

Three-Dimensional Visualization of Landau Level Electron Clouds Based on Monte Carlo Simulation

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Abstract. This study presents a comprehensive methodology for the three-dimensional visualization of electron clouds in Landau energy levels using Monte Carlo simulation techniques. Initially, this research deduces the wave function of electrons in Landau energy levels from the Schrödinger equation, solving it to obtain the eigenvalue equation for a one-dimensional harmonic oscillator containing Hermite polynomials, and then utilizes Mathematica for computational execution, resulting in the generation of intricate three-dimensional visual representations of electron clouds within these Landau levels. By integrating this approach into quantum mechanics education and research, we surpass the constraints inherent in traditional educational resources. This facilitates a visual insight, allowing students to gain a more tangible understanding of electron spatial behavior and a profound comprehension of the electron cloud's genuine physical significance. Concurrently, this study presents a comprehensive technique for rendering the three-dimensional representation of the electron cloud for generic atomic systems, employing the Monte Carlo simulation method and computational programming. This offers an innovative avenue for the advancement of visual educational tools in quantum mechanics.

Keywords: Electron Cloud in Landau Levels, Visualization, Monte Carlo Simulation.

1. Introduction

Over the past hundred years, quantum mechanics has undergone noteworthy advancements, with its applications becoming integral to daily life. Therefore, deepening students' grasp of quantum mechanics in tertiary physics education has gained paramount importance. Among the related concept in quantum mechanics for students is the spatial status of particles and the associated physical imagery. Current collegiate textbooks on quantum mechanics tend to present only the radial and angular distributions of hydrogen atom electron clouds, neglecting a holistic three-dimensional representation. Consequently, students grapple with conceiving a genuine portrayal of electron clouds [1-4]. Prior research has employed MATLAB for visualizing three-dimensional shapes of harmonic oscillators [5], while some utilized computational tools for depicting three-dimensional electron clouds in infinite potential wells [6]. Others have harnessed Mathematica for generating visuals of three-dimensional electron clouds of hydrogen atoms across varied energy states [7]. This work commences from the electron wave function in the Schrödinger equation of Landau levels. By incorporating the Monte Carlo simulation technique and utilizing Mathematica, it offers a comprehensive three-dimensional depiction of electron clouds in Landau levels. By observing these visualizations, students can attain a more profound comprehension of the electron's spatial configuration and its associated physical imagery.

Monte Carlo techniques are akin to random simulation processes and statistical experimental methodologies, employing random number sequences to mathematically emulate random events. This paper's chosen approach for simulating electron clouds in Landau levels is through rejection sampling [8-9].

Present-day university quantum mechanics courses frequently confront the issue of abstract content and elusive physical illustrations. Even post derivation of a quantum system's wave function, students find it daunting to intuitively grasp its physical representation. Conventional textbooks on quantum mechanics, while elucidating electron cloud depictions, mainly focus on radial and angular probability density functions, primarily spotlighting hydrogen atom electron clouds. Such a scope is quite narrow. Students can, at best, have a nebulous perception of the electron cloud's density, devoid of its actual three-dimensional essence. Though some current academic research present 3D visuals of electron clouds, they typically pertain only to hydrogen atoms. This research endeavors to bridge this gap. By melding the Monte Carlo simulation technique with the electron wave function in Landau levels and Mathematica programming, a three-dimensional representation of the electron clouds in Landau levels is crafted. This mitigates the prevalent constraint of most 3D electron cloud visualizations being confined to hydrogen atoms. Concurrently, we've introduced a suite of user-friendly algorithms to generate 3D depictions of electron clouds in Landau levels across diverse parameters. These algorithms, possessing significant applicability and adaptability, can be seamlessly integrated into quantum mechanics pedagogy, aiding students in grasping the spatial nature of particles.

2. Three-Dimensional Wave Functions of Electrons on Landau Levels

For a singular electron situated in a stationary state, its behavior is governed by the Schrödinger equation:

$$\hat{H}\psi = E\psi. \quad (1)$$

When accounting for a charged particle in motion within a magnetic field directed along the z-axis, the vector potential adheres to $\vec{B} = B\vec{k} = \nabla \times \vec{A}$, leading to the Hamiltonian in the Landau gauge $\vec{A} = (0, Bx, 0)$ being defined as:

$$\hat{H} = \frac{1}{2m}(\hat{p} - e\vec{A})^2 + e\phi. \quad (2)$$

Within the context of the aforementioned equation, the momentum operator is denoted by $\hat{p} = -i\hbar\nabla$, the vector potential by $\vec{A} = \vec{A}$, e stands for the electron charge, and m represents the electron mass. Given that the magnetic field is constant, it is deduced that space remains devoid of any electric field, allowing for the adoption of an equipotential surface designated as $\phi = 0$.

