04 - Addition of Angular Momentum

- Aim of Section:
  - Brief review of material on addition of angular momentum presented in previous course (PHY 373).

Introduction

- An electron possesses orbital angular momentum, $\mathbf{L}$, due to its motion in space.
- An electron also possesses an intrinsic spin angular momentum, $\mathbf{S}$.
- Hence, electron possesses total angular momentum, $\mathbf{J} = \mathbf{L} + \mathbf{S}$.
- What is the relationship between operators used to represent total angular momentum and those used to represent orbital and spin angular momentum in quantum mechanics?

Commutation Relations - I

- Three operators used to represent Cartesian components of $\mathbf{L}$ obey commutation relations that can be written in convenient vector form:

$$\mathbf{L} \times \mathbf{L} = \mathrm{i}\,\hbar\,\mathbf{L}.$$

- Likewise, three operators used to represent Cartesian components of $\mathbf{S}$ obey commutation relations:

$$\mathbf{S} \times \mathbf{S} = \mathrm{i}\,\hbar\,\mathbf{S}.$$

- Orbital angular momentum operators associated with motion through space. Spin angular momentum operators associated with internal 'motion'. Two types of motion completely unrelated. Suggests that two sets of operators commute with one another: i.e.,

$$[L_i, S_j] = 0,$$

where $i, j = 1, 2, 3$ corresponds to x, y, z.

Commutation Relations - II

- Consider
$$\mathbf{J} = \mathbf{L} + \mathbf{S}.$$
- Follows that
$$\begin{aligned}\mathbf{J}\times\mathbf{J} &= (\mathbf{L}+\mathbf{S})\times(\mathbf{L}+\mathbf{S})\\ &= \mathbf{L}\times\mathbf{L}+\mathbf{S}\times\mathbf{S}+\mathbf{L}\times\mathbf{S}+\mathbf{S}\times\mathbf{L} = \mathbf{L}\times\mathbf{L}+\mathbf{S}\times\mathbf{S}\\ &= \mathrm{i}\,\hbar\,(\mathbf{L}+\mathbf{S}) = \mathrm{i}\,\hbar\,\mathbf{J}.\end{aligned}$$
- In other words,
$$\mathbf{J}\times\mathbf{J} = \mathrm{i}\,\hbar\,\mathbf{J}.$$
- Evident that three fundamental total angular momentum operators, J_x, J_y, and J_z, obey analogous commutation relations to corresponding orbital and spin angular momentum operators.

Eigenstates of Total Angular Momentum

- Follows, by analogy with orbital and spin angular momentum, that only possible to simultaneously measure magnitude-squared of total angular momentum,

$$J^2 = J_x^2 + J_y^2 + J_z^2,$$

  and one Cartesian component of $\mathbf{J}$. Choose to measure J_z.
- Simultaneous eigenstate of J^2 and J_z written

$$J^2\,\psi_{j,m_j} = j\,(j+1)\,\hbar^2\,\psi_{j,m_j},$$

$$J_z\,\psi_{j,m_j} = m_j\,\hbar\,\psi_{j,m_j},$$

  where quantum number j can take integer or half-integer values, and quantum number m_j takes values in range

$$-j, -j+1, \cdots, j-1, j.$$

Compatible Measurements - I

- Now,

$$J^2 = (\mathbf{L} + \mathbf{S}) \cdot (\mathbf{L} + \mathbf{S}) = L^2 + S^2 + 2\,\mathbf{L} \cdot \mathbf{S},$$

which can also be written

$$J^2 = L^2 + S^2 + 2\,L_z\,S_z + L_+\,S_- + L_-\,S_+.$$

- Know that L^2 commutes with itself, and all Cartesian components of $\mathbf{L}$, and with all spin operators. Follows that

$$[J^2, L^2] = 0.$$

- Similar arguments yields

$$[J^2, S^2] = 0.$$

Compatible Measurements - II

- L_z commutes with itself, with L^2, and with all spin operators, but not with L_+ and L_-. Hence, we conclude that

$$[J^2, L_z] \neq 0.$$

- A similar argument yields

$$[J^2, S_z] \neq 0.$$

- Finally,

$$J_z = L_z + S_z,$$

where $[J_z, L_z] = [J_z, S_z] = 0$.

