

Homework is from Eisberg and Resnick (E&R) unless otherwise indicated. Please note that “questions” can be answered briefly; “problems” may be more involved. Each question usually counts 5 points; each problem counts 10 points.

1. E&R, chapter 8, problem 14.
2. E&R, chapter 8, problem 16.
3. E&R, chapter 8, problem 18.
4. E&R, chapter 9, problem 4.
5. E&R, chapter 9, problem 5.

HW #11 Solutions (Chapter 8)

14

Verify that the parities of the one-electron atom eigenfunctions Ψ_{300} , Ψ_{310} , Ψ_{320} , and Ψ_{322} are determined by $(-1)^l$.

Under a parity operation all rectangular coordinates change sign. Under spherical coordinates we have

$$r \rightarrow r$$

$$\theta \rightarrow \pi - \theta$$

$$\phi \rightarrow \pi + \phi$$

So we must show that $\Psi_{nlm}(r, \pi - \theta, \pi + \phi) = (-1)^l \Psi_{nlm}(r, \theta, \phi)$ from table 7-2 (pg 243)

$$\Psi_{300} = \frac{1}{81\sqrt{3}\pi} \left(\frac{z}{a_0}\right)^{3/2} \left(27 - 18\frac{zr}{a_0} + 2\frac{z^2 r^2}{a_0^2}\right) e^{-zr/3a_0}$$

$$P\Psi_{300} = \Psi_{300} = \Psi_{300} (-1)^{l=0} \checkmark$$

$$\Psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} \left(6 - \frac{zr}{a_0}\right) \frac{zr}{a_0} e^{-zr/3a_0} \cos\theta$$

$$P\Psi_{310} = \Psi_{310} \frac{\cos(\pi - \theta)}{\cos\theta} = \Psi_{310} \frac{-\cos(\theta)}{\cos(\theta)} = -\Psi_{310} = \Psi_{310} (-1)^{l=1} \checkmark$$

$$\Psi_{320} = \frac{1}{81\sqrt{6}\pi} \left(\frac{z}{a_0}\right)^{3/2} \frac{z^2 r^2}{a_0^2} e^{-zr/3a_0} (3\cos^2\theta - 1)$$

$$P\Psi_{320} = \Psi_{320} \frac{(3\cos^2(\pi - \theta) - 1)}{(3\cos^2(\theta) - 1)} = \Psi_{320} \frac{3(-\cos\theta)^2 - 1}{3\cos^2\theta - 1} = \Psi_{320} = \Psi_{320} (-1)^{l=2} \checkmark$$

$$\psi_{322} = \frac{1}{162\sqrt{\pi}} \left(\frac{z}{a_0}\right)^{3/2} \frac{z^2 r^2}{a_0^2} e^{-zr/3a_0} \sin^2 \sigma e^{\pm 2i\varphi}$$

$$P \psi_{322} = \psi_{322} \frac{\sin^2(\pi - \sigma)}{\sin^2 \sigma} \frac{e^{\pm 2i(\pi + \varphi)}}{e^{\pm 2i\varphi}}$$

$$= \psi_{322} \frac{(-\sin(-\sigma))^2}{\sin^2 \sigma} \frac{e^{\pm 2i\varphi}}{e^{\pm 2i\varphi}} e^{\pm 2i\pi} = \psi_{322} \cos(\pm 2\pi)$$

$$= \psi_{322} = \psi_{322} (-1)^{l=2} \checkmark$$

(16) Show that the selection rule $\Delta l = \pm 1$ is valid for transitions $n=2 \rightarrow n=1$ of the hydrogen atom.

The electric dipole matrix element has the form

$$P_{fi} = \left| \int \psi_f^* e \vec{r} \psi_i d\tau \right|$$

$$n=2, l=1, m_l = \pm 1 \rightarrow n=2, l=0, m_l=0$$

l, m_l only deal with angular part of wavefunction

$$P_{fi} = \left| \int R_f^*(r) \Theta_f^*(\sigma) \Phi_f^*(\varphi) e \vec{r} R_i(r) \Theta_i(\sigma) \Phi_i(\varphi) d\tau \right|$$

$$e \int_0^\infty R_f^*(r) R_i(r) r^3 dr = \text{Constant} = C$$

So we evaluate the rest of the integrals

$$I = \int_0^\pi \Theta_f^*(\sigma) \Theta_i(\sigma) \sin \sigma d\sigma \int_0^{2\pi} \frac{\vec{r}}{r} d\varphi \Phi_f^*(\varphi) \Phi_i(\varphi)$$

$$I_x = \int_0^{2\pi} \int_0^\pi \sin\theta \, d\theta - \sin\theta \cos\varphi \, d\varphi$$

