

Notes on Quantum Mechanics

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I. INTRODUCTION AND FUNDAMENTAL CONCEPTS

A. The birth of Quantum Theory

1. Black Body Radiation

1. Setup: Imagine a closed cavity with opaque inner walls, all held at a fixed temperature T . Suppose there's a tiny hole on the cavity

- Radiation entering the hole from outside gets absorbed after multiple reflections.
- The escaping radiation comes from the thermal equilibrium radiation inside.

What do you see?

- If the cavity is at absolute zero, you see nothing — it's perfectly black.
- If the cavity is at temperature T , you see thermal radiation, described by a frequency-dependent energy density

$$E_\omega = E_\omega(T), \quad (1)$$

where E_ω is the radiation energy density at frequency ω .

2. Failures of Classical Theories:

Rayleigh-Jeans Law (classical EM + statistical mechanics):

$$E_\omega = \frac{8\pi kT}{c^3} \omega^2. \quad (2)$$

This law is accurate at low frequencies ω , but it diverges at high ω , leading to the so-called ultraviolet catastrophe.

Wien's Law:

$$E_\omega = c_1 \omega^3 e^{-c_2 \omega/T}, \quad \text{where } \frac{c_1}{c_2} = \frac{8\pi k}{c^3}, \quad (3)$$

Matches experiment at high frequencies, but fails at low frequencies.

Neither law matches the entire experimental black body spectrum, see FIG. 1.

3. Planck's Breakthrough (1900): To explain the full spectrum, Planck proposed:

$$E_\omega = \frac{c_1 \omega^3}{e^{c_2 \omega/T} - 1}. \quad (4)$$

- This formula matches Rayleigh-Jeans at low ω and Wien's law at high ω .
- Fits experiment exactly if $c_2 = \hbar = 6.6 \times 10^{-34} J \cdot s$.

Planck introduced a revolutionary assumption:

- Energy is not radiated continuously.
- Radiation at frequency ω comes in discrete packets (quanta) of energy $E = \hbar\omega$.
- No energy is emitted at that frequency unless it's at least $\hbar\omega$.

This was the first step toward quantum theory.

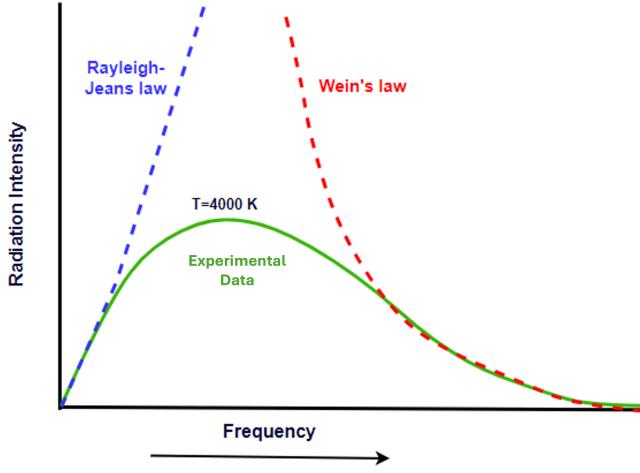


FIG. 1: Comparison of classical and experimental results for black body radiation at $T = 4000\text{K}$. The Rayleigh-Jeans law (blue, dashed) matches low-frequency behavior but diverges at high frequencies, leading to the ultraviolet catastrophe. Wien's law (red, dashed) fits the high-frequency tail but fails at low frequencies. Only the experimental curve (green) fits the full spectrum — a discrepancy that led to Planck's radiation law and the birth of quantum theory.

2. Einstein's Photon Hypothesis (1905)

Einstein extended Planck's idea and proposed that light itself consists of particles — *photons* — each with energy:

$$E = \hbar\omega. \quad (5)$$

To explain the photoelectric effect(see FIG. 2):

- Electrons are only ejected from a metal if the incoming light has frequency ω greater than a threshold.
- The electron's kinetic energy is:

$$\frac{1}{2}mv^2 = \hbar\omega - A, \quad (6)$$

where A is the work function of the material.

- Increasing light intensity increases the number of emitted electrons, but *not* their energy.

These observations cannot be explained by classical wave theory, which predicts that light shows both wave-like and particle-like properties, i.e., wave-particle duality. This duality is a cornerstone of quantum mechanics.

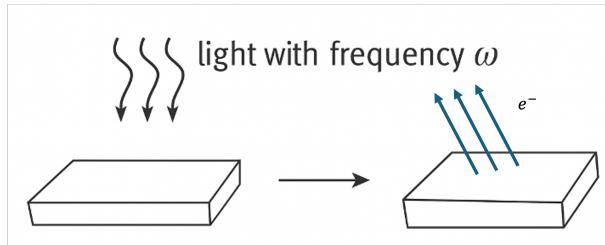


FIG. 2: In the photoelectric effect, photons with energy $\hbar\omega$ strike a metal surface. If $\hbar\omega > A$, electrons are ejected with kinetic energy $K = \hbar\omega - A$.

3. Atomic Models and the Quantum Puzzle

1. Thomson's "Plum Pudding" Model (1897): The atom is a positively charged sphere with embedded electrons (like raisins in pudding), see FIG. 3. It explains overall charge neutrality but not atomic structure or scattering experiments.

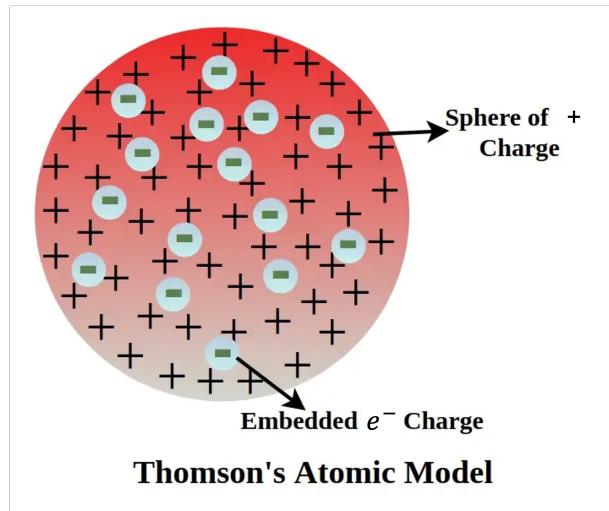


FIG. 3: J.J. Thomson's "plum pudding" model of the atom (1897). The atom is visualized as a positively charged sphere in which negatively charged electrons are embedded, like raisins in a pudding.

2. Rutherford's Nuclear Model (1911):

- Based on the gold foil experiment: most alpha particles pass through, but some scatter sharply, see FIG. 4.
- Conclusion: atoms have a dense, positively charged nucleus. Electrons orbit like planets around the sun

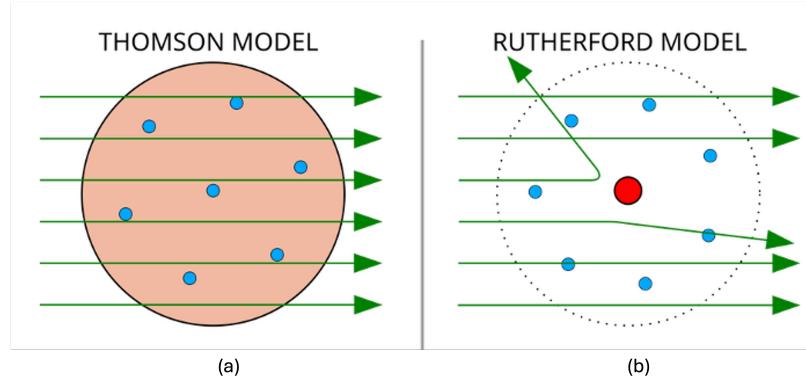


FIG. 4: Comparison of atomic scattering predictions. (a) Thomson's model predicts that alpha particles pass through with only slight deflection due to the uniform positive charge distribution. (b) Rutherford's model, with a dense central nucleus, predicts rare but large-angle deflections, which was confirmed by the gold foil experiment and inconsistent with the Thomson model.

Problem: Classical electrodynamics predicts that accelerating charges (orbiting electrons) radiate energy. The electron should spiral into the nucleus in $\sim 10^{-11} s$, therefore the atom collapses. However, real atoms are stable!

3. Bohr's Model (1913): To solve the stability problem, Bohr proposed:

- Electrons occupy discrete, stable orbits (stationary states).

- These orbits correspond to quantized energy levels E_n , see FIG. 5. The atom's energy spectrum is therefore discrete.
- Electrons emit/absorb radiation only when jumping between levels:

$$\Delta E = E_{n'} - E_n = \hbar\omega, \quad (7)$$

Bohr's model successfully explains hydrogen's spectrum and fits data well.

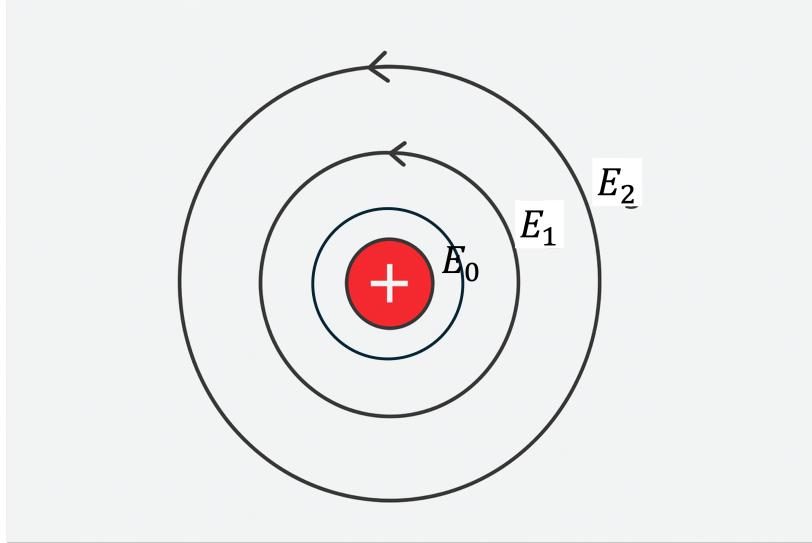


FIG. 5: Bohr model of the atom. Electrons orbit the positively charged nucleus in discrete stationary states labeled by energy levels E_0, E_1, E_2, \dots

4. A Sommerfeld's Quantization Condition: For periodic motion, the quantization rule is:

$$\oint p dq = nh, \quad n \in \mathbb{Z} \quad (8)$$

where q is the coordinate, p is the conjugate momentum, and n is the quantum number. For circular orbits (Bohr model):

$$p \cdot 2\pi r = nh \quad (9)$$

This gives quantized angular momentum and links wave ideas with orbital motion.

4. Heisenberg's matrix mechanics

1925-1927, Heisenberg, Born, and Jordan developed a formulation of quantum mechanics to replace classical quantities with matrices:

- Classical variables like position q and momentum p are promoted to operators \hat{q}, \hat{p} on a Hilbert space.
- The classical Poisson bracket becomes the commutator:

$$[\hat{q}, \hat{p}] = \hat{q}\hat{p} - \hat{p}\hat{q} = i\hbar\{q, p\} = i\hbar. \quad (10)$$

Time evolution: In the Heisenberg picture, observables evolve via:

$$\dot{A} = \{A, H\} \implies \frac{d}{dt} A_H(t) = \frac{i}{\hbar} [H_H(t), A_H(t)] + \left(\frac{\partial A_S}{\partial t} \right)_H, \quad (11)$$

- The state vectors $|\psi\rangle$ is time-indep.

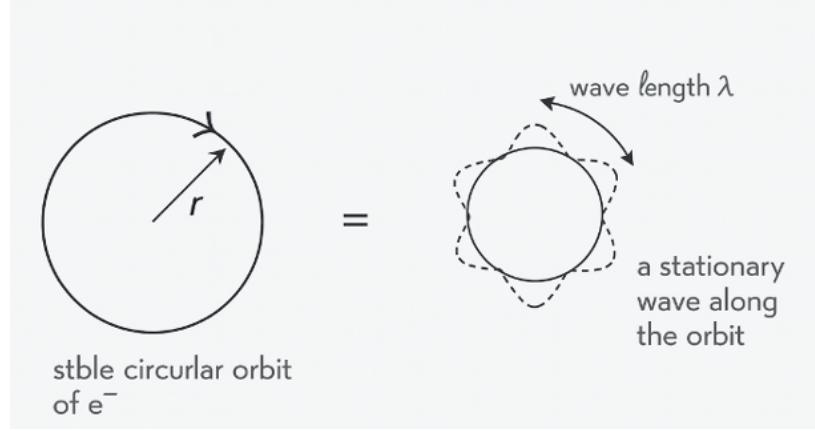


FIG. 6: Visual representation of Bohr's quantization condition from a wave perspective. A stable circular orbit of an electron corresponds to a standing wave fitting exactly along the orbit.

- Observables(operators) \hat{A} carry the time dependence. Here, “H” and “S” label observables in Heisenberg and Schrödinger picture respectively, H is the Hamiltonian.

Key insight: In quantum theory, physical quantities are not always simultaneously measurable (non-commuting operators), leading to the **Heisenberg’s Uncertainty Principle**:

$$\Delta q \Delta p \geq \frac{\hbar}{2}. \quad (12)$$

5. Schrodinger’s wave mechanics(1926)

- Inspired by de Broglie’s hypothesis (1923) that particles like electrons have wave-like properties:

$$\lambda = \frac{h}{p}, \quad \omega = \frac{E}{\hbar}, \quad (13)$$

see FIG. 6, a stable orbit corresponds to a standing wave:

$$2\pi r = n\lambda, \quad n = 1, 2, 3, \dots \implies J = pr = \frac{\hbar n}{2\pi}, \quad (14)$$

which is also the quantization condition of Bohr’s model.

- Schrödinger proposed that particles are described by a wavefunction $\psi(x, t)$, not a definite trajectory.

Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi. \quad (15)$$

This wave-based formulation is mathematically equivalent to Heisenberg’s matrix mechanics, but conceptually different.

B. Wave Nature of Particles

1. Particle-Wave Duality and de Broglie’s Hypothesis

In quantum mechanics, every matter particle is associated with a wave, described by:

$$E = \hbar\omega, \quad p = \hbar k = \frac{h}{\lambda} \quad (16)$$

This is the foundational idea of **de Broglie's hypothesis**.

Why don't we see matter waves in classical physics?

- For macroscopic objects, the associated wavelengths are extremely small, making wave-like behavior unobservable.
- For microscopic particles like electrons, the de Broglie wavelength is comparable to atomic scales $\lambda \sim$ atomic scale. Therefore, quantum effects become relevant at small scales.

Thus, quantum mechanics describes nature at the microscopic level using a wave function $\psi(x, t)$, which encodes the probability amplitude of finding a particle at position x and time t .

2. The Schrödinger Equation and Wave Functions

Quantum systems are described by a complex-valued wave function $\psi(x, t)$, which evolves according to the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = \hat{H} \psi(\vec{x}, t) \quad (17)$$

where the Hamiltonian operator \hat{H} is:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(x). \quad (18)$$

3. Superposition and Wave Packets

A single-frequency wave is given by the plane wave:

$$\psi_k(x) = e^{ikx}, \quad (19)$$

where the wave number is $k = \frac{2\pi}{\lambda}$. But real particles are not perfectly delocalized. Instead, we describe them using wave packets, which is the superpositions of plane waves:

$$\psi(x) = \sum_k a_k \psi_k(x), \quad (20)$$

or more generally, via Fourier transform:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(k) e^{ikx} dk \quad (21)$$

where $a(k)$ gives the amplitude of each wave number k , see FIG. 7. The inverse Fourier transform recovers $a(k)$ from $\psi(x)$:

$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx. \quad (22)$$

This pair of equations defines a full Fourier transform framework for wave packets.

