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### III. Spin and orbital angular momentum

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#### General Properties of Angular Momenta

Angular momentum plays a very important role in Quantum Mechanics, as it does in Classical Mechanics. The orbital angular momentum in Classical Mechanics is  $\vec{L} = \vec{R} \times \vec{P}$  or in terms of components

$$L_x = YP_z - ZP_y$$

$$L_y = ZP_x - XP_z$$

$$L_z = XP_y - YP_x.$$

In Quantum Mechanics these equations remain valid if  $P$  is replaced by the momentum operator. In addition to the orbital angular momentum we need in Quantum Mechanics to introduce new angular momenta that are intrinsic to elementary particles, namely spin. This will be discussed in detail later. There are certain fundamental properties that are common to all angular momenta (and sums of angular momenta). They all derive from the commutations relations of the components.

*Commutation Relations:* Derive the commutation relation for  $L_x$  and  $L_y$

$$\begin{aligned} [L_x, L_y] &= [YP_z - ZP_y, ZP_x - XP_z] \\ &= [YP_z, ZP_x] - [YP_z, XP_z] - [ZP_y, ZP_x] + [ZP_y, XP_z] \end{aligned}$$

Recall

$$[R_i, R_i] = 0$$

$$[P_i, P_j] = 0$$

$$[R_i, P_j] = i\hbar \delta_{ij}$$

where  $i, j \in \{x, y, z\}$ .

The last commutator can be evaluated easily:

$$\begin{aligned} \langle \vec{r} | [Z, P_z] | \psi \rangle &= Z \langle \vec{r} | P_z | \psi \rangle - P_z \langle \vec{r} | Z | \psi \rangle \\ &= \frac{\hbar}{i} z \frac{\partial}{\partial z} \langle \vec{r} | \psi \rangle - \frac{\hbar}{i} \frac{\partial}{\partial z} (z \langle \vec{r} | \psi \rangle) \\ &= -\frac{\hbar}{i} \langle r | \psi \rangle \end{aligned}$$

So

$$[Z, P_z] = i\hbar.$$

Continuing now with the calculation of  $[L_x, L_y]$  using this result gives

$$[Y P_z, Z P_x] = Y [P_z, Z] P_x = -i\hbar Y P_x$$

$$[Y P_z, X P_z] = 0 = [Z P_y, Z P_x]$$

$$[Z P_y, X P_z] = x [Z, P_z] P_y = i\hbar X P_y$$

finally gives

$$[L_x, L_y] = i\hbar(X P_y - Y P_x) = i\hbar L_z.$$

Similarly, for the other components of the angular momentum vector:

$$[L_x, L_y] = i\hbar L_z$$

$$[L_y, L_z] = i\hbar L_x$$

$$[L_z, L_x] = i\hbar L_y$$

These commutation relations can be taken as the general definition of an angular momentum vector. (The relationship to rotations in 3-D is discussed in CDL  $B_{VI}$ )

### *General Properties of an Angular Momentum $\vec{J}$ :*

The basic property of an angular momentum vector is:

$$[J_x, J_y] = i\hbar J_z$$

$$[J_y, J_z] = i\hbar J_x$$

$$[J_z, J_x] = i\hbar J_y.$$

From these relations one can easily derive:

$$[J^2, \vec{J}] = 0 \quad \text{where} \quad J^2 = J_x^2 + J_y^2 + J_z^2.$$

This, together with the commutation relations for the components, means that we can simultaneously know the *total* angular momentum and *one* of its components. The component is usually chosen to be  $J_z$ .

Instead of working with the  $J_x$  and  $J_y$  components, it is often easier to define new linear combinations of those:

$$J_+ \equiv J_x + iJ_y$$

$$J_- \equiv J_x - iJ_y.$$

The adjoints are  $J_+^\dagger = J_-$  and  $J_-^\dagger = J_+$ . These linear combinations together with  $J_z$  are the set of operators we need to deal with. The total angular momentum operator can be rewritten in terms of those three as

$$J^2 = \frac{1}{2}(J_+ J_- + J_- J_+) + J_z^2.$$

Proof:

$$\begin{aligned}
J_+J_- &= (J_x + iJ_y)(J_x - iJ_y) \\
&= J_x^2 + J_y^2 + iJ_yJ_x - iJ_xJ_y \\
&= J_x^2 + J_y^2 - i[J_x, J_y] \\
&= J_x^2 + J_y^2 + \hbar J_z \\
&= J^2 - J_z^2 + \hbar J_z
\end{aligned}$$

Similarly:

$$J_-J_+ = J^2 - J_z^2 - \hbar J_z$$

Adding the two,  $J_+J_- + J_-J_+$ , gives the above expression for  $J^2$ .

Let the eigenstates of  $J^2$  and  $J_z$  be denoted by  $|jm\rangle$ . The action of the various operators on these states (vectors) is:

$$(1) \quad J^2|jm\rangle = j(j+1)\hbar^2|jm\rangle \quad \text{with } j \in [0, \frac{1}{2}, 1, \frac{3}{2}, \dots].$$

$$(2) \quad J_z|jm\rangle = m\hbar|jm\rangle \quad \text{where } -j \leq m \leq j. \quad \text{Total of } 2j+1 \text{ values for } m.$$

(3)

$$J_-|jm\rangle = \begin{cases} \hbar\sqrt{j(j+1) - m(m-1)}|j, m-1\rangle & \text{if } m > -j \\ 0 & \text{if } m = -j \end{cases}$$

(4)

$$J_+|jm\rangle = \begin{cases} \hbar\sqrt{j(j+1) - m(m+1)}|j, m+1\rangle & \text{if } m < j \\ 0 & \text{if } m = j \end{cases}$$

All these relations can be proved using the commutation relations and operator algebra. The 'proofs' of (2) and (3) are sketched as examples:

*Prove (2):*

First, find norm of  $J_-|jm\rangle$ :

$$\begin{aligned}
\|J_-|jm\rangle\|^2 &= \langle jm|J_-^\dagger J_-|jm\rangle = \langle jm|J_+J_-|jm\rangle \\
&= \langle jm|J^2 - J_z^2 + \hbar J_z|jm\rangle = \langle jm|[j(j+1)\hbar^2 - m^2\hbar^2 + m\hbar^2]|jm\rangle \\
&= \hbar^2(j(j+1) - m(m-1)) \\
&= \hbar^2((j-m+1)(j+m))
\end{aligned}$$

Any norm must be  $\geq 0$ , that is  $(j-m+1)(j+m) \geq 0$  or  $-j \leq m \leq j+1$ .

