National Exams May 2018

17-Phys-A4, Quantum Mechanics

3 hours duration

NOTES:

1. If doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper, a clear statement of any assumptions made.
2. This is a CLOSED BOOK EXAM. Approved Casio or Sharp calculator is permitted.
3. Five (5) questions constitute a complete exam paper.
4. Each question is of equal value. Full Marking Scheme on Page 2.
5. Clarity and organization of the answers are important.
6. A number of equations and formulas, including some integrals, are provided at the end of exam questions.

Marking Scheme

Marking Scheme

1. 20 marks
2. (a) 5 marks; (b) 5 marks; (c) 5 marks; (d) 5 marks
3. 20 marks
4. (a) 7 marks; (b) 7 marks; (c) 6 marks
5. 20 marks
6. (a) 5 marks; (b) 5 marks; (c) 5 marks; (d) 5 marks
7. 20 marks

QUESTION 1

A particle of mass m is confined in a one dimensional infinite square well potential of the form:

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ +\infty, & \text{otherwise} \end{cases}$$

Use the time-independent Schrödinger equation to determine the eigenfunctions and the quantized energy levels of the system.

QUESTION 2

(a) Explain in few sentences why quantum mechanical operators representing physical observables must be Hermitian.

(b) State in words the correspondence principle in quantum mechanics.

(c) It is given that the time derivative of the expectation value of a quantum mechanical operator, A, satisfies the following relation.

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle [H, A]\rangle + \langle\frac{\partial A}{\partial t}\rangle$$

where H is the Hamiltonian operator of the system. The Hamiltonian of a particle moving in a potential $V(x)$ is of the form:

$$H = \frac{p_x^2}{2m} + V(x)$$

Use the information provided above to show that:

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}, \quad \text{and} \quad \frac{d\langle p_x\rangle}{dt} = -\langle\frac{dV(x)}{dx}\rangle$$

(d) Are the results obtained in part (c) consistent with the correspondence principle? Explain.

QUESTION 3

The spin operator for a spin 1/2 particle can be written as

$$\vec{s} = \frac{\hbar}{2}\vec{\sigma}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, with σ_x, σ_y and σ_z being the Pauli spin matrices. A neutral spin 1/2 particle with a magnetic moment $\vec{\mu}$ is placed in a uniform magnetic field $\vec{B}$. The Hamiltonian of the system is of the form

$$H = -\vec{\mu}\cdot\vec{B}$$

where $\vec{\mu} = \mu\vec{\sigma}$. If initially the spin of the particle is along the x-axis, show that the average values of the spin components are given by

$$\langle s_x \rangle = 0$$
$$\langle s_y \rangle = \frac{\hbar}{2}\sin 2\omega t$$
$$\langle s_z \rangle = \frac{\hbar}{2}\cos 2\omega t$$

where

$$\omega = \frac{\mu B}{\hbar} \quad .$$

QUESTION 4

Consider a hydrogen atom whose wave function at $t = 0$ is the given by the following expression.

$$\Psi(r,\theta,\phi; t = 0) = \frac{1}{\sqrt{14}}[\, 2\psi_{100}\,(r,\theta,\phi) - 3\psi_{200}(r,\theta,\phi) + \psi_{322}(r,\theta,\phi)]$$

Here, $\psi_{nlm}\,(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$are the normalized energy eigenfunctions of the hydrogen atom.

(a) What is the probability of finding the system in each of the following energy eigenstates: $\psi_{100}\,(r,\theta,\phi)$, $\psi_{200}\,(r,\theta,\phi)$, $\psi_{322}\,(r,\theta,\phi)$? What is the probability of finding the system in any other energy eigenstate?

(b) What is the expectation value of the energy of the system?

(c) What are the expectation values of $L^2$and L_z?

QUESTION 5

Calculate the probability that an electron in the ground state of hydrogen is outside the classically allowed region.

Note: The ground-state wave function of the hydrogen atom is given by the following expression.

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a^3}}\, e^{-\frac{r}{a}}$$

QUESTION 6

Consider a square potential barrier of the following form:

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

where $V_0 > 0$. A particle of mass m and energy $E < V_0$ is incident upon the barrier from left.

(a) Write down the time-independent Schrödinger equation and its solutions for the system in each of the following regions: (i) $x < 0$, (ii) $0 < x < a$, (iii) $x > a$.