Example: A Gauss Wave packet is

$$\psi(x) = e^{-a^2 x^2 / 2} = \frac{1}{\sqrt{2\pi}} \int a(k) e^{ikx} dk. \quad (23)$$

Its Fourier transform is:

$$a(k) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-a^2 x^2 / 2 - ikx} dk. \quad (24)$$

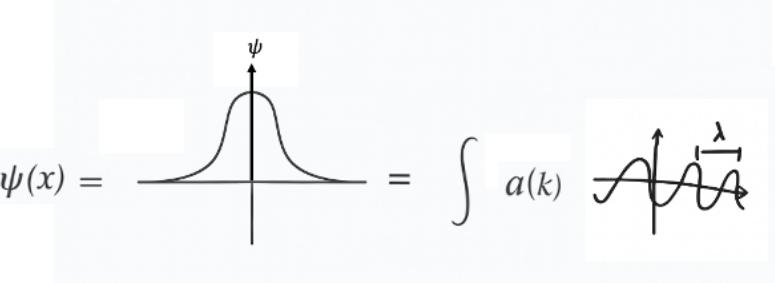


FIG. 7: A localized wave function $\psi(x)$ can be constructed as a superposition of plane waves with different wavelengths (or momenta).

This represents a localized particle in space (see FIG. 7).

Dirac Delta Function and Orthogonality: Plane waves satisfy an orthogonality relation leading to:

$$\int_{-\infty}^{\infty} e^{i(k'-k)x} dx = 2\pi\delta(k - k') \quad (25)$$

This ensures the coefficients $a(k)$ are uniquely determined by $\psi(x)$:

$$\int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx = a(k) \quad (26)$$

Warning: The delta function $\delta(k)$ is not a function in the traditional sense. It is a distribution, only defined inside integrals:

$$\int_{-\infty}^{\infty} \delta(k)f(k) dk = f(0). \quad (27)$$

4. Motion and Dispersion of Wave Packets

A general plane wave evolves as:

$$\psi_k(x, t) = e^{i(kx - \omega t)}. \quad (28)$$

Then, for a fixed phase $kx - \omega t = \text{const}$, we will have

$$kdx = \omega dt \rightarrow v_{\text{phase}} = \frac{dx}{dt} = \frac{\omega}{k} \quad (29)$$

Therefore, the phase velocity is: $v_{\text{phase}} = \frac{\omega}{k}$.

- For eEm waves, the dispersion relation is $\omega = ck \implies v_{\text{phase}} = c$. This matches the speed of light.
- For a non-relativistic particle with slow motion:

$$E = \frac{p^2}{2m} \implies \omega = \frac{\hbar k^2}{2m} \quad (30)$$

which is different from EM wave, because EM wave is photon traveling with speed of light, which is relativistic particle. The wave packet is described as:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a(k) e^{ikx - i\omega(k)t} dk. \quad (31)$$

Assuming $a(k)$ is peaked at k_0 , linearize $\omega(k)$

$$\omega(k) \approx \omega_0 + (k - k_0)\omega'_0, \quad (32)$$



FIG. 8: A wave packet $\psi(x, t)$ is formed by modulating a high-frequency carrier wave $e^{ik_0 - i\omega_0 t}$ with a slowly varying envelope. The envelope determines the spatial localization of the particle, while the carrier encodes the oscillatory behavior associated with the particle's momentum and energy.

where $\omega(k_0) = \omega_0$ and $\omega'_0 = \frac{d\omega}{dk}|_{k_0}$. Then, the wave packet in x -space is:

$$\begin{aligned}\psi(x, t) &\approx \frac{e^{ik_0 x - i\omega_0 t}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a(k) e^{i(k-k_0)x - i(k-k_0)\omega'_0 t} dk \\ &= e^{ik_0 x - i\omega_0 t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a(k) e^{i(k-k_0)(x - \omega'_0 t)} dk.\end{aligned}\quad (33)$$

Here, $e^{ik_0 x - i\omega_0 t}$ is the plane wave, and $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a(k) e^{i(k-k_0)(x - \omega'_0 t)} dk$ is the envelope of the wave packet, see FIG. 8. The envelope moves with group velocity:

$$v_g = \frac{dx}{dt} = \omega'_0 = \frac{d\omega}{dk}\Big|_{k_0}. \quad (34)$$

To see how the packet spreads over time, we expand $\omega(k)$ to second order:

$$\omega(k) \approx \omega_0 + (k - k_0) \frac{d\omega}{dk}|_{k_0} + \frac{1}{2} (k - k_0)^2 \frac{d^2\omega}{dk^2}\Big|_{k_0} \quad (35)$$

Then, the wave packet is:

$$\psi(x, t) \approx e^{i(k_0 x - \omega_0 t)} \cdot \int a(k - k_0) \cdot e^{i[\xi(x - v_g t) - \frac{1}{2}\beta\xi^2 t]} d\xi \quad (36)$$

where $\xi = k - k_0$, $v_g = \frac{d\omega}{dk}|_{k_0}$ is the group speed, and $\beta = \frac{d^2\omega}{dk^2}|_{k_0}$ measures the dispersion of the medium.

This form separates the wavefunction into a rapidly oscillating carrier $e^{i(k_0 x - \omega_0 t)}$ and a slowly varying envelope governed by the integral. To make the effect of dispersion explicit, we consider a Gaussian distribution in momentum space:

$$a(k) = e^{-k^2/(2\alpha^2)}, \quad \text{with } k_0 = 0. \quad (37)$$

Plugging this into the expression for $\psi(x, t)$, the integral can be evaluated explicitly. The resulting wave packet is:

$$\psi(x, t) = e^{-i\omega_0 t} \cdot \frac{\alpha}{\sqrt{1 + i\beta\alpha^2 t}} \cdot \exp\left(-\frac{(x - v_g t)^2 \alpha^2}{2(1 + i\beta\alpha^2 t)}\right). \quad (38)$$

Taking the modulus squared yields the probability density:

$$|\psi(x, t)|^2 = \frac{\alpha^2}{\sqrt{1 + \beta^2\alpha^4 t^2}} \cdot \exp\left(-\frac{(x - v_g t)^2 \alpha^2}{1 + \beta^2\alpha^4 t^2}\right). \quad (39)$$

This shows two key features: 1. the wave packet moves at the group velocity v_g ; 2. It spreads over time due to dispersion. The width of the packet grows as

$$\zeta(t) = \frac{\sqrt{1 + \beta^2\alpha^4 t^2}}{\alpha}. \quad (40)$$

This is analogous to the width of a Gaussian function $e^{-\frac{x^2}{2\zeta^2}}$. As time increases $t \rightarrow \infty$, the width $\zeta(t) \rightarrow \infty$, meaning the wave packet spreads out in space. This behavior is visualized in FIG. 9 and 10, which shows how the initially localized wave packet becomes broader over time due to dispersion.

Thus, while De Broglie's wave concept helps connect particles with wave-like properties, a naive interpretation of matter waves as non-spreading monochromatic waves would be incorrect.

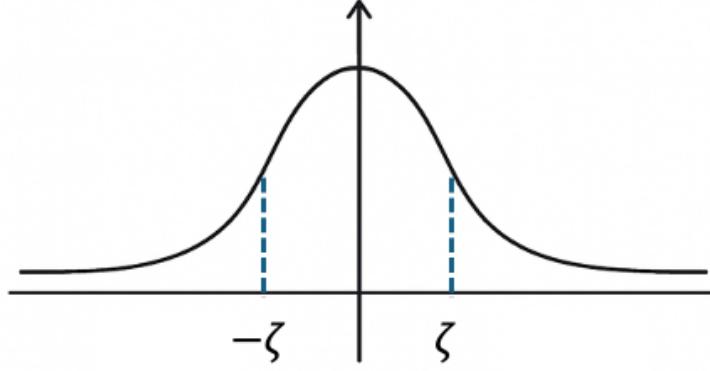


FIG. 9: Time evolution of the wave packet width $\zeta(t)$. The packet spreads over time due to the second-order dispersion.

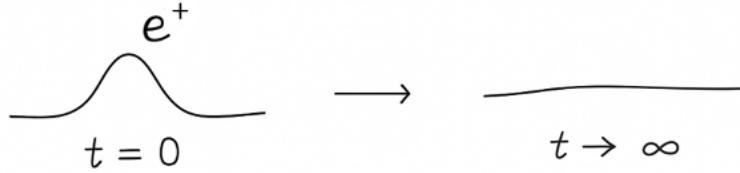


FIG. 10: Dispersion of a matter wave packet. Although initially localized, the wave packet spreads as it evolves.

II. WAVE FUNCTIONS AND THE SCHRÖDINGER EQUATION

A. Probabilistic Interpretation of the Wave Function: Born's Rule

The wave function $\psi(x, t)$ is not directly observable, but its squared magnitude describes the probability distribution of a particle in space:

$$|\psi(x, t)|^2 dx = \text{probability of finding the particle in } [x, x + dx]. \quad (41)$$

Double-slit experiment:

- Classical Particle Picture (no interference): In a double-slit experiment, a classical particle passes through slit 1 or slit 2, with respective distributions $\rho_1(x)$ and $\rho_2(x)$. The total distribution is additive:

$$\rho_{12}(x) = \rho_1(x) + \rho_2(x) \quad (42)$$

This is shown in Fig. 11.

- Wave Interpretation (interference): For classical waves (EM wave or sound wave), the wave amplitudes $\psi_1(x)$, $\psi_2(x)$ interfere:

$$I_{12}(x) = |\psi_1(x) + \psi_2(x)|^2 = |\psi_1|^2 + |\psi_2|^2 + \psi_1^* \psi_2 + \psi_1 \psi_2^* \quad (43)$$

This interference is shown in Fig. 12.

- Electrons are sent one at a time through a double-slit, the same interference pattern emerges on the detection screen, but the interpretation differs: it reflects a probability distribution. See Fig. 13.

Born's Rule and Properties of the Wave Function: For microscopic particle, e.g., e^- , we define the wavefunction $\psi(\vec{x}, t)$, and the probability amplitude satisfying

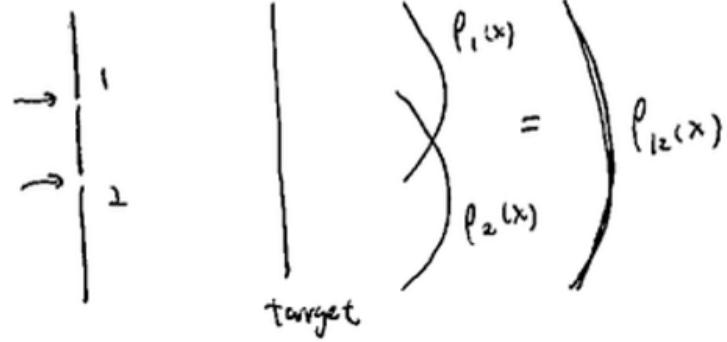


FIG. 11: Double-slit experiment interpreted as classical particles. No interference pattern appears.

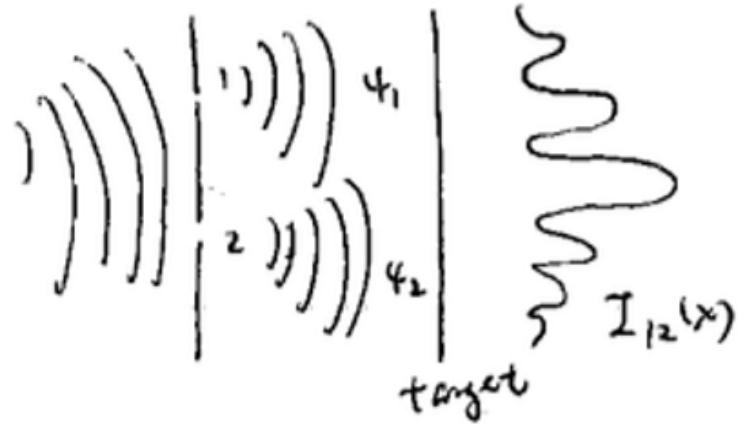


FIG. 12: Interference pattern from classical waves.

- The wave function $\psi(\vec{x}, t)$ is a complex-valued probability amplitude.
- The physical probability density is given by $|\psi(\vec{x}, t)|^2$.
- If two wavefunctions ψ_1, ψ_2 are allowed, so is their sum:

$$\psi = \psi_1 + \psi_2 \quad (44)$$

which is the superposition principle. It is also qualified as a probability amplitude of the particle.

- Probability in a volume element $\Delta x_1 \Delta x_2 \Delta x_3$ is:

$$|\psi(\vec{x}, t)|^2 \Delta x_1 \Delta x_2 \Delta x_3. \quad (45)$$

- Normalization (Born's Rule):

$$\int_{\mathbb{R}^3} |\psi(\vec{x}, t)|^2 d^3x = 1 \quad (46)$$

This is a fundamental principle in quantum mechanics.

Note: If ψ is not normalized but satisfies:

$$\int |\psi(\vec{x}, t)|^2 d^3x = N < \infty \quad (47)$$

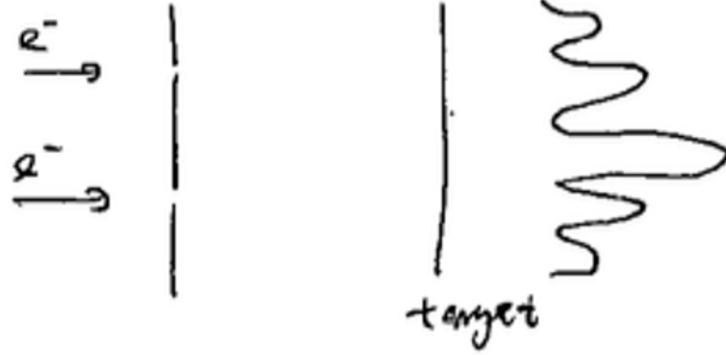


FIG. 13: Double-slit experiment with electrons. The resulting number density is a probability pattern.

we normalize it by:

$$\psi \rightarrow \frac{1}{\sqrt{N}}\psi \quad (48)$$

This interpretation, known as Born's rule, is foundational in quantum mechanics. It explains how wave behavior gives rise to probabilistic particle measurements.

B. Hilbert Space and the Structure of Quantum States

A Hilbert space is a mathematical structure used to describe quantum states. It is a complex vector space equipped with an inner product and is complete with respect to the norm induced by this inner product. Specifically, if V is a complex vector space, the inner product $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{C}$ satisfies:

- Linearity: $\langle \phi, c\psi \rangle = c\langle \phi, \psi \rangle$ and $\langle c\phi, \psi \rangle = c^*\langle \phi, \psi \rangle$ for any $c \in \mathbb{C}$.
- Conjugate symmetry: $\langle \phi, \psi \rangle = \overline{\langle \psi, \phi \rangle}$.
- Positivity: $\langle \phi, \phi \rangle \geq 0$, and equality iff $\phi = 0$.
- Cauchy-Schwarz inequality: $|\langle \phi, \psi \rangle|^2 \leq \langle \phi, \phi \rangle \langle \psi, \psi \rangle$ with norm: $\|\phi\| = \sqrt{\langle \phi, \phi \rangle}$.

Typical examples include:

- Finite-dimensional complex space \mathbb{C}^n with the Hermitian inner product:

$$\psi = (\psi_1, \psi_2, \dots, \psi_n), \quad \phi = (\phi_1, \phi_2, \dots, \phi_n), \quad \langle \phi, \psi \rangle = \sum_{i=1}^n \overline{\phi_i} \psi_i \quad (49)$$

where $\psi_i, \phi_i \in \mathbb{C}$.

- Real Euclidean space \mathbb{R}^3 with the dot product: $\mathbb{R}^3: \vec{v} \cdot \vec{u} = v_1 u_1 + v_2 u_2 + v_3 u_3$.

