MODERN PHYSICS: QUANTUM MECHANICS STUDY MATERIALS

PARTICLE ASPECT OF RADIATION

BLACKBODY RADIATION

Blackbody radiation refers to the electromagnetic radiation emitted by a black body (an idealized object that absorbs all incident electromagnetic radiation). Max Planck revolutionized physics by proposing that energy is quantized, meaning it is emitted or absorbed in discrete packets called quanta. The energy of a quantum is given by $E = hf$, where h is Planck's constant (approximately 6.626 x 10^{-34} J·s) and f is the frequency of the radiation.

Planck's Law describes the spectral radiance of a black body as a function of frequency or wavelength.

Example Problem: A black body at 6000 K has its peak emission at 500 nm. If the temperature is increased to 8000 K, what is the new peak emission wavelength? (Wien's Displacement Law: $\lambda_{max}T = constant$)

Solution Approach: Using Wien's Law, $\lambda_{max1}T_1 = \lambda_{max2}T_2$. So, $\lambda_{max2} = (\lambda_{max1}T_1) / T_2 = (500 \text{ nm} * 6000 \text{ K}) / 8000 \text{ K} = 375 \text{ nm}$.

PHOTOELECTRIC EFFECT

The photoelectric effect is the emission of electrons from a material when light shines on it. Albert Einstein explained this phenomenon by extending Planck's quantum hypothesis. He proposed that light itself consists of particles called photons, each carrying an energy $E = hf$. For an electron to be emitted, it must absorb a photon with enough energy to overcome the work function (Φ) of the material. The kinetic energy (KE_{max}) of the emitted electron is given by Einstein's photoelectric equation: $KE_{max} = hf - \Phi$.

Key concepts include:

- **Threshold Frequency (f_0):** The minimum frequency of light required to eject electrons. $hf_0 = \Phi$.
- **Stopping Potential (V_s):** The minimum negative voltage applied to the collector plate that stops the most energetic electrons from reaching it. $KE_{max} = eV_s$, where e is the elementary charge.

Example Problem: Light of frequency 8.0 x 10^{14} Hz shines on a metal surface with a work function of 2.0 eV. Calculate the maximum kinetic energy of the emitted electrons in Joules and the stopping potential in Volts. (1 eV = 1.602 x 10^{-19} J)

Solution Approach: Convert work function to Joules: $\Phi = 2.0\ eV * 1.602 \times 10^{-19}\ J/eV = 3.204 \times 10^{-19}\ J$. Calculate photon energy: $E = hf = (6.626 \times 10^{-34}\ J\cdot s) * (8.0 \times 10^{14}\ Hz) = 5.301 \times 10^{-19}\ J$. Max KE: $KE_{max} = E - \Phi = 5.301 \times 10^{-19}\ J - 3.204 \times 10^{-19}\ J = 2.097 \times 10^{-19}\ J$. Stopping potential: $V_s = KE_{max} / e = (2.097 \times 10^{-19}\ J) / (1.602 \times 10^{-19}\ C) \approx 1.31\ V$.

COMPTON EFFECT

The Compton effect is the inelastic scattering of a photon by a charged particle, usually an electron. Arthur Compton demonstrated that photons, despite being massless, carry momentum ($p = h/\lambda = E/c$) and behave like particles during collisions. When a photon scatters off an electron, it loses energy (and thus its wavelength increases), while the electron gains kinetic energy and momentum. The change in wavelength (Δλ) depends on the scattering angle (θ) and is given by the Compton scattering formula: $\Delta\lambda = \lambda' - \lambda = (h / m_e c) * (1 - \cos\theta)$, where m_e is the electron rest mass and c is the speed of light. The term $h / m_e c$ is the Compton wavelength of the electron (approximately 0.0243 Å or 2.43 x 10^{-12} m).

Example Problem: A 0.050 Å X-ray photon is scattered at an angle of 60° by an electron. What is the wavelength of the scattered photon?

