量 子 力 学 QUANTUM MECHANICS

<u>Fundamentals of quantum theory (de Broglie wavelength, uncertainty relation and photoelectric effect)</u>

1. When an electron, a proton, and an alpha particle have the same kinetic energy, show which particle has the longest de Broglie wavelength and explain the reason.
2. When an electron is enclosed in a cube of an edge length a, calculate the lowest energy of the electron using the uncertainty principle.
3. Calculate the minimum frequency of a photon causing the photoelectric effect for the hydrogen atom. Here, the binding energy of an electron in a hydrogen atom is 13 eV, the value of Planck's constant is $6.63 \times 10^{-34}\ \mathrm{J \cdot s}$, and $1\ \mathrm{eV} = 1.60 \times 10^{-19}\ \mathrm{J}$.
4. Consider that photoelectrons are produced when photons with frequency ν irradiate a metal. Show the kinetic energy E of one photoelectron in terms of the work function ϕ of the metal and Planck's constant h. Here, assume that the effect of relativity in the kinematics of an electron can be ignored.

<u>Wave functions, Schrödinger equations and potentials</u>

1. Consider a free particle of mass m confined in the region of $0 \le x \le L$ in a one-dimensional space.

   (1) Show that normalized wave functions of the particle are given by

   $$\varphi_n(x) = \sqrt{2/L}\,\sin(n\pi x/L) \quad (n = 1, 2, 3, \cdots).$$

   (2) Show that the wave functions for the different states are mutually orthogonal.

2. The time-independent Schrödinger equation for a free particle is given by

$$\hat{H}\varphi(x,y,z) = E\varphi(x,y,z),$$

where E and $\varphi(x,y,z)$ are eigenvalues and eigenfunctions of Hamiltonian $\hat{H}$, respectively. Answer the following questions.

(1) Find general solutions of $\varphi_x(x)$, $\varphi_y(y)$ and $\varphi_z(z)$ when $\varphi(x,y,z)$ is expressed by $\varphi(x,y,z) = \varphi_x(x)\,\varphi_y(y)\,\varphi_z(z)$ in the manner of separation of variables.

(2) When the particle is confined to a region of $0 \le x \le L$, $0 \le y \le L$, $0 \le z \le L$, find the $\varphi_x(x)$, $\varphi_y(y)$ and $\varphi_z(z)$.

(3) Find the eigenvalue E by using the result of question (2).

3. A particle with mass *m* and energy $E\ (<0)$ is bound in one-dimensional potential

$$V(x) = \begin{cases} \infty, & x \le 0 \quad (\text{Region I}) \\ -V_0\ (<0), & 0 < x < L \quad (\text{Region II}) \\ 0, & L \le x \quad (\text{Region III}) \end{cases}.$$

(1) Letting *k* and *k'* denote the wave numbers of the particle in the respective regions II and III, derive the wave functions.

(2) Derive the relationship between the wave numbers *k* and *k*' of question (1).

4. When a particle of mass m is bound in a one-dimensional potential $V(x) = (1/2)kx^2\ (k > 0)$, the energy eigenvalues of the particle are given by $E_n = (n + 1/2)\hbar\sqrt{k/m}\quad (n = 0, 1, 2, \cdots)$. Here, $\hbar$ is denoted by $h/2\pi$, and h is Planck's constant. Assuming that the relativistic effect in the kinematics of the particle

is ignored, answer the following questions.

(1) Explain that the value of the wave function of the particle is zero at $x = \pm\infty$.

(2) Give the time-independent Schrödinger equation for the particle.

(3) Show that the Schrödinger equation in question (2) has solutions of both odd and even functions.

(4) Assume that a solution of the Schrödinger equation in question (2) is $\psi(x) = A\exp(-\alpha x^2)$ for the ground state, where A and α (>0) are constants. Find the wave function for the ground state.

(5) Calculate the value of A normalizing $\psi(x)$ in question (4). If necessary, use the equation $\int_{-\infty}^{\infty} \exp(-x^2)\,dx = \sqrt{\pi}$.

