

Chapter 10 problems

Problem 10.1

Derive the following commutation relations:

- (a) $[\hat{L}_z, \hat{x}] = i\hbar\hat{y}$
- (b) $[\hat{L}_z, \hat{y}] = -i\hbar\hat{x}$
- (c) $[\hat{L}_z, \hat{z}] = 0$
- (d) $[\hat{L}^2, \hat{x}] = -2\hbar^2\hat{x} + 2i\hbar(\hat{L}_z\hat{y} - \hat{L}_y\hat{z})$
- (e) $[\hat{L}^2, [\hat{L}^2, \mathbf{r}]] = 2\hbar^2(\mathbf{r}\hat{L}^2 + \hat{L}^2\mathbf{r})$

Problem 10.2

The ground state wave function of a hydrogenic atom with nuclear charge Ze is $\psi_1(r) = Ae^{-r/r_1}$, where r is the distance between the electron and the nucleus and r_1 is a characteristic length scale. The electron is subject to a radially-symmetric coulomb potential given by $V(r) = -e^2/4\pi\epsilon_0\epsilon_r r$.

- (a) Find the value of the normalization constant A .
- (b) Find the value of r_1 that minimizes the energy expectation value $\langle E_1 \rangle$, and show that $\langle E_{\text{kinetic}} \rangle = -\langle E_{\text{potential}} \rangle / 2$ (which is a result predicted by the virial theorem).

- (c) Show that $r_1 = a_B/Z$ where $a_B = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$
- (d) Show that the expectation value $\langle r \rangle = 3a_B/2Z$.
- (e) Show that the expectation value of momentum $\langle p \rangle = 0$.

Problem 10.3

To calculate the spontaneous emission rate $A = 1/\tau_{\text{sp}}$ for the $2p$ to $1s$ ($|n=2, l=1, m\rangle \rightarrow |n=1, l=0, m=0\rangle$) transition in hydrogen an average over the three possible values of the quantum number m is taken so that

$$A = \frac{e^2 \omega^3}{3\hbar c^3 \pi \epsilon_0} \frac{1}{3} \sum_{m=-1}^{m=1} |\langle 2, 1, m | \hat{\mathbf{r}} | 1, 0, 0 \rangle|^2$$

where $\hbar\omega$ is the energy of the emitted photon. Since $r^2 = x^2 + y^2 + z^2$, this equation can be written as

$$A = \frac{e^2 \omega^3}{3\hbar c^3 \pi \epsilon_0} \frac{1}{3} \sum_{m=-1}^{m=1} (|\langle 2, 1, m | \hat{x} | 1, 0, 0 \rangle|^2 + |\langle 2, 1, m | \hat{y} | 1, 0, 0 \rangle|^2 + |\langle 2, 1, m | \hat{z} | 1, 0, 0 \rangle|^2)$$

- (a) Show that

$$x = r \sin(\theta) \cos(\phi) = -\sqrt{\frac{2\pi}{3}} r (Y_1^1 - Y_1^{-1})$$

$$y = r \sin(\theta) \sin(\phi) = i\sqrt{\frac{2\pi}{3}} r (Y_1^1 + Y_1^{-1})$$

$$z = r \cos(\theta) = \sqrt{\frac{4\pi}{3}} r Y_1^0$$

and rewrite each matrix element appearing in the expression for spontaneous emission in terms of a radial integral and an angular integral.

(b) Use the standard integral $\int_0^{\infty} x^n e^{-\mu x} dx = n! \mu^{-n-1}$ to show that the radial integral

$$\int_0^{\infty} r^3 R_{21}^*(r) R_{10}(r) dr = \frac{2^8}{3^4 \sqrt{6}} a_B$$

where $R_{10}(r) = 2 \left(\frac{1}{a_B} \right)^{3/2} e^{-r/a_B}$ and $R_{21}(r) = \frac{2}{\sqrt{3}} \left(\frac{1}{2a_B} \right)^{3/2} \frac{r}{2a_B} e^{-r/2a_B}$

