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Schrödinger equation for various quantum systems based on Heisenberg's uncertainty principle

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Abstract. This article establishes the proof of the Schrödinger equation for numerous quantum systems, utilizing Heisenberg's uncertainty principle. The Fourier transform connects functions in the time and frequency domains, resulting in the mathematical inequality that is the foundation of the uncertainty principle. In the part of Methods and Theory, the article derives the uncertainty principle through Fourier transforms by defining the mean and variance of angular frequency and time, and subsequently expanding the integral. This establishes the fundamental connection between time and frequency domains, illustrating the constraints imposed by quantum mechanics. In the part of Results and Application, the article applies the uncertainty principle to derive the Schrödinger equation under different conditions: free particle, particle in a box, harmonic oscillator, and hydrogen atom. For each case, the article assumes wave function solutions, uses the uncertainty in position and momentum to estimate kinetic and potential energies, and shows that the total energy matches the ground state energy derived from the Schrödinger equation. The results highlight the critical role of Heisenberg's uncertainty principle in understanding key aspects of quantum mechanics, providing a unified framework for these diverse systems.

Keywords: Fourier Transform, Heisenberg's Uncertainty Principle, Quantum Mechanics, Schrödinger Equation.

1. Introduction

Quantum mechanics is the essential theory that describes particles' behavior at the atomic and subatomic levels. It provides a framework for understanding the physical properties of nature at small scales, where classical mechanics fails to apply. The development of quantum mechanics has led to numerous technological advancements, including semiconductors, lasers, and quantum computing [1]. By describing the wave-particle duality of matter and energy, quantum mechanics reveals the probabilistic nature of physical phenomena, which is essential for the accurate prediction and manipulation of microscopic systems [1]. Heisenberg's uncertainty principle is the core of quantum mechanics, underscoring the fundamental limits of measurement and observation in the quantum realm. Mathematically, the uncertainty principle can be derived using Fourier transforms, which relate functions in the time and frequency domains. The principle can be expressed as $\Delta p \Delta x \geq \frac{\hbar}{2}$. The relationship between Heisenberg's uncertainty principle and Fourier transforms emphasizes the relationship between time and frequency domains, which is essential for comprehending the behavior of quantum systems [2]. The uncertainty principle has diverse applications in quantum mechanics, including elucidating the stability of atoms, the behavior of particles in box, and the quantization of energy levels.

This article is organized as the following. In the part of Methods and Theory, by using Fourier Transform to Prove Heisenberg uncertainty principle, it explains how the Heisenberg uncertainty principle is derived using the properties of Fourier transforms. The derivation starts with mathematical inequality and proceeds through defining the mean and variance of angular frequency and time. By interpreting these results, the uncertainty principle is established. The part of Fourier transform in time-dependent Schrödinger equation discusses the application of Fourier transforms in quantum mechanics, specifically in transitioning between the position and momentum representations of the wave function. The time-dependent Schrödinger equation, a foundational equation in quantum mechanics, is introduced, describing how a physical system's quantum state changes over time [3]. In the results and application, using Heisenberg's uncertainty principle to prove Schrödinger equation under free particle condition, it assumes a plane wave solution for a free particle and demonstrates how the uncertainty principle leads to the time-dependent Schrödinger equation.

The key steps involve recognizing the relationships between energy, momentum, and the wave function's form. When using Heisenberg's uncertainty principle to prove Schrödinger equation under particle in a box, it considers a particle confined in a one-dimensional box. It shows how the uncertainty in position and momentum aligns with the quantized energy levels obtained from the Schrödinger equation. If Heisenberg's uncertainty principle is used to prove Schrödinger equation under Harmonic Oscillator, it addresses the harmonic oscillator, verifying the ground state energy using the uncertainties in position and momentum. The results are related to the known solutions involving Hermite polynomials. By utilizing Heisenberg's uncertainty principle to prove Schrödinger equation for the hydrogen atom problem, it deals with the hydrogen atom, using the Bohr radius to estimate the uncertainties and derive the ground state energy. The result matches the solution obtained from the Schrödinger equation, demonstrating the fundamental role of the uncertainty principle in quantum mechanics.

2. Methods and Theory

2.1. Using Fourier transform to prove Heisenberg uncertainty principle

A fundamental notion in quantum physics is the Heisenberg Uncertainty Principle, which claims that it is difficult to simultaneously know the precise position and momentum of a particle [4]. This principle can be mathematically derived using Fourier transforms, which relate functions in time and frequency domains.

