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Visualization and Analysis of Three-Dimensional Linear Harmonic Oscillator

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Abstract: *Quantum mechanics holds a very important position as the theoretical foundation of the micro world. Harmonic oscillator system is a very classical model in quantum mechanics. In this paper, the wave function of a three-dimensional linear harmonic oscillator is derived based on the linear harmonic oscillator model in quantum mechanics. According to the probabilistic interpretation of quantum mechanics, we obtain the probability density function of the harmonic oscillator electron cloud. In this paper, Monte Carlo selection method is used for sampling, and Mathematica software is used to draw electron cloud images with different quantum number, so that people can intuitively see the distribution of electron cloud in three-dimensional space.*

Keywords: *Linear harmonic oscillator, Visualization, Monte Carlo simulation*

1. Introduction

In classical physics, the motion of any system near a stable equilibrium point can be approximated as a one-dimensional harmonic oscillator, such as the vibrations of diatomic molecules, atoms and ions in crystal structures, nuclear vibrations, and so on[1,2]. As one of the most important models in quantum mechanics, the study of harmonic oscillator is crucial to the exploration of the micro world. The study of harmonic oscillator motion and its related properties is of great significance in both theory and application. However, most textbooks on atomic and molecular physics and quantum mechanics only provide a rough representation of the eigenfunctions and probability density images of three-dimensional linear harmonic oscillators. Most of the existing in-depth studies use MATLAB software to draw two-dimensional images, not a complete and intuitive three-dimensional visual spatial image of the electron cloud. This makes it impossible for beginners to specifically understand the contour and density of the electron cloud distribution region of a linear harmonic oscillator. This article hopes to start from the wave function solution of the linear harmonic oscillator Schrodinger equation, use Monte Carlo simulation methods, and combine Mathematica software programming to specifically draw a three-dimensional spatial visualization image of the electron cloud of a linear harmonic oscillator, to better interpret the quantum image of the existence of microscopic particles, As an important resource for quantum mechanics courses,

Monte Carlo method is a computational method based on generating random numbers to simulate various random processes, also known as random sampling techniques or statistical testing methods. This method can realistically describe the characteristics of things and the process of physical experiments, and solve some problems that are difficult to solve by analytical methods. In this paper, the rejection sampling method of Monte Carlo method is used to simulate the electron cloud of a three-dimensional linear harmonic oscillator. Combining the powerful functions of computer graphics software, visual analysis of three-dimensional linear harmonic oscillator wave functions is carried out. In recent years, Lu Zhiheng and others have used MATLAB as a development tool and applied three-dimensional reconstruction technology [3] to achieve the appearance of the ground state and excited state electron clouds of hydrogen atoms Zhou Qunyi analyzed the distribution of electron probability density in one-dimensional linear harmonic oscillator based on MATLAB, providing an algorithm idea for electron cloud image visualization [4].

Starting from solving the Schrodinger equation to obtain the wave function solution, this paper uses Monte Carlo method to generate a series of random numbers. Finally, use Mathematica software to program and set the quantum number of the wave function to achieve visualization of the three-

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dimensional linear harmonic oscillator electron cloud [5]. By referring to the existing images of particle multidimensional electron clouds that have been studied [6,7], and by changing the quantum number, the multidimensional electron cloud images are made more intuitive, providing help for teachers to explain the relevant knowledge of three-dimensional harmonic oscillators. The content discussed in this article is of great significance for improving the teaching of linear harmonic oscillators in the course.

2. Principles and algorithms

2.1 Wave function of one-dimensional linear harmonic oscillator

In classical mechanics, the equation of motion of a linear harmonic oscillator is a simple harmonic equation of motion. First, we solve the problem of a three-dimensional isotropic harmonic oscillator in rectangular coordinates. In this case, the problem of a three-dimensional isotropic harmonic oscillator can be transformed into three independent one-dimensional harmonic oscillator problems. We consider the linear harmonic oscillator problem in quantum mechanics, which involves solving the energy levels and wave functions of the system The potential energy function of a one-dimensional linear harmonic oscillator in rectangular coordinates is *U=m ω The* Schrodinger equation for a $^{2x2/2}$ system can be written as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{m\omega^2x^2}{2}\psi=E\psi \tag{1}$$

For convenience, dimensionless variables are introduced ξ Instead of x, their relationship is:

$$\xi=\sqrt{\frac{m\omega}{\hbar}}x=\alpha x,\quad \alpha=\sqrt{\frac{m\omega}{\hbar}} \tag{2}$$

