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### Angular momentum and spin

Angular momentum is a measure of how much rotation there is in particle or in a rigid body. In quantum mechanics as well as in classical mechanics the angular momentum is given by  $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$ . In classical mechanics the time derivative is  $d\boldsymbol{L}/dt = \boldsymbol{M}$ , where  $\boldsymbol{M}$  is the torque  $\boldsymbol{r} \times \boldsymbol{F}$ . If the potential energy is rotationally invariant the force acting on the particle is in the radial direction towards/away from the centre. And the torque with respect to the point of symmetry of the potential will be zero. Hence the angular momentum of the particle  $\boldsymbol{L}$  will be a constant of the motion (time independent). This fact is for instance used when calculating planetary orbits around the sun.

In quantum mechanics the  $L^2$  operator can only take certain distinct values, the eigenvalues to the corresponding eigenstates (See Bransden Joachain, chapter 6 or Gasiorowicz, chapter 7 and supplement 7B). The values it can take are  $\hbar^2 l(l+1)$  where l is an integer l = 0, 1, 2, ...As the potential was rotational invariant the Hamiltonian will not change under an arbitrary rotation and hence eigenstates of H can also be written as eigenstates of  $L^2$  and one of its components  $L_z$  (or  $L_x$  or  $L_y$ ). The wave function can be written as:

$$u_E(\mathbf{r}) = R(r)Y_{lm}(\theta,\phi). \tag{1}$$

The quantum number m gives the eigenvalue of the z-component of the angular momentum to  $\hbar m$ . This implies that  $Y_{lm} \propto e^{(im\phi)}$ , ie along the direction of  $\phi$  is a complex wave with mwaves on a full turn around the z-axis, ie m is an integer. The possible values m can take for a given l value are m = -l, -l + 1, ..., l - 1, l, making a total of (2l + 1) different values.

We can make a graphical interpretation of the vector L for these states. The length of the vector L is

$$\sqrt{\boldsymbol{L}^2} = \hbar \sqrt{l(l+1)}.$$
(2)

Which is somewhat larger than the largest value for  $L_z$ ,  $\hbar l$ . As the operators  $L_x$  and  $L_y$  do not commute with  $L_z$  there values are not well defined. They are fully unknown  $\langle L_x \rangle = \langle L_y \rangle = 0$ if the state is an eigenstate to  $L_z$ , however the operator  $L_x^2 + L_y^2 = \mathbf{L}^2 - L_z^2$  has well determined value,  $\hbar^2 l(l+1) - \hbar^2 m^2$ .

These properties of L and the states eq. (1) are illustrated in figure (1). It is quite different from classical mechanics where the vector L is a constant pointing in a certain direction. The quantum number is referred to as the magnetic quantum number. This is because according to classical physics an orbiting electron (electrical charge) gives rise to a magnetic moment

$$\boldsymbol{\mu} = -\frac{e}{2m_e} \boldsymbol{L} \,. \tag{3}$$

In a weak magnetic field B the energy of the electron will change by the amount

$$\Delta E = -\boldsymbol{\mu} \cdot \boldsymbol{B} \,. \tag{4}$$

In quantum physics  $\boldsymbol{\mu}$  eq. (3) is an operator. Let the magnetic field be directed along the z axis,  $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ , the change to the Hamilton operator due to the magnetic field will be

$$H_1 = \frac{eB}{2m_e} L_z \,. \tag{5}$$



Figure 1: The angular momenta for the states  $Y_{lm}$  form a half circle of radius  $\hbar \sqrt{l(l+1)}$  projecting down on the z-axis at integer steps at  $\hbar(-l, -l+1, ..., l-1, l)$ . In this figure we have the following steps  $\hbar(-2, -1, 0, 1, 2)$ .

If we add a term like this the energy will change by  $B(e\hbar/2m_e)m_l$ , the wave functions will remain the same. (In classical physics the vector  $\boldsymbol{L}$  will be time dependent and will precess around the z-axis, is only  $L_z$  and  $\boldsymbol{L}^2$  are constants of the motion, whereas  $L_x$  and  $L_y$  are time dependent.