The proof starts with the following mathematical inequality:

$$\int_{-\infty}^{\infty}\left|\frac{\omega-\bar{\omega}}{2\Delta\omega^2}\hat{f}(\omega)+\frac{d\hat{f}}{d\omega}\right|^2 d\omega \geq 0 \tag{1}$$

This inequality uses properties of the Fourier transform and derives the uncertainty principle. The mean and variance can be defined as the following. The Mean and Variance of ω are $\bar{\omega}=\int_{-\infty}^{\infty}\omega\left|\hat{f}(\omega)\right|^2\frac{d\omega}{2\pi}$ and $\Delta\omega^2=\int_{-\infty}^{\infty}(\omega-\bar{\omega})^2\left|\hat{f}(\omega)\right|^2\frac{d\omega}{2\pi}$. The Mean and Variance of t are $\bar{t}=\int_{-\infty}^{\infty}t\,|f(t)|^2dt=0$ and $\Delta t^2=\int_{-\infty}^{\infty}t^2|f(t)|^2dt$. Using the above definitions to expand the integral:

$$\int_{-\infty}^{\infty}\left|\frac{\omega-\bar{\omega}}{2\Delta\omega^2}\hat{f}(\omega)+\frac{d\hat{f}}{d\omega}\right|^2 d\omega=\int_{-\infty}^{\infty}\left[\left(\frac{\omega-\bar{\omega}}{2\Delta\omega^2}\right)^2\left|\hat{f}\right|^2+\frac{\omega-\bar{\omega}}{2\Delta\omega^2}\left(\widehat{f^*}\frac{d\hat{f}}{d\omega}+\frac{d\widehat{f^*}}{d\omega}\hat{f}\right)+\left|\frac{d\hat{f}}{d\omega}\right|^2\right]d\omega \tag{2}$$

By simplifying the right-hand side, it is found that $\frac{\Delta\omega^2}{4\Delta\omega^4}\cdot 2\pi-\frac{2\pi}{2\Delta\omega^2}+2\pi\int_{-\infty}^{\infty}t^2|f(t)|^2dt\geq 0$. Combining these results, the Heisenberg uncertainty principle is

$$\Delta\omega\Delta t\geq\frac{1}{2}. \tag{3}$$

Angular frequency ω is related to momentum p by: $\omega = \frac{p}{\hbar}$. Therefore$\Delta\omega = \Delta p/\hbar$. Substituting into the uncertainty principle for angular frequency and time: $\Delta\omega\Delta t \geq \frac{1}{2}$, $\frac{\Delta p}{\hbar}\Delta t \geq \frac{1}{2}$. By multiplying both sides by $\hbar$, $\Delta p\Delta t \geq \frac{\hbar}{2}$. Interpreting Δt as Δx, it is found that $\Delta p\Delta x \geq \frac{\hbar}{2}$.

Hence, the product of the uncertainties in time and frequency domains is bounded below by a constant, which is a representation of the Heisenberg uncertainty principle. The derivation emphasizes the profound connection between time and frequency domains, as encapsulated by the Fourier transform, and their role in understanding the behavior of quantum systems.

2.2. Fourier Transform in Quantum Mechanics and Time-Dependent Schrödinger Equation

The Fourier transform can be used to turn a function of time or space into a function of frequency or momentum [5]. In quantum mechanics, the Fourier transform is used to switch between the position representation and the momentum representation of the wave function. The Fourier transform of a wave function $\psi(t)$ is given by

$$\tilde{\psi}(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(t)e^{i\omega t}\,dt \tag{4}$$

The inverse Fourier transform is:

$$\psi(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\tilde{\psi}(\omega)e^{-i\omega t}\,d\omega \tag{5}$$

The time-dependent Schrödinger equation describes how the quantum state of a physical system evolves over time [6]. It is a foundational equation in quantum mechanics and is given by:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \tag{6}$$

where $\psi(x,t)$ is denoted by the wave function of the system, $\hbar$ is denoted by the reduced Planck constant, and $\hat{H}$ is denoted by the Hamiltonian operator. For a particle in a potential $V(x)$, the Hamiltonian operator can be expressed as:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \tag{7}$$

3. Results and Application

3.1. Prove Schrödinger equation under the free particle condition

Assume a plane wave solution for a free particle

$$\psi(x,t) = Ae^{i(kx-\omega t)} \tag{8}$$

where k is the wave number, and ω is the angular frequency. Using the de Broglie relation $p = \hbar k$ and $E = \hbar\omega$, the time-dependent Schrödinger equation for a free particle is

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}. \tag{9}$$

Compute the time derivative: $\frac{\partial\psi}{\partial t} = -i\omega$ and compute the second spatial derivative: $\frac{\partial^2\psi}{\partial x^2} = -k^2$, the author can relate ω and k to Energy and Momentum.

