SOLUTION SET

Chapter 3

PARTICLE NATURE OF LIGHT – DISCRETE ENERGY LEVELS

"LASER FUNDAMENTALS"

Second Edition

By William T. Silfvast

1. Using the Bohr theory, carry out the derivation of the electron orbit radius r (eqn. 3.4) and the orbital energy E_n (eqn. 3.8) for the hydrogen atom.

From (3.2) $\quad v = \dfrac{n\hbar}{m_e r} \Rightarrow$ plug into (3.3)

$$\frac{e^2}{4\pi\epsilon_0 r^2} = \frac{m_e\left(\frac{n^2\hbar^2}{m_e^2 r^2}\right)}{r} = \frac{n^2\hbar^2}{m_e r^3}$$

$$\Rightarrow r = \frac{n^2\hbar^2 4\pi\epsilon_0}{m_e e^2} = \frac{n^2(2\pi\hbar)^2\epsilon_0}{m_e \pi e^2} = \frac{\epsilon_0 h^2}{\pi m_e e^2} n^2 = a_H n^2$$

From (3.6)

$$E = \frac{1}{2} m_e v^2 - \frac{e^2}{4\pi\epsilon_0 r}$$

but from (3.3), $\quad \frac{1}{2} m_e v^2 = \frac{1}{2}\frac{e^2 r}{4\pi\epsilon_0 r^2} = \frac{e^2}{8\pi\epsilon_0 r}$

Hence $\quad E = -\dfrac{e^2}{8\pi\epsilon_0 r}$

Using r from above:

$$E = -\frac{e^2}{8\pi\epsilon_0 r} = -\frac{e^2}{8\pi\epsilon_0\left(\frac{\epsilon_0 h^2}{\pi m_e e^2 n^2}\right)}$$

$$= -\frac{m_e e^4}{8\epsilon_0^2 h^2 n^2} = -\frac{E_0}{n^2}$$

where $E_0 = \dfrac{m_e e^4}{8\epsilon_0^2 h^2}$

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2. Compute the wavelengths for the following transitions in the hydrogen atom using the Bohr theory:

(a) $n = 2$ to $n = 1$;
(b) $n = 3$ to $n = 1$;
(c) $n = 4$ to $n = 2$;
(d) $n = 5$ to $n = 3$;
(e) $n = 6$ to $n = 4$.

From (3.11) $\frac{1}{\lambda} = R_H\left(\frac{1}{n_i^2} - \frac{1}{n_j^2}\right) = (1.0967758\times10^7)\left(\frac{1}{n_i^2} - \frac{1}{n_j^2}\right) m^{-1}$

(a) $n_j = 2$ to $n_i = 1$ $\quad \frac{1}{\lambda_{21}} = \left(\frac{1}{1^2} - \frac{1}{2^2}\right) R_H$

$\lambda_{21} = 1.2157 \times 10^{-7} m = 121.57 nm$

(b) $n_j = 3$ to $n_i = 1$ $\quad \frac{1}{\lambda_{31}} = \left(\frac{1}{1^2} - \frac{1}{3^2}\right) R_H$

$\lambda_{31} = 1.0257 \times 10^{-7} m = 102.57 nm$

(c) $n_j = 4$ to $n_i = 2$ $\quad \frac{1}{\lambda_{42}} = \left(\frac{1}{2^2} - \frac{1}{4^2}\right) R_H$

$\lambda_{42} = 4.8627 \times 10^{-7} m = 486.27 nm$

(d) $n_j = 5$ to $n_i = 3$ $\quad \frac{1}{\lambda_{53}} = \left(\frac{1}{3^2} - \frac{1}{5^2}\right) R_H$

$\lambda_{53} = 1.2822 \times 10^{-6} m = 1.2822 \mu m$

(e) $n_j = 5$ to $n_i = 4$ $\quad \frac{1}{\lambda_{54}} = \left(\frac{1}{4^2} - \frac{1}{5^2}\right) R_H$

$\lambda_{54} = 4.0523 \times 10^{-6} m = 4.0523 \mu m$

3. Compute the ionization potential for five-times ionized carbon (C^{5+}) and also compute the wavelength of the transition from $n = 3$ to $n = 2$ for that species.

