量子力学
Quantum mechanics

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Chapter 4

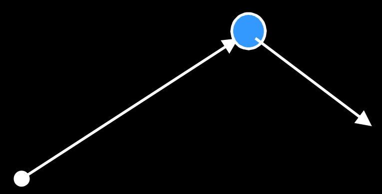
QUANTUM MECHANICS IN THREE DIMENSIONS

4.3 Angular Momentum

As we have seen, the stationary states of the hydrogen atom are labeled by three quantum numbers: *n*, *l* and *m*. The *n* is the principle quantum number which determines the energy of the state, and, *l* and *m*, are related to the orbital *angular momentum*.

In the classical theory of central forces, energy and *angular momentum* are the fundamental conserved quantities, and it plays a significant role in the quantum theory. Now we consider the *angular momentum* in quantum theory.

Classically, the angular momentum of a particle (with respect to the origin) is given by the formula



which is to say, in components,

The corresponding quantum operators are obtained by the standard prescription

In the following section we'll obtain the eigenvalues of the angular momentum by a purely *algebraic technique* reminiscent of the one we used in chapter 2 to get the allowed energies of the harmonic oscillator; it is all based on the clever exploitation of commutation relations. After that we will turn to the more difficult problem of determining the eigenfunctions.

4.3.1 Eigenvalues

(1) The momentum operators L_x, L_y , L_z and their commutation relations:

The operators L_x and L_y do not commute; in fact

$$\left[L_x, L_y\right] =$$

From the canonical commutation relations

and the other position and momentum components commute each other. So

Of course, we can calculate $[L_y, L_z]$ or $[L_z, L_x]$ as well, but there is no need to calculate these separately——we can get them immediately by cyclic permutation of the indices ($x \to y$, $y \to z$, $z \to x$):

These are the fundamental commutation relations for angular momentum; every-thing else follows from them.

Notice that L_x, L_y and L_z are incompatible observables. According to the generalized uncertainty principle,

Or

It would therefore be futile to look for states that are simultaneously eigenfunctions of L_x and L_y. *So does for other components.*

On the other hand, the square of the total angular momentum,

does commutate with the three components of *L*, for example,

Similarly, it follows, of course, that

$[L^2, L_x$

So L^2 is compatible with each component of L, and we can hope to find simultaneous eigenstates of L^2 and (say) L_z:

(2) Introduce ladder operators L_+, L_- to determine eigenvalues :

We will use a "Ladder operator" technique, very similar to the one we applied to the harmonic oscillator back in Section 2.3.1. Let

The commutator with L_z is

so

And, of course,

If f is an eigenfunction of L^2 and L_z, so

so $L_\pm f$ is an eigenfunction of L^2, with the same eigenvalue λ, and

so $L_\pm f$ is an eigenfunction of L_z with the new eigenvalue .

Therefore, as

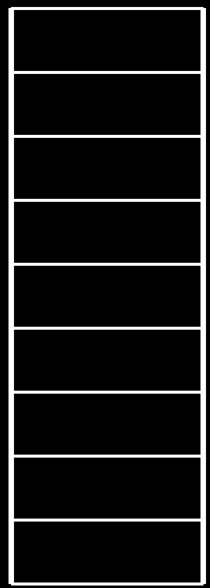
we call L_+ the "raising" operator, because it *increases* the eigenvalue of L_z by $\hbar$, and L_- the "lowering" operator, because it *lowers* the eigenvalue by $\hbar$.

For a given value of λ, then, we obtain a "ladder" of states, with each "rung" separated from its neighbors by one unit of $\hbar$ in the eigenvalue of L_z(see Figure). To ascend the ladder we apply the raising operator, and to descend, the lowering operator. But this process cannot go on forever: Eventually we're going to reach a state for which the z-component exceeds the total, and that cannot be.

There must exist a "top rung", f_t, such that

Let $l\hbar$ be the eigenvalue of L_z at this top rung (suppose):

$L_z f_t$ and



Now we calculate the following operators as

or, putting it in the other way around,

It follows that

and hence

This tells us the eigenvalue of L^2 in terms of the *maximum* eigenvalue of L_z .

