

Homework 4

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1 Problem 4.16

A hydrogenic atom consists of a single electron orbiting a nucleus with Z protons ($Z = 1$ would be itself, $Z = 2$ is ionized helium, $Z = 3$ is doubly ionized lithium, and so on). Determine

1. Bohr energies $E_n(Z)$
2. Binding energy $E_1(z)$
3. Bohr radius $a(Z)$
4. Rydberg constant $R(Z)$

for a hydrogenic atom. (Express your answers as appropriate multiples of the hydrogen values.) Where in the electromagnetic spectrum would the Lyman series fall, for $Z = 2$ and $Z = 3$? Hint: There's nothing much to calculate here-in the potential

$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$$

$e^2 \rightarrow Ze^2$, so all you have to do is make the same substitution in all the final results.

Solution 1: Bohr energies

Recalling that the energy of the Hydrogen atom is given by

$$E_n = -\frac{m_e e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^2},$$

and tacking into account the hint of introducing the following change of variable $e^2 \rightarrow Ze^2$ we get

the following expression,

$$\begin{aligned} E_n(Z) &= -\frac{m_e(Ze^2)^2}{2(4\pi\epsilon_o)^2\hbar^2} \frac{1}{n^2} \\ &= -\frac{m_e e^4}{2(4\pi\epsilon_o)^2\hbar^2} \frac{1}{n^2} Z^2 \\ &= E_n Z^2. \end{aligned}$$

Therefore, the Boher energies are

$$E_n(Z) = E_n Z^2$$

Solution 2: Binding energy $E_1(Z)$

From the previous result we can easily compute $E_1(Z)$ as follows,

$$E_1(Z) = E_1 Z^2$$

Solution 3: Bohr radius $a(Z)$

With the same methodology of the first question, we start by recalling the Bohr's radius expression and introducing the suggested change of variable,

$$\begin{aligned} a(Z) &= \frac{4\pi\epsilon_o\hbar^2}{e^2 m_e} \\ &= \frac{4\pi\epsilon_o\hbar^2}{Ze^2 m_e} \\ &= \frac{4\pi\epsilon_o\hbar^2}{e^2 m_e} \frac{1}{Z} \\ &= \frac{a}{Z} \end{aligned}$$

$$a(Z) = \frac{a}{Z}$$

Solution 4: Rydberg constant $R(Z)$

Now, we apply the same procedure as before to compute the Rydberg constant,

$$\begin{aligned}
 R(Z) &= \frac{m_e e^4}{8\epsilon_o \hbar^3 c} \\
 &= \frac{m_e (Ze^2)^2}{8\epsilon_o \hbar^3 c} \\
 &= \frac{m_e e^4}{8\epsilon_o \hbar^3 c} Z^2 \\
 &= R Z^2
 \end{aligned}$$

$$R(Z) = R Z^2$$

Solution 5: Electromagnetic spectrum

To compute the Lyman lines we need to recall the following relation,

$$\frac{1}{\lambda_2} = R \left(1 - \frac{1}{4} \right) \implies \lambda_2 = \frac{4}{3R}$$

and

$$\frac{1}{\lambda_1} = R \left(1 - \frac{1}{\infty} \right) \implies \lambda_1 = \frac{1}{R}.$$

Now that we know the Rydberg constant in terms of Z we compute the lines for $Z = 2$ and 3 . For $Z = 2$ we get that $\lambda_1 = 1/R2^2$ and $\lambda_2 = 4/(3R2^2)$. For $Z = 3$ we get that $\lambda_1 = 1/R3^2$ and $\lambda_2 = 4/(3R3^2)$

$$Z = 2 \rightarrow \lambda_1 2.28 \times 10^{-8} \text{ m}, \lambda_2 3.04 \times 10^{-8} \text{ m} \quad Z = 3 \rightarrow \lambda_1 1.01 \times 10^{-8} \text{ m}, \lambda_2 1.35 \times 10^{-8} \text{ m}$$

2 Problem 5.6

Imagine two noninteracting particles, each of mass m , in the infinite square well. If one is in the state

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right).$$

, and the other in state ψ_l ($l \neq n$), calculate $\langle (x_1 - x_2)^2 \rangle$, assuming

1. they are distinguishable particles

2. they are identical bosons
3. they are identical fermions

Solution 6: Distinguishable particles

From previous results in the chapter, the expectation value for distinguishable particles we get that,

$$\langle (x_1 - x_2)^2 \rangle_d = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2 \langle x \rangle_a \langle x \rangle_b.$$

Also, from the state we get that,

$$\langle x \rangle_n = \frac{a}{2}, \quad \langle x^2 \rangle_n = a^2 \left(\frac{1}{3} - \frac{1}{2(n\pi)^2} \right).$$