Solution Approach: Calculate the change in wavelength: $\Delta\lambda = (0.0243\ Å) * (1 - \cos 60°) = (0.0243\ Å) * (1 - 0.5) = 0.01215\ Å$. The new wavelength is $\lambda' = \lambda + \Delta\lambda = 0.050\ Å + 0.01215\ Å = 0.06215\ Å$.

WAVE ASPECT OF PARTICLES

DE BROGLIE'S HYPOTHESIS: MATTER WAVES

Louis de Broglie proposed that if light waves exhibit particle-like properties (photons), then particles like electrons should exhibit wave-like properties. He postulated that a particle with momentum p has an associated wavelength λ given by $\lambda = h/p$, where h is Planck's constant. This wavelength is known as the de Broglie wavelength.

Example Problem: Calculate the de Broglie wavelength of an electron (mass 9.11 x 10^{-31} kg) moving at a speed of 1.0 x 10^{6} m/s.

Solution Approach: First, calculate the momentum: $p = mv = (9.11 \times 10^{-31}\ kg) * (1.0 \times 10^{6}\ m/s) = 9.11 \times 10^{-25}\ kg{\cdot}m/s$. Then, calculate the wavelength: $\lambda = h/p = (6.626 \times 10^{-34}\ J{\cdot}s) / (9.11 \times 10^{-25}\ kg{\cdot}m/s) \approx 7.27 \times 10^{-10}\ m$ (or 0.727 nm).

HEISENBERG'S UNCERTAINTY PRINCIPLE

Werner Heisenberg's uncertainty principle states that there are fundamental limits to how precisely certain pairs of physical properties of a particle, known as conjugate variables, can be known simultaneously. The most famous pair is position (x) and momentum (p). The principle states: $\Delta x\, \Delta p_x \geq \hbar/2$, where Δx is the uncertainty in position, Δp_x is the uncertainty in momentum along the x-axis, and $\hbar = h/(2\pi)$ is the reduced Planck's constant.

Another important relation is between energy (E) and time (t): $\Delta E\, \Delta t \geq \hbar/2$.

Example Problem: An electron is confined to a region of space of width 1.0 nm. Estimate the minimum uncertainty in its momentum.

Solution Approach: We can approximate $\Delta x \approx 1.0\ nm = 1.0 \times 10^{-9}\ m$. Using the uncertainty principle, $\Delta p_x \geq \hbar/(2\Delta x) = (1.055 \times 10^{-34}\ J{\cdot}s) / (2 * 1.0 \times 10^{-9}\ m) \approx 5.275 \times 10^{-26}\ kg{\cdot}m/s$.

WAVE PACKET AND TIME EVOLUTION

A single de Broglie wave with infinite extent is not localized. To represent a localized particle, one needs to superimpose (add) waves of slightly different wavelengths. This superposition creates a wave packet. The wave packet represents the probability amplitude of finding the particle at a certain position. The time evolution of this wave packet is governed by the **Time-Dependent Schrödinger Equation**.

GROUP AND PHASE VELOCITIES

For a wave packet, two velocities are important:

- **Phase Velocity (v_p):** The speed at which a point of constant phase (e.g., a crest) of a monochromatic wave propagates. For a de Broglie wave, $v_p = E/p = (mc^2)/(mv) = c^2/v$, where v is the particle's velocity. Since $v < c$, $v_p > c$, which does not violate relativity as it doesn't carry information.
- **Group Velocity (v_g):** The speed at which the overall envelope (and thus the wave packet) of the wave propagates. This is the velocity of the particle. It can be shown that $v_g = d\omega/dk$, where ω is angular frequency and k is the wave number. For a relativistic particle, $v_g = v$.

Example Problem: For a non-relativistic particle of mass m and velocity v, show that $v_g = v$.

Solution Approach: Using de Broglie relations $E = \hbar\omega$ and $p = \hbar k$, we have $\omega = E/\hbar = (p^2/(2m))/\hbar = (\hbar k)^2/(2m\hbar) = \hbar k^2/(2m)$. Then, $v_g = d\omega/dk = d/dk\ (\hbar k^2/(2m)) = \hbar(2k)/(2m) = \hbar k/m$. Since $p = \hbar k$, $v_g = p/m = mv/m = v$.