Meanwhile, there is also a "bottom rung", f_b, such that

Let be the eigenvalue of L_z at this bottom rung (suppose):

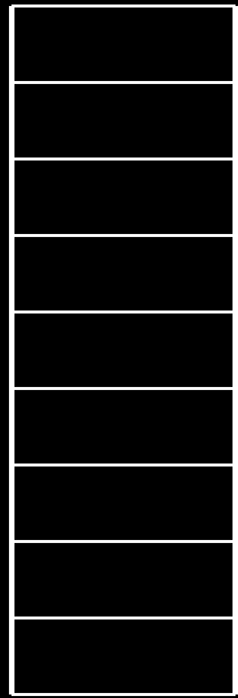
and

Then we have

and therefore

Comparing with above equation, we see that

Evidently the eigenvalues of L_z are $\mu=m\hbar$, where m goes from $-l$ to $+l$ in N integer steps. In particular, it follows that $l=-l+N$, and hence $l=N/2$, so l must be an integer or a half-integer.



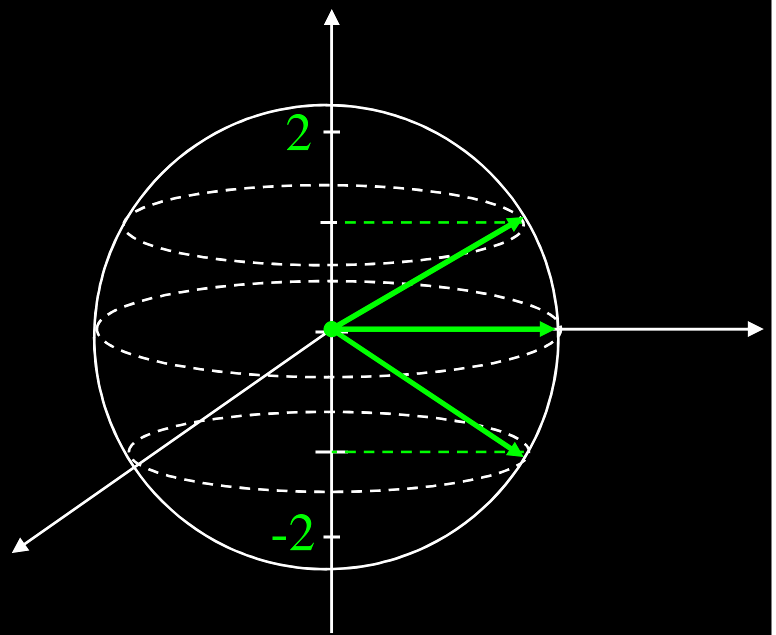
The eigenfunctions are characterized by the number l and m:

where

For a given value of l, there are $2l+1$ different values of m.

- Some people like to illustrate this result with the diagram in Figure ($l=2$). The arrows are supposed to represent possible angular momenta—in units of they all have the same length

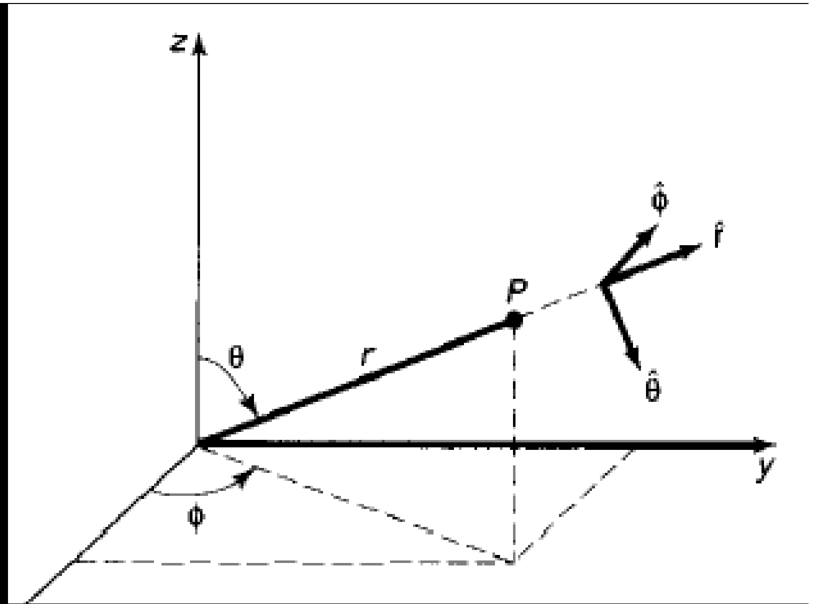
and there z components are -2,-1,0, 1,2.