For a free particle, the energy E is purely kinetic: $E = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}$. The angular frequency ω is related to the energy by $E = \hbar\omega$. Thus, $\hbar\omega = \frac{\hbar^2k^2}{2m}$. This implies $\omega = \frac{\hbar k^2}{2m}$. Substitute ω into the time derivative equation: $\frac{\partial\psi}{\partial t} = -i\left(\frac{\hbar k^2}{2m}\right)$. Rewrite the equation: $i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2k^2}{2m}$, and using the second spatial derivative: $\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{\hbar^2k^2}{2m}$, it is found that the Schrödinger equation is:

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \tag{10}$$

By assuming the wave nature of particles and using the Heisenberg uncertainty principle, it arrives at the Schrödinger equation for a free particle. The key steps involve recognizing the relationships between energy, momentum, and the wave function's form, which are all consistent with the constraints imposed by the uncertainty principle [7].

3.2. Prove Schrödinger equation under particle in a box

Consider a particle confined in a one-dimensional box of width a. The potential $V(x)$ is given by

$$V(x)=\begin{cases} 0, & \text{if } 0<\text{x}<\text{a} \\ \infty, & if\ x\leq 0\ or\ x\geq a \end{cases} \tag{11}$$

The time-independent Schrödinger equation for a particle of mass m in a potential V(x) is given by Eq. (6). When $V(x) = 0$, the equation simplifies to

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E \tag{12}$$

The solution to the Schrödinger equation where $V(x) = 0$ is given by $\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$, where n is a positive integer. The corresponding energy levels are:

$$E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}. \tag{13}$$

For a particle in the ground state $n = 1$, the wave function is:

$$\psi_1(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) \tag{14}$$

The uncertainty in position, Δx, can be approximated as: $\Delta x\approx\frac{a}{2}$. The uncertainty in momentum, Δp, can be estimated using the uncertainty principle: $\Delta p\geq\frac{\hbar}{2\Delta x}=\frac{\hbar}{a}$

To relate these uncertainties to the Schrödinger equation, the expression for the kinetic energy of the particle is: $E=\frac{p^2}{2m}$. The uncertainty in energy due to the uncertainty in momentum is: $\Delta E\approx\frac{\Delta p^2}{2m}=\frac{\hbar^2}{2ma^2}$. This energy uncertainty matches the ground state energy $E_1=\frac{\pi^2\hbar^2}{2ma^2}$. Thus, the Heisenberg uncertainty principle is consistent with the energy levels from the Schrödinger equation for a particle in a box. The ground state energy and demonstrated its alignment with the Schrödinger equation. It serves to illustrate that the uncertainty principle forms a fundamental basis for comprehending the quantization of energy levels within confined systems [8].

3.3. Prove Schrödinger equation under harmonic oscillator

The one-dimensional harmonic oscillator is given by: $V(x)=\frac{1}{2}m\omega^2x^2$. The time-independent Schrödinger equation for a particle of mass in $V(x)$ is $\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E$. For a harmonic oscillator, substituting $V(x)=\frac{1}{2}m\omega^2x^2$ gives: $\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E$. The solutions to this equation involve Hermite polynomials: $\psi_n(x)=N_ne^{-\alpha^2x^2/2}H_n(\alpha x)$, where α= $\sqrt{\frac{m\omega}{\hbar}}$. N_n is a normalization constant, and H_n are the Hermite polynomials. The corresponding energy levels are:

$$E_n=\left(n+\frac{1}{2}\right)\hbar \tag{15}$$

For the ground state ($n = 0$), the wave function is:

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$$\psi_0(x) = \left(\frac{\alpha}{\pi^{1/2}}\right)^{1/2} e^{-\alpha^2 x^2/2} \tag{16}$$

