4. A Physical Model for an Electron with Angular Momentum. An Electron in a Bohr Orbit. The Quantum Magnet Resulting from Orbital Motion.

We now have developed a vector model that allows the ready visualization of spin angular momentum in a three dimensional vectorial "spin space". We now need to come to grips with the problem of associating the spin angular momentum states with magnetic energies in the same way that we associate electronic states with electronic energies. Thus we need to associate some magnetic features with our vector model of electron spin. We have seen how to qualitatively rank the relative energy of **electronic orbitals and electronic states through electronic interactions**, so we shall develop an analogous model which will allow us to rank the relative energy of the **electronic spins and spin states through magnetic interactions**. We also need to develop a model that will allow us to visualize the interactions and couplings of electron spins which will lead to transitions between the magnetic energy levels corresponding to magnetic resonance spectroscopy and intersystem crossing.

The connection of spin structure and magnetic energy level diagrams will be made through the development of a relationship between spin angular momentum and the magnetic moment due to electron spin. The magnetic energy of the spin will depend on the coupling of the spin's magnetic moment with other magnetic moments. These couplings will both influence the energy of the electron spin magnetic energy levels and the dynamics of the electron spin transitons between magnetic energy levels.

All of the important **interactions** which bring about couplings may be classified in terms of two basic types, a so called **dipolar** interaction and a **contact** or **overlap** interaction (in analogy with the two basic types of electrostatic interactions). In addition, there are only a small number of couplings or "mechanisms" by which the two basic interactions can connect an electron spin to a magnetic moment due to some internal or external source.

We shall employ the intuitively appealing physical model of an electron executing circular motion about an axis in a Bohr orbit (Figure 4, left) to demonstrate the relationship between an electron's **orbital angular momentum** and the **magnetic moment** associated with **orbital motion**. We shall extend this model to a physical model of a spherical electron rotating about an axis (Figure 4, right) to deduce the relationship between an electron's **spin angular momentum** and the **magnetic moment** associated with **spin motion** (with appropriate quantum mechanical modifications).

Magnetic Moments Resulting from Orbital Motion of an Electron

The properties of classical magnets are all completely characterized by the magnetic moment of the magnet. Since the magnet moment is a vector quantity, all of the vectorial concepts that were discussed above for angular momentum will apply to magnetic moments!

From the simple model of an electron in a circular Bohr orbit, we shall proceed as follows:

(1) deduce from classical considerations the origin of the magnetic moment of an electron resulting from the electron's circular motion orbit about a nucleus, i.e., the magnetic moment, μ_L, that results from the electron's **orbital** angular momentum, **L**;

(2) extend this model to infer the origin of the magnetic moment of spherical electron that is spinning on a fixed axis of rotation, i.e., the magnetic moment, μ_S, that results from the electron's **spin** angular momentum, **S**;

(3) use the vector model for the spin structure of an electron and the vector model of the magnetic moment, to deduce the magnetic energy relationships between the spin structures (which define the energetic ordering of the magnetic states, and the radiationless and radiative transitions between these states).

The Magnetic Moment of an Electron is a Bohr Orbit

An electron in a Bohr atom is modeled as a point negative charge rotating in a circle about a fixed axis about a nucleus. By virtue of its constant circular motion and angular momentum, **L**, an orbiting Bohr electron produces a magnetic moment, μ_L, which can be represented by a vector coinsiding with the axis of rotation (Figure 9). This behavior is completely analogous to that of an electric current in a circular wire, which produces a magnetic moment perpendicular to the plane of the wire. Let us now see how this magnetic moment, μ_L, is related to the angular momentum of the electron, **L**, in a Bohr orbit. We are concerned with the factors determining the magnitude of the magnetic moment and its energy in a direction along the z-axis. i.e., its vectorial qualities.

Clasical considerations indicate that the magnitude of μ_L is proportional to the magnitude of **L**. From the model of the electron in the Bohr orbit the proportionality constant between **L** and μ_L can be shown to be -(e/2m), the ratio of the unit of electric charge to the electron's mass, so that a simple relationship exists between μ_L and **L** is given by eq. 7.

$$\mu_L = -(e/2m)\mathbf{L} \qquad (7)$$

The proportionality constant (e/2m), reflects the relationship between the magnetic moment and angular momentum of a Bohr orbit electron and is a fundamental quantity of quantum magnetism. It is therefore given a special symbol γ_e and the name **magnetogyric ratio** of the electron and is defined as a positive quantity. Thus, eq. 7 may be expressed as eq. 8.

$$\mu_L = -\gamma_e \mathbf{L} \qquad (8)$$

If the electron possesses one unit of angular momentum, its magnetic moment, μ_L is equal exactly to \(e/2m). This quantity may be viewed as the **fundamental unit of quantum magnetism and is given the special name of the Bohr magneton, since it was derived from the simple analysis of a Bohr atom.** We shall give the Bohr magneton a special symbol, μ_e and note that its numerical value is 9.3×10^{-20} JG^{-1}. When we see the symbol μ_e we should think of a magnetic moment generated by an electron possesing an angular momentum of exactly 1 \.