Compatible Measurements - III

- Evident that are two alternative sets of physical variables associated with angular momentum that can be simultaneously measured:
  1. L^2, S^2, L_z, S_z, J_z.
  2. L^2, S^2, J^2, J_z.
- Let $\psi^{(1)}_{l,s;m,m_s}$ be simultaneous eigenstate of L^2, S^2, L_z, S_z, J_z corresponding to eigenvalues

$$L^2\,\psi^{(1)}_{l,s;m,m_s} = l\,(l+1)\,\hbar^2\,\psi^{(1)}_{l,s;m,m_s},$$

$$S^2\,\psi^{(1)}_{l,s;m,m_s} = s\,(s+1)\,\hbar^2\,\psi^{(1)}_{l,s;m,m_s},$$

$$L_z\,\psi^{(1)}_{l,s;m,m_s} = m\,\hbar\,\psi^{(1)}_{l,s;m,m_s},$$

$$S_z\,\psi^{(1)}_{l,s;m,m_s} = m_s\,\hbar\,\psi^{(1)}_{l,s;m,m_s}.$$

Compatible Measurements - IV

- Easily seen that

$$J_z\,\psi^{(1)}_{l,s;m,m_s} = (L_z + S_z)\,\psi^{(1)}_{l,s;m,m_s} = (m + m_s)\,\hbar\,\psi^{(1)}_{l,s;m,m_s}$$
$$= m_j\,\hbar\,\psi^{(1)}_{l,s;m,m_s}.$$

- Hence,

$$m_j = m + m_s.$$

Compatible Measurements - V

- Let $\psi^{(2)}_{l,s;j,m_j}$ be simultaneous eigenstate of L^2, S^2, J^2, and J_z corresponding to eigenvalues

$$L^2\,\psi^{(2)}_{l,s;j,m_j} = l\,(l+1)\,\hbar^2\,\psi^{(2)}_{l,s;j,m_j},$$

$$S^2\,\psi^{(2)}_{l,s;j,m_j} = s\,(s+1)\,\hbar^2\,\psi^{(2)}_{l,s;j,m_j},$$

$$J^2\,\psi^{(2)}_{l,s;j,m_j} = j\,(j+1)\,\hbar^2\,\psi^{(2)}_{l,s;j,m_j},$$

$$J_z\,\psi^{(2)}_{l,s;j,m_j} = m_j\,\hbar\,\psi^{(2)}_{l,s;j,m_j}.$$

Total Angular Momentum of Electron - I

- For electron, simultaneous eigenstate of L^2 and L_z associated with angular wavefunction $Y_l^m(\theta, \phi)$. Here, l is non-negative integer, and m is integer lying in range $-l \leq m \leq l$.
- Simultaneous eigenstate of S^2 and S_z characterized by quantum numbers $s = 1/2$ and $m_s = \pm 1/2$, and associated with spinors $\chi_{1/2,\pm 1/2} \equiv \chi_\pm$.
- Can express simultaneous eigenstate of L^2, S^2, L_z, and S_z in product form
$$\psi^{(1)}_{l,1/2;m,\pm 1/2} = Y_l^m \chi_\pm.$$
- Orbital angular momentum operators act on spherical harmonic functions, Y_l^m, whereas spin angular momentum operators act on spinors, $\chi_\pm$.

Total Angular Momentum of Electron - II

- Because eigenstates $\psi^{(1)}_{l,1/2;m,\pm 1/2}$ are (presumably) orthonormal, and form a complete set, we can express eigenstates $\psi^{(2)}_{l,1/2;j,m_j}$ as linear combinations of them: e.g.,

$$\psi^{(2)}_{l,1/2;j,m+1/2} = \alpha\,\psi^{(1)}_{l,1/2;m,1/2} + \beta\,\psi^{(1)}_{l,1/2;m+1,-1/2},$$