Secondly, we can find the norm of  $J_+|jm\rangle$  in a similar way:

$$\|J_+|jm\rangle\|^2 = \hbar^2(j(j+1) - m(m+1)).$$

Therefore  $(j+m+1)(j-m) \geq 0$  or  $-(j+1) < m < j$

For both of these inequalities to be valid, we must have  $-j \leq m \leq j$ .

*Prove (3):*

Again use

$$\|J_-|jm\rangle\|^2 = \hbar^2(j(j+1) - m(m-1)).$$

This is zero when  $m = -j$ . When the norm of a vector is zero, the vector itself must be zero, so  $J_-|j-j\rangle = 0$ .

Now assume  $m > -j$ : Since  $[J^2, \vec{J}] = 0$  we have  $[J^2, J_-] = 0$  and therefore the vector  $J_-|jm\rangle$  is an eigenvector of  $J^2$ . Find the eigenvalue:

$$J^2 J_-|jm\rangle = J_- J^2|jm\rangle = j(j+1)\hbar^2 J_-|jm\rangle \quad (\text{using(1)}).$$

The eigenvalue is  $j(j+1)\hbar^2$ .

Now find  $J_z J_-|jm\rangle$ : Since

$$\begin{aligned} [J_z, J_-] &= [J_z, J_x - iJ_y] = i\hbar J_y - i(-i\hbar)J_x \\ &= -\hbar J_- \end{aligned}$$

we have

$$\begin{aligned} J_z J_-|jm\rangle &= J_- J_z|jm\rangle - \hbar J_-|jm\rangle \\ &= (m-1)\hbar J_-|jm\rangle \end{aligned}$$

So, the vector  $J_-|jm\rangle$  is an eigenvector of  $J^2$  with an eigenvalue of  $\hbar^2 l(l+1)$  and it is an eigenvector of  $J_z$  with eigenvalue  $(m-1)\hbar$ . It therefore must be proportional to the vector  $|j, m-1\rangle$ . The operator  $J_-$  is called the *Lowering Operator* because it generates a vector with one lower value of  $m$ . In the proof of (2) the norm of the new vector was found. Therefore, we have (3).

The proof of (4) is very similar, replacing  $J_-$  with  $J_+$ . Again, it can be shown that:

$$J^2 J_+|jm\rangle = j(j+1)\hbar^2 J_+|jm\rangle$$

and

$$J_z J_+|jm\rangle = \begin{cases} (m+1)\hbar J_+|jm\rangle & \text{if } m < j \\ 0 & \text{if } m = j \end{cases}$$

The operator  $J_+$  is called the *Raising Operator*.

### Stern-Gerlach Experiments:

A beam of hydrogen atoms is prepared by dissociating hydrogen molecules in a resonance cavity with a hole from which the atoms emerge. The beam is directed into a magnetic field that has been prepared in a special way.

If the atoms in the beam have magnetic moment  $\vec{M}$  then their potential energy inside the magnet with field  $\vec{B}$  is  $W = -\vec{M} \cdot \vec{B}$ . The magnetic moment can, for example, be due to the orbital angular momentum of electrons,  $\vec{M} \propto \vec{L}$ . Then the force acting on the atoms in the magnetic field is:

$$\vec{F} = -\vec{\nabla}W = \vec{\nabla}(\vec{M} \cdot \vec{B})$$

The magnet is made in such a way that the magnetic field vector  $\vec{B}$  uniformly points in the same direction inside the magnet. We choose a coordinate system such that  $\vec{B} \parallel \hat{z}$ , i.e.  $B_x = B_y = 0$ , so  $\vec{F} = \vec{\nabla}(M_z B_z)$ .

*Classically:* The angular momentum vector (and therefore also  $\vec{M}$ ) will rotate about the  $z$  axis with constant angle  $\theta$  according to the equation of motion

$$\frac{d\vec{L}}{dt} \propto \frac{d\vec{M}}{dt} \propto \vec{M} \times \vec{B}.$$

The quantity on the right hand side is the torque. This equation relating the rate of change of angular momentum to the applied torque is analogous to the Newton equation relating the rate of change of linear momentum to the applied force  $\frac{d\vec{P}}{dt} = \vec{F}$ .

So,  $M_z$  is constant but  $M_x$  and  $M_y$  oscillate rapidly and will average to zero over the time that the atom spends inside the magnet. Therefore:

$$\vec{F} = \vec{\nabla}(M_z B_z) \cong M_z \vec{\nabla} B_z$$

The magnet for this kind of experiment is made in such a way that

$$\frac{\partial B_z}{\partial x} = \frac{\partial B_z}{\partial y} = 0$$

Therefore, the force on the atom is parallel to  $\hat{z}$  and is given by  $M_z \frac{\partial B_z}{\partial z}$ . The gradient  $\frac{\partial B_z}{\partial z}$  is a property of the magnet used in the experiment and can be found by calibration.

The deflection of the atom from the initial trajectory is therefore proportional to  $M_z$ . By measuring where the atom lands on the screen  $M_z$  and, by proportionality,  $L_z$ , can be determined.

When a beam of hydrogen atoms is used in this experiment *two* well defined subbeams of hydrogen are detected on the screen (see figure above). This result is very different from the predictions of Classical Mechanics which is one broad distribution of atoms because  $\vec{M}$  can be pointing in any direction in the beam. The experiment, therefore, demonstrates quantization of the orientation of angular momentum. Furthermore, if  $\vec{M}$  results from orbital angular momentum  $\vec{L}$ , then the Quantum Mechanical prediction is that an odd number of subbeams will be formed:

$$\begin{aligned} \text{if } \ell = 0 & \text{ then one} & (m = 0) \\ \text{if } \ell = 1 & \text{ then three} & (m = -1, 0, 1) \\ \text{if } \ell = 2 & \text{ then five} & (m = -2, -1, 0, 1, 2). \end{aligned}$$

The Stern-Gerlach experiment therefore points to another source of magnetic momentum, quite different from what arises from the orbital angular momentum. From this and other experiments it has been concluded that each elementary particle has *intrinsic* angular momentum which is called *spin* and typically is denoted  $\vec{S}$ . Spin is a new degree of freedom in addition to the spacial coordinates  $(x, y, z)$ . Note that spin cannot be due to the rotation of the electron about its own axis. Rotation in  $(x, y, z)$  space would lead to an odd number of subbeams just like the orbital angular momentum.