4.3.2 Eigenfunctions

Prove:

First of all we need to rewrite L_x, L_y and L_z in spherical coordinates. Now, as



and the gradient ∇, in spherical coordinates, is:

meanwhile, so

But as

and hence

As in cartesian coordinates we use the relations

Thus

Evidently

and

We can also determine the raising and lowering operators:

In particular:

By using or we have

We are now to determine which is an eigenfunction of ,

But this is precisely the "angular equation". And it's also an eigenfunction of L_z, with the eigenvalue of $m\hbar$:

but this is equivalent to the azimuthal equation (Eq.4.21).

We have already solved this system of equations: The result is the spherical harmonic, .

Conclusion: Spherical harmonics are eigenfunctions of L^2 and L_z.

Recalling what we have done in Section 4.1 that we solved the Schrodinger equation by separation of variables, we have inadvertently constructed simultaneous eigenfunctions of the three commuting operators H, L^2 and L_z:

That is

Then at last we have

As

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(\right.\right.$$

We can rewrite the Schrodinger equation more compactly:

Question:

There is only one inconsistency between the functions

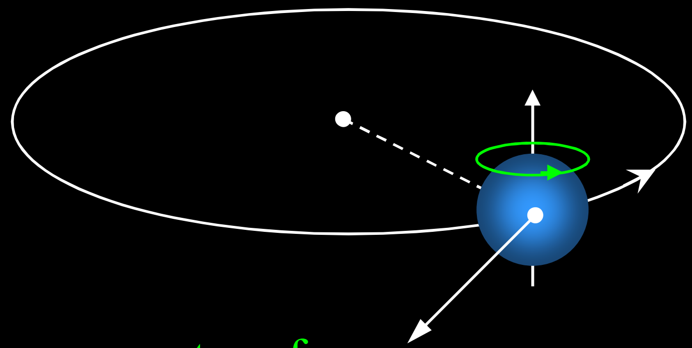
By algebraic method the angular momentum permits l to take on half-integer values, whereas separation of variables yielded eigenfunctions only for integer values. What is?

The l can be *half-integer* that is turned out to be important in the following sections. Spin!

4.4 Spin

In classical mechanics, a rigid object admits two kinds of angular momentum:

orbital angular momentum



associated with the motion of the center of mass, and ***spin***

where *I* is the *moment of inertia*, associated with the motion about the center of mass.

But, in quantum mechanics, an analogous thing happens, and there is a absolutely fundamental distinction. In addition to orbital angular momentum, associated (in the case of hydrogen) with motion of the electron around the nucleus (and described by the spherical harmonics), the electron also carries *another* form of angular momentum, which is nothing to do with motion in space (and which is not, therefore, described by any function of the position variables r, θ, Φ) but which is somewhat analogous to classical spin.

However, the electron (as far as we know) is a structureless point particle, and its spin angular momentum cannot be decomposed into orbital angular momenta of constituent parts. Suffice it to say that elementary particles carry *intrinsic* angular momentum (**S**) in addition to their "extrinsic" angular momentum (**L**).

The *algebraic* theory of spin is a carbon copy of the theory of orbital angular momentum, beginning with the fundamental commutation relations:

It follows (as before) that the eigenvectors of S^2 and S_z satisfy

and for

But this time the eigenvectors are not spherical harmonics (they are not functions of r, θ, Φ at all), and there is no a *priori* reason to exclude the half-integer values of s and m:

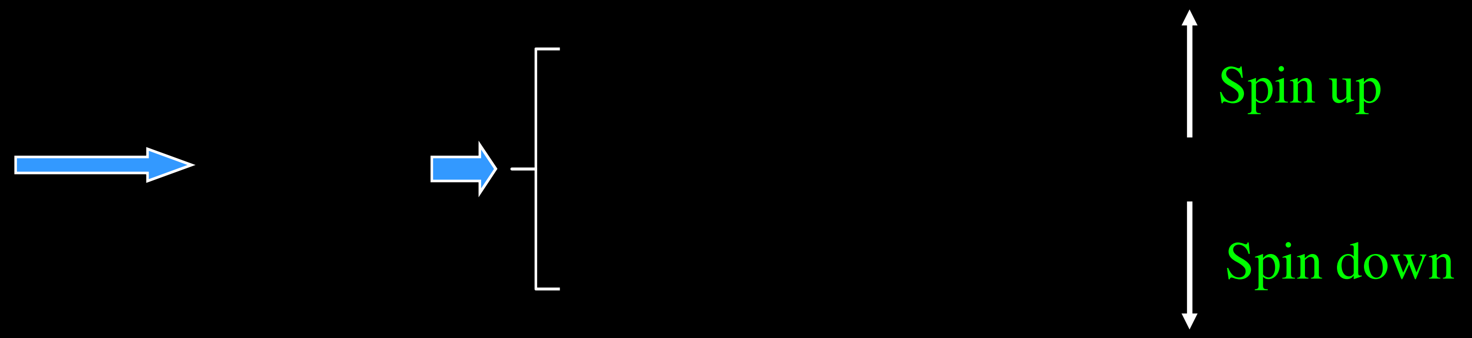
Notes:

