5 Physics 2424 Atoms

1. The probability of spontaneous transitions of a charged particle from one initial energy level to another final level is governed by the overlap integral

$$\vec{D}_o = q\int \vec{r}\,\psi_i^*\psi_f\,dV\,,$$

where q is the charge of the particle. If $\vec{D}_o = 0$ between two levels, the transition is forbidden. Searching for such forbidden transitions leads to *selection rules*. Consider the 3D infinite potential well.

(a) Show that only allowed transitions from $\psi_{n1,n2,n3}$ are to a state where two of the quantum numbers are unchanged and the other quantum number changes by an odd number like 1, 3, 5, etc.

(b) Show that the emitted photons have energies $E = p(2n - p)E_1$ where the n is the original quantum level and $n - p$ is the final quantum level and E_1 is the ground state energy of the one-dimensional potential well.

The following integral identities are useful:

$$\int_0^L \sin\left(\tfrac{n\pi x}{L}\right)\sin\left(\tfrac{m\pi x}{L}\right)dx = \frac{L}{2}\delta_{nm} \text{ and } \int_0^L x\sin\left(\tfrac{n\pi x}{L}\right)\sin\left(\tfrac{m\pi x}{L}\right)dx = \begin{cases} \dfrac{L^2}{4} & n = m \\ \dfrac{2L^2}{\pi^2}\dfrac{nm\left[(-1)^{n-m}-1\right]}{(n-m)^2(n+m)^2} & n \neq m \end{cases}$$

2. For the hydrogen atom prove the selection rules $\Delta m = 0$ or ±1 and $\Delta l = \pm1$. Remember, in spherical coordinates $\vec{r} = \mathrm{i}r\sin\theta\sin\phi + \mathrm{j}r\sin\theta\cos\phi + \mathrm{k}r\cos\theta$. Make use of symmetry where possible. The identities $\int_0^{2\pi} e^{-ib\phi}d\phi = \delta_{b0}$, $\sin\phi = \dfrac{e^{i\phi} - e^{-i\phi}}{2i}$, and $\cos\phi = \dfrac{e^{i\phi} + e^{-i\phi}}{2}$ may be of use.

3. Are L_x, L_y, L_z or L^2 eigenfunctions of $\psi(x)$ for the 3D potential well?

4. Determine $\langle r \rangle$, $\langle r^2 \rangle$, and σ_r for ψ_{100}. The integral identity $\int_0^\infty x^n e^{-ax}dx = \dfrac{n!}{a^{n+1}}$ is helpful.

5. Determine $\langle p_r \rangle$, $\langle p_r^2 \rangle$, and σ_p for ψ_{100}. Note $(p_r)_{op} = -i\hbar \dfrac{\partial}{\partial r}$ and

$$(p_r^2)_{op} = -\hbar^2 \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) = -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right).$$

6. If electrons were spinning balls, they would have moment of inertia $I = {}^2/_5 MR^2$ and spin angular momentum $S = I\omega$. The maximum speed at which the outside edge of a real ball electron could be spinning is the speed of light. Since we know $\left|\vec{S}\right| = \sqrt{s(s+1)}\hbar = \sqrt{\tfrac{3}{4}}\hbar$, what value of R does this imply? Note that experiment has shown that electrons act like point particles down to distances below 10^{-15} m.

7. The deuteron is a hydrogen atom with an extra neutron in the core. The effects the reduced mass μ in our equation for E_n. If $m_p = 1836\ m_e$ and $m_n = 1839\ m_e$, find the wavelengths of light necessary to ionize a hydrogen atom and a deuteron. What is the difference in these two wavelengths?

8. We can define the effective charge that an electron sees by the formula $E_n = Z_{eff}^2 \dfrac{E_0}{n^2}$ where E_0 = 13.6 eV. The electron configuration of sodium is $1s^2 2s^2 2p^6 3s$. If the inner electrons fully shielded the valence electron from the core, what would Z_{eff} be? How much energy would be needed to remove the valence electron from sodium in this case? The actual ionization energy of sodium is 5.1 eV. What is the true Z_{eff}?

9. Potassium has an electron configuration $1s^2 2s^2 2p^6 3s^2 3p^6 4s$ and an ionization energy of 4.3 eV. What is the true Z_{eff}? See previous question.

10. Write the electron configurations for the following, use only Fig. 7-19 of the text which shows the relative energies of the atomic shells and subshells.
a) Rubidium, Z = 37.
b) Iodine, Z = 53.