  where α and β are, as yet, unknown coefficients.
- Number of $\psi^{(1)}$ states that can appear on right-hand side of the previous expression is limited to two by constraint that $m_j = m + m_s$, and fact that m_s can only take values $\pm 1/2$.
- Assuming that $\psi^{(2)}$ eigenstates are properly normalized, we have

$$\alpha^2 + \beta^2 = 1. \tag{1}$$

Total Angular Momentum of Electron - III

- Now,

$$J^2\,\psi^{(2)}_{l,1/2;j,m+1/2} = j\,(j+1)\,\hbar^2\,\psi^{(2)}_{l,1/2;j,m+1/2}, \tag{2}$$

  where

$$J^2 = L^2 + S^2 + 2\,L_z\,S_z + L_+\,S_- + L_-\,S_+. \tag{3}$$

- Moreover,

$$\psi^{(2)}_{l,1/2;j,m+1/2} = \alpha\,Y_l^m\,\chi_+ + \beta\,Y_l^{m+1}\,\chi_-. \tag{4}$$

Total Angular Momentum of Electron - IV

- Now,

$$L_+\, Y_l^m = [l\,(l+1) - m\,(m+1)]^{1/2}\,\hbar\, Y_l^{m+1}, \tag{5}$$

$$L_-\, Y_l^m = [l\,(l+1) - m\,(m-1)]^{1/2}\,\hbar\, Y_l^{m-1}, \tag{6}$$

$$S_+\,\chi_{s,m_s} = [s\,(s+1) - m_s\,(m_s+1)]^{1/2}\,\hbar\,\chi_{s,m_s+1}, \tag{7}$$

$$S_-\,\chi_{s,m_s} = [s\,(s+1) - m_s\,(m_s-1)]^{1/2}\,\hbar\,\chi_{s,m_s-1}. \tag{8}$$

- For case of spin one-half spinors,

$$S_+\,\chi_+ = S_-\,\chi_- = 0, \tag{9}$$

$$S_\pm\,\chi_\mp = \hbar\,\chi_\pm, \tag{10}$$

$$S^2\,\chi_\pm = \frac{3}{4}\,\hbar^2\,\chi_\pm. \tag{11}$$

Total Angular Momentum of Electron - V

- (3), (5), (6), and (9)–(11) yield

$$J^2\, Y_l^m\, \chi_+ = [l\,(l+1) + 3/4 + m]\, \hbar^2\, Y_l^m\, \chi_+ \\ +[l\,(l+1) - m\,(m+1)]^{1/2}\, \hbar^2\, Y_l^{m+1}\, \chi_-, \quad (12)$$

and

$$J^2\, Y_l^{m+1}\, \chi_- = [l\,(l+1) + 3/4 - m - 1]\, \hbar^2\, Y_l^{m+1}\, \chi_- \\ +[l\,(l+1) - m\,(m+1)]^{1/2}\, \hbar^2\, Y_l^{m}\, \chi_+. \quad (13)$$

Total Angular Momentum of Electron - VI

- (2), (4), (12), and (13) yield

$$(x - m)\,\alpha - [l\,(l+1) - m\,(m+1)]^{1/2}\,\beta = 0, \tag{14}$$

$$-[l\,(l+1) - m\,(m+1)]^{1/2}\,\alpha + (x + m + 1)\,\beta = 0, \tag{15}$$

where

$$x = j\,(j+1) - l\,(l+1) - 3/4.$$

- (14) and (15) can be solved to give

$$x\,(x+1) = l\,(l+1),$$

and

$$\frac{\alpha}{\beta} = \frac{[(l-m)\,(l+m+1)]^{1/2}}{x-m}. \tag{16}$$

Total Angular Momentum of Electron - VII

- Follows that $x = l$ or $x = -l - 1$, which corresponds to $j = l + 1/2$ or $j = l - 1/2$, respectively.
- Once x is specified, (1) and (16) can be solved to give α and β.
- Obtain

$$\psi^{(2)}_{l+1/2,m+1/2} = \left(\frac{l+m+1}{2\,l+1}\right)^{1/2} \psi^{(1)}_{m,1/2} + \left(\frac{l-m}{2\,l+1}\right)^{1/2} \psi^{(1)}_{m+1,-1/2}, \tag{17}$$

$$\psi^{(2)}_{l-1/2,m+1/2} = \left(\frac{l-m}{2\,l+1}\right)^{1/2} \psi^{(1)}_{m,1/2} - \left(\frac{l+m+1}{2\,l+1}\right)^{1/2} \psi^{(1)}_{m+1,-1/2}. \tag{18}$$