SCHRÖDINGER EQUATION AND WAVEFUNCTION

THE TIME-DEPENDENT SCHRÖDINGER EQUATION (TDSE)

The TDSE is a fundamental equation in quantum mechanics that describes how the quantum state (represented by the wavefunction, Ψ) of a physical system changes over time. For a single particle of mass m in a potential $V(r, t)$, it is given by:

$$i\hbar \, \partial\Psi(r, t)/\partial t = \hat{H}\Psi(r, t)$$

where $\hat{H} = -\hbar^2/2m \, \nabla^2 + V(r, t)$ is the Hamiltonian operator, and ∇^2 is the Laplacian operator.

THE TIME-INDEPENDENT SCHRÖDINGER EQUATION (TISE)

When the potential energy V does not depend on time, the wavefunction can be separated into spatial and temporal parts: $\Psi(r, t) = \psi(r) * \varphi(t)$. This leads to the TISE, which describes the spatial distribution of a particle in a stationary state (a state where the probability density does not change with time):

$$\hat{H}\psi(r) = E\psi(r)$$

or

$$-\hbar^2/2m \, \nabla^2\psi(r) + V(r)\psi(r) = E\psi(r)$$

Here, E is the energy eigenvalue, representing the possible energy values the system can have. The solutions $\psi(r)$ are the energy eigenfunctions.

ACCEPTABILITY CONDITIONS FOR WAVE FUNCTIONS

For a wavefunction $\psi(r)$ to be physically meaningful, it must satisfy certain conditions:

- **Single-valued:** $\psi(r)$ must have only one value at each point in space.
- **Continuous:** $\psi(r)$ must be continuous everywhere.
- **Finite:** $\psi(r)$ must be finite everywhere.
- **Square-integrable:** The integral of the absolute square of $\psi(r)$ over all space must be finite ($\int|\psi(r)|^2 \, dr < \infty$). This ensures the total probability is 1.

PROBABILITY INTERPRETATION OF WAVE FUNCTION

According to the Born interpretation, the square of the absolute value of the wavefunction, $|\Psi(r, t)|^2$, represents the probability density of finding the particle at position r at time t. The probability dP of finding the particle in a small volume element dV at (r, t) is $dP = |\Psi(r, t)|^2 dV$. The total probability of finding the particle anywhere in space must be 1: $\int|\Psi(r, t)|^2 dV = 1$.

VECTOR REPRESENTATION AND DIRAC'S BRA-KET NOTATION

Quantum mechanical states can be represented as vectors in a complex vector space called Hilbert space. Each state $|\psi\rangle$ corresponds to a vector. Dirac's bra-ket notation is a convenient way to handle these vectors:

- **Ket vector:** $|\psi\rangle$ represents a state vector.
- **Bra vector:** $\langle\psi|$ is the complex conjugate transpose of the ket vector.
- **Inner product:** $\langle\varphi|\psi\rangle$ represents the inner product between two states, which corresponds to the integral $\int\varphi^*(r)\psi(r)\,dr$. This value is a complex number.

The inner product $\langle\psi|\psi\rangle$ is the norm squared of the state, which must be real and non-negative. For a normalized state, $\langle\psi|\psi\rangle = 1$.

ORTHONORMALITY OF WAVE FUNCTIONS

If ψ_n and ψ_m are two distinct eigenfunctions of a Hermitian operator (like the Hamiltonian), they are orthogonal to each other. This means their inner product is zero:

$\langle\psi_n|\psi_m\rangle = \int\psi_n^*(r)\psi_m(r)\,dr = 0$, for $n \neq m$.

A set of eigenfunctions that are mutually orthogonal and normalized to unity is called an orthonormal set.

CONCEPT OF OPERATORS

OPERATORS, EIGENFUNCTIONS, AND EIGENVALUES

In quantum mechanics, physical observables (like position, momentum, energy) are represented by linear operators. When an operator $\hat{A}$ acts on a function ψ, it transforms it into another function. If the result is proportional to the original function, then ψ is an eigenfunction of $\hat{A}$, and the proportionality constant is the eigenvalue:

$$\hat{A}\psi = a\psi$$

Here, $\hat{A}$ is the operator, ψ is the eigenfunction, and a is the eigenvalue. The eigenvalues represent the possible results of measuring the observable corresponding to the operator $\hat{A}$.