(a) From (3.13) $$E_n = -\frac{Z^2 E_0}{n^2}$$

Ionization potential from ground state of C^{5+} is:

$$E_1 = -\frac{Z^2 E_0}{1^2} = -Z^2 E_0$$

but $E_0 = 13.595\,eV$ and $Z = 6$

hence $E_1 = 6^2(13.595\,eV) = \underline{489.42\,eV}$

or $7.83 \times 10^{-17}\,J$

(b) λ_{32} for H-like C^{5+} is from (3.14):

$$\nu_{32} = \frac{c}{\lambda_{32}} = \frac{Z^2 E_0}{h}\left(\frac{1}{2^2} - \frac{1}{3^2}\right)$$

or $$\frac{1}{\lambda_{32}} = \frac{Z^2 E_0}{ch}\left(\frac{1}{2^2} - \frac{1}{3^2}\right)$$

$$\therefore \lambda_{32} = \frac{1}{R_H}\frac{1}{Z^2}\frac{1}{\left(\frac{1}{2^2} - \frac{1}{3^2}\right)}$$

$$= \underline{1.8235 \times 10^{-8}\,m = 18.235\,nm}$$

4. In the isoelectronic scaling of hydrogen-like species, what is the lowest–atomic number element that would have a possible X-ray laser transition at a wavelength shorter than 4.4 nm? (Here, consider the transition from $n = 3$ to $n = 2$ as the laser transition.)

From Problem 3:

$$\lambda_{32} = \frac{1}{Z^2}\frac{1}{R_H}\frac{1}{\left(\frac{1}{2^2}-\frac{1}{3^2}\right)} = \frac{1}{Z^2}\frac{1}{1.097\times10^7\,m^{-1}}\frac{1}{\left(\frac{1}{2^2}-\frac{1}{3^2}\right)}$$

$$= \frac{1}{Z^2}\left(6.563\times10^{-7}\,m\right) = \frac{1}{Z^2}\left(656.3\,nm\right)$$

Now $\lambda_{32} < 4.4\,nm$

$$\frac{1}{Z^2}\left(656.3\,nm\right) < 4.4\,nm$$

Hence $Z > \sqrt{\frac{656.3}{4.4}} = 12.21$

Since Z is an integer, the next larger integer is <u>13</u>

$\therefore$ $Z = 13$ which from the appendix on page 621 is <u>Aluminum</u>

5. Solve the Schrödinger equation for the energy eigenvalue of the ground state of the hydrogen atom, assuming a solution of the form $\psi_1(r) = Ce^{-\alpha r}$ (eqn. 3.38).

Schroedinger Equation:

$$\nabla^2\psi + \frac{8\pi^2\mu}{h^2}(E-V)\psi = 0 \qquad (3.29)$$

for $\psi = Ce^{-\alpha r}$ and $V = \frac{-e^2}{4\pi\epsilon_0 r}$

$$\nabla^2(Ce^{-\alpha r}) + \frac{8\pi^2\mu}{h^2}\left(E_1 + \frac{e^2}{4\pi\epsilon_0 r}\right)Ce^{-\alpha r} = 0$$

only r involved

$$\nabla^2(Ce^{-\alpha r}) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}Ce^{-\alpha r}\right) = -\frac{\alpha C}{r}e^{-\alpha r}[-\alpha r+2]$$

$$\therefore \left(C\alpha^2 + \frac{C\,8\pi^2\mu}{h^2}E_1\right)e^{-\alpha r} + \left(\frac{C2\pi\mu e^2}{\epsilon_0 h^2} - 2\alpha C\right)\frac{e^{-\alpha r}}{r} = 0$$

Each paranthesis must equal zero for all r

$$\therefore \frac{C2\pi\mu e^2}{\epsilon_0 h^2} - 2\alpha C = 0 \Rightarrow \alpha = \frac{\pi\mu e^2}{\epsilon_0 h^2} = \frac{1}{a_H}$$

and $C\alpha^2 + \frac{C\,8\pi^2\mu}{h^2}E_1 = 0 \Rightarrow E_1 = \frac{-\alpha^2 h^2}{8\pi^2\mu} = -\frac{\mu e^4}{8\epsilon_0^2 h^2} = E_1$