In quantum mechanics, the state of a particle is described by a wave function $f(x)$, which is a complex-valued function on \mathbb{R}^3 . The collection of all such wave functions forms a vector space over \mathbb{C} . That is, if $f(x)$ and $g(x)$ are wave functions, then any linear combination $c_1 f(x) + c_2 g(x)$ is also a valid wave function, where $c_1, c_2 \in \mathbb{C}$. Then, we define an inner product on this space as

$$\langle f, g \rangle = \int_{\mathbb{R}^3} \overline{f(\vec{x})} g(\vec{x}) d^3x, \quad (50)$$

which satisfies the standard properties of a complex inner product:

- Conjugate symmetry: $\langle f, g \rangle = \overline{\langle g, f \rangle}$

- Linearity in the second argument: $\langle f, c_1 g_1 + c_2 g_2 \rangle = c_1 \langle f, g_1 \rangle + c_2 \langle f, g_2 \rangle$.
- Positivity: $\langle f, f \rangle \geq 0$, with equality if and only if $f = 0$.

Moreover, the Cauchy-Schwarz inequality holds in this space:

$$\left| \int_{\mathbb{R}^3} \overline{f(x)} g(x) dx \right|^2 \leq \left(\int_{\mathbb{R}^3} |f(x)|^2 dx \right) \left(\int_{\mathbb{R}^3} |g(x)|^2 dx \right). \quad (51)$$

This ensures that the inner product $\langle f, g \rangle$ is finite as long as both functions are square-integrable, meaning

$$\|f\|^2 = \int_{\mathbb{R}^3} |f(x)|^2 dx < \infty, \quad \|g\|^2 = \int_{\mathbb{R}^3} |g(x)|^2 dx < \infty. \quad (52)$$

Physically, this condition means that $f(x) \rightarrow 0$ sufficiently fast as $|x| \rightarrow \infty$, so that the total probability is finite and can be normalized. The set of all square-integrable wave functions on \mathbb{R}^3 , i.e., all $f(x) \in \mathbb{C}$ such that

$$\int |f(x)|^2 dx < \infty, \quad (53)$$

forms a Hilbert space, denoted $L^2(\mathbb{R}^3)$. This space has the following key features:

- It is a vector space over \mathbb{C} : you can add wave functions and multiply by complex scalars.
- It is infinite-dimensional: there are infinitely many linearly independent wave functions on \mathbb{R}^3 .
- It is complete with respect to the norm $\|f\| = \sqrt{\langle f, f \rangle}$, meaning every Cauchy sequence of wave functions converges to a function within the space.

Thus, the mathematical framework for quantum states is grounded in the structure of an infinite-dimensional Hilbert space.

To construct wave functions from simple basis functions, one can consider breaking \mathbb{R} into unit intervals:

$$\mathbb{R}^1 = \bigcup_{n=-\infty}^{\infty} [n, n+1] \quad (54)$$

here we define step functions on unit intervals:

$$\chi_n(x) = \begin{cases} 1 & x \in [n, n+1] \\ 0 & \text{otherwise} \end{cases} \quad (55)$$

with

$$\int |\chi_n(x)|^2 dx = \int_n^{n+1} dx = 1. \quad (56)$$

A function like

$$\psi(x) = \sum_{n=-\infty}^{\infty} c_n \chi_n(x) \quad (57)$$

can be formed as a linear combination of these steps. However, such piecewise constant functions are not sufficient to represent general smooth functions like Gaussians. Therefore, more refined bases (e.g., Fourier modes or orthogonal polynomials) are needed to span the full Hilbert space.

C. Wave functions in Position and Momentum space

The position representation of a quantum state describes the probability of finding a particle at point \vec{x} . In this representation, $|\psi(\vec{x})|^2 d^3x$ gives the probability of finding the particle in a volume element d^3x near \vec{x} . Alternatively, the same state can be described in momentum space using a Fourier transform:

$$\psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} d^3p. \quad (58)$$

Here, $\varphi(\vec{p})$ is the momentum-space wave function. $|\varphi(\vec{p})|^2$ gives the probability density for momentum. This duality between position and momentum representations is a central aspect of quantum mechanics.

A wave function for a particle with definite momentum \vec{p} is:

$$\psi(\vec{x}) = e^{i\vec{p}\cdot\vec{x}/\hbar}, \quad (59)$$

which is completely delocalized in space. To describe a localized particle at \vec{x}_0 , we use the delta function:

$$\psi(\vec{x}) = \delta(\vec{x} - \vec{x}_0). \quad (60)$$

Any wave function can be expressed in terms of these delta functions:

$$\psi(\vec{x}) = \int \psi(x_0) \delta(\vec{x} - \vec{x}_0) d^3x_0. \quad (61)$$

The normalization condition for the wave function is:

$$\int |\psi(\vec{x})|^2 d^3x = 1 \iff \int |\varphi(\vec{p})|^2 d^3p = 1. \quad (62)$$

This equivalence can be derived using the inverse Fourier transform and integrating out the resulting delta function:

$$\varphi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-i\vec{p}\cdot\vec{x}/\hbar} \psi(\vec{x}) d^3x. \quad (63)$$

Thus, the Hilbert space of quantum mechanics not only supports the standard structure of vector spaces but also encodes both the spatial and momentum properties of quantum systems through the choice of representation.

D. Heisenberg Uncertainty Principle

In classical mechanics, a particle's motion is described by a definite trajectory. At any moment, its position $\vec{x}(t)$ and momentum $\vec{p}(t)$ are simultaneously well-defined. In quantum mechanics, however, a particle's state is described by a wave function $\psi(\vec{x})$, which gives a probability amplitude, not a deterministic trajectory. The wave function $\psi(\vec{x})$ and its Fourier transform $\varphi(\vec{p})$ (momentum space representation) are related by:

$$\varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x) e^{-ipx/\hbar} dx \quad (64)$$

Generically, if $\psi(x)$ is sharply localized in x , then $\varphi(p)$ is widely spread in p , and vice versa. Let us consider two extreme examples:

- Plane wave: $e^{ip_0x/\hbar}$. This wave has definite momentum p_0 (so $\Delta p = 0$), but the probability density in position space is uniform: $|\psi(x)|^2 = \frac{1}{2\pi\hbar}$. This implies complete uncertainty in position: $\Delta x = \infty$.
- Delta Function: $\psi(x) = \delta(x - x_0)$. The particle is localized at x_0 , so $\Delta x = 0$, but in momentum space, $\varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx_0/\hbar}$ has equal magnitude for all p , implying $\Delta p = \infty$. Proof: the variance of momentum is defined as:

$$(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 \quad (65)$$

For this wave function: $\langle p \rangle$ is undefined (integral doesn't converge); $\langle p^2 \rangle$ is also undefined (again, divergent integral). Explicitly:

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} p^2 |\varphi(p)|^2 dp = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} p^2 dp = \infty \quad (66)$$

So the standard deviation $\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$ is infinite.

These examples are idealizations. In practice, neither $\delta(x - x_0)$ nor $e^{ipx/\hbar}$ is normalizable in L^2 , and hence they are not valid wave functions in the Hilbert space. However, they illustrate the limiting behavior of the uncertainty trade-off.

A physical, square-integrable example is a Gaussian wave packet:

$$\psi(x) = e^{-\alpha^2 x^2/2} \Rightarrow |\psi(x)|^2 = e^{-\alpha^2 x^2} \quad (67)$$

The Fourier transform is also a Gaussian:

$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x) e^{-ikx} dx = \frac{1}{\alpha} e^{-k^2/(2\alpha^2)} \Rightarrow |\varphi(k)|^2 = \frac{e^{-k^2/\alpha^2}}{\alpha^2} \quad (68)$$

Here, $\Delta x \sim 1/\alpha$ and $\Delta k \sim \alpha$ so:

$$\Delta x \cdot \Delta k \sim 1 \Rightarrow \Delta x \cdot \Delta p \sim \hbar \quad (69)$$

with $pk = \hbar$. The product $\Delta x \cdot \Delta p$ is minimized for Gaussian packets.

Heisenberg proves from the matrix mechanics: $\Delta x \Delta p \geq \frac{\hbar}{2}$, which is the **Heisenberg's Uncertainty Relation**. This will be rigorously proved later in the QM course. For now, we interpret it as a fundamental limit on the precision with which position and momentum can be simultaneously known.

Interpretation and Limits

- For any microscopic particle, its position \vec{x} and momentum \vec{p} cannot both be precisely measured at the same time.
- The uncertainty principle implies that a definite trajectory (as in classical mechanics) is no longer meaningful in quantum mechanics.
- For macroscopic objects, however, $\Delta x \cdot \Delta p \gg \hbar$, so classical trajectories emerge as good approximations.
- This corresponds to the semiclassical limit $\hbar \rightarrow 0$, where quantum mechanics recovers classical mechanics as an approximation.

III. OPERATORS FOR POSITION AND MOMENTUM

A. Expectation Values and Normalization

In quantum mechanics, the squared modulus of the wave function, $|\psi(\vec{x})|^2$, gives the probability density of finding a particle at position \vec{x} . If $\psi(\vec{x})$ is normalized, then

$$\int_{\mathbb{R}^3} |\psi(\vec{x})|^2 d^3x = 1. \quad (70)$$

The expectation value of position is defined as:

$$\langle \vec{x} \rangle = \int_{\mathbb{R}^3} \vec{x} |\psi(\vec{x})|^2 d^3x = \int_{\mathbb{R}^3} \overline{\psi(\vec{x})} \vec{x} \psi(\vec{x}) d^3x. \quad (71)$$

If $\psi(\vec{x})$ is not normalized (i.e., the integral of $|\psi(\vec{x})|^2$ is finite but not equal to 1), we define the normalized wave function as:

$$\psi_{\text{norm}}(\vec{x}) = \frac{\psi(\vec{x})}{\|\psi\|}, \quad \|\psi\|^2 = \int_{\mathbb{R}^3} |\psi(\vec{x})|^2 d^3x \quad (72)$$

Then the expectation value becomes:

$$\langle \vec{x} \rangle = \frac{\int \overline{\psi(\vec{x})} \vec{x} \psi(\vec{x}) d^3x}{\int |\psi(\vec{x})|^2 d^3x}. \quad (73)$$

Similarly, for any function of \vec{x} (e.g., a potential $V(\vec{x})$), the expectation value is:

$$\langle V \rangle = \frac{\int \overline{\psi(\vec{x})} V(\vec{x}) \psi(\vec{x}) d^3x}{\int |\psi(\vec{x})|^2 d^3x}. \quad (74)$$

B. Position Operator

Recall the inner product:

$$\int_{-\infty}^{+\infty} \overline{\psi(\vec{x})} \psi(\vec{x}) d^3x = \langle \psi, \psi \rangle = \|\psi\|^2 \quad (75)$$

For the position components $\vec{x} = (x_1, x_2, x_3)$, we write:

$$\int_{-\infty}^{+\infty} \overline{\psi(\vec{x})} x_i \psi(\vec{x}) d^3x = \langle \psi, x_i \psi \rangle. \quad (76)$$

The position operator \hat{x}_i acts by multiplication:

$$\hat{x}_i \psi(\vec{x}) := x_i \psi(\vec{x}), \quad i = 1, 2, 3. \quad (77)$$

It maps a wave function to another wave function by pointwise multiplication. The expectation value in Dirac notation is:

$$\langle \hat{x}_i \rangle = \frac{\langle \psi, \hat{x}_i \psi \rangle}{\langle \psi | \psi \rangle}. \quad (78)$$

C. Momentum Operator

The momentum-space wave function is given by the Fourier transform:

$$\varphi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} e^{-i\vec{p}\cdot\vec{x}/\hbar} \psi(\vec{x}) d^3x. \quad (79)$$

The expectation value of momentum is:

$$\langle \vec{p} \rangle = \frac{\int_{\mathbb{R}^3} \overline{\varphi(\vec{p})} \vec{p} \varphi(\vec{p}) d^3p}{\int_{\mathbb{R}^3} \overline{\varphi(\vec{p})} \varphi(\vec{p}) d^3p} \quad (80)$$

Using integration by parts and the inverse transform, we find:

$$\langle \vec{p} \rangle = \int_{\mathbb{R}^3} \overline{\psi(\vec{x})} (-i\hbar\nabla) \psi(\vec{x}) d^3x = \langle \psi, (-i\hbar\nabla) \psi \rangle. \quad (81)$$

with the momentum operator defined as:

$$\hat{p}_i \psi(\vec{x}) := -i\hbar \frac{\partial}{\partial x_i} \psi(\vec{x}) \quad (82)$$

This is a derivative operator acting on the Hilbert space of wave functions. The expectation value of momentum is:

$$\langle \vec{p} \rangle = \frac{\langle \psi, \hat{p}_i \psi \rangle}{\langle \psi, \psi \rangle}. \quad (83)$$

D. Operator Formalism in QM

In general, any physical quantity $f(\vec{x}, \vec{p})$ is promoted to an operator $\hat{f}(\vec{x}, \vec{p})$ acting on wave functions. The average (expectation value) of that quantity is:

$$\langle f \rangle = \frac{\langle \psi, \hat{f} \psi \rangle}{\langle \psi, \psi \rangle} \quad (84)$$

Examples:

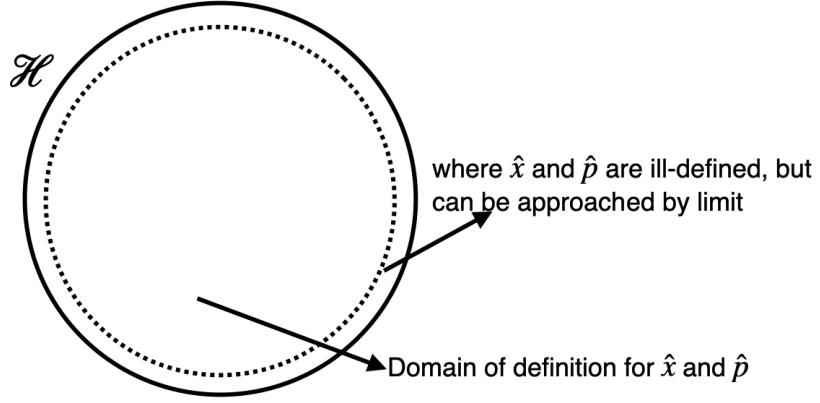


FIG. 14: Domain where \hat{x} and \hat{p} are well-defined (solid region); outside, they are ill-defined but approachable by limits.

- Kinetic energy: $T = \frac{\vec{p}^2}{2m} \Rightarrow \hat{T} = -\frac{\hbar^2}{2m} \nabla^2$.
- Potential energy: $V(\vec{x}) \Rightarrow \hat{V}\psi(\vec{x}) = V(\vec{x})\psi(\vec{x})$.
- Hamiltonian: $\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x})$.
- Angular momentum: $\vec{L} = \vec{x} \times \vec{p}$ with components:

$$\begin{aligned}\hat{L}_x &= -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right), \\ \hat{L}_y &= -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right), \\ \hat{L}_z &= -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right).\end{aligned}\tag{85}$$

E. Commutators and Uncertainty

The fundamental commutator between position and momentum operators is:

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij},\tag{86}$$

which implies the Heisenberg uncertainty relation:

$$\Delta x_i \Delta p_i \geq \frac{\hbar}{2}\tag{87}$$

F. Domains of Operators and Subtleties

Since operators like \hat{x} and \hat{p} are unbounded, they are not defined on the entire Hilbert space $L^2(\mathbb{R}^3)$, but only on dense subspaces.

- For example, the function $\psi(x) = \chi_{[0,1]}(x) = \begin{cases} 1, & x \in [0, 1] \\ 0, & x \notin [0, 1] \end{cases}$ is square-integrable and normalized:

$$\int_0^1 |\psi(x)|^2 dx = 1,\tag{88}$$

which is qualified as wave function. But it is not differentiable, so the momentum operator $\hat{p}\psi(x) = -i\hbar \frac{\partial}{\partial x} \psi(x)$ is ill-defined.

- here exist functions $\psi(x)$ such that $|\psi(x)|^2 \sim \frac{1}{|x|^{1+\epsilon}}$ as $x \rightarrow \pm\infty$, which are square-integrable, but $\hat{x}\psi(x) = x\psi(x) \sim |x|^{\frac{1}{2}-\epsilon}$ is not, because

$$|\psi(x)x|^2 \sim |x|^{1-\epsilon} \implies \int_{-\infty}^{\infty} |\psi(x)x|^2 d^3x = \infty, \quad (89)$$

So, $\hat{x}\psi(x) \notin \mathcal{H}$.

