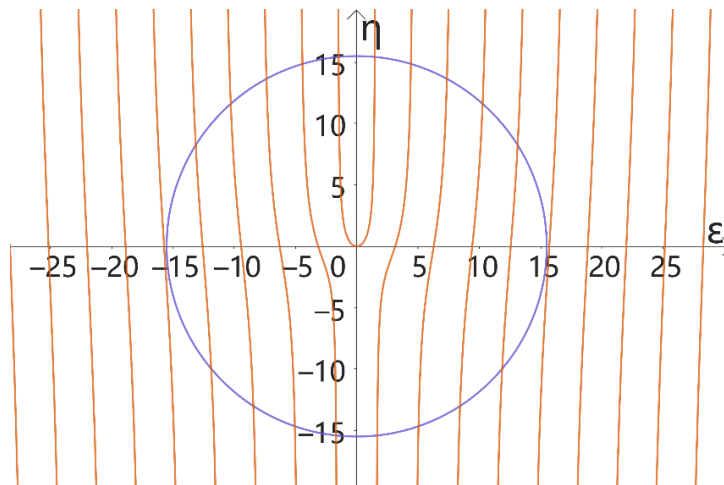


Fig. 2 The intersections of Eq. (9) and Eq. (10)

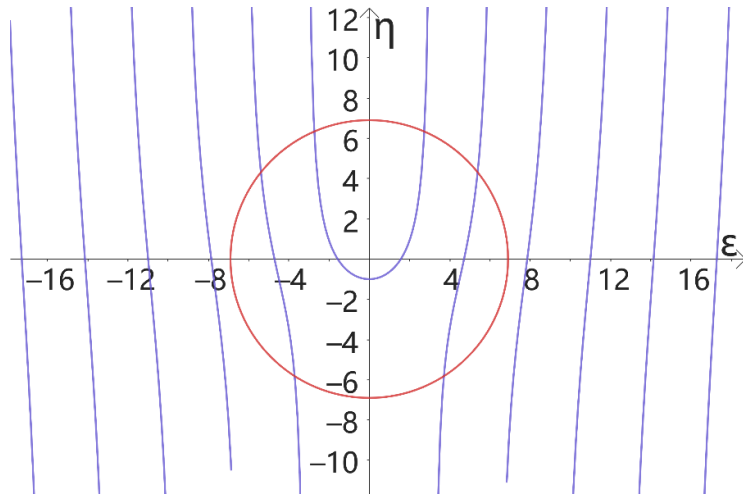


Fig. 3 The intersections of Eq. (13) and Eq. (14)

For the case of odd function, the wave function can be expressed as [9]

$$\psi(x) = \begin{cases} C_1 e^{-\kappa x}, & x < -a \\ D \sin(lx), & -a < x < a \\ C_2 e^{\kappa x}, & x > a \end{cases} \quad (11)$$

It can be deduced under the condition of ψ , ψ' are continuous at $x = a$ that $C_1 e^{-\kappa a} = D \sin(la)$ and $-\kappa C_1 e^{-\kappa a} = l \cos(la)$. Combining these two equations, it can be derived that

$$-\kappa = l \cot(la). \quad (12)$$

Similar to the case of even functions, the same transformation gives a circular equation and a transcendental equation to find their intersections. Thus, it is found that

$$-\eta = \varepsilon \cot(\varepsilon) \quad (13)$$

and

$$(\varepsilon^2 + \eta^2) = \frac{2mV_0^2 a^2}{\hbar^2}. \quad (14)$$

The intersections of Eq. (9) and Eq. (10) is shown in Fig. 3. However, the odd function case is different from the even function case when V_0 is less than a certain value. In this situation, the image has no intersection point. That is, the equation has no solution. The graphical illustration is shown in Fig. 4.

