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Solution and numerical analysis of two-dimensional time-independent Schrödinger equation based on finite difference method

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Abstract. With the continuous development and widespread use of quantum mechanics, solving the Schrödinger equation has become a hot research topic. The finite difference method has the advantages of simple calculation and high accuracy, which means that it has high potential in solving the numerical solutions of the Schrödinger equation. In this paper, we deeply explore the problem of using the finite difference method to solve the numerical solution of the time-independent Schrödinger equation, propose a solution method based on the finite difference method, and evaluate its performance under different conditions. Firstly, by analyzing the principles and characteristics of the finite difference method, we construct a difference format for the time-independent Schrödinger equation. Then, by converting the difference format of the numerical solutions of the equation into a matrix, the numerical calculation problem is transformed into a matrix eigenvalue and eigenvector problem. Finally, for different physical scenarios, the established model is numerically solved and its performance is analyzed. This study found that the constructed numerical solution method exhibits high accuracy and stability in solving the numerical solutions of the time-independent Schrödinger equation. In different physical scenarios, this method can provide satisfactory results, thus verifying the feasibility of applying the finite difference method to this problem.

Keywords: finite difference method, Schrödinger equation, numerical solution, eigenvalue.

1. Introduction

The Schrödinger equation is a fundamental equation in quantum mechanics, proposed by Austrian physicist Erwin Schrödinger in 1925 [1]. This equation describes the behavior of particles at the atomic and subatomic levels, and has been widely applied in various fields such as chemistry, physics, and materials science. The equation provides a mathematical framework for understanding the wave-like behavior of particles and their probability of existence in different states, and is divided into two types: time-dependent and time-independent. Although the equation is essential for understanding the behavior of quantum systems, its complexity and the limitations of analytical methods often make its solution challenging.

Finite difference method is a numerical technique used for approximating solutions to differential equations [2]. This method is commonly used in various fields such as physics, engineering, and finance to solve complex problems that are difficult or impossible to solve using analytical methods. The method

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divides the domain of the Schrödinger equation into a grid of discrete points and approximates the derivatives in the Schrödinger equation using finite differences, which can be easily calculated using computer algorithms.

This paper will use the finite difference method to numerically solve the second and first derivative of the time-independent Schrödinger equation in two-dimensional polar coordinates using central differences and forward differences respectively, and discuss the advantages and disadvantages of this method. In addition, this paper will provide examples of applying this method to various potential systems and discuss the accuracy of the obtained numerical solutions. Finally, this paper will discuss the potential future developments of using the finite difference method to solve the Schrödinger equation and its applications in quantum mechanics.

This paper is organized into five parts. The second part of the paper reviews the literature on the use of finite difference methods to solve physical problems, such as the previous research on finite difference methods in heat conduction and wave function. The third part of the paper will focus on the central difference format and computational method for the Schrödinger equation. The fourth part of the paper will provide examples of the method's application under different conditions and error analysis. Finally, the fifth part of the paper will summarize the research, discuss the limitations of this study, and suggest future research directions.

2. Literature review

In recent years, the finite difference method has been widely used in solving physical partial differential equations. Ge and Liu used the finite difference method to numerically solve the one-dimensional heat conduction equation in space [3]:

$$\frac{\partial u}{\partial t} = a^2 \frac{\partial^2 u}{\partial^2 x}$$

while exploring the insulation effect of double-layer glass. This equation includes five different media, namely outdoor air, outer glass, intermediate air layer, inner glass, and indoor air, corresponding to different values of a. The first-order and second-order partial derivatives of the equation were respectively discretized using backward difference and central difference, resulting in:

$$\frac{u_j^n - u_j^{n-1}}{\tau} = \alpha \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}$$

where τ is the time step, and h is the spatial step. Through numerical simulations, it was found that double-layer glass has strong thermal insulation effect.

Ge and Xu also applied the finite difference method to solve the one-dimensional source-containing equation with the following form of the heat conduction equation inverse problem [4]:

$$u_t(x,t) = Du_{xx}(x,t) + q(x)u(x,t)$$

They used the central difference method to approximate the second-order partial derivative of above equation. Then, by letting $\hat{t} = T - t, w(x,\hat{t}) = u(x,t)$, they obtained the equation:

$$w_{\hat{t}}(x_i,t) = -D\frac{w(x_i+h,\hat{t}) - 2w(x_i,\hat{t}) + w(x_i-h,\hat{t})}{h^2} + q(x_i)w(x_i,\hat{t})$$

Finally, they transformed the equation into matrix form and performed numerical simulations. They proved that this method has the characteristics of good stability and high accuracy in solving the inverse problem of heat conduction equation.

