Problem Set 6

Problem 1

1. Determine the **canonical commutation relations** for the Cartesian components of the operators $\hat{\vec{r}}$ and $\hat{\vec{?}}$:

$$\begin{aligned}
&[\hat{x}, \hat{y}], [\hat{x}, \hat{z}], [\hat{y}, \hat{z}], \\
&[\hat{x}, \hat{p}_x], [\hat{x}, \hat{p}_y], [\hat{x}, \hat{p}_z], \\
&[\hat{y}, \hat{p}_x], [\hat{y}, \hat{p}_y], [\hat{y}, \hat{p}_z], \\
&[\hat{z}, \hat{p}_x], [\hat{z}, \hat{p}_y], [\hat{z}, \hat{p}_z], \\
&[\hat{p}_x, \hat{p}_y], [\hat{p}_x, \hat{p}_z] \text{ and } [\hat{p}_y, \hat{p}_z].
\end{aligned}$$

2. Determine the fundamental commutation relations for angular momentum:

$$[\hat{L}_x, \hat{L}_y], [\hat{L}_y, \hat{L}_z], \text{ and } [\hat{L}_z, \hat{L}_x].$$

   Use the classical definition of angular momentum, $\vec{L} = \vec{r} \times \vec{p}$, which means $L_x = yp_z - zp_y$, $L_y = zp_x - xp_z$, and $L_z = xp_y - yp_x$.

Problem 2

Use separation of variables in Cartesian coordinates to solve the infinite cubical well (or "particle in a box"):

$$V(x, y, z) = \begin{cases} 0, & \text{if } x, y, z \text{ are all between 0 and } a; \\ \infty, & \text{otherwise.} \end{cases}$$

1. Find the stationary states and their corresponding energies.

2. Call the distinct energies E_1, E_2, E_3, etc., in order of increasing energy. Find the first six energies and determine their degeneracies (i.e., the number of different states that share the same energy). Note: In one dimension, one can prove that bound states are never degenerate, but in three dimensions they are very common.

3. What is the degeneracy of E_{14}, and why is this case interesting?

Problem 3

1. Use equations 2, 3, and 4 from Griffiths in the appendix to construct ${Y_0}^0$ and ${Y_2}^1$.

2. Confirm that ${Y_0}^0$ and ${Y_2}^1$ are normalized and orthogonal.

Problem 4

1. Using the tables in the appendix, construct the wavefunction ψ_{200} for the hydrogen atom.

2. Using the tables in the appendix, construct the wavefunctions ψ_{211} , ψ_{2100} and ψ_{21-1} for the hydrogen atom.

Problem 5

1. Find $\langle r \rangle$ and $\langle r^2 \rangle$ for an electron in the ground state of hydrogen. Express your answers in terms of the Bohr radius, a_0.

2. Find $\langle x \rangle$ and $\langle x^2 \rangle$ for an electron in the ground state of hydrogen. Hint: this requires no new integration. Use $r^2 = x^2 + y^2 + z^2$ and the symmetry of the ground state.

3. Find $\langle x^2 \rangle$ for an electron in the state $n = 2$, $l = 1$, and $m = 1$ of hydrogen. Hint: this state is not symmetric in x, y, z. Use $x = r \sin\theta \cos\phi$.

1 Appendix

1.1 Legendre function / polynomial

The solution is

$$\Theta(\theta) = AP_l^m(\cos\theta), \tag{1}$$

where P_l^m is the **associated Legendre function**, defined by

$$P_l^m(x) = (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_l(x), \tag{2}$$

and $P_l(x)$ is the lth **Legendre polynomial**, defined by the **Rodrigues formula**:

$$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l. \tag{3}$$

$$Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta), \tag{4}$$

where $\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m \leq 0$.

