Quantum Theory

An Olympiad Handout

Tawhid Bin Omar

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Topics Covered: Old Quantum Theory · Bohr's Postulates · Bohr–Sommerfeld Quantization · Hydrogen Atom · Wave-Particle Duality · Hilbert Space Axiomatics · Wave Function · Schrödinger Equation · Measurement Theory

Contents

1 Old Quantum Theory

Historical Context: Origins of Quantum Theory

The study of quantum theory begins with a series of experimental conclusions that could not be explained by classical theory. One of the first investigations was the analysis of thermal (blackbody) radiation. Classical theory predicted a catastrophic divergence at short wavelengths; resolving this required a radical new idea.

The classical approach (Rayleigh–Jeans) yields an energy distribution density:

Key Formula: Rayleigh–Jeans Formula

$$u(\omega, T) = \frac{\omega^3}{\pi^2 c^3} kT$$

This formula describes observations well at large wavelengths, but **fails catastrophically** at small wavelengths (the "ultraviolet catastrophe").

Definition: Planck's Quantum Hypothesis

Max Planck proposed that bodies emit energy not in a continuous spectrum, but in discrete portions proportional to the radiation frequency:

$$\varepsilon = \hbar\omega$$

This formula encapsulates **wave-particle duality**: energy is a particle characteristic, frequency is a wave characteristic.

If radiation is emitted in portions $\hbar\omega$, then energy must be an integer multiple:

$$\varepsilon_n = n\hbar\omega$$

Using the Boltzmann distribution, the probability of energy ε_n is:

$$P_n = \frac{e^{-\varepsilon_n/kT}}{\sum_n e^{-\varepsilon_n/kT}}$$

Computing the average radiation energy:

$$\langle\varepsilon\rangle = \sum_n P_n \varepsilon_n = -\hbar\omega \frac{d}{dx} \ln \sum_n e^{-nx} \bigg|_{x=\hbar\omega/kT}$$

Using $\sum_n e^{-nx} = \dfrac{1}{1 - e^{-x}}$:

Key Formula: Planck's Formula

$$u(\omega, T) = \frac{\hbar\omega}{\exp\left(\dfrac{\hbar\omega}{kT}\right) - 1} \cdot \frac{\omega^2}{\pi^2 c^3}$$

This formula agrees with all experiments. It was the **first contradiction with classical**

theory, which requires energy to be continuous.

Remark: The Photoelectric Effect

Light incident on the surface of a substance ejects electrons as though it were a stream of particles striking them, not a classical electromagnetic wave. This is the second major failure of classical physics to describe radiation.

2 Atom Structure and Bohr's Postulates

Rutherford's scattering experiment, directing electrons at a metal foil and measuring deflection, indicated the atom consists of a small, heavy nucleus with electrons orbiting it. The Coulomb interaction gives:

$$\Delta p = 2p_0 \sin\frac{\theta}{2}, \qquad \cot\frac{\theta}{2} = \frac{mv^2}{2Ze^2}\,b$$

Key Formula: Rutherford's Scattering Formula

$$\frac{dN}{N} = na\left(\frac{Ze^2}{mv^2}\right)^2 \frac{d\Omega}{\sin^4(\theta/2)}$$

Remark: The Stability Problem

Classical electrodynamics predicts that an accelerating electron must radiate, losing energy and spiraling into the nucleus. Yet atoms are stable. This contradiction motivated Bohr's postulates.

2.1 Bohr's Postulates

Axiom 1 (Discrete Orbits)

From the infinite set of possible electron orbits, electrons occupy only certain **discrete** ones, with corresponding discrete energy values. Energy is *not* a continuous function, in direct contradiction to classical mechanics.

Axiom 2 (Quantum Transitions)

Radiation is emitted or absorbed in the form of a light quantum when an electron transitions from one state to another:

$$\hbar\omega = E_n - E_m$$

2.2 Bohr–Sommerfeld Quantization

For a harmonic oscillator with energy $E = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} = n\hbar\omega$, the orbit in phase space is an ellipse.

Key Formula: Bohr–Sommerfeld Quantization Condition

$$\oint p\,dq = 2\pi\hbar n$$

For angular momentum with $p \equiv M$, $q \equiv \varphi$:

$$\boxed{M = n\hbar}$$

2.3 Hydrogen Atom Model

From $mvr = n\hbar$ and Newton's equation $\frac{mv^2}{r} = \frac{Ze^2}{r^2}$:

Key Formula: Hydrogen Atom: Bohr Model

Allowed orbit radii:

$$r_n = \frac{\hbar^2}{mZe^2} n^2$$

Energy spectrum:

$$E_n = -\frac{me^4 Z^2}{2\hbar^2 n^2}$$

2.4 Interference and Wave-Particle Duality

Definition: Wave-Particle Duality

Diffraction experiments show that not only photons but also electrons produce interference patterns when passing through slits. This means our "particles" are neither classical particles nor classical waves. They are quantum objects whose behavior we can study only probabilistically.