(c) Show that the angular integrals in (a) are

$$-\sqrt{\frac{2\pi}{3}} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (Y_1^m)^* (Y_1^1 - Y_1^{-1}) Y_0^0 \sin(\theta) d\theta d\phi = \frac{-1}{\sqrt{4\pi}} \sqrt{\frac{2\pi}{3}} (\delta_{m,1} - \delta_{m,-1})$$

$$i \sqrt{\frac{2\pi}{3}} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (Y_1^m)^* (Y_1^1 + Y_1^{-1}) Y_0^0 \sin(\theta) d\theta d\phi = \frac{i}{\sqrt{4\pi}} \sqrt{\frac{2\pi}{3}} (\delta_{m,1} + \delta_{m,-1})$$

$$\sqrt{\frac{4\pi}{3}} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (Y_1^m)^* Y_1^0 Y_0^0 \sin(\theta) d\theta d\phi = \frac{1}{\sqrt{4\pi}} \sqrt{\frac{4\pi}{3}} (\delta_{m,0})$$

(d) Combine the results of (b) and (c) to show that

$$\sum_{m=-1}^{m=1} |\langle 21m | \hat{\mathbf{r}} | 100 \rangle|^2 = 96 \left(\frac{2}{3} \right)^{10} a_B^2 = \left(\frac{32}{27} \right)^3 a_B^2$$

and that the spontaneous emission time for the 2p to 1s transition in hydrogen is $\tau_{sp} = 1.6 \text{ ns}$.

Problem 10.4

(a) Show using first-order perturbation theory that the correction to the 1s ground-state energy of a hydrogen atom subject to a uniform electric field \mathbf{E} in the z direction is zero.

(b) Show that the first-order correction to the ground-state wave function is

$$|\psi_0^{(1)}\rangle = |1, 0, 0\rangle - e|\mathbf{E}| \sum_{n \neq 1, l, m} \frac{\langle n, l, m | \hat{z} | 1, 0, 0 \rangle}{E_1 - E_n} |n, l, m\rangle$$

(c) Show to first-order in \mathbf{E} that the susceptibility for the 1s state is

$$\chi_{1s} = \frac{\langle \psi_0^{(1)} | e \hat{z} | \psi_0^{(1)} \rangle}{|\mathbf{E}|} = -2e^2 \sum_{n \neq 1, l, m} \frac{|\langle n, l, m | \hat{z} | 1, 0, 0 \rangle|^2}{E_1 - E_n}$$

Problem 10.5

(a) An electron with zero orbital angular momentum ($l = 0$) moves in a radial potential $V(r) = 0$ for $r < a$ and $V(r) = \infty$ for $r \geq a$, where a is the radius of a spherical quantum dot. Use the radial Schrödinger equation to find the eigenenergies and normalized eigenstates of the electron.

(b) Find the eigenenergies and normalized eigenstates of an electron with zero orbital angular momentum ($l = 0$) moving in a radial shell potential with $V(r) = 0$ for $a < r < b$ and $V(r) = \infty$ elsewhere.

Problem 10.6

Consider a hydrogen atom with Bohr radius a_B .

(a) Show that the radial expectation value $\langle r_{nl} \rangle$ in state ψ_{nlm} is $\langle r_{nl} \rangle = \frac{a_B}{2}(3n^2 - l(l+1))$.

(b) Show that $\langle r_{nl}^2 \rangle = \frac{n^2 a_B^2}{2}(5n^2 + 1 - 3l(l+1))$.

(c) Find an analytic expression for the spread in radial probability $\Delta r_{nl} = \sqrt{\langle r_{nl}^2 \rangle - \langle r_{nl} \rangle^2}$.

Problem 10.7

Consider the state ψ_{nlm} of hydrogen with quantum numbers $n = 2$ and $l = 1$.

(a) Calculate the numerical values of radial expectation value, $\langle r_{21} \rangle$.

(b) Calculate the value at which radial probability density reaches a maximum, r_{21}^{\max} .

(c) Calculate the numerical value in spread in radial probability, Δr_{21} , and explain why the values of $\langle r_{21} \rangle$ and r_{21}^{\max} are different.

Problem 10.8

A hydrogen atom, which in free-space has eigenstates $\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_l^m(\theta, \phi)$ where $Y_l^m(\theta, \phi)$ are the normalized spherical harmonics and n , l , and m are quantum numbers, is placed at distance $z_0 \geq 0$ in a half-space with potential $V(z \geq 0) = 0$ and $V(z < 0) = \infty$.

(a) Find the analytic expression for the ground-state wave function as $z_0 \rightarrow 0$.

(b) Find all the other eigenstates and their degeneracy as $z_0 \rightarrow 0$.