(b) The requirement of continuity of the wave function and its first derivative at the boundary points $x = 0$ and $x = a$ leads to four equations. Use the results obtained in part (a) above to write down these four algebraic equations. Describe, how you would obtain the reflection and transmission (tunneling) probabilities from these equations. (Note: You are not asked to solve the system of algebraic equations.)
(c) The tunneling probability for the case at hand turns out to be

$$T = \left[1 + \frac{V_0^2 \sinh^2(\kappa a)}{4E(V_0 - E)}\right]^{-1}$$

where, $\kappa = [2m(V_0 - E)/\hbar^2]^{1/2}$. Calculate the tunneling probability for an electron with the kinetic energy of 5 eV incident upon a barrier of height 10 eV and the width of 0.53 Å (the Bohr radius). (Note: The electron mass is, $m = 511 \times 10^3$ eV/C^2, with C = 3×10^8 m/s being the speed of light. Also, Å = 10^{-10} meters, and $\hbar = 6.58 \times 10^{-16}$ eV.s)
(d) Use the expression given in part (c) to show that for $\kappa a \gg 1$, the tunneling probability can be approximated as

$$T \cong \frac{16E(V_0 - E)}{V_0^2} e^{-2ka}$$

QUESTION 7

Consider a quantum mechanical one-dimensional simple harmonic oscillator for which the Hamiltonian is given by the following expression.

$$H_0 = \frac{p_x^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

Assume the system is further subjected to a nonlinear restoring force that can be represented by a perturbing Hamiltonian of the form:

$$H' = b\, x^4$$

where b is a positive constant.

Determine the first-order energy shift in the energy of the ground state and the first excited state of the harmonic oscillator due to the perturbation H'. Based on your results, which one of the two states receives a larger energy shift?

Note: The normalized wave-function for the ground state, $\psi_0(x)$, and the first excited state, $\psi_1(x)$, of the oscillator are given below.

$$\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}}$$

$$\psi_1(x) = \left(\frac{2\alpha^3}{\sqrt{\pi}}\right)^{\frac{1}{2}} x\, e^{-\frac{\alpha^2 x^2}{2}}$$

Here, $\alpha = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$.

You may find the following information useful.

- The fundamental commutation relation reads: $[x, p_x] = i\hbar$. From this statement it follows that:

$$[f(x), p_x] = i\hbar \frac{df}{dx} \quad , \qquad [x, g(p_x)] = i\hbar \frac{dg}{dx}$$

- The Hamiltonian operator is:

$$H = \frac{p^2}{2m} + V(\vec{r}\,) = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}\,)$$

- The Laplacian operator is:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2 \sin\theta}\left[\sin\theta \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{\sin\theta}\frac{\partial^2}{\partial \varphi^2}\right]$$

- In one dimension, the Hamiltonian becomes:

$$H = \frac{p_x^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

- The time-dependent Schrödinger equation reads:

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = H\,\Psi(\vec{r}, t)$$

- The time-independent Schrödinger equation (or the energy eigenvalue equation) is:

$$H\,\psi(\vec{r}\,) = E\,\psi(\vec{r}\,)$$

- The energy levels of the hydrogen atom are given by:

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2}, \qquad n = 1,2,3,\cdots$$

- The hydrogen wave functions are orthonormal.

$$\int_0^\infty dr\, r^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \;\; \psi^*_{nlm}(r,\theta,\phi)\;\psi_{n'l'm'}(r,\theta,\phi) = \delta_{nn'}\delta_{ll'}\,\delta_{mm'}$$

- The spherical harmonics are orthonormal.

$$\int_0^{2\pi} d\phi \int_0^\pi d\theta\, \sin\theta\; Y^*_{lm}(\theta,\phi) Y_{l'm'}(\theta,\phi) = \delta_{ll'}\delta_{mm'}$$

- The energy levels of a one-dimensional simple harmonic oscillator are given by:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \qquad n = 0,1,2,\cdots$$

where

$$\omega = \sqrt{\frac{k}{m}}$$

- The harmonic oscillator wave functions are orthonormal.

$$\int_{-\infty}^{+\infty} \psi_n^*(x)\, \psi_{n'}(x)\, dx = \delta_{nn'}$$

- The Pauli spin matrices are:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- The spin operator for a spin 1/2 particle can be expressed in terms of the Pauli spin matrices as follows:

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

- The eigenspinors of the operator S_z are:

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \chi_- = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- The first-order energy shift due to a perturbation H' is given by the following expression.

$$\Delta E = E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$$

where $|\psi_n^{(0)}\rangle$ is the eigenstate of the unperturbed Hamiltonian.

- Gaussian integrals

$$\int_0^{\infty} x^{2n}\, e^{-\frac{x^2}{a^2}}\, dx = \sqrt{\pi}\, \frac{(2n)!}{n!} \left(\frac{a}{2}\right)^{2n+1}$$

$$\int_0^{\infty} x^{2n+1}\, e^{-\frac{x^2}{a^2}}\, dx = \frac{n!}{2}\, a^{2n+2}$$

- Exponential integrals

$$\int e^{ax}\, dx = \frac{e^{ax}}{a}$$

$$\int x e^{ax}\, dx = \frac{e^{ax}}{a}\left(x - \frac{1}{a}\right)$$

$$\int x^n\, e^{ax}\, dx = \frac{x^n e^{ax}}{a} - \frac{n}{a} \int x^{n-1}\, e^{ax}\, dx$$