

Quantum Mechanics

Week 2

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1 Pre-Reading Note

Dear Students,

Welcome to the course on Quantum Mechanics. As part of your learning resources, I will prepare a series of educational materials and sheets designed to complement the lectures.

Please note that these materials are **abridged versions** of the content from the textbook *"Introduction to Quantum Mechanics By David J. Griffiths"*. They have been tailored to align with the class schedule and topics, providing you with concise summaries and key points for each topic covered.

It's important to understand that these sheets are **not standalone resources**. They are intended to be used in conjunction with the class material. For a deeper understanding and a more comprehensive view of each topic, I strongly encourage you to refer to the mentioned textbook.

The book provides detailed explanations, examples, and insights that go beyond the scope of our summaries. It will be an invaluable resource for you to solidify your understanding of Quantum Mechanics.

I cannot guarantee neither correctness nor completeness of the script. Please report any mistake directly to me.

Have fun with Quantum Mechanics!

Best regards,

Mark Benazet Castells

2 The Wave Function in Quantum Mechanics

In quantum mechanics, the wave function, denoted as $\Psi(\vec{r}, t)$, is a fundamental concept. It represents the state of a quantum system as a complex function of both position \vec{r} and time t .

2.1 Essential Characteristics of the Wave Function

The L^2 space in Quantum Mechanics, which forms a Hilbert Space (\mathcal{H}), includes all functions f for which the integral of their squared magnitude is finite, ensuring that physical probabilities are well-defined:

$$\int_{-\infty}^{\infty} |f(x)|^2 dx < \infty. \quad (1)$$

The L^2 -inner product, defined for functions f, g in this space, is essential for assessing function similarity and orthogonality:

$$\langle f, g \rangle = \int_{-\infty}^{\infty} f(x)g(x)^* dx, \quad (2)$$

where $g(x)^*$ is the complex conjugate of $g(x)$.

Properties Ensuring Hilbert Space Structure The L^2 space, with the inner product defined above, exhibits essential properties of a Hilbert space:

- **Conjugate Symmetry:** $\langle f, g \rangle^* = \langle g, f \rangle$.
- **Linearity in the Second Argument:** $\langle f, \lambda_1 g_1 + \lambda_2 g_2 \rangle = \lambda_1 \langle f, g_1 \rangle + \lambda_2 \langle f, g_2 \rangle$.
- **Conjugate Linearity in the First Argument:** $\langle \lambda_1 f_1 + \lambda_2 f_2, g \rangle = \lambda_1^* \langle f_1, g \rangle + \lambda_2^* \langle f_2, g \rangle$.
- **Positivity:** $\langle f, f \rangle \geq 0$, with equality if and only if $f = 0$ almost everywhere.
- **Cauchy-Schwarz Inequality:** $|\langle f_1, f_2 \rangle|^2 \leq \langle f_1, f_1 \rangle \langle f_2, f_2 \rangle$.

In Quantum Mechanics, the emphasis is on a specific subset of the L^2 Hilbert space where wave functions f are not only square-integrable but also normalized. This normalization criterion is pivotal, as it ensures that the wave functions represent physical states with a total probability of one. Mathematically, this is expressed as:

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = 1, \quad (3)$$

or equivalently,

$$\langle f, f \rangle = 1. \quad (4)$$

Thus, the focus is on the subset of the Hilbert space where $\langle f, f \rangle = 1$.

Example 1: Non-Square Integrable Wave Function A wave function $\psi = e^x$ over all space $x \in R$ is not square-integrable, as its integral diverges:

$$\int_{-\infty}^{\infty} |e^x|^2 dx = \int_{-\infty}^{\infty} e^{2x} dx \rightarrow \infty. \quad (5)$$

Example 2: Square Integrable and Normalizable Wave Function Consider $\psi = A \sin(\pi x)$ for $x \in [-1, 1]$ and zero elsewhere. This wave function is defined to be nonzero only within the interval $[-1, 1]$ and is zero outside this range. Hence, when integrating over all space, the contribution to the integral from outside the interval $[-1, 1]$ is zero. Therefore, the integral for square-integrability and normalization is effectively calculated only over the range where ψ is nonzero. The integral becomes:

$$\int_{-\infty}^{\infty} |A \sin(\pi x)|^2 dx = \int_{-1}^1 A^2 \sin^2(\pi x) dx = A^2, \quad (6)$$

where A can be chosen such that $A^2 = 1$ for normalization.