LINEAR OPERATORS AND COMMUTATION

An operator $\hat{A}$ is linear if $\hat{A}(c_1\psi_1 + c_2\psi_2) = c_1\hat{A}\psi_1 + c_2\hat{A}\psi_2$ for constants c_1, c_2 and functions ψ_1, ψ_2.

The **commutator** of two operators $\hat{A}$ and $\hat{B}$ is defined as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. If $[\hat{A}, \hat{B}] = 0$, the operators commute, meaning they can be applied in any order, and their corresponding observables can be measured simultaneously with arbitrary precision (their eigenfunctions are the same).

If $[\hat{A}, \hat{B}] \neq 0$, they do not commute, and there is a fundamental limit to the precision with which both observables can be known simultaneously, as expressed by the Heisenberg uncertainty principle.

Example Problem: For a free particle, the momentum operator is $\hat{p}_x = -i\hbar\, \partial/\partial x$ and the position operator is $\hat{x} = x$. Show that they do not commute.

Solution Approach: Calculate the commutator: $[\hat{x}, \hat{p}_x] = \hat{x}\, \hat{p}_x - \hat{p}_x\, \hat{x} = x(-i\hbar\, \partial/\partial x) - (-i\hbar\, \partial/\partial x)x$. Applying this to a test function $f(x)$: $(x(-i\hbar\, \partial/\partial x) - (-i\hbar\, \partial/\partial x)x)f(x) = -i\hbar\, x\, \partial f/\partial x - (-i\hbar\, (\partial f/\partial x + x\, \partial f/\partial x)) = -i\hbar\, x\, \partial f/\partial x + i\hbar\, \partial f/\partial x + i\hbar\, x\, \partial f/\partial x = i\hbar\, \partial f/\partial x$. Thus, $[\hat{x}, \hat{p}_x] = i\hbar$, which is not zero, so they do not commute.

EXPECTATION VALUE

The expectation value $\langle\hat{A}\rangle$ of an observable corresponding to the operator $\hat{A}$ for a system in a normalized state $|\psi\rangle$ is the average value of measurements of that observable on an ensemble of identically prepared systems. It is calculated as:

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle = \int \psi^*(r)\, \hat{A}\psi(r)\, dr$$

POSTULATES AND GENERAL PRINCIPLES OF QUANTUM MECHANICS

POSTULATES OF QUANTUM MECHANICS

The foundation of quantum mechanics is built upon a set of postulates:

1. **State Postulate:** The state of a quantum system is completely described by a wavefunction $\Psi(r, t)$, which is a vector in Hilbert space.
2. **Observable Postulate:** To every observable quantity in classical physics, there corresponds a linear, Hermitian operator in quantum mechanics.
3. **Measurement Postulate:** The possible results of measuring an observable are the eigenvalues of the corresponding operator. Upon measurement, the system collapses into the eigenstate corresponding to the measured eigenvalue.
4. **Probability Postulate (Born Rule):** The probability of measuring a particular eigenvalue is given by the square of the absolute value of the wavefunction's projection onto the corresponding eigenstate. For a normalized state $|\psi\rangle$ and an operator $\hat{A}$ with eigenvalue a and eigenfunction $|a\rangle$, the probability is $|\langle a|\psi\rangle|^2$.
5. **Time Evolution Postulate:** The evolution of the wavefunction in time is governed by the Time-Dependent Schrödinger Equation (TDSE): $i\hbar\, \partial\Psi/\partial t = \hat{H}\Psi$.

HERMITIAN OPERATORS

An operator $\hat{A}$ is Hermitian if it is equal to its own complex conjugate transpose (adjoint): $\hat{A}^\dagger = \hat{A}$. In integral form, this means $\int \varphi^*(r)\, \hat{A}\psi(r)\, dr = \int (\hat{A}\varphi)^*(r)\, \psi(r)\, dr$ for any valid wavefunctions φ and ψ.