Unlike the spatial coordinates, spin can only take a discrete set of values. Proportional to the spin angular momentum is a magnetic momentum,  $\vec{M}_s \propto \vec{S}$ . The deflection of the hydrogen atoms is due to the spin of the electron. The proton also has spin of equal magnitude, but the magnetic momentum due to the proton spin is much smaller and can be neglected in this experiment. The experiment was actually done originally by Stern and Gerlach on a beam of silver atoms. This also splits up into two subbeams because of the single unpaired valence electron. The magnetic momentum due to the spin of the paired core electrons cancels.

Since spin is an angular momentum it must satisfy the commutation relations

$$[S_x, S_y] = i\hbar S_z$$

$$[S_y, S_z] = i\hbar S_x$$

$$[S_z, S_x] = i\hbar S_y$$

and therefore all the general relations for angular momentum are satisfied, in particular

$$S^2 |sm\rangle = s(s+1)\hbar^2 |sm\rangle$$

$$S_z|sm\rangle = m\hbar|sm\rangle .$$

Each elementary particle has a fixed magnitude of the spin vector, given by the quantum number  $s$ . However, the projection of the spin onto one axis, typically chosen to be the  $z$ -axis, is needed in addition to the coordinates (or momenta) to fully specify the state of the particle. A complete description of spin requires relativistic Quantum Mechanics.

### Spin $\frac{1}{2}$ : Pauli Theory

Electrons, protons and neutrons have spin with  $s = \frac{1}{2}$ . This can be incorporated in non-relativistic Quantum Mechanics in a rather simple way. The projection onto the  $z$  axis can in that case only take two values,  $m = -\frac{1}{2}$  or  $m = \frac{1}{2}$ . We can therefore introduce a new variable,  $\epsilon$ , where  $\epsilon$  only can take two values  $+$  and  $-$  (or  $\uparrow$  and  $\downarrow$ ). The full set of coordinates of the electron or neutron is  $(X, Y, Z, \epsilon)$ .

The spin operators  $S^2$ ,  $S_z$ ,  $S_+$  and  $S_-$  only act on the spin variable and therefore commute with any operator acting on  $(X, Y, Z)$  space. The operators  $S^2$  and  $S_z$  form a complete set of commuting operators in spin variable space. The eigenvectors of  $S^2$  and  $S_z$  can be specified as:

$$|+\rangle_z \equiv |+\rangle \equiv \left| \frac{1}{2} \frac{1}{2} \right\rangle \quad \left( j = \frac{1}{2}, m = \frac{1}{2} \right)$$

and

$$|-\rangle_z \equiv |-\rangle \equiv \left| \frac{1}{2} -\frac{1}{2} \right\rangle \quad \left( j = \frac{1}{2}, m = -\frac{1}{2} \right)$$

By default the projection is taken along the  $z$  axis. The eigenvectors are orthonormal:

$$\langle + | - \rangle = 0$$

$$\langle + | + \rangle = \langle - | - \rangle = 1$$

and form a complete basis for spin state space:

$$|+\rangle\langle +| + |-\rangle\langle -| = 1$$

So, a general spin state can be written as:

$$|\chi\rangle = c_+ |+\rangle + c_- |-\rangle$$

As for any angular momentum vector, the raising and lowering operators can be defined:

$$S_{\pm} \equiv S_x \pm iS_y$$

and have the properties

$$S_+|+\rangle = 0 \quad S_+|-\rangle = \hbar|+\rangle$$

$$S_-|+\rangle = \hbar|-\rangle \quad S_-|-\rangle = 0.$$

(Recall

$$J_+|j m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}|j m+1\rangle$$

here

$$j = \frac{1}{2}.$$

For example set

$$m = -\frac{1}{2}.$$

Then

$$S_+|\frac{1}{2} - \frac{1}{2}\rangle = \hbar\sqrt{\frac{1}{2}\frac{3}{2} + \frac{1}{2} \cdot \frac{1}{2}}|\frac{1}{2} \frac{1}{2}\rangle = \hbar|\frac{1}{2} \frac{1}{2}\rangle \quad \text{or} \quad S_+|-\rangle = \hbar|+\rangle .)$$

Having chosen  $|+\rangle$  and  $|-\rangle$  as our basis vectors, we can describe any spin state  $|\chi\rangle = c_+|+\rangle + c_-|-\rangle$  as a vector:

$$|\chi\rangle = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

In particular:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

All the spin operators  $S_+$ ,  $S_-$ ,  $S_z$  and  $S^2$  can be represented as 2x2 matrices.

*Find the  $S_z$  Matrix:*

$$S_z|+\rangle = \frac{\hbar}{2}|+\rangle \quad \text{So:} \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

This gives  $a = \frac{\hbar}{2}$  and  $c = 0$ .

Similarly

$$S_z|-\rangle = -\frac{\hbar}{2}|-\rangle \quad \text{So:} \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

This gives  $b = 0$  and  $d = -\frac{\hbar}{2}$ . Therefore (definition of  $\sigma_z$ ):

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \frac{\hbar}{2} \sigma_z$$

*Find the  $S_+$  Matrix:* In a similar way:

$$S_+|+\rangle = 0 \quad \text{So:} \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$



This gives  $a = 0$  and  $c = 0$ .

$$S_+|- \rangle = \hbar|+ \rangle \quad \text{So : } \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

This gives  $b = 1$  and  $d = 0$ . Therefore,

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

The  $S_-$  matrix turns out to be:

$$S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Now we can find  $S_x$  and  $S_y$ :

$$\begin{aligned} S_x &= \frac{1}{2}(S_+ + S_-) \quad \text{from definition of } S_+ \text{ and } S_- \\ &= \frac{1}{2}\hbar \left[ \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right] = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv \frac{\hbar}{2}\sigma_x \\ \text{and } S_y &= -\frac{i}{2}(S_+ - S_-) = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv \frac{\hbar}{2}\sigma_y \end{aligned}$$

*Pauli matrices:*

The matrices  $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  are called the Pauli matrices. We have

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}.$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Any 2x2 matrix can be written as a linear combination of the Pauli matrices and the identity matrix.