Probability Density of a Gaussian Wave Packet

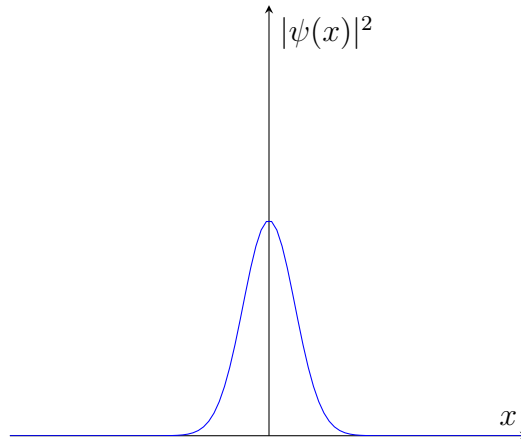


Figure 1: Plot of $|\psi(x)|^2$ illustrating the Gaussian shape centered at $x_0 = 0$ with $\sigma = 1$

3 The Schrödinger Equation

The Schrödinger Equation is a fundamental equation in quantum mechanics, analogous to Newton's second law in classical mechanics. It describes the quantum state of a particle in a potential. For a particle with mass m in a potential $V(x, t)$, the equation is called T.D.S.E. :

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x, t) \Psi(x, t), \quad (7)$$

where \hbar is the reduced Planck constant.

Components of the Schrödinger Equation

- **Reduced Planck Constant \hbar :** Connects energy and frequency, essential for quantizing physical properties.
- **Wave Function Ψ :** Represents the quantum state, evolving over time as dictated by the equation.
- **Hamiltonian Operator \hat{H} :** Represents the total energy (kinetic and potential) of the system.

3.1 Time-Dependent and Time-Independent Forms

The Schrödinger Equation comes in two variants:

- **Time-Dependent Schrödinger Equation (TDSE):** Used for dynamic systems where states change over time as seen in 7.
- **Time-Independent Schrödinger Equation (TISE):** Simplified form for stationary states:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x) \quad (8)$$

where E is the energy. This form is utilized for problems where potential does not change over time $V(x)$ like the hydrogen atom or a particle in a box.

The transition from the total wave function Ψ to ψ is a result of separating variables to solve the Schrödinger Equation under the assumption of a time-independent potential. While Ψ includes both spatial and temporal information, ψ is solely concerned with the spatial distribution of the probability density.

Our focus will be on the Time-Independent Schrödinger Equation (TISE), which allows for the exploration of stationary states within a system. These states can be linearly combined to represent any state of the system.

4 Probability in Quantum Mechanics

Quantum mechanics employs probabilities to describe the behavior of particles. The probabilities can be for both discrete and continuous outcomes, each having its own method of calculation.

4.1 Discrete Variables

For discrete outcomes, probabilities are calculated using a probability distribution function, denoted $P(j)$. For example, in a set of discrete energy levels, $P(j)$ gives the probability of finding a system in the energy level j .

4.2 Continuous Variables

In the case of continuous variables, the probability density, denoted $\rho(x)$, is used. It describes the likelihood of finding a particle in a specific range. For instance, the probability of a particle being located between positions a and b is given by:

$$P_{ab} = \int_a^b \rho(x) dx. \quad (9)$$

Example

Consider a normalized sinusoidal wave function defined as:

$$\Psi(x) = \sqrt{\frac{2}{\pi}} \sin(x)$$

The probability density function is $\rho(x) = |\Psi(x)|^2 = \frac{2}{\pi} \sin^2(x)$.