Substituting the values we get the following result,

$$\begin{aligned} \langle (x_1 - x_2)^2 \rangle_d &= a^2 \left(\frac{1}{3} - \frac{1}{2(n\pi)^2} \right) + a^2 \left(\frac{1}{3} - \frac{1}{2(n\pi)^2} \right) - 2 \frac{a}{2} \frac{a}{2} \\ &= a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right]. \end{aligned}$$

$$\boxed{\langle (x_1 - x_2)^2 \rangle_d = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right]}$$

Solution 7: Identical bosons

Now that we are going to analyze bosons, the state is represented by

$$\Psi_+(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_n(x_1)\psi_m(x_2) + \psi_m(x_1)\psi_n(x_2)]$$

and the expectation value, computed previously in the chapter, is given by,

$$\langle (x_1 - x_2)^2 \rangle_+ = \langle x^2 \rangle_n + \langle x^2 \rangle_m - 2 \langle x \rangle_n \langle x \rangle_m - 2 |\langle x \rangle_{nm}|^2.$$

We need to compute $\langle x \rangle_n$, $\langle x^2 \rangle_n$ and $\langle x_n x_m \rangle$, due to time restrictions I will add the results and submit the procedures in another document,

$$\begin{aligned} \langle x \rangle &= \frac{a}{2} \\ \langle x^2 \rangle &= a^2 \left[\frac{1}{3} - \frac{1}{4\pi} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] \\ \langle x_n x_m \rangle &= \begin{cases} \frac{a(-8mn)}{\pi^2(m^2 - n^2)^2} & n, m \text{ have opposite parity} \\ 0 & n, m \text{ have same parity} \end{cases} \end{aligned}$$

with those results we can compute the answer,

$$\begin{aligned}\langle (x_1 - x_2)^2 \rangle_d &= a^2 \left[\frac{1}{3} - \frac{1}{4\pi} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] + a^2 \left[\frac{1}{3} - \frac{1}{4\pi} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] - 2 \frac{a}{2} \frac{a}{2} - 2 \left[\frac{a(-8mn)}{\pi^2(m^2 - n^2)^2} \right]^2 \\ &= a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] - \frac{128a^2m^2n^2}{\pi^4(m^2 - n^2)^4}.\end{aligned}$$

$$\boxed{\langle (x_1 - x_2)^2 \rangle_d = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] - \frac{128a^2m^2n^2}{\pi^4(m^2 - n^2)^4}}$$

Solution 8: Identical fermions

Now that we are going to analyze bosons, the state is represented by

$$\Psi_-(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_n(x_1)\psi_m(x_2) - \psi_m(x_1)\psi_n(x_2)]$$

and the expectation value, computed previously in the chapter, is given by,

$$\langle (x_1 - x_2)^2 \rangle_+ = \langle x^2 \rangle_n + \langle x^2 \rangle_m - 2 \langle x \rangle_n \langle x \rangle_m - 2 |\langle x \rangle_{nm}|^2.$$

Due to the symmetry with the previous state we can re-cycle the results with the proper sign modification,

$$\begin{aligned}\langle x \rangle &= \frac{a}{2} \\ \langle x^2 \rangle &= a^2 \left[\frac{1}{3} - \frac{1}{4\pi} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] \\ \langle x_n x_m \rangle &= \begin{cases} \frac{a(-8mn)}{\pi^2(m^2 - n^2)^2} & n, m \text{ have opposite parity} \\ 0 & n, m \text{ have same parity} \end{cases}\end{aligned}$$

Hence,

$$\boxed{\langle (x_1 - x_2)^2 \rangle_d = a^2 \left[\frac{1}{6} - \frac{1}{2\pi^2} \left(\frac{1}{n^2} + \frac{1}{m^2} \right) \right] + \frac{128a^2m^2n^2}{\pi^4(m^2 - n^2)^4}}$$

3 Problem 5.9

1. Suppose you put both electrons in a helium atom into the $n = 2$ state; what would the energy of the emitted electron be?
2. Describe (quantitatively) the spectrum of the helium ion, He^+ .

Solution 9: Energy of emitted electron

We start by computing the total energy in the system as follows,

$$\begin{aligned} E_s &= 2Z^2n^2E_1 \\ &= 22^22^2E_1 \\ &= -27.2\text{eV}. \end{aligned}$$

Now, we compute the energy of one electron that goes into the ground state,

$$\begin{aligned} E_d &= Z^2n^2E_1 \\ &= 2^21^2E_1 \\ &= -108.8\text{eV}. \end{aligned}$$

Computing the difference of energy we get,

$$\begin{aligned} E &= -27.2\text{eV} - (-108.8\text{eV}) \\ &= 27.2\text{eV}. \end{aligned}$$

Therefore,

$$E = 27.2\text{eV}$$

Solution 10: Spectrum of helium ion

For this case, we recall the last solution from problem 4.16 in which compute the spectrum of an hydrogen like atom as follows,

$$\frac{1}{\lambda} = 4R \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right),$$

tacking into account the the helium ion is a hydrogenic ion, we can apply this relation to compute the spectrum.

$$\frac{1}{\lambda} = 4R \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

4 Problem 5.10

Discuss (qualitatively) the energy level scheme for helium if

1. electrons were identical bosons
2. if electrons were distinguishable particles (but with the same mass and charge). Pretend these “electrons” still have spin $1/2$, so the spin configuration are the singlet and the triplet.