The uncertainties in position Δx and momentum Δp for the ground state are given by: $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\hbar}{2m\omega}}$, $\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\frac{\hbar m\omega}{2}}$. For the ground state of the harmonic oscillator, it verifies the uncertainty principle $\Delta x \Delta p = \sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{\hbar m\omega}{2}} = \frac{\hbar}{2}$. The uncertainties in position and momentum are related with the energy of the harmonic oscillator: $E = \frac{\langle p^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle x^2\rangle$. For the ground state: $\langle x^2\rangle = \frac{\hbar}{2m\omega}$, $\langle p^2\rangle = \frac{\hbar m\omega}{2}$. Substituting these into the energy expression:

$$E = \frac{\hbar m\omega}{4m} + \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega} = \frac{\hbar\omega}{2}. \tag{17}$$

Thus, the energy matches the ground state energy $E_0 = \frac{1}{2}\hbar\omega$ obtained from the Schrödinger equation. It demonstrates that the limits placed on the precise position and momentum of the particle lead directly to the quantized energy levels of the harmonic oscillator [9].

3.4. *Prove Schrödinger equation for the hydrogen atom problem*

The energy for an electron in a hydrogen atom is given by the Coulomb potential: $V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$. The time-independent Schrödinger equation for the hydrogen atom in spherical dimensions is:

$$\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E \tag{18}$$

By separating variables, the radial part of the Schrödinger equation is:

$$\frac{\hbar^2}{2m}\left(\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u\right) - \frac{e^2}{4\pi\epsilon_0 r}u = Eu \tag{19}$$

For the hydrogen atom, let's assume the uncertainty in the electron's position Δr is on the order of the Bohr radius a_0: $\Delta r \approx a_0$

The uncertainty in momentum Δp can be estimated using Heisenberg's uncertainty principle:

$$\Delta p_r \approx \frac{\hbar}{\Delta r} \approx \frac{\hbar}{a_0} \tag{20}$$

The kinetic energy T can be approximated as: $T \approx \frac{(\Delta p_r)^2}{2m} = \frac{\hbar^2}{2ma_0^2}$. The potential energy V is: $V \approx -\frac{e^2}{4\pi\epsilon_0 a_0}$. The total energy E is the sum of kinetic and potential energy

$$E \approx \frac{\hbar^2}{2ma_0^2} - \frac{e^2}{4\pi\epsilon_0 a_0} \tag{21}$$

To find the ground state energy, minimize E with respect to a_0: $\frac{dE}{da_0} = 0$. Then, $\frac{\hbar^2}{ma_0^3} + \frac{e^2}{4\pi\epsilon_0 a_0^2} = 0$. Solving for a_0, it is found that $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$. Substitute a_0 back into the expression for E:

$$E = -\frac{e^2}{8\pi\epsilon_0 a_0} \tag{22}$$

This is the ground state energy of the hydrogen atom, which matches the result obtained from solving the Schrödinger equation [10].

4. Conclusion

This article demonstrates the application of Heisenberg's uncertainty principle to derive the Schrödinger equation for various quantum systems, including free particles, particles in a box, harmonic oscillators, and the hydrogen atom. By using the fundamental limits imposed by the uncertainty principle, it shows

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how the quantization of energy levels arises naturally within these systems. The proof underscores the connection between the principles of quantum mechanics and the Fourier transforms used to describe them. The derivations presented provide a clear and coherent framework for understanding the foundational aspects of quantum mechanics. With the uncertainty principle, it derives the Schrödinger equation, which manages the behavior of quantum systems. The article offers a unified approach to deriving the Schrödinger equation for different quantum systems using Heisenberg's uncertainty principle. This helps in understanding the common underlying principles that govern these systems. The use of Fourier transforms to derive the uncertainty principle and subsequently apply it to different quantum systems adds a level of mathematical rigor to the derivations, ensuring that the results are robust and consistent. However, the article has the limitations. Some derivations rely on simplifying assumptions, such as approximating uncertainties or assuming certain forms of wave functions. These assumptions, while useful for illustrative purposes, are not fully capture the complexity of real-world quantum systems. When considering the methods in more complex quantum systems, such as those with several interacting particles or external fields, it reduces constraints in the future study. Combining the analytical framework offered with numerical simulations makes it possible to provide deeper understanding and more precise predictions for a wider variety of quantum phenomena.

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