Experiments will however not give this splitting of levels. The number of levels does not match. This is due to the fact that the electron in itself possesses a magnetic moment, called spin. The electrons spin is a kind of angular momentum and is a property of the electron. Before we engulf us into a mathematical description of spin we will recapitulate the mathematical treatment of orbital angular momentum. Introduce the ladder operators  $L_+$  and  $L_-$ . These are related to the orbital angular momentum operators in the x and y direction according to,

$$L_x = \frac{1}{2} \left( L_+ + L_- \right), \quad L_y = \frac{1}{2i} \left( L_+ - L_- \right).$$
(6)

These operators have the following commutator relations:  $[L_z, L_+] = \hbar L_+, [L_z, L_-] = -\hbar L_$ and  $[L_+, L_-] = 2\hbar L_z$ . These relations can be used to show that the operator  $L_+$  increases the m quantum number by one step and that  $L_-$  decreases the m quantum number by one step according to

$$L_{+}|Y_{l,m}\rangle = \hbar \sqrt{l(l+1) - m(m+1)}|Y_{l,m+1}\rangle,$$
  

$$L_{-}|Y_{l,m}\rangle = \hbar \sqrt{l(l+1) - m(m-1)}|Y_{l,m-1}\rangle.$$
(7)

The different values are separated by unit one. One can also show the relation between the largest and smallest m value,  $m_{max}$  and  $m_{min}$ , that  $m_{min} = -m_{max} = -l$ . From this we deduce that the number of different m values is 2l + 1, and that 2l is an integer. From the relation of the operator  $L_z$  to the angle  $\phi$  we also know that the m values are integers.

# Spin

The electron has like many other particles an intrinsic angular momentum, denoted spin. The spin of the electron can be in two states, called spin up and spin down. The existence of these

two states gives rise to the Pauli principle. According to this two electrons can only have the same value of the quantum numbers n-, l- and m if they have different spin quantum numbers. Spin is also evident if we measure the energy of atoms in a magnetic field. It is important to note that spin is a property of the electron, it is not an orbital angular momentum due to some kind of motion. As to our knowledge today there are no inner parts in the electron. If there had been an inner structure of the electron we would have found (2l + 1) states, an odd number, and not two. The description of spin does hence not involve functions of the angles  $\theta$  and  $\phi$ .

Spin is an intrinsic angular momentum and we can introduce a set of operators  $S_x$ ,  $S_y$  and  $S_z$ . These have the same commutator relations as the orbital angular momentum operators. Earlier we saw that these relations led to that 2l is an integer. This implies that l is either an integer or an half integer. The spin of the electron is denoted by s. It takes the value 1/2 as the number of m values is (2s + 1) = 2. The two m states are spin up  $(m_s = 1/2)$  and spin down  $m_s = -1/2$ ). The subscript s is used to distinguish  $m_s$  from the m quantum number that is associated to the orbital motion of 3 dimensional space.

The two orthogonal and normalised state functions  $\chi_+$  and  $\chi_-$ ,

$$<\chi_{-}|\chi_{+}>=0 < \chi_{\pm}|\chi_{\pm}>=1.$$
 (8)

can be used as a set of basis functions to describe any spin state,

$$\chi = a\chi_+ + b\chi_- \,. \tag{9}$$

To fully specify  $\chi$  only two numbers are needed a and b. The state can hence be represented by the vector

$$\chi = \left(\begin{array}{c} a\\b\end{array}\right) \,. \tag{10}$$

If we let a = 1 and b = 0 (and vice verse) in eq. (9) and (10) we get

$$\chi_{+} = \begin{pmatrix} 1\\0 \end{pmatrix} \quad \chi_{-} = \begin{pmatrix} 0\\1 \end{pmatrix}. \tag{11}$$

