Problem 2. Spin-orbit coupling (10 points).

Inside atoms, besides the Column interaction there exists a term called spin-orbit (SO) coupling. The origin of SO coupling arises from relativistic Dirac equation, which is the first order relativistic correction to the non-relativistic Schrödinger Eq. (The zero-th order approximation is called Pauli Eq. that you have already seen in the midterm.) The SO coupling can be written as

$$H_{so} = f(r)\vec{\sigma}\cdot\vec{L}, \tag{4}$$

where $\vec{L}$ is the orbital angular momentum, and $f(r)$ is a scalar wavefunction that is proportional to the magnitude of radial electric field. We consider a simplified version of Eq. 4

$$H = \omega\vec{\sigma}\cdot\vec{L} \tag{5}$$

We will solve its eigenvalues and eigenstates.

We consider the spheric harmonics with orbital angular momentum l and couple with spin-$\frac{1}{2}$. we start from the basis $|lm;ss_z\rangle$ defined

$$|lm;\frac{1}{2}\frac{1}{2}\rangle = \begin{pmatrix} Y_{lm}(\theta,\phi) \\ 0 \end{pmatrix}, \quad |lm;\frac{1}{2}-\frac{1}{2}\rangle = \begin{pmatrix} 0 \\ Y_{lm}(\theta,\phi) \end{pmatrix}. \tag{6}$$

1) Prove that there are two sets of different eigenvalues $E_+ > 0$ and $E_- < 0$. What the values of E_+ and E_-?

(Hint: you may use the operator identity $\vec{\sigma}\cdot\vec{L} = \vec{J}^2 - \vec{L}^2 - \vec{S}^2$ where $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ and $\vec{J} = \vec{L}+\vec{S}$. Please note that $\vec{L}, \vec{S}$ and $\vec{J}$ are all operators.)

For the $E_\pm$-sectors, the normalized eigenstates are denoted as Y_{j_+,j_z} and Y_{j_-,j_z}, respectively, where $j_\pm = l \pm \frac{1}{2}$. They are eigenstates of total angular momentum $\vec{J}^2$ and J_z with eigenvalue $j_\pm(j_\pm+1)$ and j_z, respectively. These two sectors are called sectors with positive and negative helicitity, respectively.

2) Express $Y_{j_\pm j_z}$ as

$$Y_{j_\pm,j_z}(\theta,\phi) = \begin{pmatrix} a_{j_\pm j_z} Y_{l,m}(\theta,\phi) \\ b_{j_\pm,j_z} Y_{l,m+1}(\theta,\phi) \end{pmatrix}, \tag{7}$$

where $j_\pm = l \pm \frac{1}{2}$ and $j_z = m + \frac{1}{2}$. Derive the expressions for $a_{j_\pm,j_z}$ and $b_{j_\pm,j_z}$. Please note that $Y_{j_\pm j_z}$ need to be normalized.

Prob 2.

① $\vec{\sigma}\cdot\vec{L} = (\vec{L}+\frac{\vec{\sigma}}{2})^2 - L^2 - S^2 = \hat{J}^2 - \hat{L}^2 - \hat{S}^2$

thus eigenvalues are $j(j+1) - \ell(\ell+1) - 3/4$

for the sector of $j = j_+ = \ell + 1/2 \Rightarrow E_+ = (\ell+1/2)(\ell+3/2) - \ell(\ell+1) - 3/4$
$= \ell$

$j = j_- = \ell - 1/2 \Rightarrow E_- = (\ell - 1/2)(\ell+1/2) - \ell(\ell+1) - 3/4$
$= -(\ell+1)$.

or, another method. from $\vec{\sigma}\cdot\vec{L} = \hat{J}^2 - \hat{L}^2 - \hat{S}^2$, $\vec{\sigma}\cdot\vec{L}$ commute with $\hat{J}^2$ and $\hat{J}_z$. we consider the addition between orbital angular momentum ℓ and spin-1/2. Assum the eigenstate $\begin{pmatrix} a\, Y_{\ell m} \\ b\, Y_{\ell m+1} \end{pmatrix}$

$$\vec{\sigma}\cdot\vec{L} = \sigma_z L_z + \frac{1}{2}\left[\sigma_+ L_- + \sigma_- L_+\right]$$

$$= \begin{bmatrix} L_z & L_x - iL_y \\ L_x + iL_y & -L_z \end{bmatrix}$$

$\Rightarrow$ eigenequation

$$\begin{bmatrix} L_z & L_x - iL_y \\ L_x + iL_y & -L_z \end{bmatrix} \begin{bmatrix} a\, Y_{\ell m} \\ b\, Y_{\ell m+1} \end{bmatrix} = E \begin{bmatrix} a\, Y_{\ell m} \\ b\, Y_{\ell m+1} \end{bmatrix}$$