1. It so happens, that every elementary particle has a specific and immutable value of s, which we call the spin of that particular species: pi mesons have spin 0; electrons have spin 1/2; photons have spin 1; deltas have spin 3/2; gravitons have spin 2; and so on.

2. By contrast, the orbital angular momentum quantum number l can take on any integer value you please, and will change from one to another when the system is perturbed. But s is fixed, for any given particle, and this makes the theory of spin comparatively simple.

4.4.1 Spin 1/2

By far the most important case is s=1/2, for this is the spin of the particles that make up ordinary matter (protons, neutrons, and electrons), as well as all quarks and all leptons. Moreover, once you understand spin 1/2, it is a simpler matter to work out the formalism for any higher spin. These are just two eigenstates:



Using above two states as a basis vectors, the general state of a spin-1/2 particle can be expressed as a two-element column matrix (or spinor):

with representing spin up, and for spin down.

Meanwhile, the spin operators become 2×2 matrices, which we can work out by noting their effect on χ_+ and χ_-.

By using

➡

➡

If we write S^2 as a matrix with undetermined elements, Then the first equation says

so

The second equation says

so

Finally, we have

Similarly, we write S_z as a matrix with undetermined elements, and use

We have

Mean well for "ladder operators"

so

Now , so

Since S_x, S_y and S_z all carry a factor of $\hbar/2$, it is tidier to define

where

These are the famous Pauli spin matrices. Notice that S_x, S_y S_z, and S^2 are all *hermitian* (as they should be, since they represent observables). On the other hand, S_+ and S_- are not hermitian—evidently they are not observable.

The eigenspinors of S_z are (of course)

χ_+ (eigenvalue); (eigenvalue).

Go back

If you measure S_z on a particle in the general state

you could get spin up with probability , or spin down with probability .

Since these are the only possibilities, that is (i.e. the spinor must be normalized)

But what if, instead, you chose to measure S_x? What are the possible results, and what are their respective probabilities? According to the generalized statistical interpretation, we need to know the eigenvalues and eigenspinors of S_x. The characteristic equation of S_x is

Not surprisingly, the possible value for S_x are the same as those for S_z . The eigenspinors are obtained in the usual way:

Evidently the *normalized* eigenspinors of S_x are

(eigenvalue); (eigenvalue).

As the eigenvectors of a hermitian matrix, they span the space; the generic spinor can be expressed as a linear combination of them:

Now, if you measure S_x, the probability of getting $\hbar/2$ is $1/2|a+b|^2$, and the $-\hbar/2$ probability of getting is $1/2|a-b|^2$.

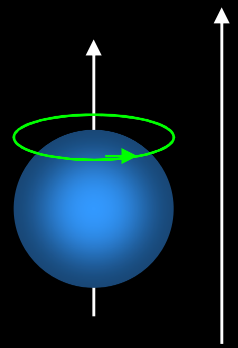
Discussion: See book on page 176.

z-component S_z ?

x-component S_x ?

4.4.2 Electron in Magnetic Field

A spinning charged particle constitutes a magnetic *dipole*.
Its *magnetic dipole moment*, $\boldsymbol{\mu}$, is proportional to its spin angular momentum, $\boldsymbol{S}$:



The proportional constant, γ, is called the *gyromagnetic ratio* and

When a magnetic dipole is placed in a magnetic field B, it experiences a *torque* , which is to line it up parallel to the field (just like a compass needle). The energy associated with this torque is

so the Hamiltonian of a spinning charged particle, at rest in a magnetic field B, is