An operator that acts on  $\chi$  gives a new state  $\chi' = A\chi$ . If the operator A is linear it can be represented by a matrix,

$$A\chi = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}.$$
 (12)

The relation between the matrix elements and the result when A acts on  $\chi_+$  and  $\chi_-$  we find from

$$A\chi_{+} = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix},$$
  

$$A\chi_{-} = \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix}.$$
(13)

The three spin operators  $S_x$ ,  $S_y$  och  $S_z$  correspond to the orbital angular momentum operators  $L_x$ ,  $L_y$  and  $L_z$ . The matrix that represents  $S_z$  can be deduced from that  $\chi_{\pm}$  are eigenstates,

$$S_z \chi_{\pm} = \pm \frac{1}{2} \hbar \chi_{\pm} \tag{14}$$

and hence  $S_z$  is diagonal,

$$S_z = \begin{pmatrix} \frac{\hbar}{2} & 0\\ 0 & -\frac{\hbar}{2} \end{pmatrix}. \tag{15}$$

The action of  $S_x = (S_+ + S_-)/2$  and  $S_y = (S_+ - S_-)/2i$  is given in a similar way as earlier from the commutator relations. Accordingly  $S_+$  and  $S_-$  act in accordance with eq. (7),

$$S_{+}\chi_{+} = 0 \quad \text{och} \quad S_{-}\chi_{-} = 0 \tag{16}$$
$$S_{+}\chi_{-} = \hbar_{1}\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - \left(-\frac{1}{2}\right)\left(-\frac{1}{2}+1\right)}\chi_{+}$$

$$S_{-\chi_{+}} = \hbar \sqrt{\frac{1}{2} \left(\frac{1}{2} + 1\right) - \left(\frac{1}{2}\right) \left(\frac{1}{2} - 1\right)} \chi_{-}$$
$$= \hbar \chi_{-}.$$
(18)

For the matrices  $S_+$  and  $S_-$  we have,

$$S_{+} = \begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix} \quad S_{-} = \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix}$$
(19)

and the matrices for  $S_x$  and  $S_y$  become,

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\\ i & 0 \end{pmatrix}.$$
 (20)

Now we turn to the physics. A charged particle with a spin has an intrinsic magnetic moment

$$\boldsymbol{\mu}_s = -\frac{g_s e}{2m_e} \boldsymbol{S} \,. \tag{21}$$

A magnetic moment such as this can be deduced from the corresponding relativistic Schrödinger equation for a charged particle with s = 1/2, the Dirac equation. The Dirac equation gives  $g_s = 2$  whereas the real value is  $g_s = 2.0023...$  Quantum fluctuations in the electromagnetic field can be accounted for the deviation.

#### The appearance of the spin in the Hamiltonian

The magnetic moment of the electron brings about many important effects. In the presence of a magnetic field there will be the following term in the Hamiltonian to account for it

$$H_1 = -\boldsymbol{\mu}_s \cdot \boldsymbol{B} = \frac{g_s e}{2m_e} \boldsymbol{S} \cdot \boldsymbol{B} \,. \tag{22}$$

If there is only an external constant magnetic field that interacts with the spin, then we can solve the dynamics of the spin degrees of freedom separately, by solely taking into account  $H_1$ . The time dependent Schrödinger equation for this part is

$$i\hbar\frac{\partial\chi}{\partial t}(t) = H_1\chi(t) \tag{23}$$

This is conveniently solved by separation of variables, just as we solved the time dependent equation previously. That is, we assume that the solution is

$$\chi(t) = \chi_0 T(t) \tag{24}$$

where  $\chi_0$  is a time independent spin state. The time dependent function T(t) comes out as  $\exp(-iEt/\hbar)$  where the energy E is given by the equation for the spin state

$$H_1\chi_0 = E\chi_0. \tag{25}$$

It is most convenient to solve (25) if the magnetic field is pointing in the z-direction. Then with  $\alpha = g_s eB/2m_e$  the Hamiltonian becomes  $H_1 = \alpha S_Z$  and the eigenstates  $(\chi_0)$  are the eigenstates of  $S_z$ , that is  $\chi_{\pm}$  and the eigenvalues,

$$E = \pm \alpha \frac{\hbar}{2} = \pm \frac{g_s eB}{2m_e} \frac{\hbar}{2} \,. \tag{26}$$

The magnetic field coming from a permanent magnet (a ferromagnetic material) comes from the spin magnetic moments of the valence electrons.