$$\begin{bmatrix} a m Y_{\ell m} + b\sqrt{(\ell+m+1)(\ell-m)}\, Y_{\ell m} \\ \left[a\sqrt{(\ell-m)(\ell+m+1)} - b(m+1)\right] Y_{\ell m+1} \end{bmatrix} = E \begin{bmatrix} a\, Y_{\ell m} \\ b\, Y_{\ell m+1} \end{bmatrix}$$

$$\Rightarrow \begin{cases} a(m-E) + b\sqrt{(\ell+m+1)(\ell-m)} = 0 \\ a\sqrt{(\ell-m)(\ell+m+1)} - b(m+1+E) = 0 \end{cases}$$

solve it $\Rightarrow E_+ = \ell$

det $= 0$ $\quad E_- = -(\ell+1)$

(2) work out the C-G coefficient

(1) j_+ sector: $\mathcal{Y}_{j_+, j_z = m+1/2} = \begin{pmatrix} a_m Y_{lm} \\ b_m Y_{l\,m+1} \end{pmatrix}$

apply $J_- = l_- + \frac{\sigma_-}{2}$

$$J_- \mathcal{Y}_{j_+ j_z} = \sqrt{(j_+ + j_z)(j_+ - j_z + 1)}\ \mathcal{Y}_{j_+, m-1/2} = \sqrt{(l+m+1)(l-m+1)}\ \mathcal{Y}_{j_+, j_z - 1}$$

$$= \sqrt{(l+m+1)(l-m+1)} \begin{pmatrix} a_{m-1} Y_{lm-1} \\ b_{m-1} Y_{lm} \end{pmatrix}$$

$$\left(l_- + \frac{\sigma_-}{2}\right) \begin{pmatrix} a_m Y_{lm} \\ b_m Y_{lm+1} \end{pmatrix} = \begin{pmatrix} a_m \sqrt{(l+m)(l-m+1)}\ Y_{lm-1} \\ (a_m + b_m \sqrt{(l-m)(l+m+1)})\ Y_{lm} \end{pmatrix}$$

$$\Rightarrow \begin{cases} \sqrt{(l+m+1)(l-m+1)}\ a_{m-1} = a_m \sqrt{(l+m)(l-m+1)} \\ \sqrt{(l+m+1)(l-m+1)}\ b_{m-1} = a_m + b_m \sqrt{(l-m)(l+m+1)} \end{cases}$$

$\Rightarrow \dfrac{a_{m-1}}{a_m} = \dfrac{\sqrt{l+m}}{\sqrt{l+m+1}}$ define $a_m = \sqrt{l+m+1} \cdot C \leftarrow$ a common constant

$\Rightarrow \sqrt{l-m+1}\ b_{m-1} = C + b_m \sqrt{l-m}$. $(m = l, l-1, \cdots, -l-1)$.

The beginning of this relation: for $m = l \Rightarrow \begin{cases} a_l = 1 \\ b_l = 0 \end{cases}$

$\Rightarrow C = \dfrac{1}{\sqrt{2l+1}}$ and then $\begin{cases} a_m = \dfrac{\sqrt{l+m+1}}{\sqrt{2l+1}} \\ b_m = \dfrac{\sqrt{l-m}}{\sqrt{2l+1}} \end{cases}$ according to recursive relation and normalization condition.

$$\Rightarrow \boxed{\mathcal{Y}_{j_+, j_z = m+1/2} = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{l+m+1}\ Y_{lm} \\ \sqrt{l-m}\ Y_{lm+1} \end{pmatrix}}$$

2 j_--sector $\mathcal{Y}_{j_-, j_z = m+1/2} = \begin{pmatrix} a'_m Y_{lm} \\ b'_m Y_{l\,m+1} \end{pmatrix}$ $m = (l-1, l-2, \dots -l)$.

$$J_- \mathcal{Y}_{j_- j_z} = \sqrt{(j_- + j_z)(j_- - j_z + 1)}\; \mathcal{Y}_{j_- j_z - 1} = \sqrt{(l+m)(l-m)} \begin{pmatrix} a'_{m-1} Y_{lm-1} \\ b'_{m-1} Y_{lm} \end{pmatrix}$$

$$\left(L_- + \frac{\sigma_-}{2}\right) \mathcal{Y}_{j_- j_z} = \begin{pmatrix} a'_m \sqrt{(l+m)(l-m+1)}\; Y_{lm-1} \\ a'_m + b'_m \sqrt{(l-m)(l+m+1)}\; Y_{lm} \end{pmatrix}$$

$$\Rightarrow \begin{cases} \sqrt{(l+m)(l-m)}\; a'_{m-1} = a'_m \sqrt{(l+m)(l-m+1)} \\ \sqrt{(l+m)(l-m)}\; b'_{m-1} = a'_m + b'_m \sqrt{(l-m)(l+m+1)} \end{cases}$$

$$\begin{cases} \dfrac{a'_{m-1}}{a_m} = \dfrac{\sqrt{l-m+1}}{\sqrt{l-m}} \qquad \text{define } a_m = \sqrt{l-m}\; C \\ \sqrt{l-m}\; b'_{m-1} = C + \sqrt{l+m+1}\; b'_m . \end{cases}$$