1. Larmor precession:

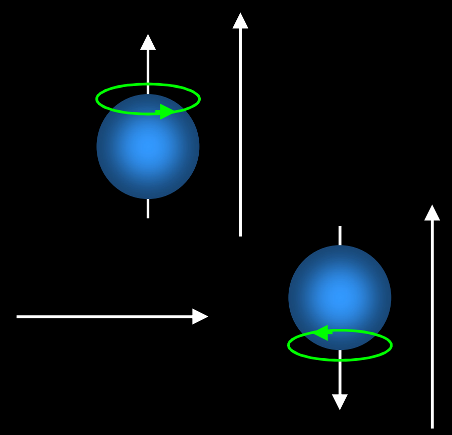
Imagine a particle of spin 1/2 at rest in a uniform magnetic field, which points in the z-direction:

The Hamiltonian, in matrix form, is

The eigenstates of H are the same as those of S_z

with the energy

with the energy



Evidently the energy is lowest when the dipole moment is parallel to the field——just as it would be classically.

Since the Hamiltonian is time-dependent, the general solution to the time-dependent Schrodinger equation,

can be expressed in terms of the stationary states:

General initial state $t=0$:

Clearly, the constant a and b are determined by the initial conditions:

with $|a|^2+|b|^2=1$.

As $|a|^2+|b|^2=1$, without essential loss of generality, we will write

where is a fixed angle whose physical significance will appear in a moment.

Thus

To get a feel for what is happening here, let's calculate the expectation value of $\boldsymbol{S}$, as a function of time:

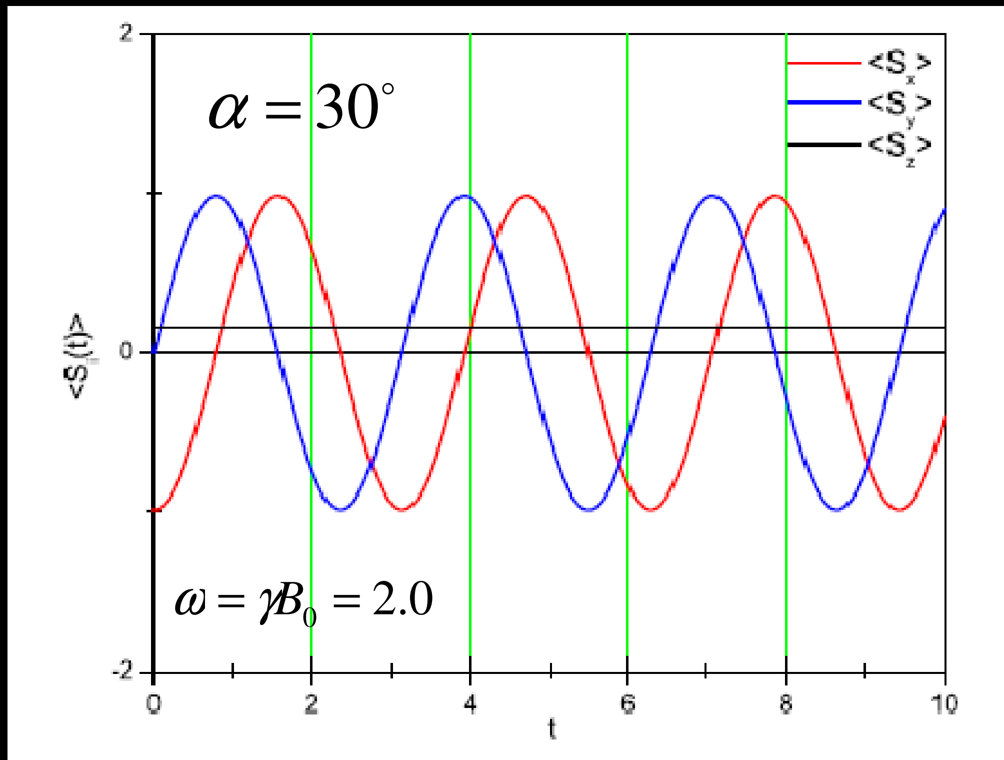
Similarly,

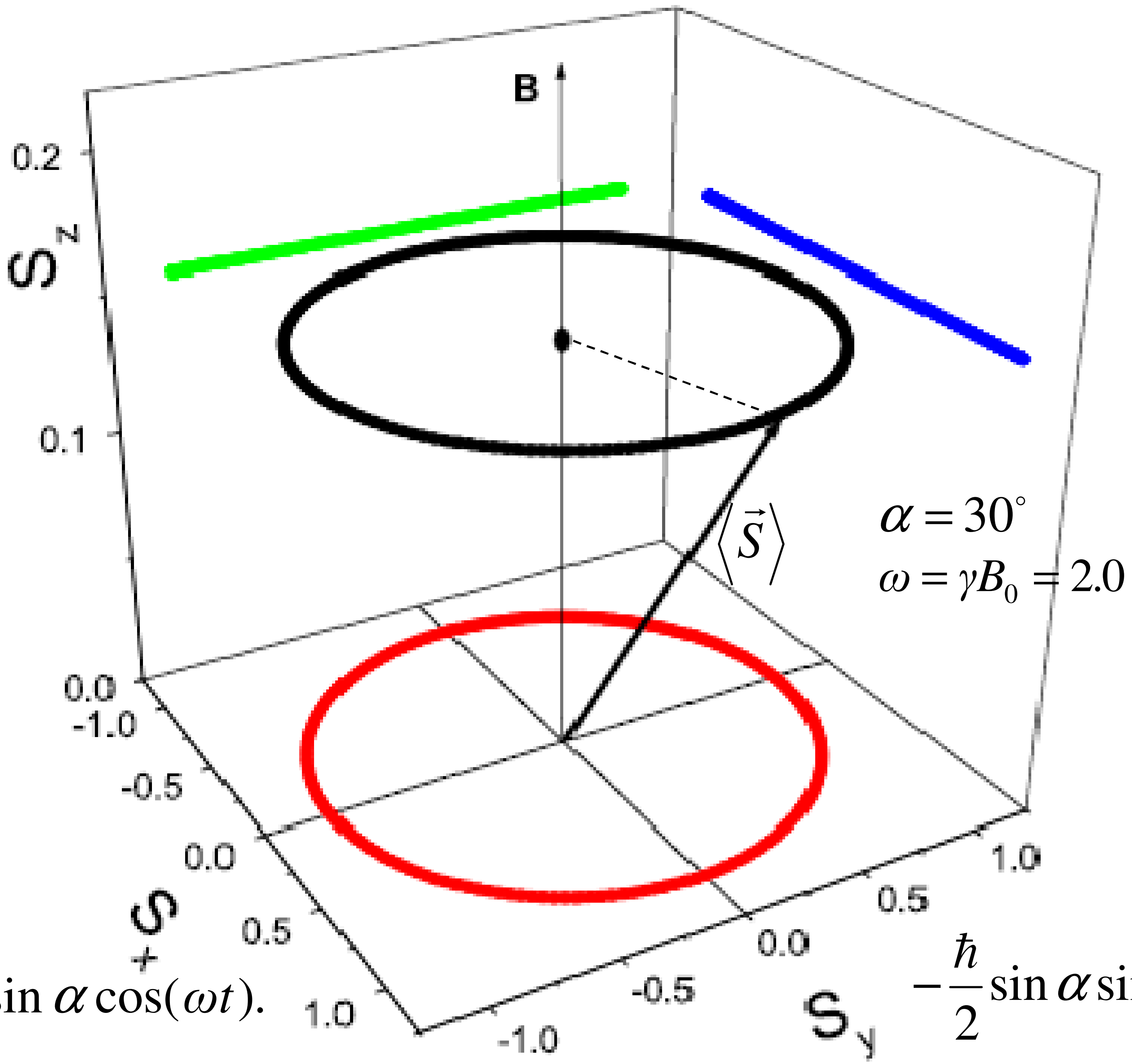
Finally, we have

$\langle S_z \rangle$

$\omega = \gamma B_0$

$\boldsymbol{\alpha}$ determine the initial state.





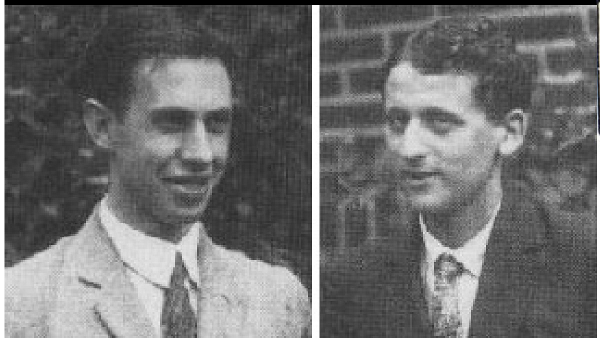
$\frac{\hbar}{2} \sin\alpha \cos(\omega t).$

