

Quick Review of Angular Momentum in Quantum Mechanics

For a “central” potential energy (i.e., one that depends only on the radial variable, r , in spherical coordinates), the solution to the Schrödinger equation can always be written as a product $\psi = R(r) Y(\theta, \phi)$. The function Y is the angular momentum eigenfunction requiring two (quantum) numbers per eigenvalue (corresponding to the two degrees of angular freedom at a given r). The first one is defined by

$$L^2 Y = \beta(\beta + 1)\hbar^2 Y \quad (1)$$

where L is the angular momentum operator, and $\beta = 0, 1, 2, \dots$ and the 2nd quantum number is defined by

$$L_z \Phi = \beta_z \hbar \Phi \quad (2)$$

where $\Delta\beta_z = 1$, and $\beta_z = 0, +/-1, +/-2, \dots$ up to a maximum magnitude of β . In other words, β defines the total angular momentum, and β_z defines its projection on the z axis. Clearly the number of β_z values for each value of β is

$$N_\beta = 2\beta + 1 \quad (3)$$

Hence, it is convenient to think of the orbital angular momentum as the vector lying on the cone shown in Fig.1. It has a fixed length of $\sqrt{\beta(\beta + 1)} \cdot \hbar$, and a fixed projection on the z axis of $\beta_z \hbar$, but a random orientation on the cone, consistent with the statistical nature of quantum mechanics. All of the possible degenerate eigenstates of \mathbf{L} are then represented by $2\beta + 1$ different cones, each having a projection on the z axis given by one of the allowed values of β_z

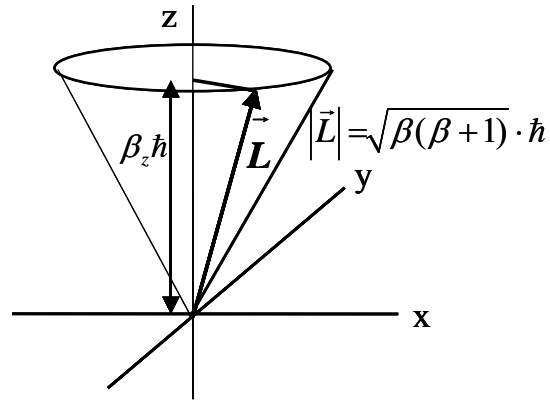


Fig. 1. Three-dimensional model of angular momentum vector of electron consistent with rules of quantum mechanics.

It is a fundamental fact of quantum mechanics that the quantization expressions (1) and (2) remain valid in form for any spin angular momentum \mathbf{S} if we replace \mathbf{L} by \mathbf{S} , L_z by S_z , and β by s , so that the operator S^2 has the eigenvalue $s(s+1)\hbar^2$ and the operator S_z has the eigenvalue $s_z\hbar$. The possible increments of s and s_z are defined by $\Delta s = 1$, $\Delta s_z = 1$, and the maximum magnitude of s_z is s , so that there are $N_s = 2s+1$ values values of s_z for each s . The key difference between spin and angular momentum is that s can be either integral or half-integral. As we saw in 215A, this apparently trivial distinction is the means for classifying all know particles in nature, not just electrons. Integral spin means the particles (called bosons) can occupy the same space-spin state and must have symmetric (with respect to particle label exchange) total wave functions, and half-integral spin means that the particles (called fermions) can not occupy the same space-spin state and must have an antisymmetric total wave function.

It is remarkable that the quantization expressions (1) to (3) remain valid in form for a total angular momentum \mathbf{J} if we replace \mathbf{L} by \mathbf{J} and L_z by J_z so that J^2 has eigenvalue $\gamma(\gamma+1)\hbar^2$ and J_z has eigenvalue $\gamma_z\hbar$. Again, the increments are given by $\Delta\gamma = 1$, $\Delta\gamma_z = 1$, so that the maximum magnitude of γ_z is γ and there are $2\gamma+1$ values values of γ_z for each γ . And just like spin angular momentum, neither γ or γ_z are necessarily integral. This makes total angular momentum difficult, in general, but relatively simple if the particles in question are electrons and there is no interaction between their orbital and

spin operators.¹ In that case, we utilize the fact that the spin for each individual electron is strictly *binary*, spin up or down along an arbitrarily chosen axis, *and has no component on any other axis*. We are then free (and wise) to choose this axis to coincide with the z axis of the angular momentum coordinate system for that electron. In this case there are just two possible total angular momentum magnitudes for that electron: (1) $|\mathbf{J}| = |\mathbf{L} + \mathbf{S}|$ and (2) $|\mathbf{J}| = |\mathbf{L} - \mathbf{S}|$. In other words, the two possible eigenvalues have $\gamma = \beta + \frac{1}{2}$, and $\gamma = \beta - \frac{1}{2}$.