*Example:* We can apply  $S_x$  to a spin pointing in the positive  $z$  direction,  $|+ \rangle$ :

$$S_x|+ \rangle = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}|- \rangle .$$

But the resulting state represents spin pointing in the negative  $z$  direction. Therefore,  $|+ \rangle$  is not eigenvector of  $S_x$ . We cannot know the  $x$  and  $z$  component of an angular momentum vector simultaneously. Applying the  $S_x$  operator again gives

$$S_x^2|+ \rangle = \frac{\hbar}{2} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar^2}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Therefore,  $|+\rangle$  is an eigenstate of  $S_x^2$ . Similarly

$$S_y^2 |+\rangle = S_z^2 |+\rangle = \frac{\hbar^2}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Applying  $S^2$  gives

$$S^2 |+\rangle = S_x^2 + S_y^2 + S_z^2 |+\rangle = \frac{3\hbar^2}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2} \left( \frac{1}{2} + 1 \right) \hbar^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Although we cannot know the value of  $S_x$  when the particle is in the state  $|+\rangle \equiv |+\rangle_z$ , we can ask what the expectation value is, i.e., the average value after repeated measurements on equivalent particles:

$$\begin{aligned} \langle S_x \rangle &= \langle \chi | S_x | \chi \rangle \\ &= \langle + | S_x | + \rangle = (1, 0) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= (1, 0) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \end{aligned}$$

There is no polarization in the  $x$  direction in the state  $|+\rangle$ .

We can use Stern-Gerlach apparatus to polarize the beam in any direction we want. If we polarize the spin in the positive  $x$  direction, i.e.,  $|\chi\rangle = |+\rangle_x$ , how can we represent the spin state in terms of our basis  $|+\rangle_z$  and  $|-\rangle_z$ ? Let  $|+\rangle_x = (a, b)$ . Then

$$S_x |+\rangle_x = \frac{\hbar}{2} |+\rangle_x \quad \text{or} \quad \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} a \\ b \end{pmatrix}$$

Therefore, we must have  $b = a$ .

So, with the proper normalization:

$$|+\rangle_x = \frac{1}{\sqrt{2}} (|+\rangle_z + |-\rangle_z) = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

Similarly, when polarized in the negative  $x$  direction

$$|-\rangle_x = \frac{1}{\sqrt{2}} (|+\rangle_z - |-\rangle_z).$$

If the beam is polarized in the  $y$  direction we get

$$|\pm\rangle_y = \frac{1}{\sqrt{2}} (|+\rangle_z \pm i |-\rangle_z)$$

### Arbitrary Orientation of the Spin:

It can be advantageous to use spherical polar coordinates. A unit vector pointing in the direction  $(\theta, \phi)$  can be represented in cartesian coordinates as

$$\hat{u} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z} .$$

The  $u$  component of the spin is:

$$\begin{aligned} S_u &= \vec{S} \cdot \hat{u} = S_x \sin \theta \cos \phi + S_y \sin \theta \sin \phi + S_z \cos \theta \\ &= \frac{\hbar}{2} \left[ \begin{pmatrix} 0 & \sin \theta \cos \phi \\ \sin \theta \sin \phi & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \sin \theta \sin \phi \\ i \sin \theta \sin \phi & 0 \end{pmatrix} + \begin{pmatrix} \cos \theta & 0 \\ 0 & -\cos \theta \end{pmatrix} \right] \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \end{aligned}$$

What are the eigenvectors of  $S_u$ ? Those correspond to polarization in the  $+$  and  $-$  direction along the  $\hat{u}$  axis.

$$S_u |+\rangle_u = \frac{\hbar}{2} |+\rangle_u$$

$$\begin{aligned} \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} &= \frac{\hbar}{2} \begin{pmatrix} a \\ b \end{pmatrix} \\ \begin{pmatrix} \cos \theta - 1 & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta - 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} &= 0 \\ \begin{pmatrix} -\sin^2 \frac{\theta}{2} & \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{-i\phi} \\ \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{i\phi} & -\cos^2 \frac{\theta}{2} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} &= 0 \end{aligned}$$

Multiply out:

$$-a \sin^2 \frac{\theta}{2} + b \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{-i\phi} = 0$$

$$a = b \frac{\cos \frac{\theta}{2}}{\sin \frac{\theta}{2}} e^{-i\phi}$$

This gives the direction of the eigenvector in the  $(|+\rangle, |-\rangle)$  plane but not its length.

Now use the normalization condition:  $|a|^2 + |b|^2 = 1$  This gives

$$|b|^2 \frac{\cos^2 \frac{\theta}{2}}{\sin^2 \frac{\theta}{2}} + |b|^2 = 1$$

$$|b|^2 = \sin^2 \frac{\theta}{2}$$

Choose the phase to be  $\frac{\phi}{2}$  so

$$b = \sin \frac{\theta}{2} e^{i\phi/2}$$

and

$$a = \cos \frac{\theta}{2} e^{-i\phi/2}.$$

The final expression for the  $|+\rangle_u$  state is

$$|+\rangle_u = \cos \frac{\theta}{2} e^{-i\phi/2} |+\rangle_z + \sin \frac{\theta}{2} e^{i\phi/2} |-\rangle_z.$$

(Check: Choose  $\hat{u} = \hat{x}$ , then  $\theta = \frac{\pi}{2}$ ,  $\phi = 0$  and get  $|+\rangle_x = \frac{1}{\sqrt{2}} (|+\rangle_z + |-\rangle_z)$  which is correct.)