The first term in this series is $\mathcal{Y}_{j_-, l-1/2}$, which should be orthogonal to $\mathcal{Y}_{j_+, l-1/2} = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{2l}\, Y_{l,l-1} \\ Y_{ll} \end{pmatrix}$.

$$\Rightarrow \mathcal{Y}_{j_-, l-1/2} = \frac{1}{\sqrt{2l+1}} \begin{pmatrix} -\, Y_{l\,l-1} \\ \sqrt{2l}\; Y_{ll} \end{pmatrix} e^{i\theta}.$$

According to convention that

$$\langle \mathcal{Y}_{j_+\, l-1/2} | L_z | \mathcal{Y}_{j_-\, l-1/2} \rangle > 0 \Rightarrow e^{i\theta} = 1.$$

i.e. $\begin{cases} a'_{l-1} = -\dfrac{1}{\sqrt{2l+1}} \\ b'_{l-1} = \dfrac{\sqrt{2l}}{\sqrt{2l+1}} \end{cases} \Rightarrow C = -\dfrac{1}{\sqrt{2l+1}}$ and thus

$$a'_m = -\frac{\sqrt{l-m}}{\sqrt{2l+1}},$$

check normalization and recursive relation

$$b'_m = \frac{\sqrt{l+m+1}}{\sqrt{2l+1}}$$

$$\Rightarrow \boxed{\mathcal{Y}_{j_- j_z = m+1/2} = \frac{1}{\sqrt{2\ell+1}} \begin{pmatrix} -\sqrt{\ell-m}\ \mathcal{Y}_{\ell m} \\ \sqrt{\ell+m+1}\ \mathcal{Y}_{\ell\, m+1} \end{pmatrix}}$$

Another method:

a) For the j_+-sector, plug in $E_+ = \ell \Rightarrow$

$$\begin{cases} a(m-\ell) + b\sqrt{(\ell+m+1)(\ell-m)} = 0 \\ a\sqrt{(\ell-m)(\ell+m+1)} - b(\ell+m+1) = 0 \end{cases} \Rightarrow \frac{a}{b} = \frac{\sqrt{\ell+m+1}}{\sqrt{\ell-m}}$$

$$\Rightarrow \quad \mathcal{Y}_{j_+, j_z} = \frac{1}{\sqrt{2\ell+1}} \begin{bmatrix} \sqrt{\ell+m+1}\ \mathcal{Y}_{\ell m} \\ \sqrt{\ell-m}\ \mathcal{Y}_{\ell, m+1} \end{bmatrix} e^{i\theta_{j_+ j_z}}$$

For the j_--sector, plug in $E_- = -(\ell+1) \Rightarrow$

$$a(m+\ell+1) + b\sqrt{(\ell+m+1)(\ell-m)} = 0 \quad \Rightarrow \quad \frac{a}{b} = -\frac{\sqrt{\ell-m}}{\sqrt{\ell+m+1}}$$

$$\Rightarrow \quad \mathcal{Y}_{j_- j_z} = \frac{1}{\sqrt{2\ell+1}} \cdot \begin{bmatrix} -\sqrt{\ell-m}\ \mathcal{Y}_{\ell m} \\ \sqrt{\ell+m+1}\ \mathcal{Y}_{\ell\, m+1} \end{bmatrix} e^{i\theta_{j_- j_z}}$$

The phase convection is not required here. we can fix the phase convention

$$\mathcal{Y}_{j_+ j_z} = \frac{1}{\sqrt{2\ell+1}} \begin{pmatrix} \sqrt{\ell+m+1}\ \mathcal{Y}_{\ell m} \\ \sqrt{\ell-m}\ \mathcal{Y}_{\ell\, m+1} \end{pmatrix} \quad \text{and}$$

$$\mathcal{Y}_{j_- j_z} = \frac{1}{\sqrt{2\ell+1}} \begin{pmatrix} -\sqrt{\ell-m}\ \mathcal{Y}_{\ell m} \\ \sqrt{\ell+m+1}\ \mathcal{Y}_{\ell\, m+1} \end{pmatrix}.$$