Homework14 答案

January 1, 2021

1.计算氢原子的强场Zeeman效应。考虑能级E_2,共8个简并态$|2lmm_s\rangle$.(1)忽略精细结构,讨论能级及其简并.(2)计算精细结构引起的能级移动到一阶微扰.(提示：证明$\langle \boldsymbol{S}\cdot\boldsymbol{L}\rangle = \hbar^2 m m_s$;在$\psi_{nlm}$下,$\langle \frac{1}{r^3}\rangle = \frac{1}{l(l+\frac{1}{2})(l+1)n^3a^3}$)

解：取高斯单位, a为玻尔半径,

(1)取外磁场为z轴方向，哈密顿量为：

$$H_0 = \frac{\hat{p}^2}{2\mu} - \frac{\alpha}{r},$$

$$H_Z = \frac{e}{2\mu}(\hat{L_z} + 2\hat{S_z})B_{ext},$$

$$H = H_0 + H_Z,$$

$$E_n = -\frac{e^2}{2n^2a},$$

$$\langle \frac{1}{r}\rangle = \frac{1}{n^2a}, \langle \frac{1}{r^2}\rangle = \frac{1}{(l+1/2)n^3a^2}$$

$[H_0, H_Z] = 0$, 可取共同本征态$|nlmm_s\rangle$, 于是能量本征值为

$$E_{nlmm_s} = -\frac{e^2}{2n^2a} + \mu_B(m+2m_s)B_{ext}$$

$n = 2$时，共分裂为5个能级，其中
$E_{2001/2}, E_{2101/2}$简并,$E_{200-1/2}, E_{210-1/2}$简并. $E_{21-11/2}, E_{211-1/2}$简并.

(2)精细结构的微扰:自旋轨道耦合H_{so}

$$H_{fs} = \frac{\alpha \boldsymbol{L}\cdot\boldsymbol{S}}{2\mu^2 r^3}$$

$$E_{so}^{(1)} = \langle nlmm_s|\frac{\alpha \boldsymbol{L}\cdot\boldsymbol{S}}{2\mu^2r^3}|nlmm_s\rangle = \frac{\alpha^2}{2\mu^2}(\langle L_x\rangle\langle S_x\rangle + \langle L_y\rangle\langle S_y\rangle + \langle L_z\rangle\langle S_z\rangle)\langle\frac{1}{r^3}\rangle.$$

在L_z, S_z表象下,$\langle L_x\rangle, \langle S_x\rangle, \langle L_y\rangle, \langle S_y\rangle$为0,自旋轨道能量修正为:

$$E_{so}^{(1)} = \frac{\alpha\hbar^2 m m_s}{2\mu^2 l(l+1/2)(l+1)n^3a^3} = \frac{\mu\alpha^4 m m_s}{2l(l+1/2)(l+1)n^3}.$$

这就是精细结构修正. 相对论修正是同意量级的，因此也可以加进来. 请参考Griffiths书.

2.计算氢原子的弱场Zeeman效应.还是考虑能级E_2,共8个简并态$|2ljm_j\rangle$.讨论能级及其简并，画出能级随磁场B的变化图。

解:

此题是考虑$B_{ext} \ll B_{int}$,精细结构主导，Zeeman效应视作微扰，好量子数为:n, l, j, m_j.

Zeeman修正项为:$H_Z = \frac{e}{2\mu}\boldsymbol{B_{ext}} \cdot (\boldsymbol{L} + 2\boldsymbol{S})$

$$E_Z = \langle nljm_j|H_Z|nljm_j\rangle = \frac{e}{2\mu}\boldsymbol{B_{ext}} \cdot \langle \boldsymbol{L} + 2\boldsymbol{S}\rangle = \frac{e}{2\mu}\boldsymbol{B_{ext}}\langle (J_z + S_z)\rangle$$

$$\langle S_z\rangle = \langle nljm_j|S_z|nljm_j\rangle$$

$$E_Z = \mu_B g_J B_{ext} m_j,$$

其中

$$g_J = \left[1 + \frac{j(j+1) - l(l+1) + 3/4}{2j(j+1)}\right] = \begin{cases} 1 + \frac{1}{2j} & j = l + 1/2 \\ 1 - \frac{1}{2j+2} & j = l - 1/2 \end{cases}.$$

$$E_{nljm_j} = -\frac{13.6eV}{n^2}\left[1 + \frac{\alpha^2}{n^2}(\frac{n}{j+1/2} - \frac{3}{4})\right]$$