5. Consider a particle with mass m and energy E, which approaches the potential

$$V(x) = \begin{cases} 0 & (x < 0) \\ V_0 \ (> E > 0) & (0 \le x) \end{cases},$$

from $x = -\infty$. The general solutions of the time-independent Schrödinger equations are given by

$$u(x) = \begin{cases} A\exp(ik_1 x) + B\exp(-ik_1 x) & (x < 0) \\ C\exp(k_2 x) + D\exp(-k_2 x) & (0 \le x) \end{cases},$$

where k_1 and k_2 are wave numbers. Ignore the relativistic effect in the kinematics of the particle, and answer the following questions.

(1) Express k_1 and k_2 using m, E, V_0 and $\hbar = h/(2\pi)$ (h: Planck's constant).

(2) Show the relationships among constants A, B, C and D under the boundary conditions at $x=0$ and $x=+\infty$.

(3) Find the reflection coefficient of the incident wave.

(4) Find the transmission coefficient of the incident wave.

(5) Explain that the probability current density in the stationary state is constant.

Hydrogen-like atom

1. The Hamiltonian for an electron in a hydrogen atom is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r},$$

where $\hbar = h/(2\pi)$ (h: Planck's constant), and m, e, ε_0 and r are electron mass, elementary charge, vacuum permittivity and distance from the hydrogen nucleus, respectively. The Laplacian ∇^2 in spherical polar coordinates (r, θ, ϕ) is described by

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}.$$

Assume that the wave function of the electron in the hydrogen atom is $\psi = \exp(-ar)$, where a is a positive constant. Answer the following questions. Use $\int_0^\infty x^z \exp(-bx)\,dx = z!/b^{z+1}$, if necessary.

(1) Find $\int \psi^* \psi \, dv$ and $\int \psi^* \hat{H} \psi \, dv$, where dv is the volume element in spherical polar coordinates and the integral expands over the entire region.

(2) Find the minimum energy expectation value and a which gives it.

2. The radial wave function $R_{\mathrm{K}}(r)$ of K shell of hydrogen atom is expressed by

$$R_{\mathrm{K}}(r) = 2(1/a_0)^{3/2} \exp(-r/a_0),$$

where a_0 is Bohr radius, and r is a distance from the nucleus. The expectation values of r and $1/r$ are denoted by $\langle r \rangle$ and $\langle 1/r \rangle$, respectively. When r_0 gives the maximal value of $r^2 R_{\mathrm{K}}^2(r)$, show that r_0 equals $1/\langle 1/r \rangle$ but disagrees with $\langle r \rangle$, and describe its physical meaning.

Expectation value and Hermitian operator

1. A particle of mass m in one-dimensional space is in the state $\psi(x,t) = \exp(ikx - i\omega t)$, where k, ω, t and $\hat{p}_{\mathrm{x}}$ are wave number, angular frequency of oscillation, time and momentum operator, respectively. And the expectation value of $\hat{A}$ is defined as $< \hat{A} > = \lim_{L\to\infty}\left(\int_{-L}^{L} \psi^* \hat{A} \psi \, dx \Big/ \int_{-L}^{L} \psi^* \psi \, dx \right)$. Find expectation values of $< x >$, $< (x - < x >)^2 >$, $< \hat{p}_{\mathrm{x}} >$ and $< (\hat{p}_{\mathrm{x}} - < \hat{p}_{\mathrm{x}} >)^2 >$ in this system.

2. When an operator $\hat{A}$ satisfies

$$\int_{-\infty}^{\infty} \psi^*(x) \hat{A} \varphi(x) dx = \int_{-\infty}^{\infty} (\hat{A}\psi(x))^* \varphi(x) dx$$

for two arbitrary functions $\psi(\phi)$ and $\varphi(\phi)$, $\hat{A}$ is called Hermitian.

(1) Show that the eigenvalues of a Hermitian operator are real.

(2) When $\hat{A}\psi(x) = a\psi(x)$ and $\hat{A}\varphi(x) = b\varphi(x)$ $(a \neq b)$ for the Hermitian operator $\hat{A}$, show $\int_{-\infty}^{\infty} \psi^*(x)\varphi(x)dx = 0$.