Subsequently, due to translational invariance along the x and z directions, the operators $\hat{p}_x$ and $\hat{p}_z$ commute with $\hat{H}$, resulting in $[\hat{p}_x, \hat{H}] = [\hat{p}_z, \hat{H}] = 0$. Along the y direction, the behavior of the electron can be approximated as a one-dimensional harmonic oscillator. Furthermore, the unconstrained momentum along the x and z directions and the harmonic motion along the y direction are independent, which allows the wave function to be expressed as a separable solution:

$$\psi(x, y, z) = e^{i(p_x x + p_z z)/\hbar} \chi(y), \quad -\infty < p_x, p_z < +\infty. \quad (3)$$

In this equation, $\chi(y)$ describes the wave function of the one-dimensional harmonic oscillator, $e^{ip_x x/\hbar}$ and $e^{ip_z z/\hbar}$ denote the plane wave solutions of the electron along the x and z directions respectively.

Conclusively, by incorporating Equations (2) and (3) into Equation (1) and simplifying, we obtain:

$$\frac{1}{2m} \left(-\hbar^2 \frac{d^2}{dy^2} \chi(y) + (p_x^2 + p_z^2) \chi(y) + e^2 B^2 x^2 \chi(y) \right) = E \chi(y). \quad (4)$$

Equation (4) can be further reduced to a one-dimensional harmonic oscillator eigenvalue equation for the variable $\chi(y)$, represented as

$$-\frac{\hbar^2}{2m} \frac{d^2}{dy^2} \chi(y) + \frac{1}{2} m \omega_c^2 (y - y_0)^2 \chi(y) = \left(E - \frac{p_z^2}{2m} \right) \chi(y). \quad (5)$$

In this equation, $y_0 = cp_x / |e| B$ represents a displacement caused by p_x , and $\omega_c = |e| B / mc$ signifies the electron's cyclotron frequency.

The eigenvalue equation (5) is solved by Hermite polynomials [10], yielding a particular solution denoted as

$$\chi_n(y - y_0) = N_n e^{-\frac{(y-y_0)^2}{2l^2}} H_n \left(\frac{y - y_0}{l} \right). \quad (6)$$

Here, $l^2 = \hbar c / |e| B$ signifies the magnetic length, and $N_n = (\sqrt{\pi} 2^n n! l)^{-\frac{1}{2}}$. Inserting equation (6) back into equation (3) provides the three-dimensional wave function of electrons on Landau levels.

In examining the quantum state distribution of electrons within Landau levels, prevailing methods predominantly emphasize analytical solutions or numerical estimations. While these methodologies offer theoretical precision, they frequently encounter computational challenges in multidimensional or intricate systems. In contrast, this research harnesses the Monte Carlo simulations, recognized for their efficiency and adaptability as numerical strategies. The strength of this technique resides in its ability to sustain manageable computational demands for expansive and multidimensional scenarios, especially when analytical solutions become untenable or computation intensive. By integrating the Monte Carlo approach with the Mathematica platform, this study not only produces three-dimensional visual depictions of the electron wave functions on Landau levels but also gains exhaustive understanding of the probability density distributions across distinct energy echelons [11]. Such a methodology enhances the comprehension of electron dynamics in quantum confinement and equips scholars with an accessible and discernible tool for examining intricate quantum occurrences.

3. Monte Carlo Simulation of Electron Clouds

To visualize the electron cloud in a three-dimensional space, this research harnesses the Monte Carlo technique, specifically employing Rejection Sampling, to delineate a sequence of spatial coordinates derived from the electron wave function. With the wave function being separable, it can be fractionated into three distinct components corresponding to Cartesian axes. For each axis component, Monte Carlo sampling is executed to ascertain the electron's spatial coordinates.

To commence, equation (3) elucidates that the wave function of electrons on the Landau level for both x and z direction adopt a specific functional form. The electrons are uniformly distributed in the y direction. Consequently, our initial focus pertains to the distribution along the y -axis. In accordance with the Rejection Sampling technique, we compute the probability density function related to the y -direction wave function $W_y(y) = |\chi(y)|^2$, along with its maximal value $L = 1/\lambda$. Subsequently, a suitable closed interval is chosen within which a uniformly distributed random number y_i is generated. Another uniformly distributed random number a_i is generated in the interval $[0,1]$ for comparison. If the condition represented by equation.

$$a_i \leq W_y(y_i) \quad (7)$$

Is satisfied, the random number is retained as a sample value; otherwise, it is discarded. This process is repeated until a sufficiently large set of sample values $\{y_1, y_2, \dots, y_n\}$ is finally obtained.