Normalize To find C

$$\int|\psi_1|^2 dv = \int_0^\infty C^2 e^{-2\alpha r}4\pi r^2 dr = \frac{C^2\,2\cdot 4\pi}{(2\alpha)^3} = 1$$

$$\Rightarrow C = \frac{\alpha^{3/2}}{\sqrt{\pi}} = \frac{1}{a_H^{3/2}\sqrt{\pi}} \Rightarrow \psi_1 = \frac{1}{\sqrt{\pi}\,a_H^{3/2}}e^{-r/a_H}$$

6. Write out the wave function for the hydrogen atom for $n = 3$, $l = 2$, and $m = +1$ using (3.65) and (3.66).

$n=3 \quad l=2 \quad m=+1$

from (3.65) $\psi_{n,l,m} = C\rho^{l} e^{-\rho/2} L_{n+l}^{2l+1}(\rho)\, P_{l}^{|m|}(\cos\theta)\, e^{im\phi}$ $\quad \rho = \frac{2r}{na_H}$

$$\psi_{3,2,+1} = C\rho^{2} e^{-\rho/2} L_5^5\, P_2^1(\cos\theta)\, e^{i\phi} \qquad \rho = \frac{2r}{3a_H}$$

from (3.66) $C = -\left\{\left(\frac{2Z}{na_H}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{1/2} \left[\frac{(2l+1)(l-|m|)!}{4\pi\,(l+|m|)!}\right]^{1/2}$

$$= -\left\{\left(\frac{2}{3a_H}\right)^3 \frac{0!}{6(5!)^3}\right\}^{1/2} \left[\frac{5}{4\pi}\,\frac{1!}{3!}\right]^{1/2}$$

$$= -\left\{\frac{8}{27a_H^3}\cdot\frac{1}{6\cdot 120^3}\right\}^{1/2}\left[\frac{5}{24\pi}\right]^{1/2}$$

$$= -\left\{\frac{1}{27\cdot 6\cdot 15\cdot 120^2 a_H^3}\cdot\frac{5}{24\pi}\right\}^{1/2} = -\frac{1}{12960\, a_H^{3/2}\sqrt{\pi}}$$

$$= -\frac{4.35\times 10^{-5}}{a_H^{3/2}}$$

From (3.57)

determine $L_5^5 \quad L_n^n = n! \therefore L_5^5 = -120$

From (3.54) $P_2^1(x) = 3x(1-x^2)^{1/2}$

$\therefore P_2^1 \cos\theta = 3\cos\theta\,(1-\cos^2\theta)^{1/2} = 3\cos\theta\sin\theta$

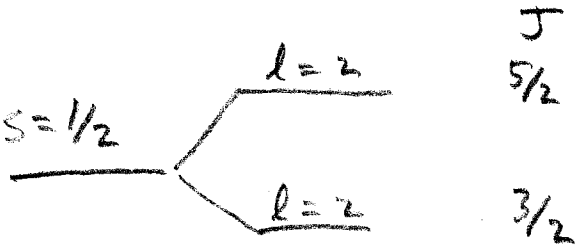
$$\therefore \psi_{3,2,1} = -\frac{4.35\times 10^{-5}}{a_H^{3/2}}\,\rho^2 e^{-\rho/2}(-120)\,3\cos\theta\sin\theta\, e^{i\phi}$$

$$= \frac{6.97\times 10^{-3}\, r^2}{a_H^{7/2}}\, e^{-r/3a_H}\cos\theta\sin\theta\, e^{i\phi}$$

7. Obtain the possible term designations for a hydrogen atom in which the electron is in the 3d level.

3d level of hydrogen

$s = 1/2 \qquad l = 2 \Rightarrow J = 5/2, 3/2$



$^2D_{5/2}, \quad ^2D_{3/2}$

8. Give the electron configuration for a lithium atom in its ground state, and write out the term designation for that state.

$1s^2\ 2s$ Li ground state

for 2s

$s = 1/2 \quad l = 0 \Rightarrow$ s state

$^{2S+1}L_J \Rightarrow {}^2S_{1/2}$

9. List the electron configurations for the following elements in their ground states: aluminum, fluorine, calcium, germanium, and krypton.