And order:

$$\lambda=\frac{2E}{\hbar\omega} \tag{3}$$

The Schrodinger equation can be rewritten as:

$$\frac{d^2\psi}{d\xi^2}+(\lambda-\xi^2)\psi=0 \tag{4}$$

This is a second order ordinary differential equation with variable coefficients We put Ψ Write it in the following form to find the solution of equation (4):

$$\psi(\xi)=e^{-\frac{\xi^2}{2}}H(\xi) \tag{5}$$

The function H to be solved in the formula(ξ) stay ξ Should be limited when limited, $H(\xi)$ And when ξ Progressive behavior at →∞ must also ensure that $\Psi(\xi)$ "Is finite, and only in this way can the standard conditions of the wave function be satisfied."

Substitute Equation (5) into Equation (1), and first find the pair of Equation (5) ξ's secondary WeChat business:

$$\frac{d\psi}{d\xi}=\left(-\xi H+\frac{dH}{d\xi}\right)e^{-\frac{\xi^2}{2}}, \tag{6}$$

$$\frac{d^2\psi}{d\xi^2}=\left(-H-2\xi\frac{dH}{d\xi}+\xi^2H+\frac{d^2H}{d\xi^2}\right)e^{-\frac{\xi^2}{2}}. \tag{7}$$

Substitute to obtain the equation satisfied:

$$\frac{d^2H}{d\xi^2}-2\xi\frac{dH}{d\xi}+(\lambda-1)H=0 \tag{8}$$

Using a series solution, expand H into ξ To find the solution of this equation. This series must contain only limited terms, ξ When → ∞ $\Psi(\xi)$ Is limited; The condition for a series to contain only limited terms is λ Odd:

$$\lambda=2n+1,\ n=0,1,2,\cdots \tag{9}$$

By substituting Equation (3), the energy level of the linear harmonic oscillator can be obtained as

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$$E_n = \hbar\omega\left(n + \frac{1}{2}\right),\ n = 0,1,2,\cdots \tag{10}$$

Therefore, the energy of a linear harmonic oscillator can only take discrete values the interval between two adjacent energy levels is $\hbar$ ω:

$$E_{n+1} - E_n = \hbar\omega \tag{11}$$

Different n or different λ, Equation (6) has different solutions $H_n(\xi)$, $H_n(\xi)$ Known as Hermitian polynomials, it can be represented by the following formula:

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \tag{12}$$

$H_n(\xi)$ The highest power of is ^{n}, and its coefficient is 2n. From Equation (10), H_n can be obtained(ξ) The following recursive relationship is satisfied:

$$\frac{dH_n}{d\xi} = 2nH_{n-1}(\xi) \tag{13}$$

$$H_{n+1}(\xi) - 2\xi H_n(\xi) + 2nH_{n-1}(\xi) = 0 \tag{14}$$

The wave function for energy E (n) is:

$$\psi_n(x) = N_n e^{-\frac{\alpha^2}{2}x^2} H_n(\alpha x) \tag{15}$$

It consists of orthogonal normalization conditions:

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_{n'}(x)dx = \delta_{n,n'} \tag{16}$$

The normalization factor N_n *is* determined as:

$$N_n = \left(\frac{\alpha}{\pi^{\frac{1}{2}}2^n n!}\right)^{\frac{1}{2}} \tag{17}$$

Of which $\Psi_N(x)$ is the wave function of a linear harmonic oscillator along the x-axis with a quantum number of n. The same is true for the *y-axis and z-axis*.

Due to the independence of directions, the corresponding wave function is the product of the wave functions in three directions:

$$\psi_n(x,y,z)=\psi_{nx}(x)\psi_{ny}(y)\psi_{nz}(z) \tag{18}$$

From the above discussion, we can obtain that the probability density function for energy E (n) is

$$W_\theta(\delta) = \psi_n(\delta)^2 \tag{19}$$

2.2 Sampling random numbers using the first type of rounding method

The electrons of a three-dimensional linear harmonic oscillator are distributed around the atomic nucleus with a certain probability and have a certain probability density distribution function [8]. In order to simulate the distribution of electrons in a linear harmonic oscillator in three-dimensional space, the first type of rejection method in Monte Carlo method is selected for sampling. Since the rectangular coordinates of the three-dimensional linear harmonic oscillator wave function are *x, y, and z*, we sample the corresponding functions to obtain the random positions of electrons.