These issues are handled rigorously using operator domains:

- The domains $\mathcal{D}(\hat{x})$ and $\mathcal{D}(\hat{p})$ are dense subsets of $L^2(\mathbb{R}^3)$.
- Even if a function is not in the domain, it can often be approximated arbitrarily well by smooth functions that are, see FIG. 15.

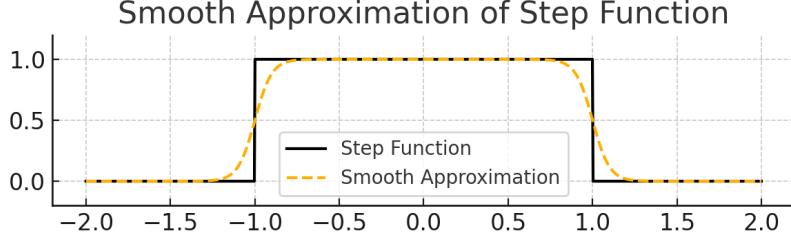


FIG. 15: Approximation of a discontinuous step function by smooth functions.

IV. TBA

A. State Superposition Principle

Given two wave functions, $\psi_1(x)$ and $\psi_2(x)$, any linear combination

$$C_1\psi_1(x) + C_2\psi_2(x) \quad (90)$$

is also a wave function. The wave function in momentum space

$$\psi(x) = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} d^3p. \quad (91)$$

- This represents a superposition of a continuous spectrum of plane waves.
- $\psi(x)$ is a state of the physical system.
- $\varphi(p)$ is the probability amplitude in momentum space, and $\psi(p)$ gives the amplitude to find the system in a state of fixed momentum p (as a plane wave).

Schrödinger's Cat Example:

$$\psi_{\text{cat}} = C_{\uparrow}\psi_{\uparrow} + C_{\downarrow}\psi_{\downarrow} \quad (92)$$

- ψ_{cat} is a state of the system (the cat).
- The Hilbert space is 2-dimensional, with basis states:
 - ψ_{\uparrow} : cat is alive.
 - ψ_{\downarrow} : cat is dead.
- Interpretation of Coefficients:

- C_{\uparrow} : probability amplitude of the system being in state ψ_{\uparrow} (cat is alive).
- C_{\downarrow} : probability amplitude of the system being in state ψ_{\downarrow} (cat is dead).
- But the system is completely described by ψ_{cat} which is a superposition. It describes all the probabilities of the system at all possible states (determine all the uncertainties).

In general, the Hilbert space is infinite-dimensional. Any state ψ of the system can be written as a superposition:

$$\psi = \sum_n C_n \psi_n \quad (93)$$

where ψ_n is the basis states of the Hilbert space, and C_n is the probability amplitude to find the system (described by ψ) in the state ψ_n .

B. Measurement Principle

Suppose your system is a single particle described by a state $\psi(x)$, and you want to measure its momentum. According to the Fourier transformation:

$$\psi(x) = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(p) e^{i\vec{p} \cdot \vec{x}/\hbar} d^3 p \quad (94)$$

where $\varphi(p)$ is probability amplitude in momentum space. $|\varphi(p)|^2$ is the probability density to measure momentum \vec{p} .

Step-by-Step Procedure: Measuring Momentum

- Goal: You want to measure momentum of a system in state ψ .
- Find the operator for momentum: $\hat{p} = -i\hbar\vec{\nabla}$.
- Solve the eigenvalue problem:

$$\hat{p} e^{i\vec{p} \cdot \vec{x}/\hbar} = \vec{p} e^{i\vec{p} \cdot \vec{x}/\hbar}. \quad (95)$$

where the eigenfunctions are $e^{i\vec{p} \cdot \vec{x}/\hbar}$, and the eigenvalues are \vec{p} .

- Expand $\psi(x)$ using the eigenfunctions:

$$\psi(x) = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(p) e^{i\vec{p} \cdot \vec{x}/\hbar} d^3 p, \quad (96)$$

where the momentum eigenfunctions form a complete basis.

- Interpretation:
 - The eigenvalues \vec{p} correspond to all possible momentum values you may obtain upon measurement.
 - The probability amplitude to obtain a specific momentum \vec{p}_0 is $\varphi(\vec{p}_0)$.
 - The probability is $|\varphi(\vec{p}_0)|^2$.
- After the measurement, you obtain p_0 which is the wave function “collapse” the corresponding eigenstate $e^{ip_0 \cdot \vec{x}/\hbar}$:

$$\psi(x) \xrightarrow[\text{get } p_0]{\text{measure } \hat{p}} e^{ip_0 \cdot \vec{x}/\hbar} \text{ collapsed}. \quad (97)$$

A general recipe of measurement principle: Given a system described by a state $\psi \in \mathcal{H}$, you want to measure a physical quantity A :

- Let $A = A^\dagger$ be a Hermitian operator. Look for the operator \hat{A} of the physical quantity $\hat{A} : \mathcal{H} \rightarrow \mathcal{H}$.
- Solve the eigenvalue problem of \hat{A} :

$$\hat{A}\psi_n = a_n \psi_n, \quad (98)$$

This guarantees real eigenvalues and orthonormal eigenfunctions.

- Expand the original state ψ using the eigenbasis ψ_n :

$$\psi = \sum_{n=1}^{\infty} c_n \psi_n \quad (99)$$

- the eigenvalues a_n are all possible value, you might obtain in the measurement of A :

$$a_n \leftrightarrow \psi_n \leftrightarrow c_n \quad (100)$$

the corresponding coefficient c_n from ψ is the probability amplitude to find $A = a_n$, where $|c_n|^2$ is the probability.

- After the measurement, ψ collapses to the eigenstate ψ_n corresponding to the output a_n :

$$\psi(x) \xrightarrow[\text{get } a_n]{\text{measure } A} \psi_n. \quad (101)$$

Examples and Understanding the Measurement Principle:

- Example 1: Normalized State and Total Probability: if $\|\psi\| = 1$, then the total probability is: $\sum_{n=1}^N |C_n|^2 = 1$. This follows from:

$$\langle \psi, \Phi \rangle = \sum_{i=1}^N \langle \psi, \psi_i \rangle \psi_i, \quad (102)$$

where $\{\psi_i\}$ is an orthonormal basis and $C_n = \langle \psi_n, \psi \rangle$.

- For any Hermitian matrix $A = A^\dagger = (A^*)^T$, its eigenvectors are orthogonal w.r.t $\langle \cdot, \cdot \rangle$, i.e.,

$$A\vec{e}_m = a_m \vec{e}_m \quad \Rightarrow \quad \langle \vec{e}_n, \vec{e}_m \rangle = \delta_{nm} \quad (103)$$

- Consider a particle in the state: $\psi(x) = e^{-x^2/2}$, we measure the kinetic energy T . Apply the Measurement Principle:

- Step 1: Find all possible values of T (i.e., the spectrum of the kinetic energy operator).
- Step 2: Find the probability to obtain a specific value T_0 .
- Step 3: Verify that the total probability is: $\sum P(T_n) = 1$.

Comments: No one truly knows why the measurement principle works. But we know it works: it provides a systematic recipe to do computation in quantum theory. All the predictions from QM using this principle agree remarkably well with experiments.

C. Schrödinger Equation

EOM for wavefunctions $\psi(\vec{x}, t)$: Let us recall the superposition principle: ψ_1, ψ_2 re wave functions, then $C_1\psi_1 + C_2\psi_2$ is also a wave function, i.e., if ψ_1, ψ_2 is the solution of E.O.M, then $C_1\psi_1 + C_2\psi_2$ is also the solution of E.O.M. Therefore, the equation of motion (EOM) must be linear.

Time-Dependent Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = \hat{H} \psi(\vec{x}, t) \quad (104)$$

For the case of a single particle:

$$\hat{H} = T + V \implies i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] \psi(\vec{x}, t) \quad (105)$$

where \hat{H} is an linear operator, i.e.,

$$\hat{H}(C_1\psi_1 + C_2\psi_2) = C_1\hat{H}\psi_1 + C_2\hat{H}\psi_2 \quad (106)$$

which holds for all operators in QM.

Motivation of Schrödinger Equation: Plane Wave Ansatz: Let us consider a free particle:

$$\psi(\vec{x}, t) = e^{i(\vec{k}\vec{x} - \omega t)/\hbar} = e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} \quad (107)$$

with the wave-particle duality:

$$\vec{p} = \hbar\vec{k}, \quad E = \hbar\omega. \quad (108)$$

From the plane wave, we have

$$\begin{aligned} -i\hbar\vec{\nabla}e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} &= \vec{p}e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}, \\ i\hbar\frac{\partial}{\partial t}e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} &= Ee^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}. \end{aligned} \quad (109)$$

where $\vec{\nabla}$ is the momentum operator, and $\frac{\partial}{\partial t}$ is the energy operator.

From Classical Energy to Quantum Equation: Classically, the free particle energy-momentum relation is

$$E = \frac{p^2}{2m} \quad (110)$$

which will be replaced by operator equation:

$$i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi. \quad (111)$$

- For $\psi = e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}$, we have

$$i\hbar\frac{\partial}{\partial t}e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} = Ee^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}, \quad -\frac{\hbar^2}{2m}\nabla^2e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} = \frac{p^2}{2m}e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}, \quad (112)$$

which shows that

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi \implies \left(E - \frac{p^2}{2m}\right)e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} = 0, \quad (113)$$

then $e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar}$ satisfies the equation iff

$$E = \frac{p^2}{2m}, \quad (114)$$

which relates to the dispersion relation $\omega = \frac{\hbar k^2}{2m}$.

Generalizing to Superposition of Plane Waves: From the wave functions

$$\psi(\vec{x}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(\vec{p}) e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} d^3p. \quad (115)$$

Then, the time evolution is

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(\vec{p}) E e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} d^3p \quad (116)$$

and the spatial part is

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(\vec{p}) \frac{p^2}{2m} e^{i(\vec{p}\cdot\vec{x} - Et)/\hbar} d^3p. \quad (117)$$

Therefore, from

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi \quad (118)$$

we will have

$$\frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(\vec{p}) \left(E - \frac{p^2}{2m} \right) e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar} d^3 p = 0. \quad (119)$$

Again, as $E = \frac{p^2}{2m}$, i.e., general solution to the equation $i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar}{2m} \nabla^2 \psi$ is

$$\psi(\vec{x}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(p) e^{i(\vec{p}\cdot\vec{x}-\frac{p^2}{2m}t)/\hbar} d^3 p \quad (120)$$

with arbitrary $\varphi(p)$. Then, we will have arbitrary superposition of plane waves $e^{i(\vec{p}\cdot\vec{x}-\frac{p^2}{2m}t)/\hbar}$ with $E = \frac{p^2}{2m}$.

If the particle moves in a potential $V(\vec{x})$, the classical total energy is:

$$E = \frac{p^2}{2m} + V(\vec{x}) \quad (121)$$

which is replaced with operators $E \rightarrow i\hbar \frac{\partial}{\partial t}$ and $\vec{p} \rightarrow -i\hbar \vec{\nabla}$:

$$i\hbar \frac{\partial}{\partial t} \psi = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] \psi \quad (122)$$

This is the Schrödinger equation for a non-relativistic single particle in a potential.

D. Conservation law of Probability in Quantum Mechanics

The total probability of finding a particle somewhere in space is always equal to 1 and does not change with time. This is ensured by the normalization condition of the wave function:

$$\int_{\mathbb{R}^3} |\psi(\vec{x}, t)|^2 d^3 x = 1 \quad (123)$$

This must hold at all times, which implies:

$$\frac{d}{dt} \int_{\mathbb{R}^3} |\psi(\vec{x}, t)|^2 d^3 x = 0 \quad (124)$$

This condition can be derived from the Schrödinger equation, which is consistent with the probabilistic interpretation of quantum mechanics when the potential is real (i.e., $V = \bar{V}$):

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi. \quad (125)$$

Taking the complex conjugate gives:

$$-i\hbar \frac{\partial \bar{\psi}}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \bar{\psi} + V \bar{\psi}, \quad (126)$$

Multiply the first equation by $\bar{\psi}$, and the second by ψ , then subtract. This leads to:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \|\psi\|^2 &= i\hbar \left(\bar{\psi} \frac{\partial \psi}{\partial t} + \psi \frac{\partial \bar{\psi}}{\partial t} \right) = -\frac{\hbar^2}{2m} (\bar{\psi} \nabla^2 \psi - \psi \nabla^2 \bar{\psi}) = -\frac{\hbar^2}{2m} (\bar{\psi} \nabla^2 \psi - \psi \nabla^2 \bar{\psi} + \nabla \psi \cdot \nabla \bar{\psi} - \nabla \psi \cdot \nabla \bar{\psi}) \\ &= -\frac{\hbar^2}{2m} [\nabla \cdot (\bar{\psi} \nabla \psi) - \nabla \cdot (\psi \nabla \bar{\psi})] = -\frac{\hbar^2}{2m} \nabla \cdot (\bar{\psi} \nabla \psi - \psi \nabla \bar{\psi}). \end{aligned} \quad (127)$$

We now define the probability density:

$$\rho = |\psi|^2, \quad (128)$$

and the probability current:

$$\vec{J} = -i\frac{\hbar}{2m}(\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}). \quad (129)$$

This gives the local **conservation law of probability**:

$$\frac{\partial\rho}{\partial t} + \nabla \cdot \vec{J} = 0. \quad (130)$$

This is known as the continuity equation for probability.

To interpret it physically, consider a finite region R in space with boundary S . Integrating over R and using the divergence theorem:

$$\frac{\partial}{\partial t} \int_R \rho d^3x + \int_R \nabla \cdot \vec{J} d^3x = \frac{\partial}{\partial t} \int_R \rho d^3x + \oint_S \vec{J} \cdot \hat{n} dS = 0, \quad (131)$$

where we use the Gauss theorem with $\int_R \nabla \cdot \vec{J} d^3x = \oint_S \vec{J} \cdot \hat{n} dS$ with \hat{n} the normal of S . The first term is the rate of change of probability inside R , and the second is the flux of probability current through the boundary. This means that any change in probability within R must be due to flow across the boundary, which is analogous to the continuity condition of fluid mechanics.

Now consider the entire space by taking $S \rightarrow \infty$:

$$\frac{\partial}{\partial t} \int_R \rho d^3x + \lim_{S \rightarrow \infty} \oint_S \vec{J} \cdot \hat{n} dS = 0. \quad (132)$$

If ψ vanishes fast enough at infinity, the boundary term disappears

$$\lim_{S \rightarrow \infty} \oint_S \vec{J} \cdot \hat{n} dS = 0. \quad (133)$$

This leads to the conclusion that the total probability in all of space is conserved:

$$\frac{\partial}{\partial t} \int_{\mathbb{R}^3} |\psi|^2 d^3x = 0. \quad (134)$$

E. Initial Value Problem and Propagator

Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right) \psi \quad (135)$$

is first-order in time. This means that once the initial condition $\psi(\vec{x}, 0)$ is given, the wave function at any later time t is completely determined.