$$\begin{aligned} P_{\frac{\pi}{4}, \frac{3\pi}{4}} &= \int_{\frac{\pi}{4}}^{\frac{3\pi}{4}} \rho(x) dx \\ &= \int_{\frac{\pi}{4}}^{\frac{3\pi}{4}} \frac{2}{\pi} \sin^2(x) dx \\ &= \frac{2}{\pi} \int_{\frac{\pi}{4}}^{\frac{3\pi}{4}} \frac{1 - \cos(2x)}{2} dx \\ &= \frac{1}{\pi} \left[x - \frac{\sin(2x)}{2} \right]_{\frac{\pi}{4}}^{\frac{3\pi}{4}} \\ &= \frac{1}{\pi} \left(\frac{3\pi}{4} - \frac{\pi}{4} - \frac{\sin(\frac{3\pi}{2})}{2} + \frac{\sin(\frac{\pi}{2})}{2} \right) \\ &= \frac{1}{\pi} \left(\frac{\pi}{2} + \frac{1}{2} + \frac{1}{2} \right) \\ &= \frac{1}{2} + \frac{1}{\pi}. \end{aligned}$$

Thus, the probability $P_{\frac{\pi}{4}, \frac{3\pi}{4}}$ of finding the particle in the range $\frac{\pi}{4} < x < \frac{3\pi}{4}$ is $\frac{\pi+2}{2\pi}$ or 81.83

5 Quantum Operators and Observables

5.1 Explanation

In quantum mechanics, operators are more than just mathematical constructs; they are the linchpins that connect the abstract Hilbert space of quantum states to measurable physical quantities. Unlike classical physics, where physical properties are directly observable, quantum operators act on state vectors in the complex Hilbert space to extract observable properties. Observables are fundamental to understanding the outcomes of quantum measurements, as they are directly associated with the eigenvalues of quantum operators.

5.2 Understanding Observables

An observable in quantum mechanics is represented by a Hermitian operator. The eigenvalues of these operators correspond to the possible outcomes of measuring the associated physical quantity. When a measurement is performed, the system's state collapses to an eigenstate of the operator, and the corresponding eigenvalue becomes the observed value. This quantization of observables is a key feature distinguishing quantum mechanics from classical physics.

5.3 Common Quantum Operators

Key operators in quantum mechanics, each representing a fundamental physical quantity, include:

- **Position Operator \hat{x} :** It acts on a state vector to yield the particle's position. Mathematically, in one dimension, it is simply \hat{x} , while in three dimensions, it is represented by $\hat{x}, \hat{y}, \hat{z}$.
- **Momentum Operator \hat{p} :** Corresponding to the particle's momentum, this operator in position representation takes the form of a differential operator, $-i\hbar \frac{\partial}{\partial x}$.
- **Hamiltonian Operator \hat{H} :** Central to the dynamics of quantum systems, this operator encapsulates the total energy (kinetic plus potential) and forms the core of the Schrödinger equation, $\hat{H}\Psi = E\Psi$.

Example

Consider a particle confined in a one-dimensional box with width L . The particle's wave functions are described by:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \dots \quad (10)$$

In this scenario, the potential energy inside the box is zero, so the Hamiltonian operator, representing only the kinetic energy, is given by:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}. \quad (11)$$

Applying \hat{H} to $\psi_n(x)$ yields:

$$\hat{H}\psi_n(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_n(x) = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L} \right)^2 \psi_n(x). \quad (12)$$

This result shows that $\psi_n(x)$ is an eigenfunction of \hat{H} with corresponding energy eigenvalue $E_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L} \right)^2$.

In the next class we will explore the profound implications of these operators and their eigenvalues in understanding quantum behavior.

6 Heisenberg Uncertainty Principle

The Heisenberg Uncertainty Principle is a famous uncertainty principle in quantum mechanics, emphasizing the intrinsic limitations in measuring position and momentum, simultaneously.

Remark: We will go deeper in the Uncertainty Principle for all non-commuting operators later on.

6.1 Mathematical Expression

The principle is quantitatively expressed as:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}, \quad (13)$$

where σ_x and σ_p represent the standard deviations (uncertainties) in position and momentum, respectively, and \hbar is the reduced Planck's constant.

6.2 Physical Interpretation

This principle arises from the wave-particle duality of quantum objects. It implies that attempting to precisely determine a particle's position (σ_x) increases the uncertainty in its momentum (σ_p), and vice versa. This is not a limitation of measurement technology but a fundamental characteristic of quantum systems.

