A little bit of angular momentum

Notes on Quantum Mechanics

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...[quote]...

Quantum aspects of angular momentum: Space quantization

The effect of angular motion appears in the radial Schrödinger equation as the repulsive centrifugal potential

$$\frac{\hbar^2 \ell(\ell+1)}{2 \, m \, r^2}$$

In classical physics kinetic energy due to motion of a mass m on an arc of radius r is

$$\frac{J^2}{2I} = \frac{J^2}{2mr^2}$$

Comparing the classical energy expression to the repulsive centrifugal potential, evidently we can identify $\ell(\ell + 1)\hbar^2$ as the squared angular momentum of the electron.

Evaluate the total centrifugal potential energy due to the motion of electrons in a mole of hydrogen atoms, assuming $\ell = 1$ (p electrons) and r = 1 Å. Answer: 735 kJ/mol.

Evaluate the total centrifugal potential energy due to the motion of electrons in a mole of hydrogen atoms, assuming $\ell = 3$ (f electrons) and r = 1 Å. Answer: 4411 kJ/mol.

We have learned that in addition to the quantum number ℓ , there is the quantum number m_{ℓ} with $2\ell + 1$ values $-\ell$, $-\ell + 1$, ..., ℓ . These values of m_{ℓ} are interpreted as the possible values, in units of \hbar , of the projection of the angular momentum vector $\vec{\ell}$ along an axis (conventionally chosen to be the *z* axis).

Since the length of $\vec{\ell}$ is $\sqrt{\ell(\ell+1)} \hbar > \ell \hbar$, but since the largest projection of $\vec{\ell}$ along z is $\ell \hbar$ (corresponding to the maximum value of m_ℓ), (1) $\vec{\ell}$ can never be exactly parallel to the z axis, and (2) it can be oriented at only $2\ell + 1$ possible angles to the z axis. The restriction on orientation of the possible orientations of $\vec{\ell}$ in space is known as *space quantization*.

Evaluate the possible angles the \vec{l} can make with the *z* axis is l = 1. Answer: 135°, 90°, 45°.

As the value of ℓ increases, $\vec{\ell}$ can be oriented closer to the *z* axis, and as ℓ becomes very large, it can be nearly parallel to the *z* axis and can take nearly arbitrary orientation with respect to the *z* axis. Thus, for very large values of ℓ , the effect of space quantization becomes insignificant.

Evaluate the minimum angle that \vec{l} can make with the *z* axis is l = 10, 100, and 1000. Answer: 17.5 ° and 5.7 °, 1.8 °.

Spin angular momentum

Electrons have an intrinsic magnetic moment that is found experimentally to be able to be aligned along a magnetic field with only two possible orientations. These alternative orientations are call *up* and *down*. Classically, a magnetic moment is equivalent to an electrical current in the plane perpendicular to the magnetic moment. Since electrons have electrical charge, when the intrinsic magnetic moment of the electron was discovered, it was first thought that it was due to the current generated by the electrically charged electron spinning on its own axis, and for this reason the magnetic moment is referred to as the *spin* of the electron. In fact, the electron is not spinning, but nonetheless has a magnetic moment and this is still referred to as the electron spin.

Since the "spin" of the electron can take just two orientation with respect to an applied magnetic field, it is interpreted as an angular momentum of quantum number s = 1/2, since then it has only two possible projection quantum numbers $m_s = -1/2$, +1/2. Since the electron is not actually spinning, its alternative spin states are not represented in terms of motion in physical space. Rather they are denoted as α for $m_s = +1/2$ and β for $m_s = -1/2$.

Angular momentum operators

A compact way of expressing the angular momentum properties of a the state of a quantum system is to label the state with the numerical values of the angular momentum quantum number J and the projection quantum number M_J as $|JM_J\rangle$. The symbol J is used when we do not need to distinguish between orbital and spin momentum. Then we can express the angular momentum properties in terms of operators for the squared angular momentum and the angular momentum projection as

$$J^{2} | J, M_{J} \rangle = J(J+1) \hbar^{2} | J, M_{J} \rangle,$$
$$J_{z} | J, M_{J} \rangle = M_{J} \hbar | J, M_{J} \rangle.$$

For example, the angular momentum properties of a d electron with $m_{\ell} = -2$ could be expressed as

$$J^{2} | J = 2, M_{J} = -2 \rangle = \ell^{2} | 2, -2 \rangle = 2 (2 + 1) \hbar^{2} | 2, -2 \rangle = 6 \hbar^{2} | 2, -2 \rangle,$$

$$J_{z} | J = 2, M_{J} = -2 \rangle = \ell_{z} | 2, -2 \rangle = -2 \hbar | 2, -2 \rangle$$

and the angular momentum properties of a spin down electron could be expressed as

$$J^2 | J = 1/2, M_J = -1/2 \rangle = s^2 \beta = 1/2 (1/2+1) \hbar^2 \beta = 3/4 \hbar^2 \beta$$

$$J_z | J = 1/2, M_J = -1/2 \rangle = s_z \beta = -1/2 \hbar \beta$$

Two other operators operators are

$$J_{\pm} = J_x \pm i J_y$$
.