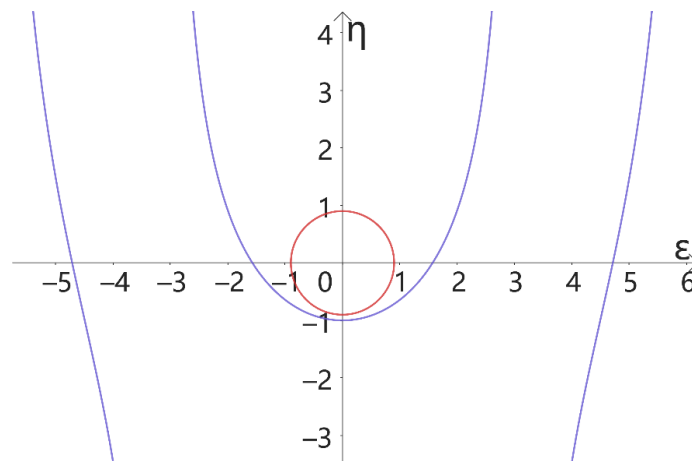


Fig. 4 The intersections of Eq. (13) and Eq. (14) when V_0 is small enough.

3. One-dimensional finite-depth asymmetric square potential well

The potential energy equation for a one-dimensional finite-depth asymmetric square potential well is given by [10]

$$\psi(x) = \begin{cases} V_1, & x < 0 \\ 0, & 0 < x < L \\ V_2, & x > L \end{cases} \quad (15)$$

The potential is shown in Fig. 5.

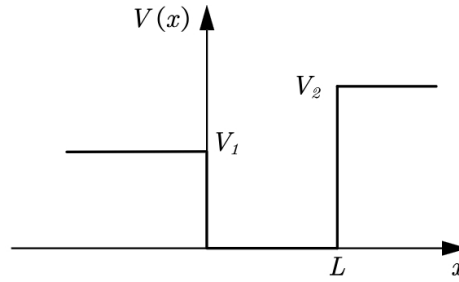


Fig. 5 One-dimensional finite-depth asymmetric square potential well

For the discrete spectrum, the energy E needs to be less than the potential energy at infinity, therefore, $E < V_1$. Its Schrödinger equation in the region of $x < 0$ is

$$\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} + (E - V_1)\psi = 0. \quad (16)$$

The wave function satisfying boundary condition $\psi(-\infty) = 0$ is $\psi(x) = C_1 e^{-\kappa_1 x}$, $\kappa_1 = \frac{1}{\hbar} \sqrt{2m(V_1 - E)}$. Its Schrödinger equation in the region $x > L$ is

$$\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} + (E - V_2)\psi = 0. \quad (17)$$

The wave function satisfying boundary condition $\psi(+\infty) = 0$ is $\psi(x) = C_2 e^{-\kappa_2 x}$, $\kappa_2 = \frac{1}{\hbar} \sqrt{2m(V_2 - E)}$. Inside the well $0 < x < L$, the Schrödinger equation is

$$\frac{\hbar}{2m} \frac{d^2\psi}{dx^2} + E\psi = 0. \quad (18)$$

Here, ψ can take the following form $\psi(x) = C \sin(kx + \delta)$, $\kappa \equiv \frac{\sqrt{2mE}}{\hbar}$. According to the continuity condition of ψ , ψ' on the edge of the potential well, it is obtained $\sin \delta = \frac{k\hbar}{\sqrt{2mV_1}}$ and $\sin(\delta + kL) = -\frac{k\hbar}{\sqrt{2mV_2}}$. After eliminating δ , the following transcendental equation is obtained as $kL = n\pi - \sin^{-1} \frac{k\hbar}{\sqrt{2mV_1}} - \sin^{-1} \frac{k\hbar}{\sqrt{2mV_2}}$. For this transcendental equation, a similar graphing method can be used to find its numerical solution.

4. Conclusion

Through the detailed study of the one-dimensional finite depth square potential well in the bound state, one finds that the depth of the potential well has a significant effect on the energy and wave function distribution of particles. If the one-dimensional symmetric finite depth square potential well is considered from the point of view of classical mechanics, there will be no particles outside the well, but it is possible from the point of view of quantum mechanics. This study provides a systematic theoretical analysis of the one-dimensional finite depth square potential well problem in bound states and provides a useful foundation for further research in related fields. On the basis of this paper,

readers can further study the more complicated cases such as the asymmetric finite depth square potential well, so as to deepen the understanding of the behavior law of particles in confined space. To conclude, this work should be a suitable reference for the readers in this area.

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