*General Spin State:*

An arbitrary spin state can be represented as

$$|\psi\rangle = \alpha |+\rangle + \beta |-\rangle.$$

We assume this vector is normalized,  $\langle \psi | \psi \rangle = 1$ , so

$$|\alpha|^2 + |\beta|^2 = 1$$

The coefficients  $\alpha$  and  $\beta$  are in general complex numbers that can be written in terms of magnitude and phase as

$$\alpha = |\alpha| e^{i \text{Arg}(\alpha)} \quad \text{and} \quad \beta = |\beta| e^{i \text{Arg}(\beta)}$$

Given that the overall phase of  $\Psi$  is arbitrary and by making use of the normalization condition above, two real numbers  $\theta$  and  $\phi$  can be used instead of  $\alpha$  and  $\beta$ . The normalization condition is satisfied if we choose a  $\theta$  such that

$$\cos \left( \frac{\theta}{2} \right) = |\alpha| \quad \text{and} \quad \sin \left( \frac{\theta}{2} \right) = |\beta|$$

Defining  $\phi$  and  $\chi$  as

$$\phi \equiv \text{Arg}(\beta) - \text{Arg}(\alpha)$$

$$\chi \equiv \text{Arg}(\beta) + \text{Arg}(\alpha)$$

we have

$$\text{Arg}(\beta) = \frac{\chi + \phi}{2}$$

$$\text{Arg}(\alpha) = \frac{\chi - \phi}{2}$$

The state can then be written as

$$|\psi\rangle = e^{i\chi/2} \left( \cos \frac{\theta}{2} e^{-i\phi/2} |+\rangle + \sin \frac{\theta}{2} e^{i\phi/2} |-\rangle \right).$$

Comparing with the  $|+\rangle_u$  expression, this is spin pointing in the  $(\theta, \phi)$  direction. This shows that any spin state can be interpreted as a vector (the spin) pointing in a definite direction  $(\theta, \phi)$ .

*Example:*

Prepare a beam of atoms with spin in the  $(\theta, \phi)$  direction. Now direct the beam into an analyzer that measures the spin along the  $x$  axis.

Find the probability of measuring  $+\frac{\hbar}{2}$ :

$${}^x P_+ = |{}_x \langle + | \psi \rangle|^2 \text{ with } |+\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$

So:

$$\begin{aligned} {}^x P_+ &= \left| \frac{1}{\sqrt{2}}(1, 1) \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\phi/2} \\ \sin \frac{\theta}{2} e^{i\phi/2} \end{pmatrix} \right|^2 \\ &= \frac{1}{2} \left( \cos^2 \frac{\theta}{2} + \sin \frac{\theta}{2} \cos \frac{\theta}{2} (e^{-i\phi} + e^{i\phi}) + \sin^2 \frac{\theta}{2} \right) \\ &= \frac{1}{2} \left( 1 + \sin \frac{\theta}{2} \cos \frac{\theta}{2} 2 \cos \phi \right) \end{aligned}$$

Find the expectation value:  $\langle S_x \rangle$

$$\begin{aligned} \langle \psi | S_x | \psi \rangle &= \frac{\hbar}{2} \begin{pmatrix} \cos \frac{\theta}{2} e^{i\phi/2}, \sin \frac{\theta}{2} e^{-i\phi/2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} e^{i\phi/2} \\ \sin \frac{\theta}{2} e^{i\phi/2} \end{pmatrix} \\ &= \frac{\hbar}{2} \left( \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{i\phi} + \cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{-i\phi} \right) \\ &= \frac{\hbar}{2} \sin \theta \cos \phi \end{aligned}$$

(Check: if  $\hat{u} = \hat{x}$ ,  $\theta = \frac{\pi}{2}$ ,  $\phi = 0$ ,  $\langle S_x \rangle = \frac{\hbar}{2}$ ). You can verify that  $\langle S_x \rangle = \frac{\hbar}{2} ({}^x P_+ - {}^x P_-)$ .

This is just the  $x$  component of a vector of length  $\frac{\hbar}{2}$  that points in the  $(\theta, \phi)$  direction. So, although any one measurement on one particle can only give  $\pm \frac{\hbar}{2}$  the average behaves like a classical angular momentum vector in  $(x, y, z)$  space.

### Larmor Precession:

In a uniform magnetic field the orientation of the spin changes periodically. Assume the uniform magnetic field is pointing in the  $\hat{z}$  direction,  $\vec{B}_0 = |\vec{B}_0| \hat{z}$ . The magnetic

moment associated with the spin,  $\vec{M} = \gamma\vec{S}$  (the proportionality constant,  $\gamma$ , is called the gyromagnetic ratio) interacts with the field. The potential energy is

$$\begin{aligned} W &= -\vec{M} \cdot \vec{B}_0 \\ &= -M_z B_0 \\ &= -\gamma B_0 S_z \end{aligned}$$

It is convenient to define  $\omega_0 \equiv -\gamma B_0$ . This quantity has the units of frequency, i.e.  $time^{-1}$ .

If we ignore the other degrees of freedom ( $x, y, z$ ) or treat them classically, then

$$H = W = \omega_0 S_z.$$

The stationary states (eigenvectors of  $H$ ) are the eigenstates of  $S_z$  since  $[H, S_z] = 0$ :

$$\begin{aligned} H|\pm\rangle &= \pm \frac{\hbar\omega_0}{2} |\pm\rangle \\ E_{\pm} &= \pm \frac{\hbar\omega_0}{2} \\ \Delta E &= \hbar\omega_0 \end{aligned}$$

However,  $S_x$  and  $S_y$  do not commute with  $H$  so  $\langle S_x \rangle$  and  $\langle S_y \rangle$  are not constants of the motion.