Aluminum

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p$

Fluorine

$1s^2\ 2s^2\ 2p^5$

Calcium

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$

Germanium

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^2$

Krypton

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6$

10. Determine the number of states and write out the term designations (eqn. 3.76) for those states that result from an outer electron configuration of 2s4p.

<u>2s 4p</u>

$2s \Rightarrow l = 0 \quad s = 1/2$

$4p \Rightarrow l = 1 \quad s = 1/2$

$L = l_1 + l_2 = 0 + 1 = 1$

$S = s_1 + s_2 = \frac{1}{2} + \frac{1}{2} = 1$

$= s_1 - s_2 = \frac{1}{2} - \frac{1}{2} = 0$

<u>$L = 1 \quad S = 1$</u>

$J = L + S = 1 + 1 = 2 \Rightarrow {}^3P_2$

$1 + 0 = 1 \Rightarrow {}^3P_1$

$1 - 1 = 0 \Rightarrow {}^3P_0$

<u>$L = 1 \quad S = 0$</u>

$J = L + S = 1 + 0 = 1 \Rightarrow {}^1P_1$

11. You are told that a short-wavelength laser is measured to have a wavelength of 30.38 nm and occurs on an H-like transition from $n = 4$ to $n = 3$. In what element does the laser action occur? Justify your answer.

$$\nu = \frac{Z^2 E_0}{h}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right) = Z^2\, 3.28\times10^{15}\left(\frac{1}{2^2} - \frac{1}{4^2}\right)$$

$$= Z^2\, 6.15\times10^{14}$$

$$Z^2 = \frac{\nu}{6.15\times10^{14}}$$

$$\nu = \frac{c}{\lambda} = \frac{3\times10^8}{30.38\times10^{-9}}$$

$$= 9.87\times10^{15}\ \text{Hz}$$

$$Z^2 = \frac{9.87\times10^{15}}{6.15\times10^{14}} = 16.048$$

$$\therefore\ Z = 4.00 \Rightarrow \boxed{\text{Be}}$$

12. The element magnesium (Mg) is vaporized to produce a gas of magnesium atoms. An electrical current is passed through the gas in order to excite the atoms to levels above the ground state. Give the complete ground-state electron configuration. Make an energy-level diagram and provide the labels of the ground state and all of the excited energy levels associated with the same n quantum number as that of the ground state. Allow only one of the outer electrons to be excited.

Mg $\quad 1s^2\,2s^2\,2p^6\,3s^2$

$3s^2 \rightarrow 3s\,3p \qquad 3s\,3d$

$\underline{3s^2} \Rightarrow \quad l=0 \quad s=1/2$
$\qquad\qquad\quad l=0 \quad s=1/2$

$S=0 \quad L=0$

$\boxed{{}^1S_0}$

$\underline{3s\,3p} \Rightarrow \quad l=0 \quad s=1/2$
$\qquad\qquad\quad l=1 \quad s=1/2$

$S=0,1 \quad L=1$

$\boxed{{}^1P_1^o \quad {}^3P^o_{2,1,0}}$

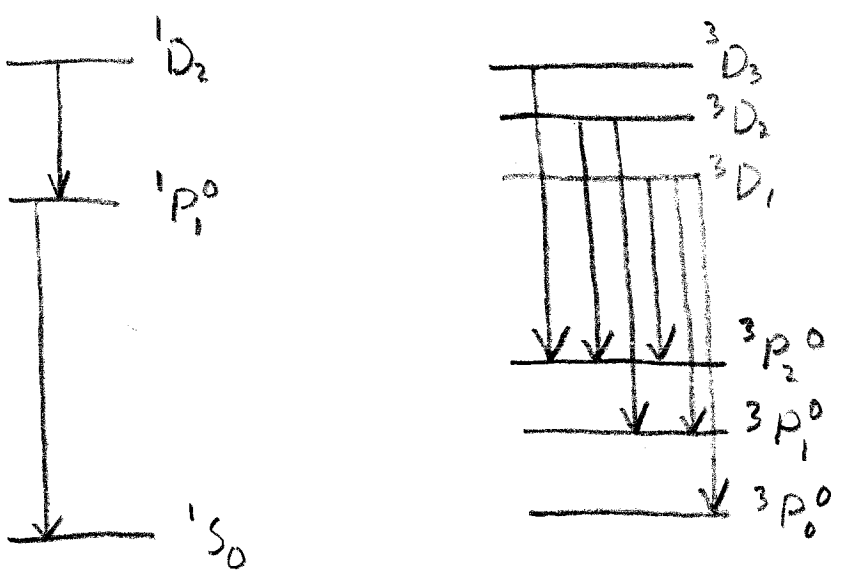
$3s\,3d \Rightarrow \quad l=0 \quad s=1/2$
$\qquad\qquad\quad l=2 \quad s=1/2$

