

**PYL112: Quantum Mechanics**

Major: Part B  
02-05-2019

II Semester 2018-19  
Answer any FIVE questions

Time: 1.5 hours  
Max. Marks: 30

NOTE: All symbols used have their usual meaning. Each question carries 6 marks. Some useful mathematical expressions are given at the end of the questions.

- 1) Calculate from first principles the Clebsch-Gordan coefficients for  $j_1 = 1$  and  $j_2 = \frac{1}{2}$ . Use the calculated coefficients to write the wave functions for the p-states of the electron  $\left(l=1, s=\frac{1}{2}\right)$  for  $j = \frac{3}{2}$   $\left(m_j = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}\right)$  and  $j = \frac{1}{2}$   $\left(m_j = \frac{1}{2}, -\frac{1}{2}\right)$ . [3+3 = 6 Marks]

- 2) Consider the radial wave function  $R_{nl}(r)$  of a hydrogen atom and its corresponding radial probability density  $P_{nl}(r)$ . Calculate the following:
- The expectation value  $\langle r \rangle_{21}$  for the hydrogen atom. Also find the value of  $r$  at which the radial probability density reaches its maximum for the state  $n=2, l=1$ . Compare these two values and comment (giving a proper reason) on their difference if any.
  - The width of the probability density distribution for  $r$  w.r.t. the above radial wavefunction. [3+2 = 5 Marks]

- 3) The wave function of an electron in a hydrogen atom is given by

$$|\psi_{21m_s}(r, \theta, \varphi)\rangle = R_{21}(r) \left[ \sqrt{\frac{2}{5}} Y_{10}(\theta, \varphi) \left| \frac{1}{2}, +\frac{1}{2} \right\rangle + \sqrt{\frac{3}{5}} Y_{11}(\theta, \varphi) \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \right]$$

Where  $\left| \frac{1}{2}, \pm \frac{1}{2} \right\rangle$  are the spin state vectors.

- Calculate  $\hat{J}_z |\psi_{21m_s}(r, \theta, \varphi)\rangle$ , i.e., the z-component of the electron's total angular momentum.
- If you measure  $\hat{J}^2$ , what values will you obtain? What are the corresponding probabilities?
- If you measure the z-component of the electron's orbital angular momentum, what values will you obtain? What are the corresponding probabilities?
- Calculate  $\langle \psi_{21m_s} | \hat{L}_- | \psi_{21m_s} \rangle$  and  $\langle \psi_{21m_s} | \hat{S}_z | \psi_{21m_s} \rangle$ . [1+3+1+2 = 7 Marks]

- 4) Consider the electron's spin operator:  $\hat{S} = \frac{\hbar}{2} \vec{\sigma}$ , where the components of  $\vec{\sigma}$  are the Pauli spin matrices.

- Find the eigenvalues and eigenstates of  $\hat{S}$  in the direction of a unit vector  $\vec{n}$ ; assume  $\vec{n}$  lies in the  $xz$  plane.
- Find the probability of measuring  $\hat{S}_z = +\frac{\hbar}{2}$ . [3+2 = 5 Marks]

Handwritten notes and diagrams:

- A diagram showing a 3D coordinate system with x, y, and z axes. A unit vector  $\vec{n}$  is shown in the xz-plane, making an angle  $\alpha$  with the z-axis and  $\beta$  with the x-axis. The components of  $\vec{n}$  are  $n_x = \sin \alpha \cos \beta$ ,  $n_z = \cos \alpha$ , and  $n_y = \sin \alpha \sin \beta$ .
- Equation:  $A\psi = \lambda\psi$
- Equation:  $\frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$
- Equation:  $\langle \psi | \hat{S}_z | \psi \rangle$
- Equation:  $\frac{\hbar}{2} \begin{pmatrix} \cos \alpha & \sin \alpha \cos \beta \\ \sin \alpha \sin \beta & -\cos \alpha \end{pmatrix}$
- Equation:  $\begin{pmatrix} \cos \alpha & \sin \alpha \cos \beta \\ \sin \alpha \sin \beta & -\cos \alpha \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$
- Equation:  $\begin{pmatrix} \cos \alpha - \lambda & \sin \alpha \cos \beta \\ \sin \alpha \sin \beta & -\cos \alpha - \lambda \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$
- Equation:  $\begin{pmatrix} \cos \alpha - \lambda & \sin \alpha \cos \beta \\ \sin \alpha \sin \beta & -\cos \alpha - \lambda \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
- Equation:  $\frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- 5) Consider a system under translational symmetry.
- (i) Use an appropriate form (stating proper reasons) of the operator  $\hat{T}(\varepsilon)$  for an *infinitesimal* translation by  $\varepsilon$  and show that momentum is the generator of such translations. Give proper reasons in each step.
- (ii) What does translational *invariance* imply? Show that momentum for the system is conserved under translational *invariance*.
- (iii) What should be the form of the operator  $\hat{T}(a)$  for a finite translation by 'a'? Deduce it from part (i) above. [3+2+2 = 7 Marks]