Zhan et al. used the finite difference method to solve the heat conduction equation with a nonlinear convection term in a one-dimensional spatial model [5]:

$$u_t(x,y) - u_{xx}(x,t) + |u_x(x,t)|^p = f(x,t)$$

They used forward difference for the first-order derivative term and central difference for the second-order derivative term. Let f_j^n represent $f(x_j,t_n)$, the equation can be written as:

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$$\frac{u_j^{n+1}-u_j^n}{\tau}-\frac{u_{j+1}^n+u_{j-1}^n-2u_j^n}{h^2}+\left|\frac{u_{j+1}^n-u_j^n}{h}\right|^p=f_j^n$$

Then, they performed numerical calculations to investigate the influence of the exponent parameter p on the numerical difference solution. They compared the calculated results with the actual results and calculated the L_2 norm of the exact solution u^{exact} and the numerical solution u^{app}, given by $L_2 = ||u^{\text{exact}} - u^{\text{app}}||_2$, as well as the infinite norm $L_\infty = ||u^{\text{exact}} - u^{\text{app}}||_\infty$, to represent the error. They found that when $p > 1$, the error of the numerical solution of the equation is close at different times. When $p < 1$, the error of the numerical solution of the equation increases with time.

LHP de Assis and EC Romao used fourth-order difference methods in cylindrical and spherical coordinate systems to discretize the heat conduction equation [6]:

$$\rho c_p\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}\right)=k\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)\right)+\dot{q}$$

and

$$\rho c_p\left(\frac{\partial T}{\partial t}+v_r\frac{\partial T}{\partial r}\right)=k\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)\right)+\dot{q}$$

The time derivative terms in above equations were discretized using the Crank-Nicolson method to obtain:

$$T^{n+1}=0.5\Delta t\begin{bmatrix}\alpha\left(\frac{\partial^2 T^{n+1}}{\partial r^2}\right)+\left(\frac{\alpha}{r}-v_r\right)\left(\frac{\partial T^{n+1}}{\partial r}\right)+\left(\frac{\dot{q}}{\rho c_p}\right)^{n+1}\\+\alpha\left(\frac{\partial^2 T^n}{\partial r^2}\right)+\left(\frac{\alpha}{r}-v_r\right)\left(\frac{\partial T^n}{\partial r}\right)+\left(\frac{\dot{q}}{\rho c_p}\right)^n\end{bmatrix}+T^n$$

and

$$T^{n+1}=0.5\Delta t\begin{bmatrix}\alpha\left(\frac{\partial^2 T^{n+1}}{\partial r^2}\right)+\left(\frac{2\alpha}{r}-v_r\right)\left(\frac{\partial T^{n+1}}{\partial r}\right)+\left(\frac{\dot{q}}{\rho c_p}\right)^{n+1}\\+\alpha\left(\frac{\partial^2 T^n}{\partial r^2}\right)+\left(\frac{2\alpha}{r}-v_r\right)\left(\frac{\partial T^n}{\partial r}\right)+\left(\frac{\dot{q}}{\rho c_p}\right)^n\end{bmatrix}+T^n$$

Then, the spatial derivative terms were discretized using fourth-order central differences:

$$\frac{\partial T}{\partial r}=\frac{-T_{i+2}+8T_{i+1}-8T_{i-1}+T_{i-2}}{12\Delta r}$$

and

$$\frac{\partial^2 T}{\partial r^2}=\frac{-T_{i+2}+16T_{i+1}-30T_i+16T_{i-1}-T_{i-2}}{12\Delta r^2}$$