$-\frac{\hbar}{2} \sin\alpha \sin(\omega t),$

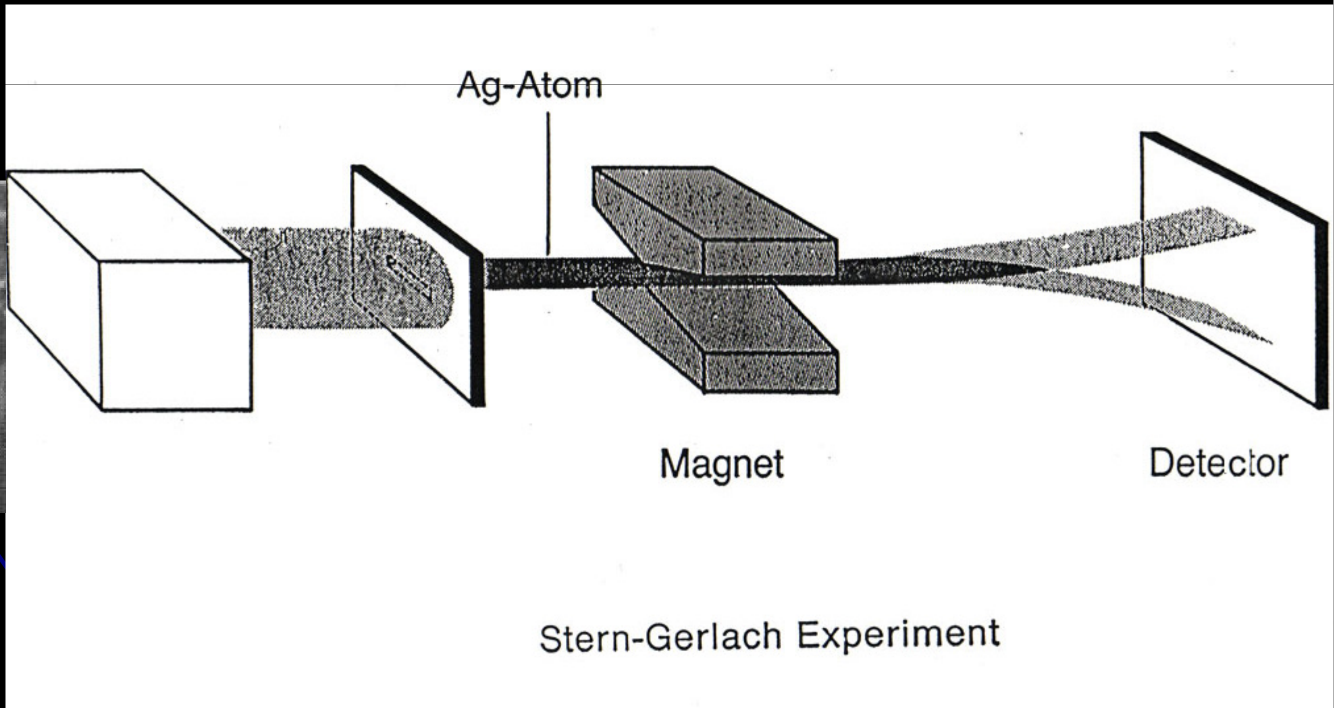
Evidently $\langle S \rangle$ is tilted at a constant angle to the z-axis, and precesses about the field at the *Larmor frequency*

just as it would classically.