Example: Free Particle Propagation: For a free particle, the potential is zero: $V(\vec{x}) = 0$. The Schrödinger equation becomes:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi \quad (136)$$

The general solution is a superposition of plane waves:

$$\psi(\vec{x}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \varphi(\vec{p}) e^{i(\vec{p} \cdot \vec{x} - Et)/\hbar} d^3p \quad \text{with} \quad E = \frac{p^2}{2m}. \quad (137)$$

To find the coefficients $\varphi(\vec{p})$, use the inverse Fourier transform of the initial wave function:

$$\varphi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(\vec{x}', 0) e^{-i\vec{p} \cdot \vec{x}'/\hbar} d^3x' \quad (138)$$

Substitute this into the solution:

$$\begin{aligned}\psi(\vec{x}, t) &= \frac{1}{(2\pi\hbar)^3} \int d^3x' d^3p \psi(\vec{x}', 0) e^{i[\vec{p} \cdot (\vec{x} - \vec{x}') - \frac{\vec{p}^2}{2m}t]/\hbar}, \\ &= \int G(\vec{x} - \vec{x}', t - 0) \psi(\vec{x}', 0) d^3x'.\end{aligned}\quad (139)$$

We define the propagator or Green's function $G(\vec{x} - \vec{x}', t)$ such that:

$$\psi(\vec{x}, t) = \int G(\vec{x} - \vec{x}', t) \psi(\vec{x}', 0) d^3x' \quad (140)$$

The propagator is given by:

$$G(\vec{x} - \vec{x}', t) = \frac{1}{(2\pi\hbar)^3} \int e^{i\vec{p} \cdot (\vec{x} - \vec{x}')/\hbar} e^{-i\frac{\vec{p}^2}{2m}t/\hbar} d^3p \quad (141)$$

This shows how each component in momentum space evolves and contributes to the wave function at time t . More general, we can write it as:

$$\psi(\vec{x}, t) = \int G(\vec{x} - \vec{x}', t - t') \psi(\vec{x}', t') d^3x' \quad (142)$$

with the propagator or Green's functions:

$$G(\vec{x} - \vec{x}', t - t') = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\vec{p} \cdot (\vec{x} - \vec{x}')/\hbar} e^{-i\frac{\vec{p}^2}{2m}(t-t')/\hbar} \quad (143)$$

Remarks and Physical Interpretation:

- The propagator determines how the wave function at time t is built from the initial state.
- If the initial state is a delta function (i.e., particle localized at $\vec{x}' = 0$):

$$\psi(\vec{x}, 0) = \delta(\vec{x}) \Rightarrow \psi(\vec{x}, t) = G(\vec{x}, t) \quad (144)$$

So the Green's function describes the time evolution of a point source.

- After evaluating the integral, the free particle propagator is:

$$G(\vec{x} - \vec{x}', t - t') = \left(\frac{m}{2\pi i \hbar (t - t')} \right)^{3/2} \exp \left[\frac{im}{2\hbar} \frac{(\vec{x} - \vec{x}')^2}{t - t'} \right] \quad (145)$$

This result captures how a wave packet spreads over time during free evolution in three-dimensional space.

F. Stationary States and Time-Independent Schrödinger Equation

To better understand the dynamics of quantum systems, we often solve the Schrödinger equation using separation of variables. We start from the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] \psi(\vec{x}, t) \quad (146)$$

Assume a solution of the form:

$$\psi(\vec{x}, t) = f(t) \phi(\vec{x}) \quad (147)$$

Substitute into the Schrödinger equation:

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = \frac{1}{\phi(\vec{x})} \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] \phi(\vec{x}) = E \quad (148)$$

Since the left-hand side depends only on t , and the right-hand side only on \vec{x} , both must equal a constant, denoted E — the energy. This gives two equations: 1. the time part

$$i\hbar \frac{df(t)}{dt} = Ef(t) \quad \Rightarrow \quad f_E(t) = e^{-iEt/\hbar}, \quad (149)$$

and the spatial part (the time-independent Schrödinger equation):

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] \phi_E(\vec{x}) = E\phi_E(\vec{x}) \quad (150)$$

So the full solution becomes

$$\psi_E(\vec{x}, t) = \phi_E(\vec{x}) e^{-iEt/\hbar} \quad (151)$$

This is called a stationary state because its probability density is independent of time:

$$|\psi_E(\vec{x}, t)|^2 = |\phi_E(\vec{x})|^2 \quad (152)$$

Examples:

- For free particle $V(x) = 0$, the time-independent equation becomes:

$$-\frac{\hbar^2}{2m} \nabla^2 \phi = E\phi \quad (153)$$

A solution is

$$-\frac{\hbar^2}{2m} \nabla^2 \phi_E(x) = E\phi_E(x) \implies \phi_E(x) = e^{ipx/\hbar}, \quad E = \frac{p^2}{2m} \quad (154)$$

These are plane waves with continuous energy spectrum. However, they are not square-integrable (i.e., not normalizable).

- Bound States in a Potential ($V \neq 0$): For potentials like the harmonic oscillator or finite wells, the spectrum is discrete:

$$E_0, E_1, E_2, \dots \quad (155)$$

Each eigenfunction $\phi_n(\vec{x})$ is normalizable and corresponds to a well-defined energy.

In a stationary state, expectation values of observables are constant in time:

$$\langle A \rangle_{\psi(t)} = \int \overline{\psi(\vec{x}, t)} \hat{A} \psi(\vec{x}, t) d^3x = \int \overline{\phi_E(\vec{x})} \hat{A} \phi_E(\vec{x}) d^3x \quad (156)$$

So:

$$\frac{d}{dt} \langle A \rangle = 0 \quad (157)$$

Any observable whose operator commutes with the Hamiltonian is a conserved quantity.

Even if the system is not in a stationary state, we can expand any solution $\Psi(\vec{x}, t)$ as a superposition:

$$\Psi(\vec{x}, t) = \sum_E C_E \phi_E(\vec{x}) e^{-iEt/\hbar}. \quad (158)$$

This still satisfies the Schrödinger equation, due to linearity. However, unless only one energy eigenvalue is present, the state is not stationary - interference between different energy components can cause time-dependent probability densities and expectation values.

V. BOUND STATES IN 1D POTENTIALS

A. The Infinite Square Well

We consider a particle in a 1D infinitely deep square potential well with potential $V(x) = \begin{cases} 0 & x \in [0, a] \\ \infty & x < 0 \text{ or } x > a \end{cases}$. The Schrödinger Equation is

$$\hat{H}\phi_E = E\phi_E \Rightarrow \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi_E = E\phi_E \quad (159)$$

with the boundary conditions:

$$\phi(0) = \phi(a) = 0. \quad (160)$$

We solve the differential equation inside the well:

$$\frac{d^2\phi_E}{dx^2} + \frac{2mE}{\hbar^2} \phi_E = 0 \quad (161)$$

Define:

$$k^2 = \frac{2mE}{\hbar^2} \Rightarrow \frac{d^2\phi_E}{dx^2} + k^2\phi_E = 0. \quad (162)$$

The general solution inside the well is:

$$\phi_E(x) = C_+ e^{ikx} + C_- e^{-ikx} \quad (163)$$

which is the combination of exponentials. Then, we can apply boundary conditions:

- At $x = 0$: $\phi_E(0) = C_+ + C_- = 0 \Rightarrow C_- = -C_+$.
- At $x = a$: $\phi_E(a) = C_+ (e^{ika} - e^{-ika}) = 0 \Rightarrow \sin(ka) = 0$

This gives the quantization condition:

$$k = \frac{n\pi}{a}, \quad n = 1, 2, 3, \dots \quad (164)$$

where k is discrete. The energy levels are

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad (165)$$

Therefore, the normalized eigenfunctions are:

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad x \in [0, a] \quad (166)$$

Summary of the infinite square well:

- The eigenvalues E_n are discrete, and we have the discrete spectrum $\{E_n\}$.
- The full set $\{\phi_n(x)\}$ forms an orthonormal basis for the Hilbert space $L^2(0, a)$.
- This is useful as an idealized model for bound particles.

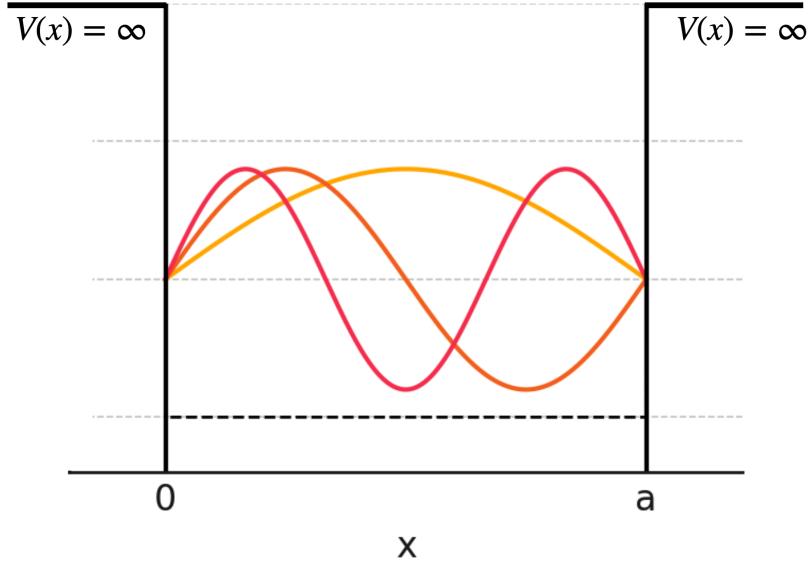


FIG. 16: The infinite well

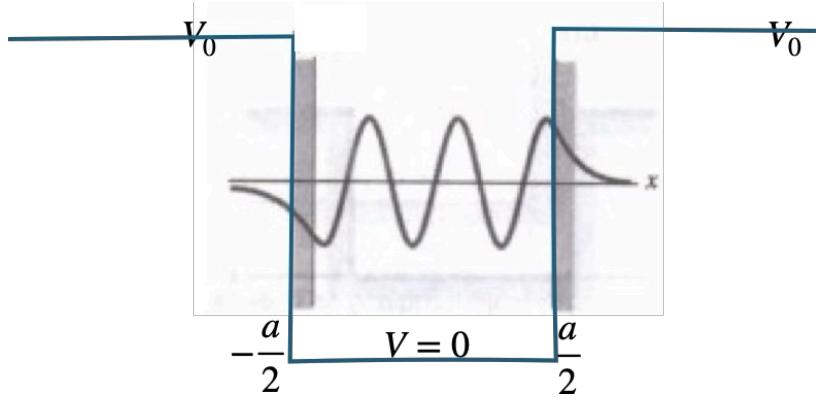


FIG. 17: The Finite square well

B. The Finite Square Well

Symmetric potential well, see FIG. 17:

$$V(x) = \begin{cases} 0 & \text{for } |x| \leq \frac{a}{2} \\ V_0 & \text{for } |x| > \frac{a}{2} \end{cases} \quad (167)$$

Solving the Time-Independent Schrödinger Equation:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi(x) = E\phi(x) \quad (168)$$

Region-by-Region Analysis:

- Region I $|x| \geq \frac{a}{2}$: Schrödinger equation becomes

$$\frac{d^2\phi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\phi = 0. \quad (169)$$

which is still similar to free EOM. Let $\phi = e^{ikx}$, we have

$$\left[-k^2 + \frac{2m}{\hbar^2}(E - V_0) \right] e^{ikx} = 0 \implies k^2 = \frac{2m}{\hbar^2}(E - V_0). \quad (170)$$

Now you have 2 possibilities:

- If $E > V_0$: $k \in \mathbb{R}$, this is classically allowed. The solution is oscillatory

$$k = \pm \sqrt{\frac{2m}{\hbar^2} (E - V_0)} \quad (171)$$

which is the free particle behavior, and we have

$$\phi_E(x) = e^{\pm ikx}. \quad (172)$$

We apply the free-particle boundary condition, allowing oscillatory solutions: $\phi \sim e^{ikx}$.

- If $E < V_0$ (classically forbidden): Classically, $E < V_0$ implies the kinetic energy is negative, so no particle is allowed. However, in QM, the wavefunction does not vanish, the exponential decay is allowed, leading to the tunneling effect. We define

$$k = i\beta, \quad \beta_{\pm} = \pm \sqrt{\frac{2m}{\hbar^2} (V_0 - E)}. \quad (173)$$

The solution becomes exponential in the classically forbidden region $|x| > \frac{a}{2}$:

$$\phi_E(x) = e^{-\beta_{\pm} x}. \quad (174)$$

We impose the bound-state condition: $\phi(x) \rightarrow 0$ as $|x| \rightarrow \infty$. This selects the decaying exponential:

- * For $x > a/2$: $\phi_E(x) = e^{-\beta_{+} x}$ with $\beta_{+} = \sqrt{\frac{2m}{\hbar^2} (V_0 - E)}$, and β_{-} is unphysical.
- * For $x < -a/2$: $\phi_E(x) = e^{\beta_{-} x}$ with $\beta_{-} = -\sqrt{\frac{2m}{\hbar^2} (V_0 - E)}$, and β_{+} is unphysical

Remarks:

- The boundary condition at infinity selects the physical solution (decaying exponential).
- Even in the classically forbidden region, the wavefunction is nonzero — this reflects non-zero quantum probability density.
- In the limit $V_0 \rightarrow \infty$, the solution outside the well vanishes exponentially, recovering the infinite square well case.
- Region II: inside the well $|x| \leq a/2$. The potential is symmetric and constant, so the Schrödinger equation becomes:

$$\frac{d^2\phi}{dx^2} + k^2\phi(x) = 0, \quad \text{with } k = \sqrt{\frac{2mE}{\hbar^2}}. \quad (175)$$

The general solution is

$$\phi(x) = C_1 e^{ikx} + C_2 e^{-ikx}. \quad (176)$$

Since the potential satisfies $V(x) = V(-x)$, we can use the parity Lemma: If $V(x) = V(-x)$, then the eigenfunctions $\phi(x)$ can be chosen to have definite parity:

- Even parity: $\phi(-x) = \phi(x)$,
- Odd parity: $\phi(-x) = -\phi(x)$.

Thus, we can rewrite the general solution as:

- Even parity: $\phi(x) \propto \cos(kx)$,
- Odd parity: $\phi(x) \propto \sin(kx)$.

To find the allowed energies E , we match the wavefunction and its derivative at $x = a/2$ between the inner (oscillatory) and outer (exponentially decaying) regions. In the outside region $x > a/2$, where $E < V_0$, the solution is:

$$\phi(x) \propto e^{-\beta_+ x}, \quad \beta_+ = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (177)$$

We use the continuity of the logarithmic derivative:

$$\left. \frac{\phi'(x)}{\phi(x)} \right|_{x=a/2^-} = \left. \frac{\phi'(x)}{\phi(x)} \right|_{x=a/2^+}. \quad (178)$$

- Even Parity States: Inside the well:

$$\phi(x) \propto \cos(kx) \implies \frac{\phi'}{\phi} = -k \tan(kx) \quad (179)$$

Outside the well:

$$\phi(x) \propto e^{-\beta_+ x} \implies \frac{\phi'}{\phi} = -\beta_+ \quad (180)$$

Matching at $x = a/2$ gives

$$k \tan(ka/2) = \beta_+ = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}, \quad k = \frac{\sqrt{2mE}}{\hbar}. \quad (181)$$

This transcendental equation determines the allowed energies E for even parity states.

- Odd Parity States: Inside the well:

$$\phi(x) \propto \sin(kx) \implies \frac{\phi'}{\phi} = k \cot(kx) \quad (182)$$

Outside the well:

$$\phi(x) \propto e^{-\beta_+ x} \implies \frac{\phi'}{\phi} = -\beta_+ \quad (183)$$

Matching at $x = a/2$ gives

$$k \cot(ka/2) = -\beta_+ = -\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}, \quad k = \frac{\sqrt{2mE}}{\hbar}. \quad (184)$$

This gives the condition for the allowed energy levels E of odd parity eigenstates.

Summary

- The symmetry of the potential lets us separate the problem into even and odd solutions.
- Matching the wavefunction's logarithmic derivative at $x = a/2$ gives two transcendental equations.
- Each equation (one for even, one for odd) determines a discrete set of allowed energy levels E .

C. Tunneling Through a Potential Barrier

We consider a particle approaching a 1D square potential barrier defined as:

$$V(x) = \begin{cases} V_0 & \text{for } x \in [0, a] \\ 0 & \text{otherwise} \end{cases} \quad (185)$$

See FIG. 18. Suppose the particle is incident from the left with energy $E < V_0$, so classically it cannot pass through the barrier:

$$E = \frac{1}{2}mv^2 + V \implies \text{no transmission if } E < V_0 \quad (186)$$

However, in QM, tunneling is possible. The time-independent Schrödinger equation is:

$$\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \phi(x) + V(x)\phi(x) = E\phi(x) \quad (187)$$

We divide space into three regions and solve separately in each:

- Region I ($x < 0$): Free particle

$$\phi(x) = e^{ikx} + Re^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}. \quad (188)$$

Here, e^{ikx} is the incoming wave, R is the reflection coefficient, and Re^{-ikx} is the reflected wave.