Second-order central differences were used at the boundaries. Substituting the discretized spatial derivatives into the time-discretized equations yields:

$$\left(\frac{-\alpha\Delta t}{2\Delta r^2}+\frac{\alpha\Delta t}{4r\Delta r}-\frac{v_r\Delta t}{4\Delta r}\right)T_{i-1}^{n+1}+\left(1+\frac{\alpha\Delta t}{\Delta r^2}\right)T_i^{n+1}-\left(\frac{\alpha\Delta t}{2\Delta r^2}+\frac{\alpha\Delta t}{4r\Delta r}-\frac{v_r\Delta t}{4\Delta r}\right)T_{i+1}^{n+1}=\frac{0.5\Delta t\dot{q^{n+1}}}{\rho c_p}+$$
$$\left(\frac{\alpha\Delta t}{2\Delta r^2}-\frac{\alpha\Delta t}{4r\Delta r}+\frac{v_r\Delta t}{4\Delta r}\right)T_{i-1}^n+\left(1-\frac{\alpha\Delta t}{\Delta r^2}\right)T_i^n+\left(\frac{\alpha\Delta t}{2\Delta r^2}+\frac{\alpha\Delta t}{4r\Delta r}-\frac{v_r\Delta t}{4\Delta r}\right)T_{i+1}^n+\frac{0.5\Delta t\dot{q^n}}{\rho c_p}$$

and

$$\left(\frac{-\alpha\Delta t}{2\Delta r^2}+\frac{\alpha\Delta t}{2r\Delta r}-\frac{v_r\Delta t}{4\Delta r}\right)T_{i-1}^{n+1}+\left(1+\frac{\alpha\Delta t}{\Delta r^2}\right)T_i^{n+1}-\left(\frac{\alpha\Delta t}{2\Delta r^2}+\frac{\alpha\Delta t}{2r\Delta r}-\frac{v_r\Delta t}{4\Delta r}\right)T_{i+1}^{n+1}=\frac{0.5\Delta t\dot{q^{n+1}}}{\rho c_p}+$$
$$\left(\frac{\alpha\Delta t}{2\Delta r^2}-\frac{\alpha\Delta t}{2r\Delta r}+\frac{v_r\Delta t}{4\Delta r}\right)T_{i-1}^n+\left(1-\frac{\alpha\Delta t}{\Delta r^2}\right)T_i^n+\left(\frac{\alpha\Delta t}{2\Delta r^2}+\frac{\alpha\Delta t}{2r\Delta r}-\frac{v_r\Delta t}{4\Delta r}\right)T_{i+1}^n+\frac{0.5\Delta t\dot{q^n}}{\rho c_p}$$

Numerical calculations were performed on this result, and it was found that this differencing method

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has high efficiency and low error in both cylindrical and spherical coordinate systems, as compared to the exact solutions.

In addition to the heat conduction equation, the finite difference method is also often used to solve wave equations. Si and Chen used central difference to solve the one-dimensional wave equation [7]:

$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2} + f(x,t)$$

Let $\Delta x = h, \Delta t = \tau$ and use the central difference to transform the above equation into:

$$u_j^{k+1} = s^2\left(u_{j-1}^k + u_{j+1}^k\right) + 2\left(1 - s^2\right)u_j^k - u_j^{k-1} + \tau f\left(x_j, t_k\right)$$

where $s = \frac{a\tau}{h}$ and the authors then conducted numerical simulations to study the vibration of a spring with a length of $1m$, fixed at one end, and oscillating with a period of $T = 1s$ under external force at the other end. The vibration equation at that point is given by:

$$u(1,t) = sin(2\pi t)$$

The propagation speed of the vibration is $a = 1m/s$. We take $\tau = 0.05s, h = 0.05m$. The equation obtained is:

$$u_j^{k+1} = u_{j-1}^k + u_{j+1}^k - u_j^{k-1}$$

with initial conditions $u_j^0 = 0, u_j^1 = 0$. Finally, it was found that this method can easily and quickly calculate the numerical solution of the wave equation and is applicable to different initial and boundary conditions.

Zhang used Taylor expansion to derive a three-point central difference scheme for the two-dimensional wave equation [8]:

$$\frac{\partial^2 u}{\partial t^2} = a\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

by substituting the expansions of each term into the equation:

$$u_{j,k}^{n+1} \approx 2u_{j,k}^n - u_{j,k}^{n-1} + \frac{a\tau^2}{h^2} \cdot \left(u_{j+1,k}^n + u_{j,k+1}^n - 4u_{j,k}^n + u_{j-1,k}^n + u_{j,k-1}^n\right)$$

To derive a five-point central difference scheme, the author introduced the following approximation for the second-order derivative:

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{j,k}^n = c_1 u_{j-2,k}^n + c_2 u_{j-1,k}^n + c_3 u_{j,k}^n + c_4 u_{j+1,k}^n + c_5 u_{j+2,k}^n + o\left(\Delta x^6\right)$$

and solved for the coefficients, which are found to be $c_1 = -\frac{1}{12\Delta x^2}$, $c_2 = \frac{4}{3\Delta x^2}$, $c_3 = -\frac{5}{2\Delta x^2}$, $c_4 = \frac{4}{3\Delta x^2}$, $c_5 = -\frac{1}{12\Delta x^2}$, respectively. By substituting these coefficients into the above equation, a fourth-order, five-point central difference scheme for the second-order derivative $\frac{\partial^2 u}{\partial x^2}$ is obtained. Then, by incorporating this scheme into the second-order approximation for $\frac{\partial^2 u}{\partial t^2}$, the author derived the five-point difference scheme for the wave equation:

$$u_{j,k}^{n+1} = \frac{a\tau^2}{12h^2}\left(-u_{j-2,k}^n + 16u_{j-1,k}^n - 60u_{j,k}^n + 16u_{j+1,k}^n - u_{j+2,k}^n - u_{j,k-2}^n + 16u_{j,k-1}^n + 16u_{j,k+1}^n - u_{j,k+2}^n\right) - 2u_{j,k}^n - u_{j,k}^{n-1}$$

Comparing the five-point and three-point central difference schemes, the author found that the former improves the accuracy of the approximate solution from second order with respect to the spatial variable to fourth order, while maintaining the same accuracy with respect to the time variable.

Sun and Wang used finite difference method to study the deflection equation of a charged thin film

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in an electronic capacitor under fixed boundary conditions [9]:

$$\varepsilon^2 \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} - \Delta u = -\lambda \frac{1}{u^2}$$

where u represents the deflection of the thin film, ε^2 is the ratio of inertial damping force, and $\lambda > 0$ is a control parameter. When λ is smaller than the critical voltage λ^*, the thin film can reach a steady state in finite time, which means there exists a stable solution. Therefore, obtaining the steady state solution of the equation is crucial for determining λ^*. First, the bounded region is divided into an $M \times N$ rectangular grid, and the equation is transformed into:

$$(\widetilde{u_t})_i^{j+\frac{1}{2}} - (\widetilde{u_{xx}})_i^{j+\frac{1}{2}} = -\left(\frac{\lambda}{\widetilde{u^2}}\right)_i^{j+\frac{1}{2}}$$

By Taylor expanding at $(i\Delta x, j\Delta t)$ and simplifying, the difference format is obtained:

$$\left[1 - \frac{\Delta t}{2}\frac{2\lambda}{\left(\widetilde{u_i^j}\right)^3}\right]\delta_t \widetilde{u_i^{j+\frac{1}{2}}} - \delta_x^2 \widetilde{u_i^{j+\frac{1}{2}}} = -\frac{\lambda}{\left(\widetilde{u_i^j}\right)^2} + O\left(\Delta x^2 + \Delta t^2\right)$$

It is proved that this format converges to second order in time and space in the discrete l^2 space, and is unconditionally stable in the energy norm. Finally, numerical simulations are conducted and compared with the numerically exact solution, which verifies the effectiveness of this difference format.

Qiao et al. discretized the Schrödinger equation using the five-point finite difference formula in the finite difference method [10]:

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

The discretized equation is obtained as follows:

$$-\frac{\hbar^2}{2m}\frac{1}{12h^2}(-\psi_{i-2} + 16\psi_{i-1} - 30\psi_i + 16\psi_{i+1} - \psi_{i+2}) = E\psi(x)$$

Then, the kinetic energy and potential energy terms in this expression were transformed into matrix form:

$$\begin{pmatrix} -30a + V(x_1) & 16a & -a & & & & & \\ 16a & -30a + V(x_2) & 16a & -a & & & & \\ -a & 16a & -30a + V(x_3) & 16a & -a & & & \\ & & & \ddots & & & & \\ & & & & -a & 16a & -30a + V(x_{n-2}) & 16a & -a \\ & & & & & -a & 16a & -30a + V(x_{n-1}) & 16a \\ & & & & & & -a & 16a & -30a + V(x_n) \end{pmatrix}$$

where $a = -\frac{\hbar^2}{24mh^2}$ and subsequently, the numerical solution of the equation was obtained by setting non-dimensional parameters and solving for the eigenvalues of the matrix. The eigenvalues calculated by the five-point difference method were found to be in good agreement with the analytical solutions obtained using wave mechanics.