$$= \int_0^\pi \sin^2\theta \, d\theta \int_0^{2\pi} \cancel{\cos\varphi} \, d\varphi = 0 \quad \checkmark$$

$$I_y = \int_0^\pi \sin^2\theta \, d\theta \int_0^{2\pi} \sin\varphi \cancel{\cos\varphi} \, d\varphi = 0 \quad \checkmark$$

$$\Delta l \neq 0$$

$$I_z = \int_0^\pi \sin\theta \cancel{\cos\theta} \int_0^{2\pi} d\varphi = 0 \quad \checkmark$$

$$\text{for } n=2, l=1, m_l=0 \rightarrow n=1, l=0, m_l=0$$

$$I_x = \int_0^{2\pi} \int_0^\pi \cos\theta \, d\theta \, d\varphi \sin\theta \cos\varphi \sin\theta$$

$$= \int_0^\pi \cos\theta \sin^2\theta \, d\theta \int_0^{2\pi} \cancel{\cos\varphi} \, d\varphi$$

$$= 0$$

$$I_y = \int_0^\pi \cos\theta \sin^2\theta \, d\theta \int_0^{2\pi} \sin\varphi \cancel{\cos\varphi} \, d\varphi = 0$$

$$I_z = \int_0^\pi \cos^2\theta \sin\theta \int_0^{2\pi} d\varphi = -\cos^3\theta \Big|_0^\pi \cdot 2\pi$$

$$= 4\pi \neq 0 \quad \text{transition allowed}$$

for $n=2, l=1, m_l=\pm 1 \rightarrow n=1, l=0, m_l=0$

$$I_x = \int_0^{2\pi} \int_0^\pi \sin^2 \theta e^{\pm i\varphi} \sin \theta \cos \varphi d\theta d\varphi$$

$$= \int_0^\pi \sin^3 \theta d\theta \int_0^{2\pi} e^{\pm i\varphi} \cos \varphi d\varphi$$

$$= \left[-\frac{1}{3} \cos \theta (\sin^2 \theta + 2) \right]_0^\pi \int_0^{2\pi} e^{\pm i\varphi} \left(\frac{e^{i\varphi} + e^{-i\varphi}}{2} \right) d\varphi$$

$$= -\frac{1}{3} (-1 - (+1))(2) \int_0^{2\pi} \frac{e^{i\varphi(1\pm 1)} + e^{-i\varphi(\pm 1-1)}}{2} d\varphi$$

$$\stackrel{+1}{=} -\frac{4}{3} \left[\int_0^{2\pi} \frac{e^{2i\varphi} + 1}{2} d\varphi \right]$$

$$= -\frac{2}{3} (2\pi - 0) = -\frac{4\pi}{3}$$

$$-1 = -\frac{4}{3} \left[\int_0^{2\pi} \frac{1 + e^{i\varphi^2}}{2} d\varphi \right] = -\frac{4\pi}{3} \neq 0 \quad \begin{matrix} \text{transition} \\ \text{allowed} \end{matrix}$$

$$I_y = \int_0^\pi \sin^3 \theta d\theta \int_0^{2\pi} e^{\pm i\varphi} \sin \varphi d\varphi$$

$$= -\frac{4}{3} \int_0^{2\pi} \left[\frac{e^{\pm i\varphi}}{2i} (e^{i\varphi} - e^{-i\varphi}) d\varphi \right]$$

$$\stackrel{+1}{=} -\frac{4\pi i}{3} \neq 0$$

$$\stackrel{-1}{=} \frac{4\pi i}{3}$$

$$I_z = \int_0^\pi \sin^2 \theta \cos \theta d\theta \int_0^{2\pi} e^{\pm i\varphi} d\varphi = 0$$

18) a) Calculate rate for $n=1 \rightarrow n=0$ transitions in a simple harmonic oscillator carrying charge e .

$$\mathcal{E} \approx 10^3 \text{ J/m}^2$$

For a harmonic oscillator

$$\psi_0 = A_0 e^{-u^2/2} \quad u = \frac{[(em)^{1/4} / \hbar^{1/2}]}{\alpha} X$$

$$\psi_1 = A_1 u e^{-u^2/2}$$

$$\nu = \frac{1}{2\pi} \sqrt{\frac{e}{m}}$$

$$du = \alpha dx$$

$$P_{10} = \int \psi_1^* e x \psi_0 dx$$

$$1 = \int \psi_0 \psi_0 dx = A_0^2 \int e^{-u^2} du \frac{1}{\alpha} = \frac{A_0^2}{\alpha} \sqrt{\pi}$$