However, the force that keeps the spins of the valence electrons in ferromagnetic materials to point in the same directions is remarkably not due to the electromagnetic interaction between magnetic moments. It is a property of the wave function.

Also neutrons and protons are particles with spin (s = 1/2). They interact with a magnetic field in just the same way as the electron though their  $g_s$ -values are somewhat bigger and the electron mass is replaced by the nucleon mass. The magnetic interaction between the magnetic moment of a proton (or some other nucleus) and a magnetic field is the basis of nuclear magnetic resonance (NMR). When a microwave with a frequency such that the photon energy  $h\nu$  is equal to the energy separation between the two spin states,

$$h\nu = g_p \frac{eB\hbar}{2m_N} \tag{27}$$

then the microwave radiation is absorbed by the protons. NMR is used in chemistry as the resonance condition is slightly changed by chemical bonds. This change gives rather detailed information on the molecular structure. NMR is also used in the medicinal science under the name magnetic resonance imaging (MRI).

The intrinsic magnetic moment of the electron (21) gives rise to several interesting phenomena, among some: permanent magnets. Their interaction to a magnetic field is given in equation (22). It also gives rise to that the spin part and spatial part of the wave function influence each other. Classically we know that something that moves in an electric field also will sense a magnetic field. This magnetic field interacts with a magnetic dipole that moves in an electric field. It turns out that this magnetic field for the electron is proportional to  $\boldsymbol{L}$  the orbital angular momentum. The contribution to the Hamilton operator will be proportional  $\boldsymbol{L} \cdot \boldsymbol{S}$ .

This gives rise to a coupling between the orbital motion and the spin. As one discusses the quantum mechanical state of the electron one should take both spin and the wave function  $\psi(\mathbf{r})$ . Generally the state can be written

$$\Psi(\boldsymbol{r}) = \psi_{+}(\boldsymbol{r})\chi_{+} + \psi_{-}(\boldsymbol{r})\chi_{-} = \begin{pmatrix} \psi_{+}(\boldsymbol{r}) \\ \psi_{-}(\boldsymbol{r}) \end{pmatrix}.$$
(28)

This is the general form of the composite wave function if there is a coupling between spin and orbital angular momentum. This can be simplified if spin and orbital motion are independent of each other. In this case we can form the product (independent degrees of freedom)

$$\Psi(\boldsymbol{r}) = \psi(\boldsymbol{r})\chi = \psi(\boldsymbol{r})\begin{pmatrix} a\\b \end{pmatrix}.$$
(29)

The  $L \cdot S$  contribution to the Hamilton operator gives rise to states like

$$f(r) \begin{pmatrix} aY_{l,m_l-1} \\ bY_{l,m_l} \end{pmatrix} = f(r) \left[ aY_{l,m_l-1}\chi_+ + bY_{l,m_l}\chi_- \right] \,. \tag{30}$$

The operator for the total angular momentum along the z axis is  $L_z + S_z$  and is usually denoted by  $J_z$ . The state above is an eigenfunction of  $J_z$  as this operator commutes with the  $L \cdot S$ -term.

There are for a given value of  $J_z$  two different eigenstates to  $L \cdot S$  that correspond to spin and orbital angular momentum pointing the same or opposing directions, see figure 2.



Figure 2: Addition of the vectors  $\boldsymbol{L}$  and  $\boldsymbol{S}$  to form the composite vector  $\boldsymbol{J}$ .