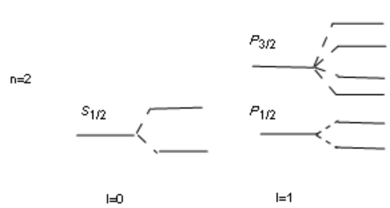
以上公式合并了相对论效应. 不考虑相对论相应也可。

对于n=2，不同能级的分裂为:

$$2S_{1/2} : -3.4eV(1 + \frac{5\alpha^2}{16}) + 2\mu_B m_j B_{ext}$$

$$2P_{1/2} : -3.4eV(1 + \frac{\alpha^2}{16}) + \frac{2}{3}\mu_B m_j B_{ext}$$

$$2P_{3/2} : -3.4eV(1 + \frac{\alpha^2}{16}) + \frac{4}{3}\mu_B m_j B_{ext}$$



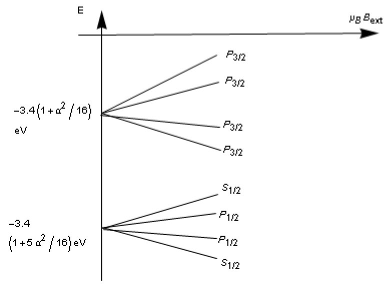


Figure 1: 能级图

3.计算氢原子E_3能级的Stark效应

解:

共有9个简并的态$|300\rangle, |310\rangle, |320\rangle, |311\rangle, |321\rangle, |31-1\rangle, |32-1\rangle, |322\rangle, |32-2\rangle$.
安顺序排成第一到第九个基矢.

$$H_S = eE_{ext}z = eE_{ext}r\cos\theta$$

$$\cos\theta Y_{lm} = a_{lm}Y_{l+1,m} + a_{l-1,m}Y_{l-1,m}, a_{lm} = \sqrt{\frac{(l+1)^2-m^2}{(2l+1)(2l+3)}}$$

$$\langle nlm|z|nl^{'}m^{'}\rangle = \langle nl|r|nl^{'}\rangle(a_{l^{'}m^{'}}\delta_{l,l^{'}+1} + a_{l^{'}-1,m^{'}}\delta_{l,l^{'}-1})\delta_{mm^{'}}, \langle nlm|z|nl^{'}m^{'}\rangle = \langle nl^{'}m^{'}|z|nlm\rangle$$

只需计算:$\langle 300|z|310\rangle, \langle 310|z|320\rangle, \langle 31\pm1|z|32\pm1\rangle$.

由:

$$\int_0^\infty R_{30}R_{31}r^3dr = -9\sqrt{2}a, \int_0^\infty R_{31}R_{32}r^3dr = -\frac{9\sqrt{5}}{2}a.$$

$$\langle 300|z|310\rangle = -3\sqrt{6}a, \langle 310|z|320\rangle = -3\sqrt{3}a, \langle 31\pm1|z|32\pm1\rangle = -(9/2)a.$$

矩阵为:

$$\begin{pmatrix} 0 & 3\sqrt{6} & 0 & & & & & & \\ 3\sqrt{6} & 0 & 3\sqrt{3} & & & & & & \\ 0 & 3\sqrt{3} & 0 & & & & & & \\ & & & 0 & 9/2 & & & & \\ & & & 9/2 & 0 & & & & \\ & & & & & 0 & 9/2 & & \\ & & & & & 9/2 & 0 & & \\ & & & & & & & 0 & \\ & & & & & & & & 0 \end{pmatrix}$$

分块求得本征值为: $\lambda = 0, \pm 9. \pm 9/2$,因此能量与简并度为:

0　3重简并
$(9/2)aeE_{ext}$　2重简并
$-(9/2)aeE_{ext}$　2重简并
$9aE_{ext}$　无简并
$-9aE_{ext}$　无简并