Let the initial direction of the spin be  $(\theta_0, \phi_0)$ , so

$$|\psi(0)\rangle = \cos \frac{\theta_0}{2} e^{-i\phi_0/2} |+\rangle + \sin \frac{\theta_0}{2} e^{i\phi_0/2} |-\rangle.$$

The time evolution of this state can be found as follows. Since the Hamiltonian is time independent, time separates from the other degrees of freedom and we can expand in the stationary states. The stationary states correspond to a certain energy,  $E_n$ , and can be written as  $|\chi_{n\tau}\rangle$ . It is possible to have more than one state with this same energy, so a second index  $\tau$  is needed to label the various states of same energy  $E_n$ . Then the time dependent state can be written as

$$|\psi(t)\rangle = \sum_n \sum_{\tau} c_{n\tau} e^{-iE_n t/\hbar} |\chi_{n\tau}\rangle.$$

The first sum is over energy levels,  $n$ , and the second sum is over states  $\tau$  with energy  $E_n$ . Here we only have two energy levels and one state for each level, so

$$\begin{aligned} |\psi(t)\rangle &= \cos \frac{\theta_0}{2} e^{-i\phi_0/2} e^{-iE_+t/\hbar} |+\rangle \\ &\quad + \sin \frac{\theta_0}{2} e^{i\phi_0/2} e^{-iE_-t/\hbar} |-\rangle \\ &= \cos \frac{\theta_0}{2} e^{-i(\phi_0+w_0t)/2} |+\rangle + \sin \frac{\theta_0}{2} e^{i(\phi_0+w_0t)/2} |-\rangle. \end{aligned}$$

In this linear combination of stationary states, the phase of the expansion coefficients changes with time. Comparing this with the form for the state with an arbitrary spin direction, we see that the state  $|\psi(t)\rangle$  corresponds to a spin pointing in a direction  $(\theta(t), \phi(t))$  with

$$\begin{aligned} \theta(t) &= \theta_0 \\ \phi(t) &= \phi_0 + w_0t. \end{aligned}$$

A calculation of the expectation values gives

$$\begin{aligned} \langle S_z \rangle_{(t)} &= \langle \psi(t) | S_z | \psi(t) \rangle = \frac{\hbar}{2} \cos \theta_0 \quad (\text{time independent}) \\ \langle S_x \rangle_{(t)} &= \langle \psi(t) | S_x | \psi(t) \rangle = \frac{\hbar}{2} \sin \theta_0 \cos(\phi_0 + w_0t) \\ \langle S_y \rangle_{(t)} &= \langle \psi(t) | S_y | \psi(t) \rangle = \frac{\hbar}{2} \sin \theta_0 \sin(\phi_0 + w_0t) \end{aligned}$$

The expectation values behave like components of a classical momentum vector in coordinate space that precesses about the  $z$  axis. This time dependence of the spin in a uniform magnetic field is called *Larmor Precession*.

### Rabi's formula

In a uniform magnetic field  $\vec{B}$  that points in an arbitrary direction, the Hamiltonian of a spin 1/2 particle is

$$H = -\gamma \vec{B} \cdot \vec{S} = -\gamma(B_x S_x + B_y S_y + B_z S_z)$$

or, using the Pauli matrices

$$= -\frac{\gamma \hbar}{2} \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}.$$

Alternatively, we can define a unit vector  $\hat{u}$  in the direction of the field,  $\vec{B} \parallel \hat{u}$ . Using polar and azimuthal angles  $(\theta, \phi)$  to give the direction, the Hamiltonian becomes

$$H = \underbrace{-\gamma|B|}_{\text{def } \omega} S_u = \frac{\omega \hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}$$

The angles  $\theta$  and  $\phi$  can be obtained from the components of the field as

$$\tan \theta = \frac{|B_{\perp}|}{|B_z|} = \frac{\sqrt{B_x^2 + B_y^2}}{|B_z|} \quad 0 \leq \theta < \pi$$

$$\tan \phi = \frac{B_y}{B_x} \quad 0 \leq \phi < 2\pi$$

The eigenstates of the Hamiltonian  $H = \omega S_u$  are  $|+\rangle_u$  and  $|-\rangle_u$  with energy  $E_+$  and  $E_-$  with an energy gap of  $\hbar\omega = E_+ - E_-$ .

A useful problem to analyze is the following: We start with a uniform magnetic field  $\vec{B}_0$  in the  $\hat{z}$  direction and the spin is initially in the  $|+\rangle$  state. Then another field  $\vec{b}$  is added perpendicular to  $\vec{B}_0$ . The question is: After how long a time is the spin in the  $|-\rangle$  state? After the field  $\vec{b}$  has been turned on the eigenstates are no longer  $|+\rangle$  and  $|-\rangle$  but rather  $|+\rangle_u$  and  $|-\rangle_u$  where  $\hat{u}$  points in the direction of the *total* field  $\vec{B} = \vec{B}_0 + \vec{b}$ .

The spin up state in the  $\hat{u}$  direction is

$$|+\rangle_u = \cos \frac{\theta}{2} e^{-i\phi/2} |+\rangle + \sin \frac{\theta}{2} e^{i\phi/2} |-\rangle.$$

The negative  $u$  direction is  $(\pi - \theta, \phi + \pi)$  so the spin down state is:

$$\begin{aligned} |-\rangle_u &= \sin \frac{\theta}{2} e^{-i\phi/2} e^{-i\pi/2} |+\rangle + \cos \frac{\theta}{2} e^{i\phi/2} e^{i\pi/2} |-\rangle \\ &= i \left( -\sin \frac{\theta}{2} e^{-i\phi/2} |+\rangle + \cos \frac{\theta}{2} e^{i\phi/2} |-\rangle \right) \end{aligned}$$

These are the stationary states. The initial state is not a stationary state

$$|\psi_{(0)}\rangle = |+\rangle$$

after the field  $\vec{b}$  is turned on. We will have Larmor precession about the total field  $\vec{B} =$



$\vec{B}_0 + \vec{b}$  with angular velocity  $\omega = -\gamma|B|$ .

If at time  $t$  the spin vector makes an angle  $\alpha$  with the  $z$  axis, then

$$|\psi(t)\rangle = \cos \frac{\alpha}{2} e^{i\beta/2} |+\rangle + \sin \frac{\alpha}{2} e^{i\beta/2} |-\rangle$$

(where  $\beta$  is some phase) and the probability of finding it in the state  $|-\rangle$  (i.e. that a measurement of the projection of the spin onto the  $z$  axis gives  $-\frac{\hbar}{2}$ ) is

$$P_{+-}(t) = \sin^2 \frac{\alpha}{2}.$$

The subscript here on the probability  $(+-)$  indicates first the initial state  $(+)$  and then the final state  $(-)$ . A trigonometric relation gives

$$\cos \alpha = \cos^2 \theta + \sin^2 \theta \cos \omega$$

so

$$P_{+-}(t) = \frac{1}{2} \sin^2 \theta (1 - \cos \omega t).$$

Recall the definition of  $\omega$

$$\omega = \frac{E_+ - E_-}{\hbar}.$$

This result is sometimes called *Rabi's Formula*.