- Region II: $0 \leq x \leq a$ (Barrier region). The general solution is

$$\phi(x) = Ae^{\beta x} + Be^{-\beta x}, \quad \beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (189)$$

The solution is exponential since $E < V_0$.

- Region III: $x > a$ (free region), the solution is

$$\phi(x) = Se^{ikx} \quad (190)$$

where S is the transmission coefficient, and Se^{ikx} is the transmitted wave.

To determine the coefficients A, B, R, S , we impose continuity of the wavefunction and its derivative at $x = 0$ and $x = a$:

- At $x = 0$:

$$\begin{cases} \phi(0^-) = \phi(0^+) \Rightarrow 1 + R = A + B \\ \phi'(0^-) = \phi'(0^+) \Rightarrow ik(1 - R) = \beta(A - B) \end{cases} \quad (191)$$

- At $x = a$:

$$\begin{cases} \phi(a^-) = \phi(a^+) \Rightarrow Ae^{\beta a} + Be^{-\beta a} = Se^{ika} \\ \phi'(a^-) = \phi'(a^+) \Rightarrow \beta(Ae^{\beta a} - Be^{-\beta a}) = ikSe^{ika} \end{cases} \quad (192)$$

These four equations fully determine A, B, R, S . The transmission amplitude S can be expressed (after solving the system) as:

$$S = \frac{-2ik/\beta}{(1 - \frac{k^2}{\beta^2}) \sinh(\beta a) - 2i\frac{k}{\beta} \cosh(\beta a)}. \quad (193)$$

As we expect:

$$V_0 \rightarrow \infty \implies \beta \rightarrow \infty \implies S \rightarrow 0 \quad (194)$$

which has no transmission. When

$$a \rightarrow \infty \implies S \rightarrow 0, \quad (195)$$

which shows tunneling probability vanishes. This shows that tunneling probability decreases exponentially with both the height and width of the barrier.

The coefficient satisfies

$$|R|^2 + |S|^2 = 1, \quad (196)$$

This ensures conservation of probability and is valid in time-independent scattering theory.

Summary: Quantum Tunneling

- Even when $E < V_0$, there is a non-zero probability for the particle to pass through the barrier.
- Tunneling is a purely quantum effect, impossible in classical mechanics.
- Tunneling can explain many physical phenomena such as: Alpha decay in nuclear physics; Electron tunneling in semiconductors; Quantum devices like tunnel diodes.

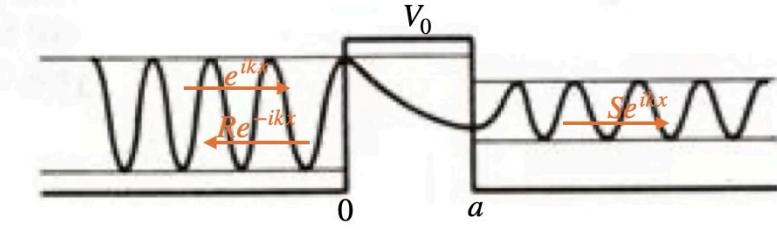


FIG. 18: The tunneling through a potential barrier

D. 1D Harmonic Oscillator

The potential is:

$$V(x) = \frac{1}{2}m\omega^2x^2 \quad (197)$$

where m is the mass of oscillator, and ω is the frequency. The time-independent Schrödinger equation is:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2 \right] \phi(x) = E\phi(x) \quad (198)$$

We impose the boundary condition:

$$\phi(x) \rightarrow 0 \quad (199)$$

as $x \rightarrow \pm\infty$. To change of variables, we define the dimensionless variable:

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x \quad \text{and} \quad \lambda = \frac{2E}{\hbar\omega} \quad (200)$$

Then the Schrödinger equation becomes:

$$\frac{d^2\phi}{d\xi^2} + (\lambda - \xi^2)\phi = 0 \quad (201)$$

As $\xi \rightarrow \pm\infty$, the dominant balance gives:

$$\frac{d^2\phi}{d\xi^2} - \xi^2\phi = 0 \quad \Rightarrow \quad \phi(\xi) \sim e^{\pm\xi^2/2} \quad (202)$$

To satisfy the boundary condition, we discard the growing exponential and keep:

$$\phi(\xi) \sim e^{-\xi^2/2}. \quad (203)$$

This motivates us to write

$$\phi(\xi) = e^{-\xi^2/2}u(\xi) \quad (204)$$

Then,

$$\frac{d^2u}{d\xi^2} - 2\xi \frac{du}{d\xi} + (\lambda - 1)u = 0. \quad (205)$$

This is the Hermite differential equation, and its solutions are Hermite polynomials $u(\xi) = H_n(\xi)$, provided:

$$\lambda_n = 2n + 1, \quad n = 0, 1, 2, \dots \quad (206)$$

The energy eigenvalues are

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega \quad (207)$$

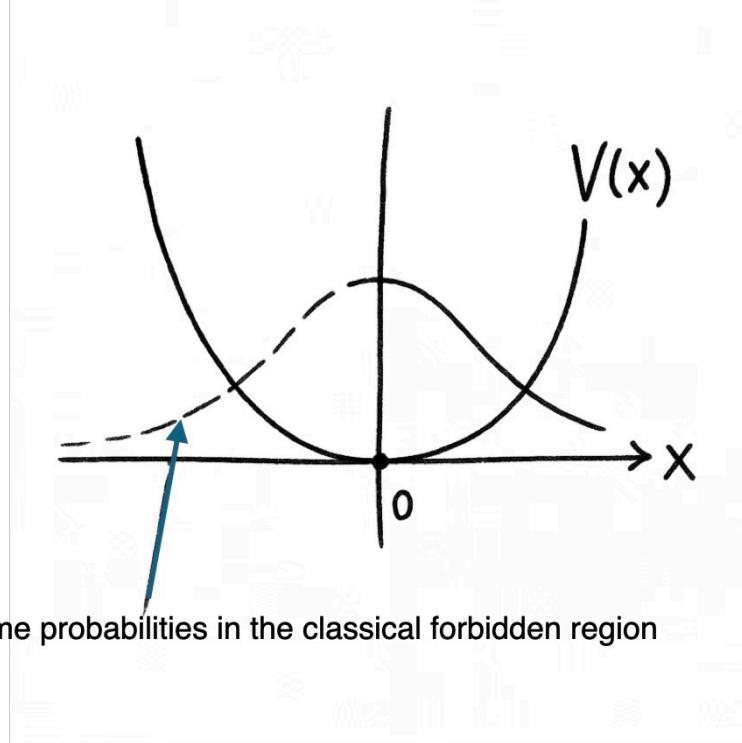


FIG. 19: Some probabilities in classical forbidden region

and the eigenfunctions are

$$\phi_n(x) = \mathcal{N}_n e^{-\xi^2/2} H_n(\xi), \quad \xi = \sqrt{\frac{m\omega}{\hbar}} x. \quad (208)$$

Some important properties are

- The ground state energy: the lowest energy (zero-point energy) is:

$$E_0 = \frac{1}{2}\hbar\omega \neq 0, \quad (209)$$

and the ground state wavefunction is

$$\phi_0(x) \propto e^{-\xi^2/2} = e^{-\frac{m\omega x^2}{2\hbar}}, \quad (210)$$

which is Gaussian distribution. Classically, a particle with $E = 0$ sits at the bottom of the potential well ($x = 0$). But in QM, due to the uncertainty principle, zero energy is forbidden. There is always non-zero spread in position and momentum, see FIG. 19.

- The polynomials satisfy:

$$\int_{-\infty}^{\infty} H_m(\xi) H_n(\xi) e^{-\xi^2} d\xi = \sqrt{\pi} 2^n n! \delta_{mn} \quad (211)$$

Therefore, the eigenfunctions $\phi_n(x)$ are orthonormal in $L^2(\mathbb{R})$:

$$\int_{-\infty}^{\infty} \phi_m(x) \phi_n(x) dx = \delta_{mn} \quad (212)$$

- Since \hat{H} is Hermitian:

$$\hat{H} \phi_n = E_n \phi_n \Rightarrow \langle \phi_m, \phi_n \rangle = \delta_{mn} \quad (213)$$

- Parity: The potential is even: $V(x) = V(-x)$, so parity is conserved. Each eigenstate has definite parity:

$$\hat{P}\phi_n(x) := \phi_n(-x) = (-1)^n\phi_n(x) \quad (214)$$

ϕ_n is even when n is even, and odd when n is odd.

VI. OPERATORS IN QUANTUM MECHANICS

An operator is a linear map on a vector space V , or more generally, on a Hilbert space $\mathcal{H} = \langle V, \langle \cdot, \cdot \rangle \rangle$, i.e., $\hat{O} : \mathcal{H} \rightarrow \mathcal{H}$ and satisfies the linearity condition:

$$\hat{O}(c_1\psi_1 + c_2\psi_2) = c_1\hat{O}\psi_1 + c_2\hat{O}\psi_2, \quad (215)$$

for any $\psi_1, \psi_2 \in \mathcal{H}$ and scalars $c_1, c_2 \in \mathbb{C}$.

Example: the momentum operator

$$\hat{\vec{p}} = -i\hbar\vec{\Delta} \quad (216)$$

It satisfies linearity:

$$\hat{\vec{p}}(c_1\psi_1 + c_2\psi_2) = -i\hbar\vec{\Delta}(c_1\psi_1 + c_2\psi_2) = c_1(-i\hbar\vec{\Delta})\psi_1 + c_2(-i\hbar\vec{\Delta})\psi_2 = c_1\hat{\vec{p}}\psi_1 + c_2\hat{\vec{p}}\psi_2 \quad (217)$$

Thus, all physical quantities in quantum mechanics are represented by linear operators.

A. Properties and Operations on Operators

- Identity Operator

$$\hat{I}\psi = \psi \quad \forall \psi \in \mathcal{H} \quad (218)$$

- Equality of Operators: Two operators \hat{A}, \hat{B} are equal if $\hat{A}\psi = \hat{B}\psi$ for any $\psi \in \mathcal{H}$.
- Sum of Operators

$$(\hat{A} + \hat{B})\psi = \hat{A}\psi + \hat{B}\psi \quad (219)$$

Example: The Hamiltonian operator can be written as

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad (220)$$

- Product of Operators:

$$(\hat{A}\hat{B})\psi = \hat{A}(\hat{B}\psi) \quad (221)$$

In general, operators do not commute $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. Example:

$$(\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\psi = x \left(-i\hbar \frac{\partial}{\partial x} \right) \psi + i\hbar(x\psi) = i\hbar\psi \quad \Rightarrow \quad [\hat{x}, \hat{p}_x] = i\hbar\hat{I}. \quad (222)$$

However,

$$(\hat{y}\hat{p}_x - \hat{p}_x\hat{y})\psi = y \left(-i\hbar \frac{\partial}{\partial x} \right) \psi + i\hbar(y\psi) = 0 \quad \Rightarrow \quad [\hat{y}, \hat{p}_x] = 0. \quad (223)$$

This leads to the canonical commutation relation:

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}\hat{I}. \quad (224)$$

- Inverse operator: If $\hat{A}\psi = \phi$ then $\hat{A}^{-1}\phi = \psi$ as

$$\hat{A}^{-1}\hat{A} = \hat{I}, \quad \hat{A}\hat{A}^{-1} = \hat{I} \quad (225)$$

Not all operators are invertible. If both \hat{A}, \hat{B} are invertible:

$$(\hat{A}\hat{B})^{-1} = \hat{B}^{-1}\hat{A}^{-1} \quad (226)$$

The inverse, if it exists, is unique.

- Functions of Operators: If a function $F(x)$ is analytic, then we can define $F(\hat{x})$ by power series:

$$F(\hat{x}) = \sum_{n=0}^{\infty} \frac{F^{(n)}(0)}{n!} \hat{x}^n \implies F(\hat{x}) = \sum_{n=0}^{\infty} \frac{F^{(n)}(0)}{n!} \hat{x}^n \quad (227)$$

Example: The translation operator:

$$F\left(\frac{d}{dx}\right) = e^{a\frac{d}{dx}} = \sum_{n=0}^{\infty} \frac{a^n}{n!} \frac{d^n}{dx^n} \Rightarrow e^{a\frac{d}{dx}} \psi(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{dx^n} \psi(x) \cdot a^n = \psi(x+a) \quad (228)$$

Similarly, for two operators \hat{A}, \hat{B} , we can define:

$$F(\hat{A}, \hat{B}) = \sum_{m,n=0}^{\infty} \frac{F^{(n,m)}(0,0)}{n!m!} \hat{A}^n \hat{B}^m, \quad F^{(n,m)}(0,0) = \frac{\partial^m}{\partial x^m} \frac{\partial^n}{\partial x^n} F(x, y) \quad (229)$$

- Hermitian Conjugate: For a Hilbert space $\mathcal{H} = \langle V, \langle \cdot, \cdot \rangle \rangle$. The Hermitian conjugate \hat{A}^\dagger satisfies:

$$\langle \psi, \hat{A}^\dagger \phi \rangle = \langle \hat{A}\psi, \phi \rangle, \quad \psi, \phi \in \mathcal{H}. \quad (230)$$

B. Commutators

The commutator of two operators \hat{A}, \hat{B} is defined as:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (231)$$

The properties of commutators:

- Antisymmetry: $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$
- Linearity: $[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$
- Leibniz Rule: $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$
- Jacobi Identity: $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$.
- $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$.

C. Angular momentum

Angular momentum is defined as:

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} \quad (232)$$

its components are:

$$\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x. \end{aligned} \quad (233)$$

They satisfy the commutation relations:

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k, \quad i = x, y, z. \quad (234)$$

where ϵ_{ijk} is the Levi-Civita symbol, with full antisymmetry:

$$\epsilon_{ijk} = -\epsilon_{jik} = -\epsilon_{ikj} = -\epsilon_{kji}. \quad (235)$$

The total angular momentum is:

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \quad (236)$$

and it commutes with each component:

$$[\hat{L}^2, \hat{L}_i] = 0. \quad (237)$$

In spherical coordinates:

$$\begin{aligned} \hat{L}_x &= i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right), \\ \hat{L}_y &= i\hbar \left(-\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right), \\ \hat{L}_z &= -i\hbar \frac{\partial}{\partial \phi} \end{aligned} \quad (238)$$

All independent of r . The total angular momentum becomes:

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]. \quad (239)$$

Coordinate relations used:

$$\begin{aligned} x &= r \sin \theta \cos \phi, & y &= r \sin \theta \sin \phi, & z &= r \cos \theta. \\ r &= \sqrt{x^2 + y^2 + z^2}, & \theta &= \tan^{-1} \sqrt{x^2 + y^2}/2, & \phi &= \tan^{-1}(y/x). \end{aligned} \quad (240)$$

D. Hermitian Operator

An operator \hat{A} is Hermitian if: $\langle \psi, \hat{A}\phi \rangle = \langle \hat{A}\psi, \phi \rangle$ for all $\psi, \phi \in \mathcal{H}$. In brief: $\hat{A}^\dagger = \hat{A}$. Example:

- For \hat{x} ,

$$\begin{aligned} \langle \psi, \hat{x}_i \phi \rangle &= \int d^3x \overline{\psi(x)} \hat{x}_i \phi(x) = \int d^3x x_i \overline{\psi(x)} \phi(x) \\ &= \int d^3x \overline{\hat{x}_i \psi(x)} \phi(x) = \langle \hat{x}_i \psi, \phi \rangle \end{aligned} \quad (241)$$

So \hat{x} is Hermitian.