3 New Quantum Theory: Axiomatic Foundations

Historical Context: Motivation

Experiments in the USSR showed that electrons emitted in small portions land at random, yet different, points on a screen. Over many repetitions, some points are hit more often and some never. This motivates a *probabilistic* framework for quantum mechanics.

Definition: State of a Quantum System

The **state** of a quantum system is defined by a *complete set of simultaneously measurable observables* (a complete set of commuting observables, CSCO). These are the degrees of freedom of the state. States may be:

- **Pure states:** Fully characterized by interaction with this system alone.
- **Mixed states:** Systems in interaction with the environment; require density matrix formalism.

3.1 Axiom 1: Hilbert Space

Axiom 1 (State Space)

A pure state of the quantum system is associated with an element $|\Psi\rangle$ of an abstract **Hilbert space**.

Definition: Hilbert Space

An abstract Hilbert space is an **infinite-dimensional, separable, complete** (in the Cauchy sense), **Euclidean linear space over** $\mathbb{C}$.

- **Linear:** Sums and scalar multiples remain in the space.
- **Euclidean:** Inner product is defined: $\langle\Psi_1|\Psi_2\rangle = \int_{-\infty}^{+\infty} \Psi_1^* \, \Psi_2 \, d^3x$
- **Complete:** Any element can be approximated by a linear combination: $|\Psi\rangle = \sum_i c_i \, |\Psi_i\rangle$ (Superposition Principle)
- **Separable:** Possesses a countable orthonormal basis.

Remark: Superposition of States

The completeness relation $|\Psi\rangle = \sum_i c_i \, |\Psi_i\rangle$ expresses the **principle of superposition**: before measurement, a particle exists in a superposition of all possible states simultaneously.

3.2 Wave Function

Definition: Wave Function and Its Representations

The wave function exists in two conjugate representations connected by Fourier transform:

- **Coordinate representation** $\Psi(x)$: $|\Psi(x)|^2$ is the probability density of finding the particle at x.
- **Momentum representation** $\Psi(p)$: $|\Psi(p)|^2$ gives the momentum probability density.

$$\Psi(p) = \int_{-\infty}^{+\infty} \Psi(x) \, e^{-ipx/\hbar} \, dx$$

3.3 Axiom 2: On Measurement

Axiom 2 (Observables as Operators)

Physical quantities are associated with **linear operators**. The eigenvalues of these operators give the possible measurement outcomes; the corresponding eigenstates are the states after measurement.

$$\hat{A} \, \Psi = a \, \Psi$$

3.4 Axiom 3: Quantization

Axiom 3 (Canonical Quantization)

Given a classical quantity $A(p, q, t)$, the corresponding quantum operator is $\hat{A}(\hat{p}, \hat{q}, t)$, where operators satisfy the **canonical commutation relation**:

$$[\hat{p},\, \hat{q}] = i\hbar$$

The solution is:

$$\hat{q} = q \cdot \text{(multiplication)}, \qquad \hat{p} = -i\hbar\nabla$$

Key Formula: Hamiltonian Operator and Energy Eigenvalue Equation

$$H = \frac{p^2}{2m} + U(r) \quad \longrightarrow \quad \hat{H} = -\frac{\hbar^2}{2m}\Delta + U(r)$$

Energy eigenvalue equation (time-independent Schrödinger equation):

$$\hat{H}\Psi = E\Psi \qquad \Longleftrightarrow \qquad -\frac{\hbar^2}{2m}\Delta\Psi + U(r)\Psi = E\Psi$$

3.5 Axiom 4: The Schrödinger Equation

Axiom 4 (Time Evolution – Schrödinger Equation)

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\Delta\Psi(x,t) + U(x)\Psi(x,t)}$$

This equation governs the time evolution of the quantum state.

Definition: Heisenberg Picture

Alternatively, one can fix the state and evolve the operators:

$$\frac{d\hat{F}}{dt} = \frac{\partial\hat{F}}{\partial t} + \frac{i}{\hbar}[\hat{H},\, \hat{F}]$$

The two pictures (Schrödinger and Heisenberg) are equivalent.