We can only use the first type of rounding method to select random numbers within a finite interval, but the sampling interval of the linear harmonic oscillator wave function tends to infinity, in order to meet the rounding range of the first type of rounding method. For coordinates in the x direction, we need to truncate the value range of x. By adjusting different value ranges, we ultimately retain 80% of the electrons in the x direction to be taken to the corresponding range, and determine the value range of x *to* be $x \in [-x_m, x_m]$. Truncating the range here ensures that the electron cloud image is relatively complete.

First, we will perform the following steps to select x:

1) Write the probability density function expression $W_R(x)$ of the electron, and calculate its maximum value M in the value range $[-x_m, x_m]$

2) Select a uniform random number x_1 *in the* [0,1] interval to construct a random number uniformly

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distributed in [- x_m, x_m] $\delta = x_m * x_1$

3) Then select a uniform random number x_2 *in the* [0,1] interval, and judge whether $x2 \leq WR(\delta)/M$ is satisfied. If the above inequality is satisfied, proceed to the next step; If not, return to the previous step.

4) Select $x_3 = \delta$ As a sampling value

Using the same method, we sample *y, z*.

By using the rounding method, we can obtain three independent arrays $\{X_i\}$,$\{Y_i\}$,$\{Z_i\}$, and construct the three sets of sampled values into the rectangular coordinates (x_i, y_i, z_i) of the electron.

3. Result

3.1 Visualization of the three-dimensional linear harmonic oscillator electron cloud

According to Equations (15) to (19), we used Mathematica software to draw three-dimensional linear harmonic wave function simulation diagrams under different particle numbers in rectangular coordinates, and obtained probability density histograms under the following three rectangular coordinates. See Figure 3 and Figure 4. The three-dimensional electron cloud visualization image is obtained as shown in Figure 4. The electron cloud image output by Mathematica software is not limited by the size of quantum numbers, but can be inputted with a set of quantum numbers of arbitrary size that meet the value range.

In the image of the electron cloud, each marker point represents the possible spatial location of the electron. Studying the distribution of electron clouds can roughly observe the density of points within a certain region. The denser the points in the selected region, the greater the probability of electrons appearing in this region. However, we must use the histogram of probability density distribution to analyze and explain the laws by comparing electron cloud images under different quantum number values.

3.2 Analysis

From the previous analysis, we can know that when n is determined. The value is constant 1, so that the corresponding wave function and probability density can be calculated.

Figure 1, Figure 2, and Figure 3 show the probability density image of a one-dimensional linear harmonic oscillator with quantum number n=0,1,2.

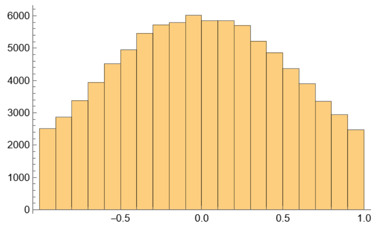

Figure 1: Histogram of probability distribution of one-dimensional linear harmonic oscillator with n=0

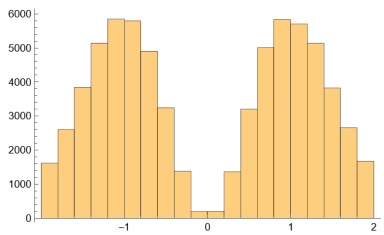

Figure 2: Histogram of probability distribution of n=1 one-dimensional linear harmonic oscillator

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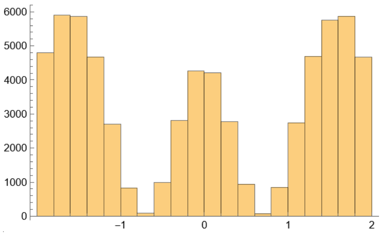
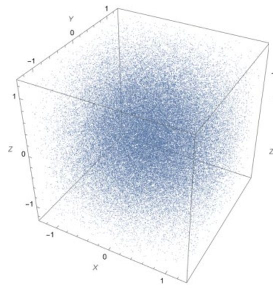
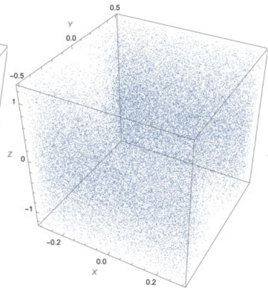


Figure 3: Histogram of probability distribution of one-dimensional linear harmonic oscillator with n=2

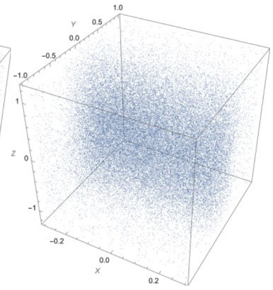
Combining the theoretical derivation of three-dimensional harmonic oscillators, using Mathematica software to draw the wave function probability density of linear harmonic oscillators under different quantum numbers, the electron cloud visualization images of three-dimensional linear harmonic oscillators under 10 conditions are obtained.