- Here, have neglected common superscripts $l, 1/2$ for sake of clarity: e.g., $\psi^{(2)}_{l+1/2,m+1/2} \equiv \psi^{(2)}_{l,1/2;l+1/2,m+1/2}$.

Total Angular Momentum of Electron - VIII

- Previous two equations can be inverted to give

$$\psi^{(1)}_{m,1/2} = \left(\frac{l+m+1}{2\,l+1}\right)^{1/2} \psi^{(2)}_{l+1/2,m+1/2} + \left(\frac{l-m}{2\,l+1}\right)^{1/2} \psi^{(2)}_{l-1/2,m+1/2}, \tag{19}$$

$$\psi^{(1)}_{m+1,-1/2} = \left(\frac{l-m}{2\,l+1}\right)^{1/2} \psi^{(2)}_{l+1/2,m+1/2} - \left(\frac{l+m+1}{2\,l+1}\right)^{1/2} \psi^{(2)}_{l-1/2,m+1/2}. \tag{20}$$

$l = 1$ States - I

- As an example, consider $l = 1$ states.
- Eigenstates of L^2, S^2, L_z, and S_z denoted $\psi^{(1)}_{m,m_s}$. Because m can take values $-1, 0, 1$, whereas m_s can take values $\pm 1/2$, there are clearly six such states. That is, $\psi^{(1)}_{1,\pm 1/2}$, $\psi^{(1)}_{0,\pm 1/2}$, and $\psi^{(1)}_{-1,\pm 1/2}$.
- Eigenstates of L^2, S^2, J^2, and J_z denoted $\psi^{(2)}_{j,m_j}$. Because j can take values $l + 1/2 = 3/2$ and $l - 1/2 = 1/2$, there are also six such states. That is, $\psi^{(2)}_{3/2,\pm 3/2}$, $\psi^{(2)}_{3/2,\pm 1/2}$, and $\psi^{(2)}_{1/2,\pm 1/2}$.

$l = 1$ States - II

- According to (17)–(20) various different states interrelated as follows:

$$\psi^{(2)}_{3/2,\pm 3/2} = \psi^{(1)}_{\pm 1,\pm 1/2}, \tag{21}$$

$$\psi^{(2)}_{3/2,1/2} = \sqrt{\frac{2}{3}}\,\psi^{(1)}_{0,1/2} + \sqrt{\frac{1}{3}}\,\psi^{(1)}_{1,-1/2}, \tag{22}$$

$$\psi^{(2)}_{1/2,1/2} = \sqrt{\frac{1}{3}}\,\psi^{(1)}_{0,1/2} - \sqrt{\frac{2}{3}}\,\psi^{(1)}_{1,-1/2}, \tag{23}$$

$$\psi^{(2)}_{1/2,-1/2} = \sqrt{\frac{2}{3}}\,\psi^{(1)}_{-1,1/2} - \sqrt{\frac{1}{3}}\,\psi^{(1)}_{0,-1/2}, \tag{24}$$

$$\psi^{(2)}_{3/2,-1/2} = \sqrt{\frac{1}{3}}\,\psi^{(1)}_{-1,1/2} + \sqrt{\frac{2}{3}}\,\psi^{(1)}_{0,-1/2}. \tag{25}$$