Fortunately, the same reasoning applies to a system of electrons such as all the electrons occupying a shell in an atom.² It is simply a binary addition process! Each electron contributes two possible total momentum eigenvalues corresponding to the two possible magnitudes $\gamma_1 = \beta_1 + s_1 = \beta_1 + 1/2$ and $\gamma_1 = \beta_1 - s_1 = \beta_1 - 1/2$. When combined with the two possible total angular momentum values for the second electron, we get (by combinatorial reasoning) 2^n unique total momentum total angular momentum quantum numbers. Stated more generally, when a system (e.g., one electron) having total momentum quantum number γ_1 is combined with another non-interacting system having total momentum quantum number γ_2 , the resulting total angular momentum quantum number has a maximum value of $\gamma_1 + \gamma_2$ and a minimum value of $|\gamma_1 - \gamma_2|$. This generalization is a very important result of quantum mechanics called the angular momentum addition theorem. It works for arbitrary particles and integral or half-integral values of γ . In this book we will only use it for electrons

Energy in Angular Momentum

Given the quantum picture of total angular momentum \mathbf{J} , the magnetic-dipole potential energy is

$$U_{PE} = -\mathbf{m} \cdot \mathbf{B}_{local} = g \mu_B \mathbf{J} \cdot \mathbf{B} = \gamma_j g \mu_B \mathbf{J} \cdot \mathbf{B}_{local} \quad (4)$$

¹ An approximation known in atomic physics as the L-S approximation.

² For an excellent introduction to shell theory and other aspects of atomic physics, see R. Eisberg and R. Resnick, "Quantum Physics" (Wiley, New York, 1974).

In other words, for \mathbf{J} pointed anywhere in the upper hemisphere of Fig. 1 (the polar axis now being defined parallel to \mathbf{B}_{local}), the potential energy is positive. And for \mathbf{J} pointed anywhere in the lower hemisphere, the potential energy is negative. According to quantum mechanics, γ_j must have $2J + 1$ equally spaced values corresponding to $2J + 1$ equally spaced energy levels. For example: if $J = 3/2$, then

$$\gamma_j = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \quad (5)$$

representing four equally spaced quantum levels.

Since spins are hidden variables within atoms, and atoms are generally distinguishable, we can apply the *Boltzmann* statistics to determine the microscopic magnetic moment and related macroscopic quantities.³ The probability of a magnetic moment being aligned along \mathbf{B} is

$$\langle \mathbf{m} \rangle = \frac{\sum_j^{2J+1} \mathbf{m}_j \exp[-U_j/k_B T]}{\sum_j^{2J+1} \exp[-U_j/k_B T]} = \frac{\sum_j^{2J+1} g \mu_B m_j \mathbf{z} \cdot \exp[\gamma_j \mu_B B/k_B T]}{\sum_j^{2J+1} \exp[\gamma_j \mu_B B/k_B T]} \quad (6)$$

This is a ratio of partial sums that can be shown to be:

$$|\langle \mathbf{m} \rangle| = gJ \mu_B B_J(x). \quad (7)$$

where B_J is called the *Brillouin function*, and x is given by

$$B_J(x) \equiv \frac{2J+1}{2J} \coth\left[\frac{(2J+1)x}{2J}\right] - \frac{1}{J} \coth\left(\frac{x}{2J}\right) \quad (8)$$

where

$$x = gJ \mu_B B/k_B T \quad (9)$$

³ A fact that seems peculiar at first until one recalls that there is nothing inherently classical or quantum mechanical about the Boltzmann statistics.

Because the Boltzmann statistics always favors the lower energy states over the higher ones, the mean magnetic moment will contain more weighting for $\langle m \rangle$ along \mathbf{B} than for the opposite case. So we expect the mean magnetic dipole moment to be *paramagnetic*.

The magnetization, polarizability, and susceptibility are then given by

$$\langle \mathbf{M} \rangle = n \langle \mathbf{m} \rangle = ngJ\mu_B B_J(x), \quad (10)$$

$$\alpha_m \equiv \frac{|\mathbf{m}|}{|\mathbf{B}_{local}|} = \frac{gJ\mu_B B_J(x)}{\mathbf{B}_{local}}, \quad (11)$$

and

$$\chi_m \approx n\alpha_m\mu_0 \quad (12)$$

where the last step follows by assuming $n\alpha_m b\mu_0 \ll 1$ – an assumption that will become invalid in ferromagnetic solids. In the high-temperature limit, one can approximate from (7), (8), (11), and (12),

$$\chi_m \approx \frac{nJ(J+1)g^2\mu_B^2\mu_0}{3k_B T} \equiv \frac{np^2\mu_B^2\mu_0}{3k_B T} \equiv \frac{C}{T} \quad (13)$$

where $p \equiv g\sqrt{J(J+1)}$ and C is the Curie constant and defined by

$$C = \frac{np^2\mu_B^2\mu_0}{3k_B}. \quad (14)$$

Eqn (13) is called the Curie law, and is generally regarded as the hallmark of paramagnetism.