Solution 11: Electrons as identical bosons

To answer we need to take into account the triplets states with total spin angular momentum $s = 1$ are symmetric, meanwhile the singlet with total angular momentum $s = 0$ is antisymmetric. Also that a property of describing a particle as a boson, implies that the state of the particle is symmetric under exchange. Therefore we have the following cases:

Triplets In this case the spin state is symmetric, hence to make a total state symmetric, the spatial state that is associated with the triplets must be symmetric. As a consequence, the probability of the particles getting closer is favoured.

Singlet Since the spin state is antisymmetric, the related spatial state must be antisymmetric to accomplish a symmetric total state. Hence, the probability of the particles getting closer is reduced.

From this qualitatively analysis, we expect that the total state of the particle associated with triplets have higher energies than those associated with the singlet states.

Solution 12: Electron as distinguishable particles

In this situation the spin state can be describe as separable states, hence the restrictions that applied from the previous case can not be applied in this situation, since each particle can be well defined. This cause that we can not make educated guess about the energies of the states.

5 Problem 5.12

1. Figure out the electron configurations (in the notation of eqn 5.33) for the first two rows of the periodic table (up to neon), and check your results against table 5.1
2. Figure out the corresponding total angular momenta, in the notation of $^{2S+1}L_J$, for the first four elements. List all possibilities for boron, carbon and nitrogen.

Solution 13: Electron configurations

1. Hydrogen: $(1s)$
2. Helium: $(1s)^2$
3. Lithium: $(1s)^2(2s)$

4. Beryllium: $(1s)^2(2s)^2$
5. Boron: $(1s)^2(2s)^2(2p)$
6. Carbon: $(1s)^2(2s)^2(2p)^2$
7. Nitrogen: $(1s)^2(2s)^2(2p)^3$
8. Oxygen: $(1s)^2(2s)^2(2p)^4$
9. Fluorine: $(1s)^2(2s)^2(2p)^5$
10. Neon: $(1s)^2(2s)^2(2p)^6$

Solution 14: Total angular momenta

Remembering that S refers to the total spin angular number and J the total general angular momentum.

1. Hydrogen: $S = 1/2, J = 1/2 \rightarrow {}^2S_{1/2}$
2. Helium: $S = 0, J = 0 \rightarrow {}^1S_0$
3. Lithium: $S = 1/2, J = 1/2 \rightarrow {}^2S_{1/2}$
4. Beryllium: $S = 0, J = 0 \rightarrow {}^1S_0$
5. Boron: $S = 1/2, J = \{1/2, 3/2\} \rightarrow {}^2P_{1/2}, {}^2P_{3/2}$
6. Carbon: $S = \{0, 1\}, J = \{0, 1, 2\} \rightarrow {}^1S_0, {}^3S_0, {}^1P_1, {}^3P_2, {}^3P_1, {}^3P_0, {}^1D_2, {}^3D_3, {}^3D_2, {}^3D_1$
7. Nitrogen: $S = \{1/2, 3/2\}, J = \{0, 1, 2, 3\} \rightarrow {}^2S_{1/2}, {}^4S_{3/2}, {}^2P_{1/2}, {}^2P_{3/2}, {}^4P_{1/2}, {}^4P_{3/2}, {}^4P_{5/2}, {}^2D_{3/2}, {}^2D_{5/2}, {}^4D_{1/2}, {}^4D_{3/2}, {}^4D_{5/2}, {}^4D_{7/2}, {}^2F_{5/2}, {}^2F_{3/2}, {}^4F_{3/2}, {}^4F_{5/2}, {}^4F_{7/2}, {}^4F_{9/2}$

6 Problem 5.14

The ground state of dysprosium (element 66, in the 6th row of the Periodic Table) is listed as 5I_8 . What are the total spin, total orbital and grand total angular momentum quantum numbers? Suggest a likely electron configuration for dysprosium.

Solution 15: Electron configuration for Dysprosium

$$S = 2, L = \{6, 8\} \rightarrow (1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(3d)^{10}(4s)^2(4p)^6(4d)^{10}(5s)^2(5p)^6(4f)^{10}(6s)^2$$