#### Expectation values and probabilities

How do we calculate an expectation value of a spin? The Stern–Gerlach experiment is an example of how one can split spin state into its constituent parts  $\chi = a\chi_+ + b\chi_-$  such that

$$\Psi_1 = \psi(x) \begin{pmatrix} a \\ b \end{pmatrix} \quad \to \quad \Psi_2 = \begin{pmatrix} \psi(x - x_1)a \\ \psi(x - x_2)b \end{pmatrix}.$$
(31)

The spin up and down components are directed towards different positions in (real) space. In the vicinity of  $x_1$  only particles with 'spin up' occur and in the area of  $x_2$  one only finds



Figure 3: Schematic view of an initial spin mixed state (top figure) is split into its two constituent parts spin up  $(x_1)$  and spin down  $(x_2)$  (bottom figure).

particles with spin down. In an area where there is only one spin state is abundant, spin can be ignored. In any of the areas  $x_1$  or  $x_2$  spin is unchanged. The probability to find an electron in the vicinity of say  $x_1$  should be proportional to  $\int dx |a\psi(x-x_1)|^2$ . From this we can conclude that the probability to find spin up (spin down) in the initial state  $\Psi_1$  is given by

$$P(\uparrow) = |a|^2, \quad P(\downarrow) = |b|^2.$$
(32)

We have used that  $\int dx |\psi(x)|^2 = 1$ , and as there are only possible values the z component of the spin can take the sum of these probabilities is

$$|a|^2 + |b|^2 = 1 \tag{33}$$

The expectation value of  $S_z$  is given by

$$\langle S_z \rangle = \frac{\hbar}{2} |a|^2 - \frac{\hbar}{2} |b|^2 \tag{34}$$

This can be expressed in the following general form

$$\langle S_n \rangle = (a \ b)^* S_n \begin{pmatrix} a \\ b \end{pmatrix}$$
 (35)

where  $S_n$  on the right side is the matrix that represents the spin operator in the direction n, say x, y, z or any other direction.

If we would measure the spin in the y direction, what would the possible outcomes be of such a measurement and their probabilities? The values you can obtain are the eigenvalues of the  $S_y$  matrix. The probabilities will be the coefficients of the two possible spin states, the eigenstates of the operator (matrix)  $S_y$ .

- **Example 1.** What is the probability to find a value larger than zero if one measures along the y direction on a spin state  $\chi = \chi_+$  ?
- **Solution:** The original state  $\chi = \chi_+$  is a spin up state to the operator  $S_z$ . We are asked to measure along the y axis. To answer the question we can rewrite the initial state into the eigenstates of the operator  $S_y$ .

We start by solving the eigenvalue/eigenvector equation.

$$\frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$
(36)

This equation will only have non trivial solutions for certain values of  $\lambda$ . we find by rewriting the equation into an homogeneous set of equations.

$$\begin{pmatrix} -\lambda & -i\frac{\hbar}{2} \\ i\frac{\hbar}{2} & -\lambda \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0.$$
(37)

A nontrivial solution will appear if the determinant is zero.

$$(-\lambda)^2 - (-i)\frac{\hbar}{2}i\frac{\hbar}{2} = 0.$$
(38)

The eigenvalues  $\lambda_{1,2}$  are  $\pm \frac{\hbar}{2}$ . The probability to find a positive outcome is the same as the probability to find the value  $\frac{\hbar}{2}$ . This probability will be given by the coefficient for this state in the expansion of the initial state in the new eigenstates as mentioned above.

We now need to find the eigenvectors to achieve this we solve the equation (36),

$$\lambda = \frac{\hbar}{2} \to \left(\begin{array}{c} \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} \end{array}\right) \quad \lambda = -\frac{\hbar}{2} \to \left(\begin{array}{c} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{array}\right). \tag{39}$$

The amplitude, A, for this state is found by the scalar product between the eigenvector and the state  $\chi$ ,

$$A = \left(\frac{1}{\sqrt{2}} \ \frac{i}{\sqrt{2}}\right) * \left(\begin{array}{c} 1\\0\end{array}\right) \tag{40}$$

The probability to find a positive value is  $|A|^2 = 0.5$ .