- For $\hat{p}_i = -i\hbar \frac{\partial}{\partial x_i}$,

$$\begin{aligned} \langle \psi, \hat{p}_i \phi \rangle &= \int d^3x \overline{\psi(x)} (-i\hbar) \frac{\partial}{\partial x_i} \phi(x) = -i\hbar \int d^3x \left(-\frac{\partial}{\partial x_i} \right) \overline{\psi(x)} \phi(x) - i\hbar \int d^3x \frac{\partial}{\partial x} \left(\overline{\psi(x)} \phi(x) \right) \\ &= \int d^3x \left(i\hbar \frac{\partial}{\partial x_i} \right) \overline{\psi(x)} \phi(x) = \int d^3x \overline{\left(-i\hbar \frac{\partial}{\partial x_i} \psi(x) \right)} \phi(x) = \langle \hat{p}_i \psi, \phi \rangle. \end{aligned} \quad (242)$$

So \hat{p}_i is Hermitian.

Lemmas:

- $(\hat{A} + \hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger$.
- $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.

Therefore, if \hat{A}, \hat{B} are Hermitian, Then $(\hat{A} + \hat{B})^\dagger = \hat{A} + \hat{B}$, so $\hat{A} + \hat{B}$ is Hermitian. But $(\hat{A}\hat{B})^\dagger = \hat{B}\hat{A} \neq \hat{A}\hat{B}$ unless $[\hat{A}, \hat{B}] = 0$, so $\hat{A}\hat{B}$ is Hermitian only if they commute.

Example: We consider the angular momentum operator: $\vec{L} = \hat{\vec{x}} \times \hat{\vec{p}}$. In components:

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \quad (243)$$

Since $\hat{y}, \hat{z}, \hat{p}_y, \hat{p}_z$ are Hermitian, \hat{L}_x is also Hermitian. Similarly, \hat{L}_y, \hat{L}_z are Hermitian.

$$[\hat{y}, \hat{p}_z] = [\hat{z}, \hat{p}_y] = 0. \quad (244)$$

Kinetic energy operator: $\hat{T} = \frac{\hat{p}^2}{2m} \Rightarrow \hat{T}^\dagger = \left(\frac{\hat{p}^2}{2m}\right)^\dagger = \frac{(\hat{p}^\dagger)^2}{2m} = \frac{\hat{p}^2}{2m} = \hat{T}$.

Angular momentum squared:

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \Rightarrow (\hat{L}^2)^\dagger = \hat{L}^2 \text{ since } (\hat{L}_i^2)^\dagger = \hat{L}_i^2 \quad (245)$$

Potential energy operator:

$$\hat{V}(x) = \sum_{n=0}^{\infty} \frac{1}{n!} V^{(n)}(0) \hat{x}^n \text{ with real coefficients} \Rightarrow \hat{V}(x)^\dagger = \hat{V}(x) \quad (246)$$

This uses the fact that:

$$(\hat{x}^n)^\dagger = (\hat{x} \cdots \hat{x})^\dagger = \hat{x} \cdots \hat{x} = \hat{x}^n \quad (247)$$

Therefore, we have

$$\hat{H} = \hat{T} + \hat{V} \text{ is Hermitian} \quad (248)$$

Caution: If $c, d \in \mathbb{C}$, then $(c\hat{A} + d\hat{B})^\dagger = \bar{c}\hat{A}^\dagger + \bar{d}\hat{B}^\dagger$. So $c\hat{A} + d\hat{B}$ is Hermitian only if $c, d \in \mathbb{R}$. Therefore, $\hat{V}(x)^\dagger = \hat{V}(x)$ only if the Taylor coefficients of $V(x)$ are all real, i.e., $V(x)$ must be a real potential. If $V(x)$ is complex, then \hat{H} is not Hermitian. In QM, all physical observables must be Hermitian operators because:

$$\langle \hat{O} \rangle = \langle \psi, \hat{O}\psi \rangle = \langle \hat{O}\psi, \psi \rangle = \overline{\langle \psi, \hat{O}\psi \rangle} = \overline{\hat{O}} \Rightarrow \langle \hat{O} \rangle \in \mathbb{R} \quad (249)$$

i.e., expectation values are real and can be observed.

1. Eigenvalues and Eigenstates of Hermitian Operators

Given a Hermitian operator \hat{A} , we define the eigenvalue equation:

$$\hat{A}\psi = a\psi \quad (250)$$

where $a \in \mathbb{C}$ is a parameter of the equation. This equation may or may not have nontrivial solutions (i.e., $\psi \neq 0$). For certain values a_n (where $n = 0, 1, 2, \dots$), the equation

$$\hat{A}\psi_n = a_n\psi_n \quad (251)$$

has nontrivial solutions. We call a_n the **eigenvalue** and ψ_n the **eigenstate**.

Example 1: Momentum Operator Let $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$. The eigenvalue equation becomes:

$$-i\hbar \frac{\partial}{\partial x} \psi = p_x \psi \quad (252)$$

This is a differential equation on $\psi(x)$ defined on $x \in (-\infty, \infty)$. To ensure physically acceptable solutions, we require $\psi(x)$ to remain finite over the whole domain. General solution is:

$$\psi(x) = Ce^{ip_x x/\hbar} = Ce^{i\frac{\text{Re}(p_x)x}{\hbar} - i\frac{\text{Im}(p_x)x}{\hbar}} \quad C \in \mathbb{C} \quad (253)$$

If $\text{Im}(p_x) \neq 0$, $\psi(x)$ diverges as $x \rightarrow \pm\infty$ and is thus unphysical. Therefore, the eigenvalue equation has nontrivial solutions only when $p_x \in \mathbb{R}$. The eigenstates are:

$$\psi_p = Ce^{ipx/\hbar} \quad (254)$$

Example 2: Angular Momentum Operator \hat{L}_z Let $\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$. Then:

$$-i\hbar \frac{\partial}{\partial \phi} \psi(r, \theta, \phi) = l_z \psi(r, \theta, \phi), \quad l_z \in \mathbb{C}. \quad (255)$$

The general solution is:

$$\psi(r, \theta, \phi) = C(r, \theta) e^{il_z \phi/\hbar} \quad (256)$$

Because ϕ is an angular variable defined on $[0, 2\pi]$, we impose periodic boundary condition:

$$\begin{aligned} \psi(r, \theta, \phi + 2\pi) &= \psi(r, \theta, \phi) \\ \Rightarrow C(r, \theta) e^{il_z(\phi+2\pi)/\hbar} &= C(r, \theta) e^{il_z \phi/\hbar} \cdot e^{i2\pi l_z/\hbar} \Rightarrow e^{i2\pi l_z/\hbar} = 1 \end{aligned} \quad (257)$$

This implies the eigenvalues are

$$\frac{l_z}{\hbar} = m \in \mathbb{Z} \Rightarrow l_z = m\hbar \quad (258)$$

and the eigenstates are

$$\psi_m(r, \theta, \phi) = C(r, \theta) e^{im\phi}. \quad (259)$$

Remarks:

1. For \hat{p} or \hat{L}_z , all eigenvalues are real. The eigenstates are defined upto a scaling C .
2. Boundary conditions are crucial for differential equations $\hat{A}\psi = a\psi$.

2. Physical Observables and Hermitian Operators

For a physical observable, it is a Hermitian operator $\hat{A} = \hat{A}^\dagger$, all eigenvalues are real.

Proof: Assume $\hat{A}\psi_n = a_n\psi_n$, and we normalize ψ_n such that $\langle \psi_n, \psi_n \rangle = 1$.

$$\langle \psi_n, \hat{A}\psi_n \rangle = a_n \langle \psi_n, \psi_n \rangle = a_n \in \mathbb{R} \Rightarrow \langle A \rangle \in \mathbb{R} \quad (260)$$

This shows the average value of observable \hat{A} is the eigenvalue a_n in eigenstate ψ_n .

Let us consider the quantum fluctuation $\langle \Delta A^2 \rangle$ in eigenstate ψ_n :

$$\langle \Delta A^2 \rangle = \langle (\hat{A} - \langle A \rangle)^2 \rangle = \langle \psi_n, (\hat{A} - a_n)^2 \psi_n \rangle = \langle \psi_n, (\hat{A}^2 - 2a_n\hat{A} + a_n^2) \psi_n \rangle = 0 \quad (261)$$

- If you measure observable \hat{A} in its eigenstate ψ_n , what you get is the eigenvalue a_n with no quantum fluctuation. Your measurement output is fixed to be a_n .
- If the state ψ is a superposition $\psi = \sum_n c_n \psi_n$, then the probability to get a_n is $|c_n|^2$.
- If $\psi = \psi_n$, then $c_n = 1$, all other $c_{m \neq n} = 0$.

3. Orthogonality of Eigenstates

Given $\hat{A}\psi_n = a_n\psi_n$ and $\hat{A}\psi_m = a_m\psi_m$ with $a_n \neq a_m$:

$$\langle \psi_m, \hat{A}\psi_n \rangle = a_n \langle \psi_m, \psi_n \rangle \quad \text{and} \quad \langle \hat{A}\psi_m, \psi_n \rangle = a_m \langle \psi_m, \psi_n \rangle \quad (262)$$

Subtracting:

$$(a_n - a_m) \langle \psi_m, \psi_n \rangle = 0 \Rightarrow \langle \psi_m, \psi_n \rangle = 0 \quad (263)$$

Therefore, ψ_m and ψ_n are orthogonal.

Example 1 \hat{L}_z Eigenstates: Let $\hat{L}_z\psi_m = m\hbar\psi_m$, where $m \in \mathbb{Z}$. Then:

$$\psi_m = C(r, \theta)e^{im\phi} \quad (264)$$

The inner product:

$$\begin{aligned} \langle \psi_m, \psi_n \rangle &= \int_0^{2\pi} d\phi \overline{C(r, \theta)} C'(r, \theta) e^{i(n-m)\phi} = 0 \quad \text{for } m \neq n \\ &\Rightarrow \langle \psi_m, \psi_n \rangle = \delta_{mn} \end{aligned} \quad (265)$$

after normalization (orthonormal set).

Examples 2 Momentum Operator \hat{p} :

$$\hat{p}\psi_p = p\psi_p, \quad \psi_p = Ce^{ipx/\hbar}, \quad \psi_{p'} = C'e^{ip'x/\hbar}, \quad p, p' \in \mathbb{R} \quad (266)$$

Then, we have

$$\begin{aligned} \langle \psi_p, \psi_{p'} \rangle &= \bar{C}C' \int_{-\infty}^{\infty} dx e^{i(p'-p)x/\hbar} \\ &\Rightarrow \langle \psi_p, \psi_{p'} \rangle = \delta(p - p') \end{aligned} \quad (267)$$

Then, after normalization, we have

$$\psi_p = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad (268)$$

which shows that $\psi_p, \psi_{p'}$ are orthogonal.

Orthogonality:

- For the discrete eigenvalues a_n , it is normalizable in the state ψ_n , we have

$$\langle \psi_n, \psi_m \rangle = \delta_{mn}. \quad (269)$$

- or the discrete eigenvalues p , it is normalizable in the state ψ_p , we have

$$\langle \psi_p, \psi_{p'} \rangle = \delta(p - p') \quad (270)$$

Example 3 Kinetic Energy Operator

$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}, \quad (271)$$

we have

$$\hat{T}\psi = T\psi \Rightarrow -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = T\psi \quad (272)$$

Therefore, we have

$$\begin{aligned} \psi &\propto \psi_p = e^{ipx/\hbar}, \\ \hat{T}\psi_p &= \frac{p^2}{2m}\psi_p \Rightarrow T = \frac{p^2}{2m} \end{aligned} \quad (273)$$

However, $\psi_{-p} = e^{-ipx/\hbar}$ also satisfies:

$$\hat{T}\psi_{-p} = \frac{p^2}{2m}\psi_{-p} \quad (274)$$

Then, we have both

$$\hat{T}\psi_p = \frac{p^2}{2m}\psi_p, \quad \hat{T}\psi_{-p} = \frac{p^2}{2m}\psi_{-p} \quad (275)$$

Therefore $T = \frac{p^2}{2m}$ is a degenerate eigenvalue, and the eigenstate is not unique.

Eigenstates ψ_p, ψ_{-p} are orthogonal:

$$\langle \psi_p, \psi_{-p} \rangle \propto \delta(p + p) = 0, \quad (276)$$

if $p \neq 0$, the eigenspace spanned by ψ_p, ψ_{-p} which is 2-dimensional.

In general, $\hat{A}\psi_{n\alpha} = a_n\psi_{n\alpha}$ may have degeneracy, e.g., $\hat{A}\psi_{n\alpha} = a_n\psi_{n\alpha}$, with $m = 1, 2, \dots$, $\alpha = 1, \dots, \dim V_m$. Here, we have $\langle \psi_{m\alpha}, \psi_{n\beta} \rangle = \delta_{mn}\delta_{\alpha\beta}$ orthogonal.

- For different $m \neq n$: $\langle \psi_{m\alpha}, \psi_{n\beta} \rangle = 0$
- For same m , different $\alpha \neq \beta$: $\langle \psi_{m\alpha}, \psi_{m\beta} \rangle = 0$
- For same (m, α) : $\langle \psi_{m\alpha}, \psi_{m\alpha} \rangle = 1$

Theorem: If $[\hat{A}, \hat{B}] = 0$ then \hat{A}, \hat{B} share the same set of eigenstates (\hat{A}, \hat{B} can be simultaneously diagonalized).

Proof:

$$\hat{A}\psi_m = a_n\psi_m, \quad \psi_m \in V_m, \quad (277)$$

there maybe degeneracy, i.e., $\dim V_m \geq 1$.

$$\hat{A}\hat{B}\psi_m = a_n\hat{B}\psi_m \Rightarrow \hat{B}\psi_m \in V_m \quad (278)$$

Then \hat{B} leaves the eigenspace V_m invariant. \hat{B} now can be viewed as an Hermitian operator on V_m . We consider the eigenvalue equation:

$$\hat{B}\phi_m = b_m\phi_m, \quad \phi_m \in V_m \quad (279)$$

here b_m is the eigenvalue of \hat{B} on V_m . and the eigenstates are $\phi_{m\alpha}$. Then,

$$\hat{B}\phi_{m\alpha} = b_\alpha\phi_{m\alpha} \quad \hat{A}\phi_{m\alpha} = a_m\phi_{m\alpha},$$

Thus $\phi_{m\alpha}$ are eigenstates shared by \hat{A} and \hat{B} , and

$$\langle \phi_{m\alpha}, \phi_{n\beta} \rangle = \delta_{mn}\delta_{\alpha\beta} \quad (280)$$

We define $V_{m\alpha}$ the eigenspace corresponding to eigenvalues a_m of \hat{A} and b_α of \hat{B} .

E. (\hat{L}^2, \hat{L}_z) Eigenstates

The total angular momentum operator \hat{L}^2 and the z -component \hat{L}_z are defined as:

$$\begin{aligned} \hat{L}^2 &= -\hbar^2 \left[\frac{1}{\sin\theta} \partial_\theta (\sin\theta \partial_\theta) + \frac{1}{\sin^2\theta} \partial_\varphi^2 \right] \\ \hat{L}_z &= -i\hbar\partial_\varphi \end{aligned}$$

Consider wavefunction $\psi(\theta, \varphi)$ on the sphere:

$$\langle \psi, \psi' \rangle = \int_0^\pi d\theta \int_0^{2\pi} d\varphi \sin\theta \overline{\psi(\theta, \varphi)} \psi'(\theta, \varphi).$$

Let us assume separation of variables:

$$\psi(\theta, \varphi) = \Theta(\theta)e^{im\varphi}, \quad m = 0, \pm 1, \pm 2, \dots$$

Then, let $l^2 = \lambda\hbar^2$, we have:

$$\hat{L}^2\psi = l^2\psi, \Rightarrow -\hbar^2 \left[\frac{1}{\sin\theta} \partial_\theta (\sin\theta \partial_\theta \Theta) + \frac{1}{\sin^2\theta} (-m^2)\Theta \right] = \lambda\hbar^2\Theta$$

Let $\zeta = \cos\theta$, then $\zeta \in [-1, 1]$ due to $\theta \in [0, \pi]$:

$$(1 - \zeta^2) \frac{d^2}{d\zeta^2}\Theta - 2\zeta \frac{d\Theta}{d\zeta} + \left(\lambda - \frac{m^2}{1 - \zeta^2} \right) \Theta = 0$$

This is the Legendre equation. Θ should be finite at $\zeta = \pm 1$ requires:

$$\lambda = l(l+1), \quad l = 0, 1, 2, \dots, \quad |m| \leq l$$

The solution is $\Theta_{lm}(\theta) \propto P_l^m(\zeta)$, which is the associated Legendre polynomial.