3. Methodology

Consider the time-independent Schrödinger equation in two-dimensional Cartesian coordinates:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi + V(x,y)\psi = E\psi \tag{1}$$

Transforming equation (1) into polar coordinates, we have:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right)\psi + V(r,\theta)\psi = E\psi \tag{2}$$

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For the two-dimensional isotropic problem, we have $\frac{\partial^2\psi}{\partial\theta^2} = 0, V(r,\theta) = V(r)$. Therefore, equation (2) can be simplified as:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial r^2}\right)\psi + V(r)\psi = E\psi \tag{3}$$

where $0 < r < R$ and discretizing the continuous equation, we choose a series of equidistant discrete points $r_1, \cdots, r_{n-1}, r_n$, with the expression for each point given by $r_j = \left(j-\frac{1}{2}\right)h$, where h is the spatial step size. The corresponding wave function values at each point are $\psi(r_1), \psi(r_2), \cdots, \psi(r_{n-1}), \psi(r_n)$, which for convenience, we denote as $\psi_1, \cdots, \psi_{n-1}, \psi_n$.

We use forward difference method to approximate the first-order derivative and obtain the expression:

$$\frac{\partial\psi_j}{\partial r} = \frac{\psi_{j+1}-\psi_j}{h} \tag{4}$$

We use central difference method to approximate the second-order derivative and obtain the expression:

$$\frac{\partial^2\psi_j}{\partial r^2} = \frac{\psi_{j-1}-2\psi_j+\psi_{j+1}}{h^2} \tag{5}$$

where h is the spatial step size.

Substitute the obtained derivative expressions (4) and (5) into the discrete equation (3) and use $\left(j-\frac{1}{2}\right)h$ to represent r_j. We can then rearrange the equation to obtain:

$$-\frac{\hbar}{2m}\left(\frac{1}{\left(j-\frac{1}{2}\right)h^2}\left(-\psi_j+\psi_{j+1}\right)+\frac{1}{h^2}\left(\psi_{j-1}-2\psi_j+\psi_{j+1}\right)\right)+V\left(\left(j-\frac{1}{2}\right)\cdot h\right)\psi_j = E\psi_j \tag{6}$$

Combining like terms in equation (6), we obtain:

$$-\frac{\hbar}{2m}\left(\frac{1}{h^2}\psi_{j-1}+\frac{-2j}{\left(j-\frac{1}{2}\right)h^2}\psi_j+\frac{j+\frac{1}{2}}{\left(j-\frac{1}{2}\right)h^2}\psi_{j+1}\right)+V\left(\left(j-\frac{1}{2}\right)\cdot h\right)\psi_j = E\psi_j \tag{7}$$

The equation can be expressed in matrix form as $T\psi + V\psi = H\psi$, where T is the coefficient matrix of the kinetic energy term:

$$T = \frac{\hbar}{2m}\begin{pmatrix} \frac{2}{\left(1-\frac{1}{2}\right)\cdot h^2} & -\frac{1+\frac{1}{2}}{\left(1-\frac{1}{2}\right)h^2} & & & \\ -\frac{1}{h^2} & \frac{4}{\left(2-\frac{1}{2}\right)\cdot h^2} & -\frac{2+\frac{1}{2}}{\left(2-\frac{1}{2}\right)h^2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{h^2} & \frac{2\cdot(n-1)}{\left((n-1)-\frac{1}{2}\right)\cdot h^2} & -\frac{(n-1)+\frac{1}{2}}{\left((n-1)-\frac{1}{2}\right)h^2} \\ & & & -\frac{1}{h^2} & \frac{2\cdot n}{\left(n-\frac{1}{2}\right)\cdot h^2} \end{pmatrix} \tag{8}$$

V is the coefficient matrix of the potential energy term:

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$$V = \begin{pmatrix} V\left(\frac{1}{2}\cdot h\right) & & & & \\ & V\left(\frac{3}{2}\cdot h\right) & & & \\ & & \ddots & & \\ & & & V\left(\left(n-\frac{3}{2}\right)\cdot h\right) & \\ & & & & V\left(\left(n-\frac{1}{2}\right)\cdot h\right) \end{pmatrix} \tag{9}$$

ψ is the vector of wave function values at each point: $\psi = (\psi_1 \quad \psi_2 \quad \cdots \quad \psi_{n-1} \quad \psi_n)^T$.