$S=0 \quad L=2 \quad J=2$

$\boxed{{}^1D_2}$

$S=1 \quad L=2 \quad J=3,2,1$

$\boxed{{}^3D_{3,2,1}}$



13. Obtain the spectroscopic designation and diagram the energy levels for the following three electronic configurations:

$$1s^2 2s^2, \qquad 1s^2 2s2p, \qquad 1s^2 2s3d.$$

$1s^2 2s^2 \rightarrow$ $\quad s = 1/2 - 1/2 \quad l = 0, 0$

$$\boxed{{}^1S_0}$$

$1s^2 2s\,2p \rightarrow$ $\quad s = 1/2 \quad l = 0$

$s = 1/2 \quad l = 1$

$S = \frac{1}{2} + \frac{1}{2} = 1, \quad L = 0 + 1 = 1 \quad J = 2, 1, 0$

$$\boxed{{}^3P^o_{2,1,0}}$$

$S = \frac{1}{2} - \frac{1}{2} = 0 \quad l = 0 + 1 = 1 \quad J = 1$

$$\boxed{{}^1P^o_1}$$

$1s^2 2s\,3d \rightarrow$ $\quad s = 1/2 \quad l = 0$

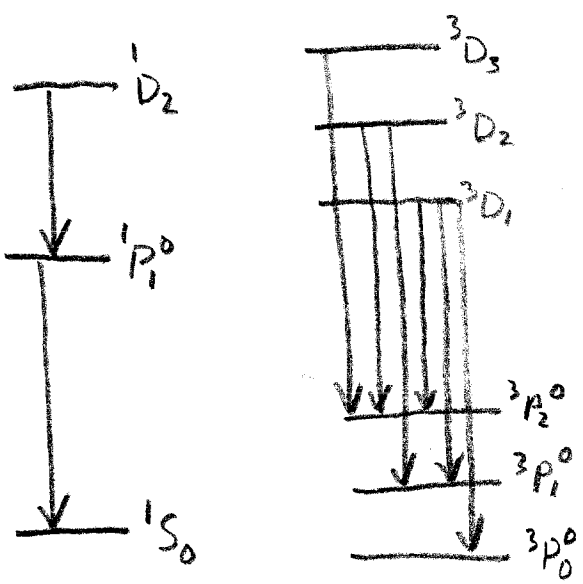
$s = 1/2 \quad l = 2$

$S = \frac{1}{2} + \frac{1}{2} = 1 \quad L = 0 + 2 = 2 \quad J = 3, 2, 1$

$$\boxed{{}^3D_{3,2,1}}$$

$S = \frac{1}{2} - \frac{1}{2} = 0 \quad L = 0 + 2 = 2 \quad J = 2$

$$\boxed{{}^1D_2}$$



14. Determine the number of energy levels and the term designations for those levels of an atom in a state in which the two outer electrons are 2s and 2p.

2s 2p

$s = 1/2 \quad l = 0$

$s = 1/2 \quad l = 1$

$S = \frac{1}{2} + \frac{1}{2} = 1 \qquad L = 0 + 1 = 1 \qquad J = 2, 1, 0$

$\boxed{{}^3P^o_{2,1,0}}$

$S = \frac{1}{2} - \frac{1}{2} = 0 \qquad L = 0 + 1 = 1 \qquad J = 1$

$\boxed{{}^1P^o_1}$

4 states