Evaluation:

$$\Theta_{00}(\theta) = \frac{1}{\sqrt{4\pi}}, \quad \Theta_{10}(\theta) = \sqrt{\frac{3}{4\pi}} \cos\theta, \quad \Theta_{1\pm 1}(\theta) = \sqrt{\frac{3}{8\pi}} \sin\theta, \quad \dots$$

Orthogonality:

$$\int_{-1}^1 d\zeta P_l^m(\zeta) P_{l'}^m(\zeta) = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll'}$$

Normalization:

$$\Theta_{lm} = (-1)^m \sqrt{\frac{2l+1}{2} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) \implies \int_0^\pi d\theta \sin\theta \overline{\Theta_{lm}} \Theta_{l'm} = \delta_{ll'}$$

Full Eigenfunctions:

$$\psi_{lm}(\theta, \varphi) = \Theta_{lm}(\theta)e^{im\varphi} = (-1)^m \sqrt{\frac{2l+1}{2} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\varphi}$$

with

$$\begin{aligned} \hat{L}^2\psi_{lm} &= l(l+1)\hbar^2\psi_{lm}, \\ \hat{L}_z\psi_{lm} &= m\hbar\psi_{lm}, \end{aligned} \quad l = 0, 1, 2, \dots, m = -l, \dots, l$$

The spherical Harmonic $\psi_{lm}(\theta, \varphi)$ are eigenstates of (\hat{L}^2, \hat{L}_z) with simultaneous eigenspace V_{lm} is 1-dimensional and no degeneracy. The eigenspace of \hat{L}^2 is V_l has $(2l+1)$ dimensions. Here V_l are spanned by $\{\psi_{lm}\}_{m=-l}^l$.

Orthonormality:

$$\langle \psi_{lm}, \psi_{l'm'} \rangle = \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta \overline{\psi_{lm}(\theta, \varphi)} \psi_{l'm'}(\theta, \varphi) = \delta_{ll'} \delta_{mm'}$$

F. Complete Set of Physical Observables

We consider the time-independent Schrödinger equation:

$$\hat{H}\psi = E\psi, \quad \psi \in \mathcal{H}. \quad (281)$$

Solving the eigenvalue problem:

$$\hat{H}\phi_n = E_n\phi_n, \quad (282)$$

we find the energy eigenstates and eigenvalues. However, E_n may be degenerate, so the dimension of the eigenspace V_n can be greater than one:

$$\dim V_n > 1. \quad (283)$$

To resolve this degeneracy, we seek another physical observable \hat{A} (Hermitian), such that $[\hat{A}, \hat{H}] = 0$. Then:

$$\hat{A}\hat{H}\phi_n = \hat{H}\hat{A}\phi_n = E_n\hat{A}\psi_n \implies \hat{A}\phi_n \in V_n, \quad (284)$$

so \hat{A} leaves V_n invariant. We view \hat{A} as a Hermitian operator acting on V_n , and solve its eigenvalue problem:

$$\hat{A}\phi_{n\alpha} = a_\alpha\phi_{n\alpha}, \quad (285)$$

$$\hat{H}\phi_{n\alpha} = E_n\phi_{n\alpha}. \quad (286)$$

These $\phi_{n\alpha}$ are simultaneous eigenstates of \hat{H} and \hat{A} , spanning a subspace $V_{n\alpha} \subseteq V_n$. The degeneracy is partially resolved:

$$\dim V_{n\alpha} < \dim V_n. \quad (287)$$

If $\dim V_{n\alpha} > 1$, we look for another observable \hat{B} (Hermitian), such that:

$$[\hat{B}, \hat{H}] = [\hat{B}, \hat{A}] = [\hat{A}, \hat{H}] = 0. \quad (288)$$

Then \hat{B} also leaves $V_{n\alpha}$ invariant, and we solve:

$$\begin{aligned} \hat{B}\hat{H}\phi_{n\alpha} &= \hat{H}\hat{B}\phi_{n\alpha} = E_n\hat{B}\psi_{n\alpha}, \\ \hat{A}\hat{B}\phi_{n\alpha} &= \hat{B}\hat{A}\phi_{n\alpha} = a_\alpha\hat{B}\psi_{n\alpha} \implies \hat{B}\phi_{n\alpha} \in V_{n\alpha}, \end{aligned} \quad (289)$$

Then, we solve the eigen-equations for \hat{B} on $V_{n\alpha}$, we will have

$$\hat{B}\phi_{n\alpha\mu} = b_\mu\phi_{n\alpha\mu}, \quad (290)$$

yielding a further refined simultaneous eigenspace $\phi_{n\alpha\mu} \in V_{n\alpha\mu}$. We have:

$$\hat{H}\phi_{n\alpha\mu} = E_n\phi_{n\alpha\mu}, \quad \hat{A}\phi_{n\alpha\mu} = a_\alpha\phi_{n\alpha\mu}, \quad \hat{B}\phi_{n\alpha\mu} = b_\mu\phi_{n\alpha\mu}. \quad (291)$$

For the simultaneous eigenspace $\phi_{n\alpha\mu} \in V_{n\alpha\mu}$, we further reduce the dimension::

$$\dim V_{n\alpha\mu} < \dim V_{n\alpha} < \dim V_n. \quad (292)$$

but $\dim V_{n\alpha\mu}$ might still be greater than one. We can continue this process by introducing observables \hat{C}, \hat{D}, \dots that all commute with $\hat{H}, \hat{A}, \hat{B}, \dots$ and mutually commute, until:

$$\dim V_{n\alpha\mu\dots} = 1. \quad (293)$$

This gives a complete set of observables:

$$\{\hat{H}, \hat{A}_1, \hat{A}_2, \dots\}, \quad (294)$$

where all \hat{A}_i commute with \hat{H} and with each other:

$$[\hat{A}_i, \hat{H}] = [\hat{A}_i, \hat{A}_j] = 0. \quad (295)$$

such that

$$\hat{H}\psi = E\psi, \quad \hat{A}_i\psi = a^{(i)}\psi \quad (296)$$

and the simultaneous eigenspace is one-dimensional without degeneracy.

Example 1 Free Particle in 1D: Consider a free particle with Hamiltonian:

$$\hat{H} = \hat{T} = \frac{\hat{p}^2}{2m}. \quad (297)$$

We know:

$$\hat{T}e^{ipx/\hbar} = \frac{p^2}{2m}e^{ipx/\hbar}, \quad \hat{T}e^{-ipx/\hbar} = \frac{p^2}{2m}e^{-ipx/\hbar}, \quad (298)$$

so the eigenspace of \hat{H} with eigenvalue $p^2/(2m)$ is two-dimensional as the eigenspace V_p being spanned by $\{e^{ipx/\hbar}, e^{-ipx/\hbar}\}$.

Now consider the momentum operator \hat{p} :

$$[\hat{H}, \hat{p}] = 0. \quad (299)$$

We have:

$$\hat{T}e^{ipx} = \frac{p^2}{2m}e^{ipx}, \quad \hat{p}e^{ipx} = pe^{ipx}, \quad (300)$$

$$\hat{T}e^{-ipx} = \frac{p^2}{2m}e^{-ipx}, \quad \hat{p}e^{-ipx} = -pe^{-ipx}. \quad (301)$$

Thus, the simultaneous eigenspace of (\hat{T}, \hat{p}) with eigenvalue $(p^2/2m, p)$ is one-dimensional. (\hat{T}, \hat{p}) gives a complete set of observables for the free particle.

The eigenvalue of a Hermitian operator is usually called a **quantum number**. For a complete set of observables $\{\hat{H}, \hat{A}_1, \dots\}$, their eigenvalues $\{E, a^{(1)}, a^{(2)}, \dots\}$ are called **good quantum numbers**, since they uniquely label a one-dimensional eigenspace.

Simultaneous eigenstates are labeled as:

$$\psi_{E, a^{(1)}, a^{(2)}, \dots}, \quad (302)$$

where:

$$\hat{H}\psi_{E, a^{(1)}, \dots} = E\psi_{E, a^{(1)}, \dots}, \quad (303)$$

$$\hat{A}_1\psi_{E, a^{(1)}, \dots} = a^{(1)}\psi_{E, a^{(1)}, \dots}, \quad (304)$$

$$\hat{A}_2\psi_{E, a^{(1)}, a^{(2)}, \dots} = a^{(2)}\psi_{E, a^{(1)}, a^{(2)}, \dots}, \quad \text{etc.} \quad (305)$$

VII. REPRESENTATION IN QM

A vector \vec{v} in 3D space is independent of the basis, but its representation changes with the choice of basis. Choosing a basis $\hat{x}, \hat{y}, \hat{z}$:

$$\vec{v} = v_x \hat{x} + v_y \hat{y} + v_z \hat{z} \equiv (v_x, v_y, v_z) \quad (306)$$

Choosing another basis $\hat{x}', \hat{y}', \hat{z}'$:

$$\vec{v} = v'_x \hat{x}' + v'_y \hat{y}' + v'_z \hat{z}' \equiv (v'_x, v'_y, v'_z) \quad (307)$$

So the vector is the same, but its representation (components) depends on the basis.

In QM, the state $\psi \in \mathcal{H}$ is infinite-dimensional Hilbert space. Its representation depends on the chosen basis (representation).

Given a Hermitian operator \hat{A} with eigenstates $\{\psi_n\}$:

$$\hat{A}\psi_n = a_n\psi_n, \quad n = 1, 2, \dots, \infty \quad (308)$$

Any state ψ can be expanded as:

$$\psi = \sum_n c_n \psi_n \equiv (c_1, c_2, \dots) \quad (309)$$

The set $\{c_n\}$ is the representation of ψ in the representation of $\{\psi_n\}$ or \hat{A} -representation.

Compute the inner product:

$$\langle \psi_m | \phi \rangle = \langle \psi_m | \sum_n c_n \psi_n \rangle = \sum_n c_n \langle \psi_m | \psi_n \rangle = c_m, \quad (310)$$

which shows that the representation of ψ in the \hat{A} -representation is $\langle \psi_m, \psi \rangle$ where ψ_m is the eigenstate of \hat{A} .

Example: In momentum representation (\hat{p} -representation):

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \phi(p) e^{ipx/\hbar}, \quad \phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dx \psi(x) e^{-ipx/\hbar} \quad (311)$$

In position representation (\hat{x} -Representation):

$$\hat{x}\delta(x - x_0) = x_0\delta(x - x_0), \quad (312)$$

We can expand a state ψ in position representation:

$$\psi(x) = \langle x | \psi \rangle = \int_{-\infty}^{\infty} dx_0 \delta(x - x_0) \psi(x_0) \quad (313)$$

where $\psi(x_0)$ is the representation of the state ψ in position representation. We see that a state ψ should be understood as a vector, the wave function $\psi(x)$ or $\varphi(p)$ are actually representations. analogous:

- $\vec{v} \iff$, which is the Dirac ket.
- $(v_1, v_2, v_3) \iff \psi(x)$ or $\varphi(p)$ are representatives depend on representation.

1. Operator in representation

Given a representation $\{\psi_m\}_{m=1}^{\infty}$ basis, we can define:

$$\hat{A}\psi_m = a_m \psi_m, \quad \psi = \sum_m c_m \psi_m \quad (314)$$

Then $c_m = \langle \psi_m, \psi \rangle \equiv (c_1, c_2, \dots)$. Any operator \hat{O} acts on a state $\psi = \sum_n c_n \psi_n$:

$$\psi' = \hat{O}\psi = \sum_n c_n \hat{O}\psi_n = \sum_{m,n} O_{mn} c_n \psi_m \quad (315)$$

where $O_{mn} = \langle \psi_m | \hat{O} | \psi_n \rangle$ is the matrix element of the operator \hat{O} in the representation. And the matrix notation is:

$$b_m = \sum_n O_{mn} c_n \quad (316)$$

in the representation of $\{\psi_n\}$. The notation here is

- Any state ψ can be represented as (c_1, c_2, \dots) .
- Any operator \hat{O} can be represented as a matrix O_{mn} which is $\infty - \text{dim}$.
- $\hat{O}\psi = \psi'$ is represented as a matrix-vector multiplication:

$$\begin{pmatrix} O_{11} & O_{12} & O_{13} & \dots \\ O_{21} & O_{22} & O_{23} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix} \quad (317)$$

2. Change of representations

Suppose we have two orthonormal bases $\{\psi_n\}_{n=1}^\infty$ and $\{\phi_m\}_{m=1}^\infty$. The two representations of a state ψ are:

$$\begin{aligned}\psi &= \sum_n c_n \psi_n = (c_1, c_2, \dots) \\ \psi &= \sum_m \tilde{c}_m \phi_m = (\tilde{c}_1, \tilde{c}_2, \dots)\end{aligned}\tag{318}$$

Transformation matrix:

$$\tilde{c}_m = \langle \phi_m | \psi \rangle = \langle \phi_m | \sum_n c_n \psi_n \rangle = \sum_n \langle \phi_m | \psi_n \rangle c_n = \sum_n U_{mn} c_n,\tag{319}$$

where $U_{mn} = \langle \phi_m | \psi_n \rangle$. Then the inverse transformation is:

$$c_n = \langle \psi_n | \psi \rangle = \langle \psi_n | \sum_m \tilde{c}_m \phi_m \rangle = \sum_m \langle \psi_n | \phi_m \rangle \tilde{c}_m = \sum_m (U^{-1})_{nm} \tilde{c}_m\tag{320}$$

which implies:

$$U^{-1} U = I\tag{321}$$

Moreover, the matrix elements:

$$(U^{-1})_{nm} = \langle \phi_n | \psi_m \rangle = \overline{U}_{mn} \iff U^{-1} = U^\dagger\tag{322}$$

which is an unitary matrix or unitary operator. The $\infty - \text{dim}$ matrix in a representation is an operator. Let us consider two states $\psi, \phi \in \mathcal{H}$ in a given representation $\{\psi_n\}$ and an operator \hat{O} , we can compute the inner product in two representations:

$$\langle \psi | \hat{O} \phi \rangle = \sum_{m,n} \overline{b_m} d_n \langle \psi_m, \psi_n \rangle = \sum_n \overline{b_n} d_n\tag{323}$$

where we have used the matrix representation of \hat{O} :

$$\begin{aligned}b_n &= \sum_m O_{nm} c_m, & \psi &= \sum_m c_m \psi_m, \\ d_n &= \sum_m O_{nm} f_m, & \phi &= \sum_m f_m \psi_m.\end{aligned}\tag{324}$$

If \hat{O} is unitary, $\iff \langle \hat{O}\psi, \hat{O}\phi \rangle = \langle \psi, \phi \rangle$. Notice that given a representation $\{\psi_n\}_{n=1}^\infty$, the inner product is defined as:

$$\langle \psi, \phi \rangle = \sum_{m=1}^{\infty} \overline{c_m} f_m\tag{325}$$

same as inner product on \mathbb{C}^N as $N \rightarrow \infty$. We can view the Hilbert space \mathcal{H} in QM is abstract. The state ψ is a vector in the abs \mathcal{H} with abstract inner product $\langle \psi, \phi \rangle$.

Summary of representations

- Given a representation: $\langle \psi, \phi \rangle = \sum_{m=1}^{\infty} \overline{c_m} f_m$.
 - The components (c_1, c_2, \dots) depend on the basis.
 - An operator \hat{O} is represented by a matrix whose entries are computed using inner products in the given basis.
 - Representations are equivalent to choosing different coordinate systems in Hilbert space.
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