Let $a = \frac{\hbar}{2m}$ and based on $T + V = H$, we can obtain:

$$H = \begin{pmatrix} a\frac{2}{\left(1-\frac{1}{2}\right)\cdot h^2} + V\left(\frac{1}{2}\cdot h\right) & -a\frac{1+\frac{1}{2}}{\left(1-\frac{1}{2}\right)h^2} & & & \\ -a\frac{1}{h^2} & a\frac{4}{\left(2-\frac{1}{2}\right)\cdot h^2} + V\left(\frac{3}{2}\cdot h\right) & -a\frac{2+\frac{1}{2}}{\left(1+\frac{1}{2}\right)h^2} & & \\ & \ddots & & & \\ & & -a\frac{1}{h^2} & a\frac{2\cdot(n-1)}{\left((n-1)-\frac{1}{2}\right)\cdot h^2} + V\left(\left(n-\frac{3}{2}\right)\cdot h\right) & -a\frac{(n-1)+\frac{1}{2}}{\left((n-1)+\frac{1}{2}\right)h^2} \\ & & & -a\frac{1}{h^2} & a\frac{2\cdot n}{\left(n-\frac{1}{2}\right)\cdot h^2} + V\left(\left(n-\frac{1}{2}\right)\cdot h\right) \end{pmatrix} \tag{10}$$

With these transformations, the numerical solution of the Schrödinger equation is transformed into the problem of finding the eigenvalues and corresponding eigenvectors of the equation $H\psi = E\psi$.

4. Numerical experiment

For convenience, let a be a non-dimensional parameter of 1, and obtain the total energy matrix H:

$$H = \begin{pmatrix} \frac{2}{\left(1-\frac{1}{2}\right)\cdot h^2} + V\left(\frac{1}{2}\cdot h\right) & -\frac{1+\frac{1}{2}}{\left(0+\frac{1}{2}\right)h^2} & & & \\ -\frac{1}{h^2} & \frac{4}{\left(2-\frac{1}{2}\right)\cdot h^2} + V\left(\frac{3}{2}\cdot h\right) & -\frac{2+\frac{1}{2}}{\left(1+\frac{1}{2}\right)h^2} & & \\ & \ddots & & & \\ & & -\frac{1}{h^2} & \frac{2\cdot(n-1)}{\left((n-1)-\frac{1}{2}\right)\cdot h^2} + V\left(\left(n-\frac{3}{2}\right)\cdot h\right) & -\frac{(n-1)+\frac{1}{2}}{\left((n-1)+\frac{1}{2}\right)h^2} \\ & & & -\frac{1}{h^2} & \frac{2\cdot n}{\left(n-\frac{1}{2}\right)\cdot h^2} + V\left(\left(n-\frac{1}{2}\right)\cdot h\right) \end{pmatrix} \tag{11}$$

Assuming a spatial step size of $h = 0.01$ and a study area of $0.005 \le r \le 0.995$, we divide this circular two-dimensional space into 99 equal parts, with a total of $n = 100$ calculation positions. We set up three different potential energy equations representing three electric potential fields, which are:

Uniform electric potential field equation:

$$V_1(r) = \begin{cases} 5000, & 0 < r < 1 \\ \infty, & otherwise \end{cases} \tag{12}$$

Distance-positive linear electric potential field equation:

$$V_2(r) = \begin{cases} 10000r, & 0 < r < 1 \\ \infty, & otherwise \end{cases} \tag{13}$$

Distance-negative linear electric potential field equation:

$$V_3(r) = \begin{cases} -10000r + 10000, & 0 < r < 1 \\ \infty, & otherwise \end{cases} \tag{14}$$

The average potential values of these three electric potential fields are all 5000. Among them, the first one is a uniform electric potential field, where the electric potential is equal at every position. The second and third electric potential fields are both linear electric potential fields, but the difference is that

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the electric potential of the second potential field is positively correlated with distance, while the electric potential of the third potential field is negatively correlated with distance.

By substituting the equations of the above three electric potential fields into a central matrix, three different models are obtained accordingly. Then, the corresponding r values of each position are respectively substituted into the three models to obtain three 100×100 matrices. Using the eig method in numpy to calculate the matrix, 100 eigenvalues and corresponding eigenvectors are obtained.

Select the first three eigenvalues and their corresponding eigenvectors. Plot the square of the modulus of each eigenvector and its corresponding r value in a two-dimensional graph to obtain probability density images.