Several of the results above one could have guessed without doing any calculations. But the calculation illustrates how quantum mechanical principles are applied in a spin calculation.

**Example 2.** What are the eigenstates to a spin operator in the direction given by the vector  $\mathbf{n} = (\sin \theta, 0, \cos \theta)$ ?

**Solution:** The spin operator  $S_n$  is given by the scalar product

$$S_{\mathbf{n}} = \mathbf{S} \cdot \mathbf{n} = S_x n_x + S_y n_y + S_z n_z \,. \tag{41}$$

Hence its matrix will be

$$S_{\mathbf{n}} = \frac{\hbar}{2} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & -\cos\theta \end{pmatrix}.$$
(42)

It is simple to check that the eigenvalues are  $\pm \hbar/2$ . The eigenvectors are (the calculation is straight forward and similar to the one above in Example 1).

$$\lambda = \frac{\hbar}{2} \rightarrow \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) \end{pmatrix} \quad \lambda = -\frac{\hbar}{2} \rightarrow \begin{pmatrix} \sin(\frac{\theta}{2}) \\ -\cos(\frac{\theta}{2}) \end{pmatrix}.$$
(43)

## The Stern-Gerlach experiment

The intrinsic magnetic moment of the electron is pointing in the same direction as the spin of the electron. Magnetic fields may be used to probe the spin of the particle. The Stern-Gerlachs experiment (1921) is an example of this.

Stern and Gerlach used in inhomogeneous magnetic field as shown in figure 4. It



Figure 4: Illustration of the inhomogeneous magnetic field in the magnets of a Stern-Gerlach apparatus.

is important that the field is not homogeneous as this would only rotate a magnetic dipole and not accelerate it.

They let neutral silver atoms move through the magnetic field along a certain distance. Silver atoms have a single valence electron 5s (n=5, l=0) in their electron configuration. The other shells are filled and will not contribute to the magnetic moment of the atom. The magnetic moment of the silver atom will originate from the intrinsic moment of the single valence electron. (The contribution from the nucleus is negligible.) The magnetic energy  $-\mu \cdot \mathbf{B}$  depends on the atoms position along the z axis. This will result in a force on the atom tending to move it along the z axis.

$$\mathbf{F} = \nabla \mu \cdot \mathbf{B} = \nabla (\mu_x B_x + \mu_z B_z). \tag{44}$$

If the particle is centred in the x direction and moving along the y axis and the magnetic field is pointing in the z direction the particle will be deflected either along the positive or negative direction of the z axis depending on the orientation of its spin.

$$\mathbf{F} = \mu_z \frac{\partial B_z}{\partial z} \tag{45}$$

We can use classical arguments for forces and tracks of the atoms as long as the magnetic field varies little within the length scale set by the de Broglie wave length of the silver atom. The silver atoms will exit the Stern–Gerlach apparatus in two beams as shown in figure 5. If two Stern–Gerlach apparatuses are place in series the first on can be used as a spin filter selecting a known spin state (along one direction) into the second. This setup is shown in figure 6. This set up is used to investigate properties of spin states.



Figure 5: The splitting of an electron beam into its two constituent spin parts in a Stern–Gerlach magnet.



Figure 6: Spin filters made from Stern–Gerlach magnets. The filter lets just one spin direction pass as indicated by the arrows. To the left the beam passes the filters as they both accept spin up. In the middle the beam is blocked as the first filter lets spin up pass but the second filter lets only spin down pass which is no longer present. To the right the first filter lets spin up pass but the second filter is probing an orthogonal direction and the spin up beam from filter one has to be expanded in eigenstates for filter number two, and hence part of the beam will pass.