These operators raise (J_+) or lower (J_-) the value of the *z* projection quantum number M_J by one unit,

$$J_{\pm} | J, M_J \rangle = \sqrt{J(J+1) - M_J(M_J \pm 1)} \hbar | J, M_J \pm 1 \rangle,$$

and so are referred to as the raising (J_+) and lowering (J_-) operators. Since there is a maximum possible value of M_J , the effect of the raising operator on a state with $M_J = J$ is said to annihilate the state. For example,

$$s_{+} \alpha = \sqrt{1/2(1/2+1) - 1/2(1/2+1)} \hbar | 1/2, 3/2 \text{ (not possible !)} = 0$$

Similarly, since there is a minimum possible value of M_J , the effect of the lowering operator on a state with $M_J = -J$ is to annihilate the state. For example,

$$s_{-}\beta = \sqrt{1/2(1/2+1) + 1/2(-1/2-1)}\hbar |1/2, -3/2 \text{ (not possible !)} = 0$$

Show that $s_+ \beta = \hbar \alpha$ and that $s_- \alpha = \hbar \beta$.

Composite spin angular momentum

Angular momenta can combine together. An important example are the four symmetrized spin states of two electrons,

state₁ =
$$\alpha(1) \alpha(2)$$

state₂ = $\beta(1) \beta(2)$
state₃ = $\alpha(1) \beta(2) + \alpha(2) \beta(1)$
state₄ = $\alpha(1) \beta(2) - \alpha(2) \beta(1)$

The challenge is to determine what the are the values of the total angular momentum quantum number J and the projection quantum number M_z for such a combination.

The way to determine the angular momentum properties of these combined spin states is to introduce the total spin momentum,

$$\vec{S} = \vec{s_1} + \vec{s_2},$$

and then to determine the effect of the operators for the squared total spin momentum

$$S^{2} = (\overrightarrow{s_{1}} + \overrightarrow{s_{2}}) \cdot (\overrightarrow{s_{1}} + \overrightarrow{s_{2}}) = s_{1}^{2} + s_{2}^{2} + 2 \overrightarrow{s_{1}} \cdot \overrightarrow{s_{2}},$$

and z projection of the total spin momentum,

$$S_z = s_{1z} + s_{2z},$$

on each of the symmetrized states of two spins.

For example, it will turn out below that the effect of S^2 on the two spin state state₁ is S^2 state₁ = $2\hbar^2$ state₁. Since we know the general the eigenvalue of S^2 is $S(S + 1)\hbar^2$, we can conclude by setting 2 = S(S + 1) that S = 1, and so that state₁ corresponds to a total spin angular momentum quantum number of 1.

In a similar way, we can determine value of the spin projection quantum number M_z by determining the effect of S_z on each of the combined spin states. In particular, it will turn out below that S_z state₁ = \hbar state₁. Since the general eigenvalue of S_z is $M_z \hbar$, this result means that $M_z = 1$ for state 1.

These results mean that state₁ can be represented as $|S, M_z\rangle = |1, 1\rangle$.

Total spin momentum z projection

To evaluate the effect of the total spin momentum z projection, we need to evaluate the effect of S_z on each of the states.

Use the expression for S_z to show that the effect of S_z on state₁ is S_z state₁ = \hbar state₁ and so that $M_S = 1$ for state₁.

Evaluate the effect of S_z on state₂, state₃, and state₄ to show that their values of M_S are -1, 0, and 0, respectively.

Squared total spin momentum

To evaluate the effect of the total angular momentum operator

$$S^{2} = (\overrightarrow{s_{1}} + \overrightarrow{s_{2}}) \cdot (\overrightarrow{s_{1}} + \overrightarrow{s_{2}}) = s_{1}^{2} + s_{2}^{2} + 2 \overrightarrow{s_{1}} \cdot \overrightarrow{s_{2}},$$

on a two spin state, we need to express $2 \vec{s_1} \cdot \vec{s_2}$ in terms of operators whose effect on spin states we know. We do this using raising and lowering operators each spin.

Show that $2(s_{1x}s_{2x} + s_{1y}s_{2y}) = s_{1+}s_{2-} + s_{1-}s_{2+}$, and so that $2\vec{s_1} \cdot \vec{s_2} = 2s_{1z}s_{2z} + s_{1+}s_{2-} + s_{1-}s_{2+}$

Using the result of the previous problem, we can express the total angular momentum operator as

$$S^{2} = (\vec{s_{1}} + \vec{s_{2}}) \cdot (\vec{s_{1}} + \vec{s_{2}}) = s_{1}^{2} + s_{2}^{2} + 2 s_{1z} s_{2z} + s_{1+} s_{2-} + s_{1-} s_{2+}$$

Use this expression to show that the effect of S^2 on state₁ is S^2 state₁ = $2\hbar^2$ state₁, and similarly for state₂ and state₃.

Based on the result of the previous problem, show that S = 1 for state₁, state₂, and state₃.

Use the expression for S^2 above to show that the effect of S^2 on state₃ is S^2 state₄ = 0 and so that S = 0 for state₄

Composite spin state labels

We have already anticipate that state₁ = $\alpha(1) \alpha(2)$ can be represented as $|S, M_z\rangle = |1, 1\rangle$.

Use the values that you have determined for *S* and M_S to verify that the following $|S, M_S\rangle$ labelling of the other three composite spin states.

state₂ = $\beta(1) \beta(2) = |1, -1\rangle$

state₃ = $\alpha(1) \beta(2) + \alpha(2) \beta(1) = |1, 0\rangle$

state₄ =
$$\alpha(1)\beta(2) - \alpha(2)\beta(1) = |0, 0\rangle$$