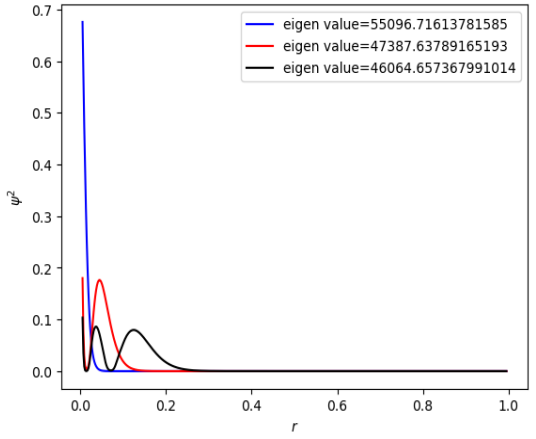

Figure 1. Several probability density functions with V_1.

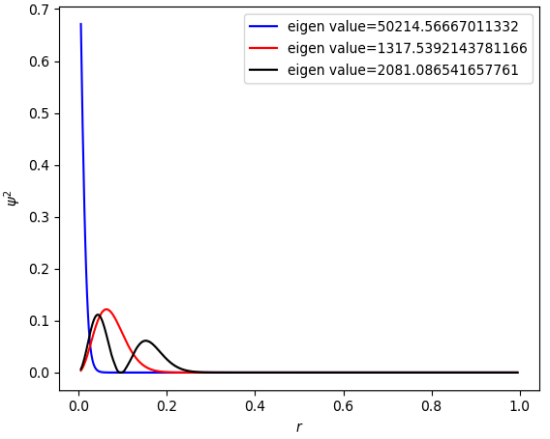

Figure 2. Several probability density functions with V_2.

By comparing Figure 1 and Figure 2, it can be observed that the positively correlated electric potential field has a stretching effect on the probability density image. Under this electric potential field, the peak of the Schrödinger equation shifts towards the far end. By comparing the Figure 1 and Figure 3, it can be observed that the negatively correlated electric potential field has a compressing effect on the probability density image. Under this electric potential field, the peak of the Schrödinger equation shifts towards the near end.

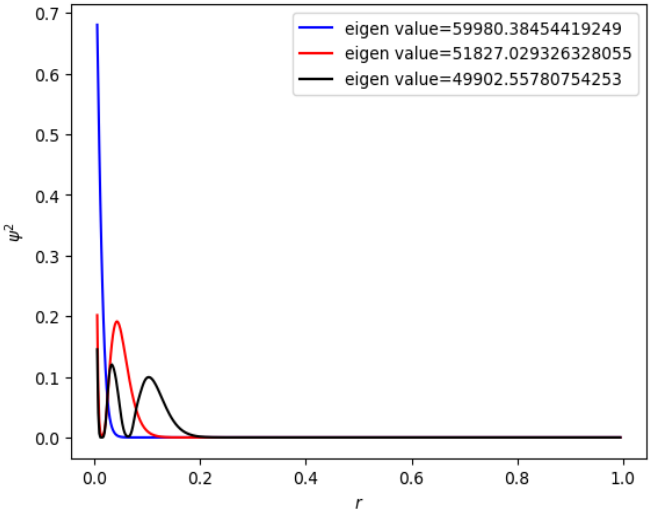

Figure 3. Several probability density functions with V_3.

5. Conclusion

This article discusses numerical solutions for the two-dimensional time-independent Schrödinger equation with isotropic properties. The equation is discretized using forward and central difference

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methods to represent first and second derivative terms, respectively. The kinetic energy and potential energy terms of the equation are then transformed into matrices, converting the problem of solving the Schrödinger equation into the problem of solving matrix eigenvalues and eigenvectors. This method has the advantages of being computationally simple, fast, and highly accurate under different conditions.
The method used in this paper weakens the dependence on the physical dimension, so that this method can obtain the qualitative characteristics of the Schrödinger equation solution and greatly simplify the calculation process at the same time. However, in more complex practical problems, the potential field environment of particles, the measurement of particle-related motion parameters, the coordination of dimensions and the precise determination of energy levels are all important factors that affect the theoretical research of the Schrödinger equation and its practical application. There is a certain room for improvement in the above aspects, which need to be paid attention to in the further development of the Schrödinger equation definite solution problem.

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