### Magnetic Resonance:

If the field  $\vec{b}$  is time varying within the  $xy$  plane

$$\vec{b}(t) = b_0(\cos \omega t \hat{x} + \sin \omega t \hat{y})$$

representing, for example, the magnetic field in an electromagnetic wave, then the probability of the spin having gone from  $|+\rangle$  to  $|-\rangle$  will be large for certain times  $t$  if  $\omega \simeq \omega_0$  ( $\omega_0$  is the Larmor angular velocity of the  $\vec{B}_0$  field). Then even a very weak rotating field  $\vec{b}(t)$  is able to reverse the direction of the spin. This is because the applied field is in *resonance* with the Larmor precession. This can be seen in the following way: The Hamiltonian is

$$H(t) = \omega_0 S_z + \omega_1(\cos \omega t S_x + \sin \omega t S_y)$$

where  $\omega_0 \equiv -\gamma|\vec{B}_0|$  and  $\omega_1 \equiv -\gamma|\vec{b}|$ . The time dependent spin state can be represented in the  $|+\rangle$ ,  $|-\rangle$  basis as

$$\begin{aligned} |\psi(t)\rangle &= a_+(t)|+\rangle + a_-(t)|-\rangle \\ &= \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}. \end{aligned}$$

The time dependence of the state manifests itself in the time dependence of the expansion coefficients. Using the Pauli matrices for  $S_z$ ,  $S_x$ , and  $S_y$  the Hamiltonian can be written in matrix form as

$$H = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & \omega_0 \end{pmatrix}.$$

The time dependent Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

can be written in matrix form as:

$$i\hbar \begin{pmatrix} \frac{da_+(t)}{dt} \\ \frac{da_-(t)}{dt} \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{i\omega t} & \omega_0 \end{pmatrix} \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}$$

Multiplying this out gives two equations:

$$i \frac{da_+(t)}{dt} = \frac{\omega_0}{2} a_+(t) + \frac{\omega_1}{2} e^{i\omega t} a_-(t)$$

and

$$i \frac{da_-(t)}{dt} = \frac{\omega_1}{2} e^{i\omega t} a_+(t) - \frac{\omega_0}{2} a_-(t).$$

The problem is reduced to finding the functions  $a_+(t)$  and  $a_-(t)$ . The time dependence in the coefficients of the two equations can be eliminated by defining new functions

$$\begin{aligned} c_+(t) &\equiv e^{i\omega t/2} a_+(t) \\ c_-(t) &\equiv e^{i\omega t/2} a_-(t) \end{aligned}$$

This transformation corresponds to going to a coordinate system that rotates with angular velocity  $\omega$  about the z axis. Substituting this into the two equations (1) and (2) gives

$$i \frac{d}{dt} c_+(t) = -\frac{\Delta\omega}{2} c_+(t) + \frac{\omega_1}{2} c_-(t)$$

and

$$i \frac{d}{dt} c_-(t) = \frac{\omega_1}{2} c_+(t) + \frac{\Delta\omega}{2} c_-(t)$$

where  $\Delta\omega$  is defined as the difference between the frequency of the applied field and the Larmor precession in the stationary field,  $\Delta\omega \equiv \omega - \omega_0$ . By analogy with procedure used above to reduce the time dependent Schrödinger equation to two coupled differential equations in time, but now applying that procedure in reverse, we can see that this set of equations corresponds to a time dependent Schrödinger equation

$$i\hbar \frac{d}{dt} |\tilde{\psi}(t)\rangle = \tilde{H} |\tilde{\psi}(t)\rangle$$

for the state

$$|\tilde{\psi}(t)\rangle = c_+(t)|+\rangle + c_-(t)|-\rangle$$

where the Hamiltonian is time *independent*

$$\tilde{H} = \frac{\hbar}{2} \begin{pmatrix} -\Delta\omega & \omega_1 \\ \omega_1 & \Delta\omega \end{pmatrix}.$$

This Hamiltonian corresponds to a fixed, time independent field in the new rotating coordinate system. Again we ask the question: Given that the state of the spin is  $|+\rangle$  at time  $t = 0$ , what is the probability  $P_{+-}(t)$  that we will find this spin in the state  $|-\rangle$  at time  $t$ ? Since initially we have

$$|\psi(0)\rangle = |+\rangle$$

then  $a_+(0) = 1$  and  $a_-(0) = 0$ . By definition of  $c_+$  and  $c_-$  we also have

$$|\tilde{\psi}(0)\rangle = |+\rangle.$$

At time  $t$ , the probability is

$$\begin{aligned} P_{+-}(t) &= |\langle -|\psi(t)\rangle|^2 = |a_-(t)|^2 \\ &= |c_-(t)|^2 = |\langle -|\tilde{\psi}(t)\rangle|^2 \end{aligned}$$

but this is given by Rabi's formula

$$\begin{aligned} P_{+-}(t) &= \frac{1}{2} \sin^2 \theta \left( 1 - \cos \left( \frac{E_+ - E_-}{\hbar} t \right) \right) \\ &= \sin^2 \theta \sin^2 \left[ \frac{(E_+ - E_-)t}{2\hbar} \right]. \end{aligned}$$

By comparing the Hamiltonian  $\tilde{H}$  to the Hamiltonian for the previous case where the applied field  $b$  is time independent, we get

$$\sin^2 \theta = \frac{\omega_1^2}{\omega_1^2 + \Delta\omega^2}$$

and

$$\frac{E_+ - E_-}{\hbar} = \sqrt{\omega_1^2 + \Delta\omega^2}$$

So, finally

$$P_{+-}(t) = \frac{\omega_1^2}{\omega_1^2 + \Delta\omega^2} \sin^2 \left( \sqrt{\omega_1^2 + \Delta\omega^2} \frac{t}{2} \right)$$

If  $\Delta\omega = 0$  the probability becomes 1 at certain times irrespective of how large  $\omega_1$  is. That means even a very small applied time dependent field can reverse the spin if the frequency is right. This corresponds to a resonance between the applied field  $\vec{b}$  and the Larmor precession of the spin in the uniform external field. Away from resonance,  $P_{+-}$  is never large. For example, if  $\Delta\omega = 3\omega_1$ , then  $P_{+-}(t)$  is never larger than 0.1.