In the aforementioned procedure, it is critical to select a suitable closed interval. It is pertinent to note that although equation (6) prescribes a potentially infinite range for the variable in question, a specific decay factor $\exp[-(y - y_0)^2 / 2l^2]$ ensures that the wave function attenuates rapidly as it departs from a focal point y_0 , approaching zero. In addition, given that Rejection Sampling is effective only within a finite interval, the section is limited to the vicinity of this focal point. For this study purposes, the selected interval $[-2, 2]$ assures that over a 90% likelihood exists for the particle's presence within this span.

Figure 1 (a)-(d) offers a visual interpretation of the coordinate sampling results. The curve depicted signifies the probability density function (6), while the histogram illustrates the frequency distribution of the set of radial random point samples. The x-axis in the figure reflects the radial distance from y to y_0 . By adjusting both the orbital quantum number l and the principal quantum number n , varying probability density functions for the y-axis, contingent on diverse parameters, can be derived.

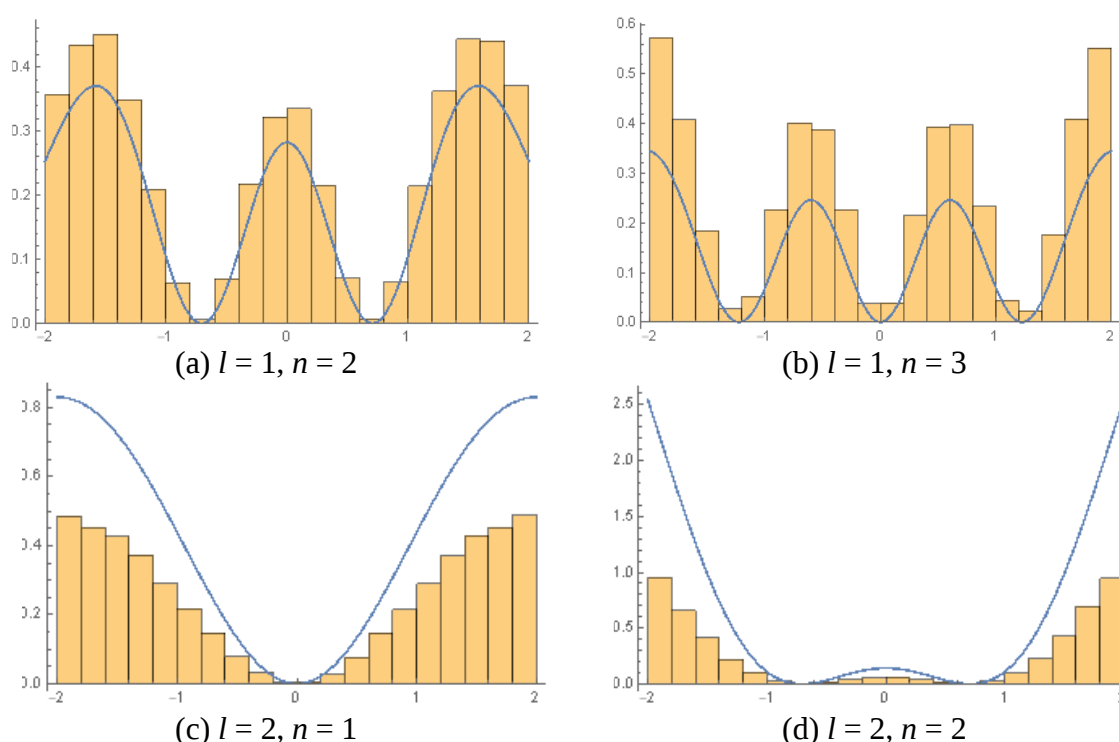


Figure 1. The results of sampling in the y direction

Figure 1 illustrates the electron probability density in the y direction when $l = 1, n = 2$; $l = 1, n = 3$; $l = 2, n = 1$; $l = 2, n = 2$. Based on the aforementioned sampling results, a Mathematica program was written to generate corresponding three-dimensional electron cloud images. Figures 2-5 display front views, top views, and default views of the electron clouds for the four sets of Landau levels described.