Example

For an electron with a position uncertainty of 1 nm (1×10^{-9} m), the minimum uncertainty in its momentum (σ_p) can be calculated using the Heisenberg formula:

Given:

$$\begin{aligned} \sigma_x &= 1 \times 10^{-9} \text{ m}, \\ \hbar &= 1.05 \times 10^{-34} \text{ Js}. \end{aligned}$$

The minimum uncertainty in momentum is:

$$\begin{aligned} \sigma_p &\geq \frac{\hbar}{\sigma_x} \\ &= \frac{1.05 \times 10^{-34}}{1 \times 10^{-9}} \\ &\approx 5.25 \times 10^{-26} \text{ kg m/s}. \end{aligned}$$

This calculation illustrates the significant momentum uncertainty for an electron confined to such a small region, demonstrating the core concept of the Heisenberg Uncertainty Principle in quantum mechanics.

6.3 Intuition Behind the Heisenberg Uncertainty Principle

The Heisenberg Principle principle can be intuitively understood by examining the probability densities of different wave functions.

Probability Density of a Gaussian Wave Packet

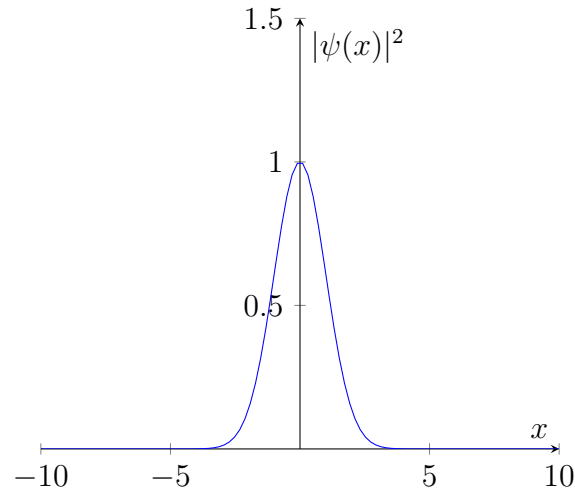


Figure 2: Plot of $|\psi(x)|^2$ illustrating the Gaussian shape centered at $x_0 = 0$ with $\sigma = 1$

The Gaussian wave packet, characterized by a bell-shaped curve, represents a state where the position of the particle is relatively well-defined (within the width of the packet), but its momentum is less certain. This is due to the Fourier transform relationship between position and momentum representations in quantum mechanics.

Probability Density of a Sinusoidal Wave Function

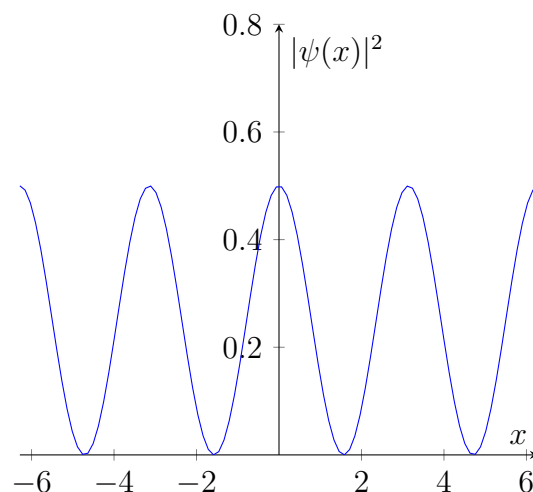


Figure 3: Plot of $|\psi(x)|^2$ for a sinusoidal wave, showing a periodically varying probability density, indicative of a less defined position but more defined momentum.

Conversely, the sinusoidal wave function demonstrates a state with a more defined momentum (evidenced by its regular wavelength), but an indeterminate position, as the probability density is spread uniformly.

7 Ehrenfest Theorem

The Ehrenfest Theorem asserts that the expectation values in quantum mechanics obey classical mechanics, implying:

$$\langle p \rangle = m \langle v \rangle = m \frac{d\langle x \rangle}{dt} \quad (14)$$