1.2 Tables of Legendre Polynomials and Radial Wave Functions

Table 1: The first few spherical harmonics, $Y_l^m(\theta,\phi)$

Spherical Harmonic	Expression
Y_0^0	$\left(\frac{1}{4\pi}\right)^{1/2}$
Y_1^0	$\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$
$Y_1^{\pm1}$	$\mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta e^{\pm i\phi}$
Y_2^0	$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$
$Y_2^{\pm1}$	$\mp\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$
$Y_2^{\pm2}$	$\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta e^{\pm 2i\phi}$
Y_3^0	$\left(\frac{7}{16\pi}\right)^{1/2}(5\cos^3\theta-3\cos\theta)$
$Y_3^{\pm1}$	$\mp\left(\frac{21}{64\pi}\right)^{1/2}\sin\theta(5\cos^2\theta-1)e^{\pm i\phi}$
$Y_3^{\pm2}$	$\left(\frac{105}{32\pi}\right)^{1/2}\sin^2\theta\cos\theta e^{\pm 2i\phi}$
$Y_3^{\pm3}$	$\mp\left(\frac{35}{64\pi}\right)^{1/2}\sin^3\theta e^{\pm 3i\phi}$

Table 2: The first few Laguerre polynomials, $L_q(x)$.

Polynomial	Expression
L_0	1
L_1	$-x+1$
L_2	x^2-4x+2
L_3	$-x^3+9x^2-18x+6$
L_4	$x^4-16x^3+72x^2-96x+24$
L_5	$-x^5+25x^4-200x^3+600x^2-600x+120$
L_6	$x^6-36x^5+450x^4-2400x^3+5400x^2-4320x+720$

Table 3: Some associated Laguerre polynomials, $L_q^p(x)$.

Polynomial	Expression
L_0^0	1
L_1^0	$-x+1$
L_2^0	x^2-4x+2
L_0^1	1
L_1^1	$-2x+4$
L_2^1	$3x^2-18x+18$
L_0^2	2
L_1^2	$-6x+18$
L_2^2	$12x^2-96x+144$
L_0^3	6
L_1^3	$-24x+96$
L_2^3	$60x^2-600x+1200$

Table 4: The first few radial wave functions for hydrogen, $R_{nl}(r)$.

Radial Function	**Expression**
R_{10}	$2a_0^{-3/2}\exp(\frac{-r}{a_0})$
R_{20}	$\left(\frac{1}{\sqrt{2}}\right)a_0^{-3/2}\left(1-\frac{1}{2}\frac{r}{a_0}\right)\exp(\frac{-r}{2a_0})$
R_{21}	$\left(\frac{1}{\sqrt{24}}\right)a_0^{-3/2}\frac{r}{a_0}\exp(\frac{-r}{2a_0})$
R_{30}	$\left(\frac{2}{\sqrt{27}}\right)a_0^{-3/2}\left(1-\frac{2}{3}\frac{r}{a_0}+\frac{2}{27}\left(\frac{r}{a_0}\right)^2\right)\exp(\frac{-r}{3a_0})$
R_{31}	$\left(\frac{8}{27\sqrt{6}}\right)a_0^{-3/2}\left(1-\frac{1}{6}\frac{r}{a_0}\right)\frac{r}{a_0}\exp(\frac{-r}{3a_0})$
R_{32}	$\left(\frac{4}{81\sqrt{30}}\right)a_0^{-3/2}\left(\frac{r}{a_0}\right)^2\exp(\frac{-r}{3a_0})$
R_{40}	$\frac{1}{4}a_0^{-3/2}\left(1-\frac{3}{4}\frac{r}{a_0}+\frac{1}{8}\left(\frac{r}{a_0}\right)^2-\frac{1}{192}\left(\frac{r}{a_0}\right)^3\right)\exp\left(-\frac{r}{4a_0}\right)$
R_{41}	$\frac{\sqrt{5}}{16\sqrt{3}}a_0^{-3/2}\left(1-\frac{1}{4}\frac{r}{a_0}+\frac{1}{80}\left(\frac{r}{a_0}\right)^2\right)\frac{r}{a_0}\exp\left(-\frac{r}{4a_0}\right)$
R_{42}	$\frac{1}{64\sqrt{5}}a_0^{-3/2}\left(1-\frac{1}{12}\frac{r}{a_0}\right)\left(\frac{r}{a_0}\right)^2\exp\left(-\frac{r}{4a_0}\right)$
R_{43}	$\frac{1}{768\sqrt{35}}a_0^{-3/2}\left(\frac{r}{a_0}\right)^3\exp\left(-\frac{r}{4a_0}\right)$