Properties of Hermitian Operators:

- Their eigenvalues are always real numbers, corresponding to measurable quantities.
- Eigenfunctions corresponding to distinct eigenvalues are orthogonal.

Example Problem: Show that the momentum operator $\hat{p}_x = -i\hbar\, d/dx$ is Hermitian on the interval [a, b].

Solution Approach: We need to show $\int_a^b \varphi^*(x)\, \hat{p}_x\, \psi(x)\, dx = \int_a^b (\hat{p}_x\varphi)^*(x)\, \psi(x)\, dx$. Starting with the left side: $\int_a^b \varphi^*(x)\, (-i\hbar\, d\psi/dx)\, dx = -i\hbar \int_a^b \varphi^*(x)\, d\psi/dx\, dx$. Using integration by parts: $[\varphi^*(x)\psi(x)]_a^b - \int_a^b (d\varphi^*/dx)\, \psi(x)\, dx$. If we assume the boundary terms vanish (e.g., wavefunctions are zero at boundaries or periodic), this becomes $-\int_a^b (d\varphi^*/dx)\, \psi(x)\, dx$. Since $(\hat{p}_x\varphi)^* = (-i\hbar\, d\varphi/dx)^* = i\hbar\, d\varphi^*/dx$, the right side is $\int_a^b (i\hbar\, d\varphi^*/dx)\, \psi(x)\, dx = i\hbar \int_a^b (d\varphi^*/dx)\, \psi(x)\, dx$. Thus, $-i\hbar \int_a^b (d\varphi^*/dx)\, \psi(x)\, dx = -(i\hbar \int_a^b (d\varphi^*/dx)\, \psi(x)\, dx)$. Wait, need to be careful with the sign. Let's retry integration by parts.

Left side: $\int_a^b \varphi^*(x)\, (-i\hbar\, d\psi/dx)\, dx = -i\hbar \int_a^b \varphi^*(x)\, d\psi/dx\, dx$. Integration by parts ($u = \phi^*$, $dv = d\psi/dx\, dx \Rightarrow du = d\phi^*/dx\, dx$, $v = \psi$): $-i\hbar\, [\varphi^*(x)\psi(x)]_a^b - (-i\hbar) \int_a^b (d\varphi^*/dx)\, \psi(x)\, dx$. Assuming boundary terms are zero: $i\hbar \int_a^b (d\varphi^*/dx)\, \psi(x)\, dx$. Now, consider the right side: $\int_a^b (\hat{p}_x\varphi)^*(x)\, \psi(x)\, dx = \int_a^b (-i\hbar\, d\varphi/dx)^*(x)\, \psi(x)\, dx = \int_a^b (i\hbar\, d\varphi^*/dx)\, \psi(x)\, dx = i\hbar \int_a^b (d\varphi^*/dx)\, \psi(x)\, dx$. The two sides are equal, so $\hat{p}_x$ is Hermitian (under appropriate boundary conditions).

EXPANSION IN EIGENFUNCTIONS

A crucial property of operators corresponding to physical observables is that their eigenfunctions form a complete set. This means any arbitrary, well-behaved wavefunction $\Phi(r)$ can be expanded as a linear combination (a sum or integral) of the eigenfunctions $\psi_n(r)$ of a given operator $\hat{A}$:

$$\Phi(r) = \Sigma_n\, c_n\, \psi_n(r)$$

where c_n are coefficients. If the eigenfunctions are orthonormal, these coefficients can be found using the inner product: $c_n = \langle\psi_n|\Phi\rangle = \int \psi_n^*(r)\Phi(r)\, dr$.

EIGENFUNCTIONS OF COMMUTING OPERATORS

If two operators $\hat{A}$ and $\hat{B}$ commute (i.e., $[\hat{A}, \hat{B}] = 0$), then there exists a complete set of common eigenfunctions that are eigenfunctions of both operators simultaneously. This means that the corresponding physical quantities can be measured simultaneously with arbitrary precision.