**Table 1:** Spherical Harmonics and their expressions in Cartesian coordinates.

$Y_{lm}(\theta, \varphi)$	$Y_{lm}(x, y, z)$
$Y_{00}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}}$	$Y_{00}(x, y, z) = \frac{1}{\sqrt{4\pi}}$
$Y_{10}(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos \theta$	$Y_{10}(x, y, z) = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$
$Y_{1,\pm 1}(\theta, \varphi) = \mp \sqrt{\frac{3}{8\pi}} e^{\pm i\varphi} \sin \theta$	$Y_{1,\pm 1}(x, y, z) = \mp \sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$
$Y_{20}(\theta, \varphi) = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$	$Y_{20}(x, y, z) = \sqrt{\frac{5}{16\pi}} \frac{3z^2 - r^2}{r^2}$
$Y_{2,\pm 1}(\theta, \varphi) = \mp \sqrt{\frac{15}{8\pi}} e^{\pm i\varphi} \sin \theta \cos \theta$	$Y_{2,\pm 1}(x, y, z) = \mp \sqrt{\frac{15}{8\pi}} \frac{(x \pm iy)z}{r^2}$
$Y_{2,\pm 2}(\theta, \varphi) = \sqrt{\frac{15}{32\pi}} e^{\pm 2i\varphi} \sin^2 \theta$	$Y_{2,\pm 2}(x, y, z) = \mp \sqrt{\frac{15}{32\pi}} \frac{x^2 - y^2 \pm 2ixy}{r^2}$

**Table 2:** First few radial wave functions  $R_n(r)$  of the hydrogen atom

$R_{10}(r) = 2a_0^{-3/2} e^{-r/a_0}$	$R_{21}(r) = \frac{1}{\sqrt{6a_0^3}} \frac{r}{2a_0} e^{-r/2a_0}$
$R_{20}(r) = \frac{1}{\sqrt{2a_0^3}} \left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0}$	$R_{31}(r) = \frac{8}{9\sqrt{6a_0^3}} \left(1 - \frac{r}{6a_0}\right) \left(\frac{r}{3a_0}\right) e^{-r/3a_0}$
$R_{30}(r) = \frac{2}{3\sqrt{3a_0^3}} \left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right) e^{-r/3a_0}$	$R_{32}(r) = \frac{4}{9\sqrt{30a_0^3}} \left(\frac{r}{3a_0}\right)^2 e^{-r/3a_0}$

**Table 3:** First few Legendre polynomials and associated Legendre functions.

Legendre Polynomials	Associated Legendre Functions
$P_0(\cos \theta) = 1$	$P_1^1(\cos \theta) = \sin \theta$
$P_1(\cos \theta) = \cos \theta$	$P_2^1(\cos \theta) = 3 \cos \theta \sin \theta$
$P_2(\cos \theta) = (3 \cos^2 \theta - 1)/2$	$P_2^2(\cos \theta) = 3 \sin^2 \theta$
$P_3(\cos \theta) = (5 \cos^3 \theta - 3 \cos \theta)/2$	$P_3^1(\cos \theta) = 3 \sin \theta (5 \cos^3 \theta - 1)/2$
$P_4(\cos \theta) = (35 \cos^4 \theta - 30 \cos^2 \theta + 3)/8$	$P_3^2(\cos \theta) = 15 \sin^2 \theta \cos \theta$
$P_5(\cos \theta) = (63 \cos^5 \theta - 70 \cos^3 \theta + 15 \cos \theta)/8$	$P_3^3(\cos \theta) = 15 \sin^3 \theta$

**Table 4:** First few Laguerre polynomials and associated Laguerre polynomials.

Laguerre polynomials $L_k(r)$	Associated Laguerre polynomials $L_k^N(r)$
$L_0 = 1$	
$L_1 = 1 - r$	$L_1^1 = -1$
$L_2 = 2 - 4r + r^2$	$L_2^1 = -4 + 2r, \quad L_2^2 = 2$
$L_3 = 6 - 18r + 9r^2 - r^3$	$L_3^1 = -18 + 18r - 3r^2, \quad L_3^2 = 18 - 6r, \quad L_3^3 = -6$
$L_4 = 24 - 96r + 72r^2 - 16r^3 + r^4$	$L_4^1 = -96 + 144r - 48r^2 + 4r^3,$ $L_4^2 = 144 - 96r + 12r^2, \quad L_4^3 = 24r - 96, \quad L_4^4 = 24$
$L_5 = 120 - 600r + 600r^2 - 200r^3$ $+ 25r^4 - r^5$	$L_5^1 = -600 + 1200r - 600r^2 + 100r^3 - 5r^4,$ $L_5^2 = 1200 - 1200r + 300r^2 - 20r^3,$ $L_5^3 = -1200 + 600r - 60r^2, \quad L_5^4 = 600 - 120r,$ $L_5^5 = -120$