$I = 1$ States - III

- Furthermore,

$$\psi^{(1)}_{\pm 1,\pm 1/2} = \psi^{(2)}_{3/2,\pm 3/2}, \tag{26}$$

$$\psi^{(1)}_{1,-1/2} = \sqrt{\frac{1}{3}}\,\psi^{(2)}_{3/2,1/2} - \sqrt{\frac{2}{3}}\,\psi^{(2)}_{1/2,1/2}, \tag{27}$$

$$\psi^{(1)}_{0,1/2} = \sqrt{\frac{2}{3}}\,\psi^{(2)}_{3/2,1/2} + \sqrt{\frac{1}{3}}\,\psi^{(2)}_{1/2,1/2}, \tag{28}$$

$$\psi^{(1)}_{0,-1/2} = \sqrt{\frac{2}{3}}\,\psi^{(2)}_{3/2,-1/2} - \sqrt{\frac{1}{3}}\,\psi^{(2)}_{1/2,-1/2}, \tag{29}$$

$$\psi^{(1)}_{-1,1/2} = \sqrt{\frac{1}{3}}\,\psi^{(2)}_{3/2,-1/2} + \sqrt{\frac{2}{3}}\,\psi^{(2)}_{1/2,-1/2}. \tag{30}$$

$l = 1$ States - IV

- If we know that electron in $l = 1$ state characterized by $m = 0$ and $m_s = 1/2$ [i.e., state represented by $\psi^{(1)}_{0,1/2}$] then, according to (28), measurement of total angular momentum will yield $j = 3/2$, $m_j = 1/2$ with probability $2/3$, and $j = 1/2$, $m_j = 1/2$ with probability $1/3$.
- Suppose we make such a measurement, and obtain result $j = 3/2$, $m_j = 1/2$. As a result of measurement, electron is thrown into corresponding eigenstate, $\psi^{(2)}_{3/2,1/2}$. Follows from (22) that subsequent measurement of L_z and S_z will yield $m = 0$, $m_s = 1/2$ with probability $2/3$, and $m = 1$, $m_s = -1/2$ with probability $1/3$.

Two-Electron States - I

- Consider system consisting of two electrons. Suppose that system does not possess any orbital angular momentum.
- Let $\mathbf{S}_1$ and $\mathbf{S}_2$ be spin angular momentum operators of the first and second electrons, respectively, and let

$$\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$$

  be total spin angular momentum operator.
- By analogy with previous analysis, possible to simultaneously measure either S_1^2, S_2^2, S^2, and S_z, or S_1^2, S_2^2, S_{1z}, S_{2z}, and S_z.
- Let quantum numbers associated with measurements of S_1^2, S_{1z}, S_2^2, S_{2z}, S^2, and S_z be s_1, m_{s_1}, s_2, m_{s_2}, s, and m_s, respectively.

Two-Electron States - II

- Because both electrons are spin one-half particles, $s_1 = s_2 = 1/2$, and s_{1z}, $s_{2z} = \pm 1/2$.
- Furthermore, by analogy with previous analysis,

$$m_s = m_{s_1} + m_{s_2}.$$

- Saw that when spin l is added to spin $1/2$ then possible values of total angular momentum quantum number are $j = l \pm 1/2$.
- By analogy, when spin $1/2$ is added to spin $1/2$ then possible values of total spin quantum number are $s = 1/2 \pm 1/2$.
- In other words, two-electron state (with zero orbital angular momentum) either possesses overall spin $s = 1$, or overall spin $s = 0$.

Two-Electron States - III

- To be more exact, there are three possible $s = 1$ states (corresponding to $m_s = -1, 0, 1$), and one possible $s = 0$ state (corresponding to $m_s = 0$).
- Three $s = 1$ states are known as triplet states, whereas $s = 0$ state known as singlet state.
- Triplet states take form:

$$\chi^{(2)}_{1,-1} = \chi^{(1)}_{-1/2,-1/2},$$

$$\chi^{(2)}_{1,0} = \frac{1}{\sqrt{2}}\left(\chi^{(1)}_{-1/2,1/2} + \chi^{(1)}_{1/2,-1/2}\right),$$

$$\chi^{(2)}_{1,1} = \chi^{(1)}_{1/2,1/2}.$$

- Singlet state written

$$\chi^{(2)}_{0,0} = \frac{1}{\sqrt{2}}\left(\chi^{(1)}_{-1/2,1/2} - \chi^{(1)}_{1/2,-1/2}\right).$$