### Two Level Systems:

The formalism developed for a spin  $\frac{1}{2}$  particle and results such as Rabi's formula can be used whenever the quantum problem at hand is such that we can confine ourselves to two states and ignore all others. Using the two states  $|\phi_1\rangle$  and  $|\phi_2\rangle$  as a basis and taking the origin of energy scale to be  $(H_{11} + H_{22})/2$ , the Hamiltonian becomes

$$H = \begin{pmatrix} \frac{1}{2}(H_{11} - H_{22}) & H_{12} \\ H_{21} & -\frac{1}{2}(H_{11} - H_{22}) \end{pmatrix}$$

This is analogous to the Hamiltonian of a spin  $\frac{1}{2}$  in a magnetic field where

$$\begin{aligned} H_{11} - H_{22} &\leftrightarrow -\gamma\hbar B_z \\ |H_{21}| &\leftrightarrow -\gamma\hbar B_{\perp}/2 \end{aligned}$$

Some examples of such systems are: the  $H_2^+$  molecule (see CDL p. 412) and the inversion of the  $NH_3$  molecule (CDL  $G_I V$ ).

### Spinors:

We have so far been discussing spin while ignoring other degrees of freedom (or, by assuming they can be treated classically such as the translational motion in a Stern-Gerlach experiment). More generally, we need to work with a wavefunction that is a function of all coordinates, the spacial coordinates and the spin. That is, we need to incorporate spin into the wave function.

<u>Before:</u> $ \vec{r}\rangle$ $\psi(\vec{r}) = \langle \vec{r}   \psi \rangle$	<u>Now, with Spin:</u> $ \vec{r} \epsilon\rangle$ $\psi_{\epsilon}(\vec{r}) = \langle \vec{r} \epsilon   \psi \rangle$
---	--

For spin  $\frac{1}{2}$  particles, we can expand  $\psi_{\epsilon}(\vec{r})$  in terms of the two basis states for spin

$$\psi_{\epsilon}(\vec{r}) = \psi_{+}(\vec{r}) |+\rangle + \psi_{-}(\vec{r}) |-\rangle.$$

With the understanding that  $|+\rangle$  and  $|-\rangle$  is the basis, the wave function can be represented as a vector

$$[\psi](\vec{r}) = \begin{pmatrix} \psi_{+}(\vec{r}) \\ \psi_{-}(\vec{r}) \end{pmatrix}.$$

This is called a **spinor**.

If the Hamiltonian does not involve the spin, then the spinor factorizes into a spatial part and a spin part

$$\begin{aligned} [\psi](\vec{r}) &= \phi(\vec{r})\chi(\epsilon) \\ &= \phi(\vec{r}) \begin{pmatrix} c_+ \\ c_- \end{pmatrix} \end{aligned}$$

using the expansion  $\chi(\epsilon) = c_+|+\rangle + c_-|-\rangle$ .

*Example:* A free particle with polarization in the positive  $x$  direction is represented by the spinor

$$[\psi](\vec{r}) = (Ae^{i\vec{k}\cdot\vec{r}} + Be^{-i\vec{k}\cdot\vec{r}}) \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle).$$

A free particle spinor with an arbitrary spin polarization is

$$[\psi](\vec{r}) = (Ae^{i\vec{k}\cdot\vec{r}} + Be^{-i\vec{k}\cdot\vec{r}}) \frac{1}{\sqrt{2}} (c_+|+\rangle + c_-|-\rangle).$$

We can easily calculate the expectation values for the spin components, for example

$$\langle S_x \rangle = \frac{\langle \psi | S_x | \psi \rangle}{\langle \psi | \psi \rangle}$$

where

$$\langle \psi | S_x | \psi \rangle = \frac{1}{2} (c_+^* c_-^*) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

and

$$\langle \psi | \psi \rangle = \frac{1}{2} (|c_+|^2 + |c_-|^2)$$

so

$$\langle S_x \rangle = \frac{\hbar}{2} \frac{c_+^* c_- + c_-^* c_+}{|c_+|^2 + |c_-|^2}.$$

Note that if  $|\psi\rangle$  is not normalized it is necessary to divide by the norm  $\langle \psi | \psi \rangle$  so that the value of  $\langle S_x \rangle$  is between  $-\frac{\hbar}{2}$  and  $\frac{\hbar}{2}$ .

More generally, the Hamiltonian couples  $\vec{r}$  and the spin. This happens for example when the potential is different for the two spin components  $V = V_\epsilon(\vec{r})$  or the Hamiltonian explicitly involves the spin operators, such as  $\omega_0 S_z$ . When the Hamiltonian is diagonal in the  $|+\rangle, |-\rangle$  basis, the problem simplifies greatly. Then we can solve the Schrödinger equation separately for each of the two spin components to obtain the functions  $\psi_+(\vec{r})$  and

$\psi_-(\vec{r})$ . The full spinor is then found as a linear combination of those functions in such a way as to satisfy boundary conditions.

*Example:*  $H$  atom scattering from a surface with uniform magnetic field.

*Interpretation of Spinors:* Given a spinor

$$[\psi](\vec{r}) = \begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}$$

we can find the probability that the particle is in an infinitesimal volume element around  $\vec{r}$  with spin up in the  $\hat{z}$  direction as

$$\frac{dP(\vec{r}, +)}{d^3r} = |\langle \vec{r}, + | \psi \rangle|^2 = |\psi_+(\vec{r})|^2.$$

Similarly we can ask about the polarization in the positive  $\hat{x}$  direction by left multiplying by

$$\frac{1}{\sqrt{2}}(|\vec{r}, + \rangle + |\vec{r}, - \rangle)$$

instead of  $|\vec{r}, + \rangle$ . If we do not care about the spin and simply ask about the probability of finding the particle at  $\vec{r}$ , then we must sum over the spin components:

$$\frac{d^3P(\vec{r})}{dr^3} = |\psi_+(\vec{r})|^2 + |\psi_-(\vec{r})|^2$$