$$A_0 = \frac{\alpha^{1/2}}{\pi^{1/4}}$$

$$1 = \int \psi_1 \psi_1 dx = A_1^2 \int_0^\infty u^2 e^{-u^2} \frac{du}{\alpha} = A_1^2 \left[-\frac{1}{2} u e^{-u^2} \right]_0^\infty - \int_0^\infty \left(-\frac{1}{2}\right) e^{-u^2} du$$

$$= A_1^2 \frac{\sqrt{\pi}}{4\alpha} \quad A_1 = \frac{2\alpha^{1/2}}{\pi^{1/4}}$$

$$P_{10} = \int_0^\infty \left(\frac{\alpha^{1/2}}{\pi^{1/4}} \right) \left(\frac{2\alpha^{1/2}}{\pi^{1/4}} \right) e^{-u^2/2} e x dx e^{-u^2/2} u$$

$$= \frac{2e\alpha}{\sqrt{\pi}} \int_0^\infty e^{-u^2} u^2 \frac{du}{\alpha^2}$$

$$= \frac{2e\alpha}{\sqrt{\pi}} \frac{\sqrt{\pi}}{4\alpha^2} = \frac{2e}{\alpha}$$

$$P_{10}^2 = \frac{4e^2}{\alpha^2}$$

$$R = \frac{16\pi^3 \nu^3}{3\epsilon_0 h c^3} \rho_{fi}^2 \quad (8-43)$$

$$= \frac{16\pi^3 \left(\frac{1}{2\pi} \sqrt{\frac{e}{m}} \right)^3}{3\epsilon_0 h c^3} \left(\frac{4e^2 \hbar}{(em)^{1/2}} \right)$$

$$= \frac{32\pi^2 \epsilon e^2 \hbar}{3\epsilon_0 h c^3 m^2} = \frac{16\pi}{3} \frac{(10^3 \text{ J/m}^2) (1.6 \times 10^{-19} \text{ C})^2}{(3 \times 10^8 \text{ m/s})^3 (2 \times 10^{-27} \text{ kg})^2 (8.85 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2})}$$

$$\approx 4.5 \times 10^5 \frac{\text{transitions}}{\text{second}} \quad \text{varies with molecular mass}$$

$$b) \quad \tau = \frac{1}{R} \approx 2.23 \times 10^{-6} \text{ s}$$

- ④ Verify the eigenfunction of example 9-2 is antisymmetric with respect to a change of labels of two particles.

$$\Psi_A = \frac{1}{\sqrt{3}!} \left[\Psi_\alpha(1) \Psi_\beta(2) \Psi_\gamma(3) + \Psi_\beta(1) \Psi_\gamma(2) \Psi_\alpha(3) \right. \\ \left. + \Psi_\gamma(1) \Psi_\alpha(2) \Psi_\beta(3) - \Psi_\gamma(1) \Psi_\beta(2) \Psi_\alpha(3) \right. \\ \left. - \Psi_\beta(1) \Psi_\alpha(2) \Psi_\gamma(3) - \Psi_\alpha(1) \Psi_\gamma(2) \Psi_\beta(3) \right]$$

All combination orders of α, β, γ are present in positive and negative sign terms symmetrically for each indices. So we only have to show that Ψ_A is antisymmetric under exchange of two indices.

$$\Psi_A \xrightarrow{\alpha \leftrightarrow \beta} \Psi'_A = \frac{1}{\sqrt{3}} \left[-\Psi_\beta(1) \Psi_\alpha(2) \Psi_\gamma(3) - \Psi_\beta(1) \Psi_\gamma(2) \Psi_\alpha(3) \right. \\ \left. + \Psi_\gamma(1) \Psi_\alpha(2) \Psi_\beta(3) + \Psi_\gamma(1) \Psi_\beta(2) \Psi_\alpha(3) \right. \\ \left. + \Psi_\beta(1) \Psi_\alpha(2) \Psi_\gamma(3) + \Psi_\alpha(1) \Psi_\gamma(2) \Psi_\beta(3) \right] \checkmark$$

⑤ If two particles are in the same state then

Ψ_A in 9-2 becomes

for ex. ($\alpha = \beta$)

$$\begin{aligned}\Psi_A = \frac{1}{\sqrt{3}} [& \cancel{\Psi_\alpha(1) \Psi_\alpha(2)} \Psi_\beta(3) + \Psi_\alpha(1) \cancel{\Psi_\beta(2)} \Psi_\alpha(3) \\ & + \Psi_\beta(1) \Psi_\alpha(2) \cancel{\Psi_\alpha(3)} - \Psi_\beta(1) \cancel{\Psi_\alpha(2)} \Psi_\alpha(3) \\ & - \cancel{\Psi_\alpha(1) \Psi_\alpha(2)} \Psi_\beta(3) - \cancel{\Psi_\alpha(1) \Psi_\beta(2)} \Psi_\alpha(3)] = 0 \checkmark\end{aligned}$$