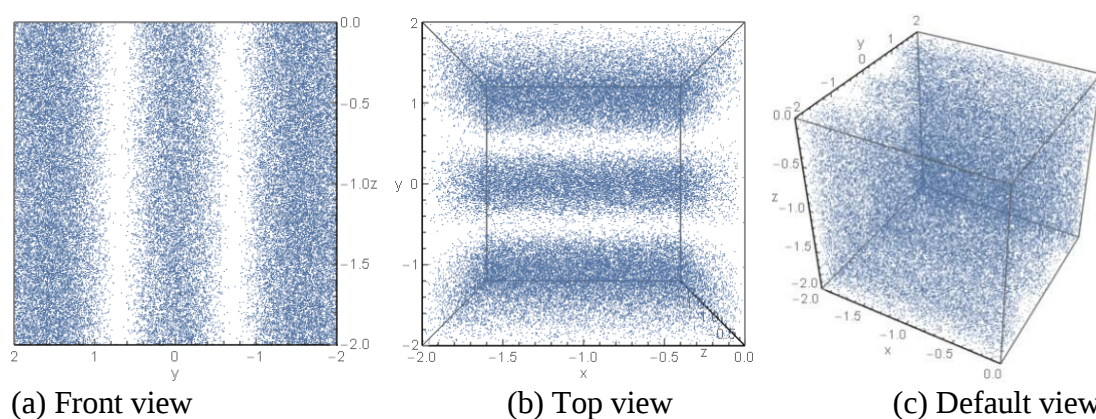


Figure 2. The 3D image of the electron cloud with $l = 1, n = 2$

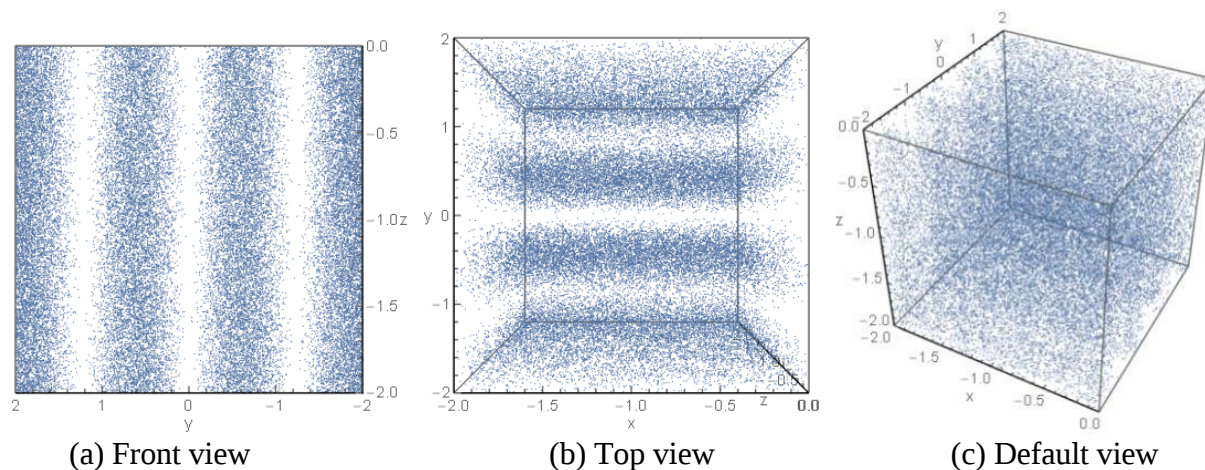


Figure 3. The 3D image of the electron cloud with $l = 1, n = 3$

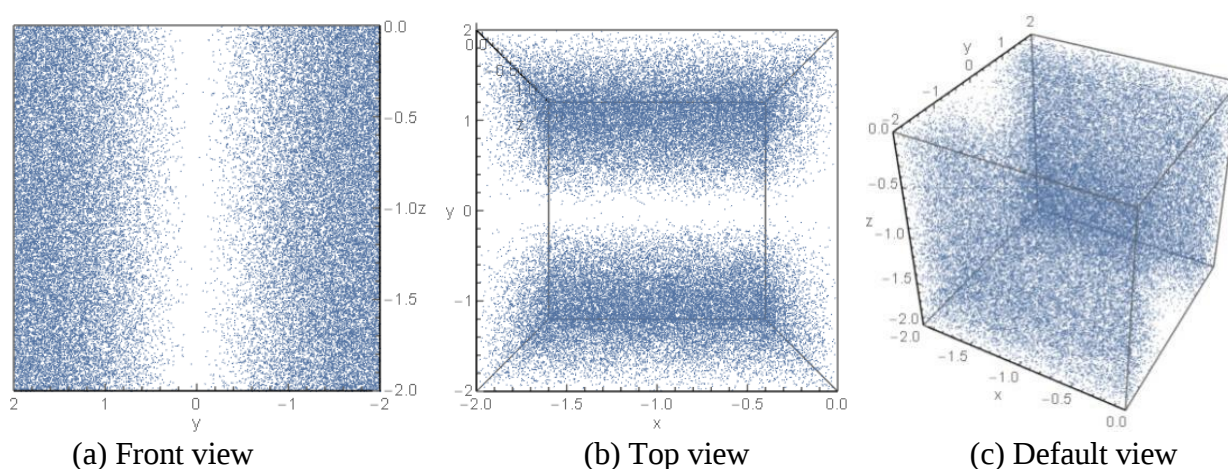


Figure 4. The 3D image of the electron cloud with $l = 2, n = 1$

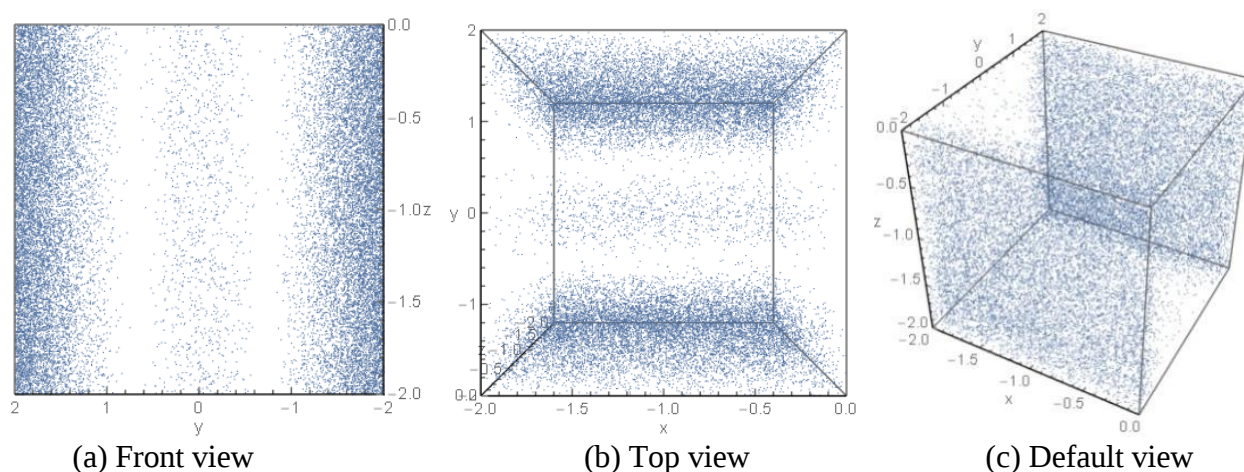


Figure 5. The 3D image of the electron cloud with $l = 2, n = 2$

Figures 2-5 illustrate that the integration of probability density function plots and scatter plots reveal the electron cloud's distinct periodic striped distribution in space. This distribution bears resemblance to the interference patterns observed in light's double-slit experiments. Maintaining a constant l and increasing n results in reduced spacing between the stripes, causing a denser electron cloud. In contrast, with a fixed n and an elevated l , the spacing between the stripes expands, resulting in a more diffuse electron cloud. More specifically, a comparison between figures 5 and 4 reveals that the latter contains two stripes, whereas the former encompasses three. The stripes in figure 5 are more closely spaced, signaling a more compact electron cloud. Drawing a parallel between figures 3 and 2, the former

presents four stripes while the latter depicts three. In figure 3, the stripe distribution is distinctly tighter, reflecting a denser electron cloud arrangement.

4. Conclusion

Utilizing Monte Carlo simulations, this research deciphered the wave functions of a stationary solitary electron as dictated by the Schrödinger equation. Executed the above procedure within the Mathematica software framework, the approach facilitating the three-dimensional visualization of electron clouds at Landau levels. The efficient application of Monte Carlo techniques minimized computational demands while offering clearer perspectives on electron dynamics. This methodology paves the way for fresh, practical investigations into the configurations and foundational principles of diverse atoms. Moreover, amalgamating these simulations with visual computer graphics for instructional use could elevate educational efficacy, making the idea of electron clouds more accessible and resonant for learners.

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