Total Angular momentum

Dipanjan Mazumdar

Sept 2019

1 Motivation

So far, somewhat deliberately, in our prior examples we have worked exclusively with the spin angular momentum and ignored the orbital component. This is acceptable for $L = 0$ systems such as filled shell atoms, but properties of partially filled atoms will depend both on the orbital and the spin part of the angular momentum. Also, when we include relativistic corrections to atomic Hamiltonian, both spin and orbital angular momentum enter directly through terms like $\vec{L}.\vec{S}$ called the spin-orbit coupling. So instead of focusing only on the spin or orbital angular momentum, we have to develop an understanding as to how they couple together. One of the ways is through the total angular momentum defined as

$$\vec{J} = \vec{L} + \vec{S} \tag{1}$$

We will see that this will be very useful in many cases such as the real hydrogen atom where the eigenstates after including the fine structure effects such as spin-orbit interaction are eigenstates of the total angular momentum operator.

2 Vector model of angular momentum

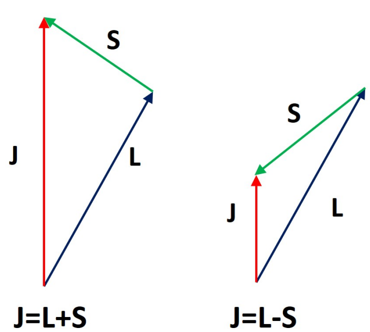

Figure 1: Maximum and minimum values of angular momentum using the vector model

Let us first develop an intuitive understanding of the total angular momentum through the vector model which is a semi-classical approach to "add" angular momenta using vector algebra. We shall first ask, knowing $\vec{L}$ and $\vec{S}$, what are the maxmimum and minimum values of $\hat{J}$. This is simple to answer using the vector model since vectors can be added or subtracted. Therefore, the extreme values are $\vec{L}+\vec{S}$ and $\vec{L}-\vec{S}$ as seen in figure 1.[1] Therefore, the total angular momentum will take up values between $l+s$ and $|l-s|$.

$$|l - s| \leq j \leq l + s \tag{2}$$

where j represents the magnitude of $\vec{J}$ which will translate to the eigenvalue in quantum mechanical language. With the vector model, we can construct other quantities that will be useful later on such as $\vec{J}\cdot\vec{J}$,

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

$$\implies \vec{L}.\vec{S} = \frac{\vec{J}^2 - \vec{L}^2 - \vec{S}^2}{2} \tag{3}$$

The quantity $\vec{L}\cdot\vec{S}$ is new and will appear in later sections. Also, it is worth mentioning that operators $\hat{L}$, $\hat{S}$ commute with each other since they belong to different vector spaces.

[1] Note that the $-\vec{S}$ vector corresponds to the $S_z = -1/2$ state.

2.1 Magnetic moment and energy associated with total angular momentum

In the case of non-zero L and S the total magnetic moment vector for associated with spin-1/2 systems such as electrons will be

$$\vec{\mu} = \vec{\mu}_L + \vec{\mu}_S = \gamma(\vec{L} + 2\vec{S}) = \gamma(\vec{J} + \vec{S}) \tag{4}$$

Where $\vec{L}$ and $\vec{S}$ are the orbital and spin angular momentum for electronic system under consideration. So interestingly the magnetic moment is not along the L, or S or J direction, but along the $J + S$ direction (or anti-parallel to $J + S$ to be precise since $\gamma = -|e|/2m_e$).

We want to convert this expression into the form $g_j\gamma\vec{J}$ if possible where g_j will be the effective g-factor. Or to be more precise, we assert that

$$\langle\hat{J} + \hat{S}\rangle = g_j\langle\hat{J}\rangle \tag{5}$$

This can be done by projecting onto $\vec{J}$ using the vector model, *i.e.*,[2]

$$(\vec{J} + \vec{S}) \cdot \vec{J} = g_j\vec{J} \cdot \vec{J} \implies g_j = \frac{(\vec{J} + \vec{S}) \cdot \vec{J}}{J^2}$$

We can manipulate the LHS by noting

$$(\vec{J} + \vec{S}) \cdot \vec{J} = (\vec{L} + 2\vec{S}) \cdot (\vec{L} + \vec{S}) = L^2 + 2S^2 + 3L \cdot \vec{S} = \frac{3}{2}J^2 + \frac{1}{2}(S^2 - L^2)$$

In quantum mechanics, $\langle\hat{J}^2\rangle = j(j + 1)\hbar^2$ similar to $\hat{L}^2$ and $\hat{S}^2$ and therefore

$$\boxed{g_j = \frac{3}{2} + \frac{s(s + 1) - l(l + 1)}{2j(j + 1)}} \tag{6}$$

The above g factor is called the Lande-g factor. It is easy to check for $l = 0$ and $s = 1/2$, g_j reduces to 2, which is the electronic g-factor. Therefore, the energy of the system under consideration when a magnetic field is applied in the z-direction $= B_o\hat{k}$ is

$$E = -\vec{\mu} \cdot \vec{B} = -g_j\gamma\vec{J} \cdot \vec{B_0} = -g_j\gamma J_z B_0 = g_j\mu_B m_j B_0 \tag{7}$$

where m_j is the quantum number associated with the $\hat{J}_z$ operator.

The magnitude of the magnetic moment is given by

$$|\vec{\mu}| = g_j\gamma|\vec{J}| = g_j\gamma\hbar\sqrt{J(J + 1)} = g_j\mu_B\sqrt{J(J + 1)} \tag{8}$$

2.2 Hund's third rule

Apart from the two rules specifying how to calculate the spin and orbital angular momentum of atom, there is a third Hund's rule that specifies the total angular momentum of an atom. Even though quantum mechanically j can take any value between $l + s$ to $|l - s|$ (implying a number of degenerate states), atoms usually pick either the highest or lowest value depending on the electronic configuration due the presence of degeneracy-breaking spin-orbit interaction. Hund's third rule takes this into account and can be summerized as follows:

- $J = |L - S|$ for less or equal to half-filled shell.
- $J = L + S$ for greater than half filled shell.

where we are using the notation that $L = \sum m$, and $S = \sum s_z$ following Hund's first and second rule.

Example: Consider Carbon atom with a $1s^2 2s^2 2p^2$ configuration and $L = 1$, $S = 1$. Since the p-shell is less than half-filled, $J = 0$. But oxygen with a $2p^4$ configuration also has $L = 1$, $S = 1$, but $J = 2$ since it is more than half-filled.

[2] This is justified when J is a good quantum number (a constant of motion) instead of $\vec{L}$ or $\vec{S}$. $\vec{L}$ and $\vec{S}$ precess around $\vec{J}$. Therefore, only the projection of $\vec{S}$ and $\vec{L}$ on $\vec{J}$, the z-component in Fig 1, is non-zero. The x and y component of $\vec{L}$ and $\vec{S}$ average to zero due to precession. In this scenario, we will consider the precession of $\vec{J}$ around the external magnetic field.