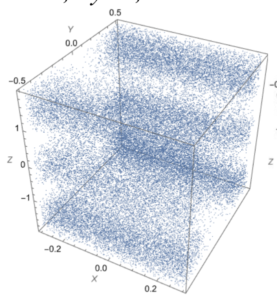
a.nx=0; ny=0; nz=0



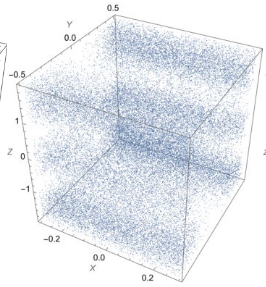
b.nx=0; ny=1; nz=0



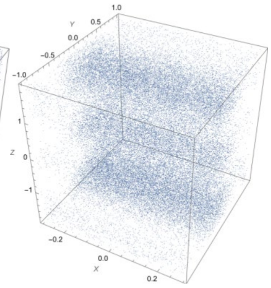
c.nx=0; ny=2; nz=0



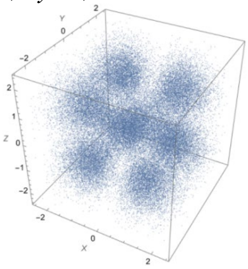
d.x=0; ny=1; nz=1



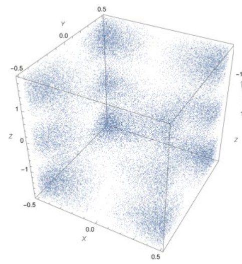
e.nx=0; ny=1; nz=2



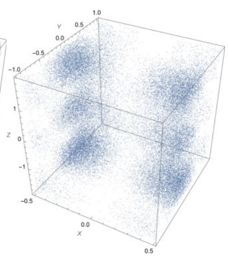
f.nx=0; ny=2; nz=2



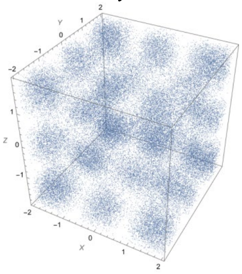
g.nx=1; ny=1; nz=1



h.nx=1; ny=1; nz=2



i.nx=1; ny=2; nz=2



j.nx=2; ny=2; nz=2

Figure 4: Image of electron cloud of three-dimensional spatial linear harmonic oscillator

Using mathematical programming, we simulated linear harmonic oscillator electron clouds with different quantum numbers in three-dimensional coordinates.

As shown in Fig 4 (a), when n is 0, the electron cloud image is a uniform sphere. And we can also

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draw the above conclusions theoretically by observing the geometric symmetry of the electron cloud image in Fig4(g), Fig4(j), and three-dimensional space n when they are 1 and 2.

The images of different quantum numbers in the remaining three-dimensional space, such as Fig4(b), Fig4(c), Fig4(d), Fig4(e), Fig4(f), Fig4(h), and Fig4(i), intuitively display the electron cloud distribution characteristics of three-dimensional linear harmonic oscillator, providing a good display for people to understand the electron cloud distribution of three-dimensional linear harmonic oscillator

4. Summary

In this paper, the wave function solution of a one-dimensional linear harmonic oscillator is obtained. Using the first type of rejection method, three-dimensional spatial visualization images of electron clouds with different quantum numbers of a three-dimensional linear harmonic oscillator are plotted using Mathematica software. In most textbooks, students cannot directly observe the distribution of atomic electron clouds, but using programs to visually simulate electron clouds can intuitively experience the morphology of microscopic particles. This article provides a feasible research idea for solving the probability distribution of microscopic particles by simulating the visualized electron clouds of linear harmonic oscillators with different quantum numbers in three-dimensional space, thereby further helping us understand the quantum mechanical model [9,10]. The study of three-dimensional linear harmonic oscillators in this paper is more helpful for people to understand and master abstract concepts.

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