Eqs. 7 and 8 show:

(1) the vector representing the magnetic moment, μ_L, and orbital angular momentum , **L**, are co-linear (they are equivalent through a proportionality factor);

(2) the vector that represents the magnetic moment of an electron is opposite in direction to that of the angular momentum vector (recall that a negative sign relating vectors means that the vectors possess orientations 180^o apart);

(3) the proportionality factor γ_e allows us to deduce that the magnitude of the magnetic moment due to orbital motion is directly proportional to the charge of the electron and inversely proportional to its mass.

The reason that Eqs. 7 and 8 are so important is that they allow us to visualize both the angular momentum, which must be strictly conserved in all magnetic transitions and the magnetic moment which provides the interactions which determine magentic energies and which "trigger" radiationless and radiative magnetic transitions to occur. Figure 9 presents such a vectorial description (the Figure is schematic only so that the sizes of the vectors are unitless and not to any particular scale).

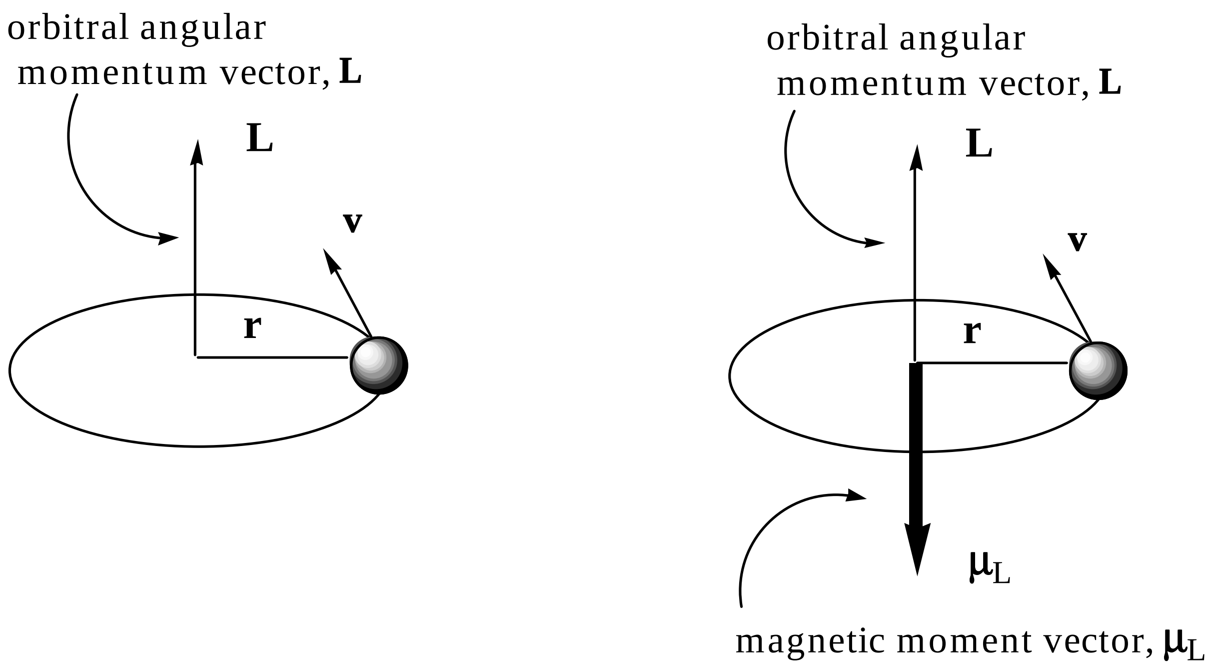

Figure 9. The vector model for the orbital angular momentum and the magnetic moment due to an electron in a Bohr orbit. The direction of the magnetic moment vector is opposite that of the direction of the angular momentum vector for an electron. The units of **L** are \ and the units of μ_L are J-G^{-1}.

We now need to proceed to deduce the magnetic moment is associated with an electron spin. We shall start with the results deduced from the electron in a Bohr orbit and transfer these ideas to the model of a rotating sphere, and determine what modifications of the model are necessary.

