Homework for Chapter 5

Xiping Hu

https://hxp.plus/

April 14, 2020

1. He 原子的两个电子处在 2p3d 电子组态. 问可能组成哪几种原子态? 用原子态的符号表示之. 已知电子间是 L8 耦合.

$$\begin{cases} s_1 = s_2 = \frac{1}{2} \\ l_1 = 1 \\ l_2 = 2 \end{cases} \Rightarrow \begin{cases} L = 3, 2, 1 \\ S = 1, 0 \end{cases}$$

So that the atom has the following 12 states

2. 已知 He 原子两电子被分别激发到 2p 和 3d 轨道,其所构成的原子态为 3D ,问这两电子的轨道角动量 p_{i_1} 与 p_{i_2} 之间的夹角,自旋角动量 p_{s_1} 与 p_{s_2} 之间夹角分别是多少?

$$\begin{cases} L = 2 \\ S = 1 \\ l_1 = 1 \\ l_2 = 2 \end{cases} \Rightarrow \begin{cases} p_{l1} = \sqrt{l_1 (l_1 + 1)} \hbar = \sqrt{2} \hbar \\ p_{l2} = \sqrt{l_2 (l_2 + 1)} \hbar = \sqrt{6} \hbar \\ P_l = \sqrt{L (L + 1)} \hbar = \sqrt{6} \hbar \end{cases}$$

$$P_L^2 = p_{l1}^2 + p_{l2}^2 + 2p_{l1}p_{l2}\cos\theta \Rightarrow \cos\theta = \frac{P_L^2 - p_{l1}^2 - p_{l2}^2}{2p_{l1}p_{l2}} \Rightarrow \theta = 106^\circ$$

- 3. 锌原子(Z=30)的最外层电子有两个,基态时的组态是 4s4s. 当其中有一个被激发,考虑两种情况:
 - (1) 那电子被激发到 5s 态,
 - (2) 它被激发到 4p 态.

试求出在 LS 耦合情况下这两种电子组态分别组成的原子状态. 画出 相应的能级图. 从(1)和(2)情况形成的激发态向低能级跃迁分别各有几种光谱跃迁?

Q1 When the electrons is in 4s5s

$$\begin{cases} s_1 = s_2 = \frac{1}{2} \\ l_1 = 0 \\ l_2 = 0 \end{cases} \Rightarrow \begin{cases} S = 0, 1 \\ L = 0 \end{cases}$$

The possible transitions are

$$5^{1}S_{0} \rightarrow 4^{1}P_{1}$$

 $5^{3}S_{1} \rightarrow 4^{3}P_{0}$
 $5^{3}S_{1} \rightarrow 4^{3}P_{1}$
 $5^{3}S_{1} \rightarrow 4^{3}P_{2}$
 $4^{3}P_{2} \rightarrow 4^{3}S_{1}$

Q2 When the electrons is in 4s5p

$$\begin{cases} s_1 = s_2 = \frac{1}{2} \\ l_1 = 0 \\ l_2 = 1 \end{cases} \Rightarrow \begin{cases} S = 0, 1 \\ L = 0, 1 \end{cases}$$

The possible transitions are

$$4^1P_1 \to 4^1S_0$$

4. 试以两个价电子 $l_1=2$ 和 $l_2=3$ 为例证明,不论是 LS 耦合还 是 jj 耦合都给出同样数目的可能状态.

L-S coupling has 20 states

$$S = 0, 1$$

$$L = 1, 2, 3, 4, 5$$

$$S = 0 \quad S = 1$$

$$L = 1 \quad {}^{1}P_{1} \quad {}^{3}P_{0,1,2}$$

$$L = 2 \quad {}^{1}D_{2} \quad {}^{3}D_{1,2,3}$$

$$L = 3 \quad {}^{1}F_{3} \quad {}^{3}F_{2,3,4}$$

$$L = 4 \quad {}^{1}G_{4} \quad {}^{3}G_{3,4,5}$$

$$L = 5 \quad {}^{1}H_{5} \quad {}^{3}H_{4,5,6}$$

jj coupling has 20 states as follows, as well

$$j_1 = \frac{5}{2} \qquad j_1 = \frac{3}{2}$$

$$j_2 = \frac{7}{2} \quad J = 6, 5, 4, 3, 2, 1 \quad J = 5, 4, 3, 2$$

$$j_2 = \frac{5}{2} \quad J = 5, 4, 3, 2, 1, 0 \quad J = 4, 3, 2, 1$$

6. 已知 He 原子的一个电子被激发到 2p 轨道,而另一个电子 还在 1s 轨道. 试作出能级跃迁图来说明可能出现哪些光谱线的跃迁.

$$\begin{cases} s_1 = s_2 = \frac{1}{2} \\ l_1 = 1 \\ l_2 = 0 \end{cases} \Rightarrow \begin{cases} L = 1 \\ S = 1, 0 \end{cases}$$

So that the atom has the following 12 states

The possible transitions are

$$2^{1}P_{1} \to 1^{1}S_{0}$$

$$2^{1}P_{1} \to 2^{1}S_{0}$$

$$2^{3}P_{0} \to 2^{3}S_{1}$$

$$2^{3}P_{1} \to 2^{3}S_{1}$$

$$2^{3}P_{2} \to 2^{3}S_{1}$$

8. Pb 原子基态的两个价电子都在 6p 轨道, 若其中一个价电子被激发到 7s 轨道, 而其价电子间相互作用属于 jj 耦合。问此时 Pb 原子可能有哪些状态?

jj coupling has 20 states as follows, as well

$$j_1 = \frac{3}{2} j_1 = \frac{1}{2}$$

$$j_2 = \frac{1}{2} J = 2, 1 J = 1, 0$$