3.6 Key Conclusions on Measurement

Remark: Discreteness and Quantization

- For any localized micro-object (confined to a finite region), the spectrum of measurable quantities is **discrete**.
- Quantities change in “portions” — they are **quantized**.
- Even a “continuous” spectrum is really an extremely dense discrete spectrum.

Remark: Degrees of Freedom

To obtain complete information about a quantum system's state, it is generally necessary to measure **more than one quantity**. The number of required independent measurements equals the number of degrees of freedom of the system.

4 Problems

Problem 1 — Photoelectric Effect

A metal plate is irradiated with light that knocks electrons out of it. Analyze the resulting photoelectric effect.

Problem 2 — Work Function from Current-Voltage Graph

Monochromatic radiation with power $P = 0.18$ W falls on the cathode of a vacuum tube and produces a photocurrent. On average, 1 out of 25 photons knocks out an electron. A graph of current vs. voltage between anode and cathode is given. Find the **work function** of electrons from the cathode material.

Problem 3 — Light Pressure on a Moving Mirror

A moving robot carries a perfectly reflecting mirror (reflection coefficient ≈ 1) past a fixed, powerful light source. A sensor records the light pressure force on the mirror. At some moment the force reaches a maximum $F_m = 0.8$ nN; after time $t = 2.60$ s it becomes $F = 0.1$ nN. The robot moves at $v = 2$ m/s and the mirror area is $S = 10$ cm^2. Find:

(a) The minimum distance from the source to the mirror during the motion.

(b) The power of the source.

Problem 4 — Hydrogen Atom Transitions

The energy levels of hydrogen: $E_n = -E_1/n^2$, where $E_1 \approx -13.6$ eV. A ground-state hydrogen atom absorbs a photon with wavelength $\lambda_1 \approx 103$ nm. It then returns to the ground state by emitting two photons with wavelengths λ_2 and λ_3. Find λ_2 and λ_3.

Problem 5 — Compton Scattering

One of the most striking demonstrations of the corpuscular nature of light is the Compton effect: a photon scattering off an electron transfers part of its momentum and thus undergoes a wavelength shift ("redshift"). Derive the change in photon wavelength $\Delta\lambda$ as a function of scattering angle.

Problem 6 — Harmonic Oscillator Ground State Energy

Using the **Heisenberg uncertainty relation** $\Delta x\,\Delta p \geq \hbar/2$, determine the minimum energy of a quantum harmonic oscillator.

Problem 7 — Kvantik the Quantum Kitten

In the quantum world, a kitten named Kvantik can be in a superposition of two box states:

$$|\Psi\rangle = a\,|1\rangle + b\,|2\rangle$$

Monday: The wave function is $|\Psi\rangle = \frac{1}{\sqrt{3}}\,|1\rangle + b\,|2\rangle$.
Find the probability of finding Kvantik in box 1 and box 2.
Tuesday: The probability of finding Kvantik in box 2 is 3 times that of box 1.
Determine the coefficients of the wave function.

Problem 8 — Double-Slit Electron

An electron's state in the double-slit experiment is:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\,|L\rangle + \frac{i}{\sqrt{2}}\,|R\rangle$$

Probability amplitudes from left/right slit at point X: $Ae^{i\varphi_1}$, $Ae^{i\varphi_2}$ with $\varphi_2 - \varphi_1 = \pi/2$.
Find the probability of the electron hitting point X.

Problem 9 — Photon Polarization

A photon is in a superposition of $|\leftrightarrow\rangle$ (horizontal) and $|\updownarrow\rangle$ (vertical) polarization. It is known that:

- Probability of detecting $+45$ polarization: 0.5
- Probability of detecting -45 polarization: 0.25

Can you determine the probabilities of finding the photon in each basis state?

Problem 10 — Advanced Problems

Problems on: the **potential barrier**, the **hydrogen atom**, and a **particle in a magnetic field**.

Problem 11 — Quantum Tunneling Current

Two parallel metal plates (area S, separation $L = 2$ nm) in vacuum, voltage $U = 10$ V.
All electrons have energy $\varepsilon = 1.5$ eV, work function = 2 eV.
Tunneling probability:

$$D \approx \exp\left(-\frac{4\sqrt{2m}}{3\hbar eE}\,(A-\varepsilon)^{3/2}\right)$$

At $t = 0$, there are 10^{12} electrons on the plate.

(a) Find the number of electrons that transfer in 0.01 s.

(b) Estimate the average current over 0.01 s.

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