Electron Spin Angular Momentum and the Magnetic Moment Associated with Magnetic Moment Associated with Electron Spin

An electron in isolation possesses several simple properties: mass, electron charge, spin angular momentum, and a magnetic moment. There is no question that the electron is a quantum particle and as such will possess many properties which are quite unusual and unpredictable from observations of classical particles. Nonetheless, there is a clear visualization that is possible if we take as a model for the electron a material particle of definite size and spherical shape with a negative electric charge distributed over its surface. The properties of mass and charge are clearly articulated in this simple model. In order to understand the angular momentum of the electron resulting from its spin motion, it is intuitively natural to assume that since the mass of the electron is fixed and since its spin angular momentum is quantized and fixed, the spherical electron must spin about an axis with a fixed velocity, **v** (Figure 10). It is also quite natural to apply the results relating the orbital angular momentum of an electron to a magnetic moment due to its orbital motion to infer the relationship of the spin angular momentum of an electron to a magnetic moment due to its spin motion.

However, we should not be too surprised if the electron spin angular momentum has some differences because **there is no simple classical analogue of electron spin**. From the model of orbital angular momentum, the concept of electron spin angular momentum was devised to explain atomic spectra and was empirical in origin. Since the electron is a charged particle, we expect that as a result of its spinning motion, it will generate a magnetic moment, μ_S, in analogy to the magnetic moment generated by an electron in a Bohr orbit. A direct analogy with the relationship of orbital angular momentum and magnetic moment (Eq. 8) would suggest that the magnetic moment of the spinning electron should be equal to $\gamma_e\mathbf{S}$, i.e., the magnetic moment due to spin should be directly proportional to the value of the spin and the proportionality constant should be γ_e. However, experimental evidence and a deeper theory show that this is not quite the case and that for a free electron and that Eq. 9 applies.

$$\mu_S = -g_e\gamma_e\mathbf{S} \qquad (9)$$

In Eq. 9 g_e is a dimensionless constant called the g factor or g value of the free electron. and has an experimental value of ca 2. Thus, the simple model which attempts to transfer the properties of an orbiting electron to a spinning electron, is incorrect by a factor of 2. This flaw are is not of concern for the qualitative features of spin.

The following important conclusions can now be made:

(1) since spin is quantized and the spin vector and the magnetic moment vectors are directly related by eq. 9, **the magnetic moment associated with spin, as the angular momentum from which it arises is quantized in magnitude and orientation**;

(2) since the energy of a magnetic moment depends on its orientation in a magnetic field, **the energies of various quantized spin states will depend on the orientation of the spin vector in a magnetic field**;

(3) the vectors μ_S and **S** are both positioned in a cone of orientation which depends on the value of M_S (Figure 10, right);

(4) in analogy to the relationship of the orbital angular momentum and the magnetic moment derived from orbtial motion, the vectors μ_S and **S** are antiparallel (Figure 10, left).

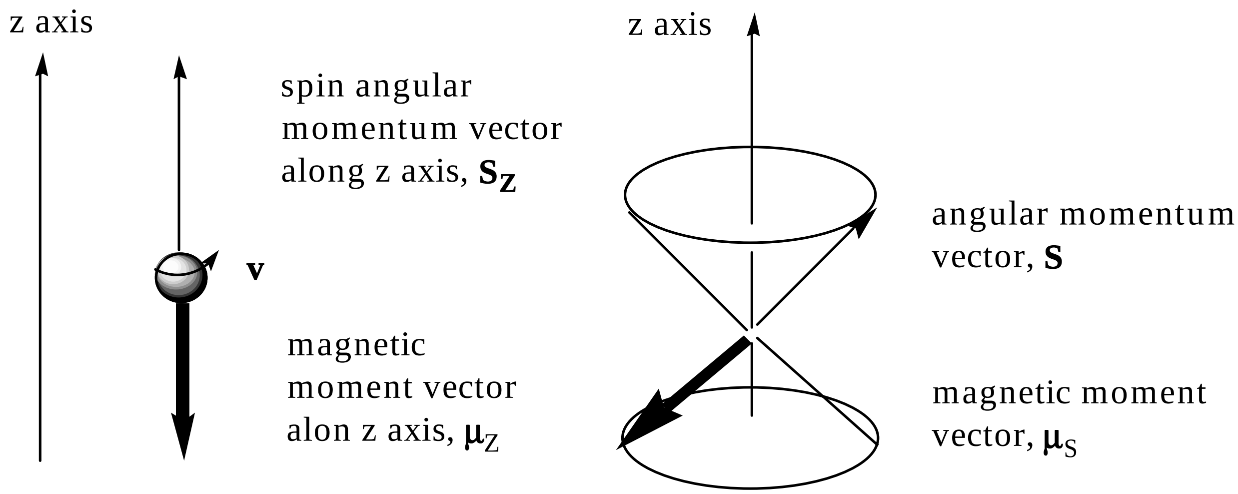

Figure 10. Vector representation of the spin angular momentum, **S**, and the magnetic moment associated with spin, μ_S. The two vectors are colinear, but antiparallel.