2. The Stern-Gerlach experiment:

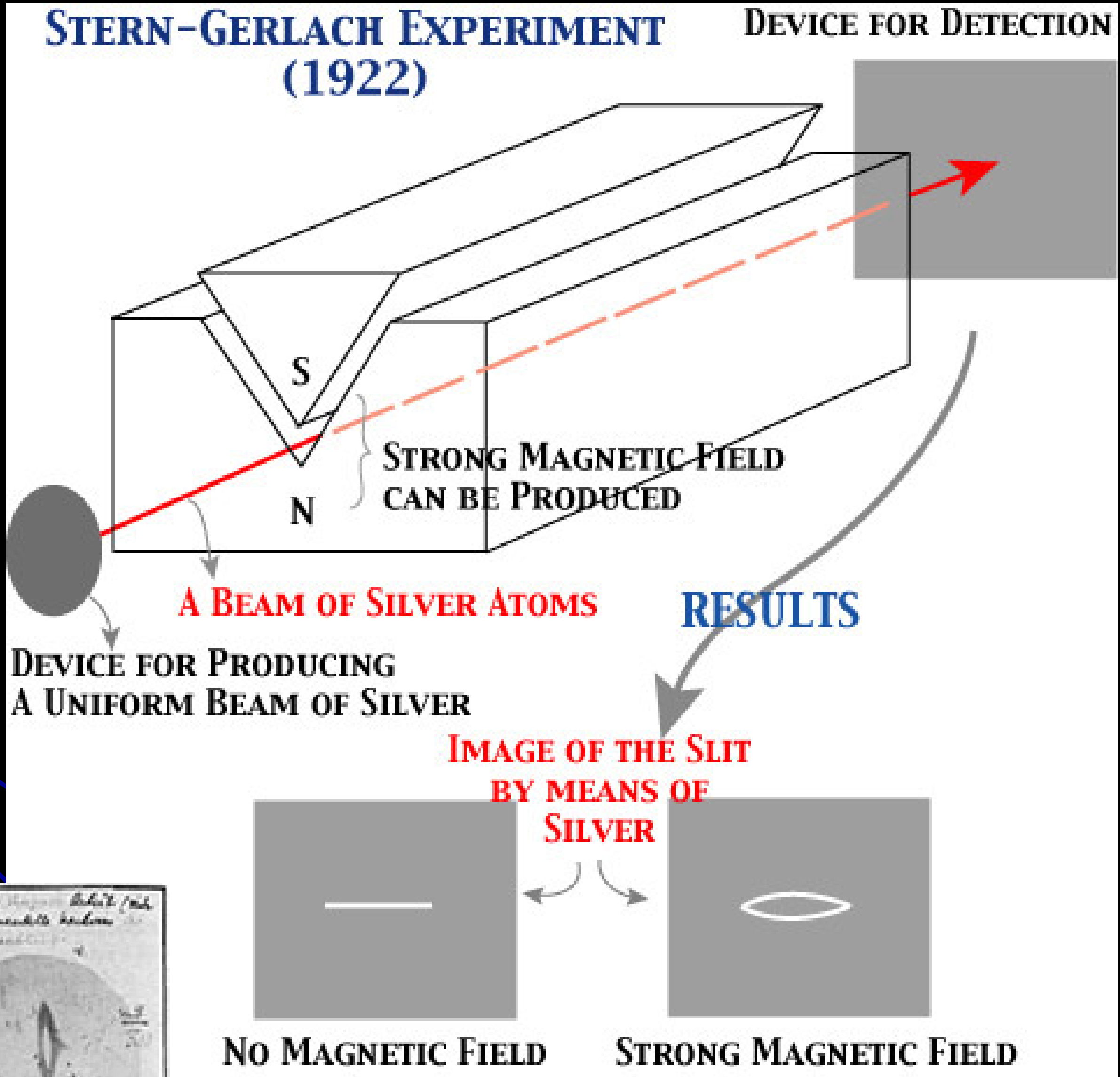


Stern-Gerlach

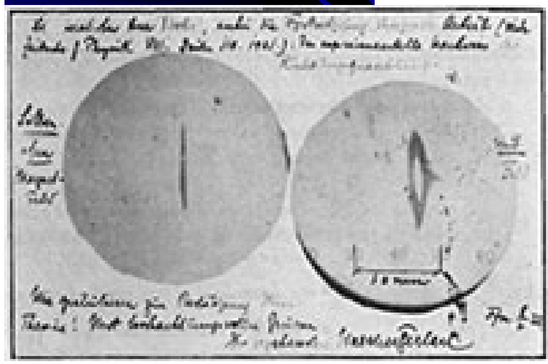


Stern-Gerlach Experiment

Stern



Gerlach



Experimental conditions:

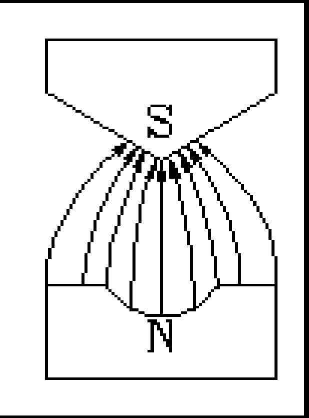
(1) A heavy neutral atomic beam — Ag atom, for example.

Using neutral atom is to avoid the large-scale deflection that would otherwise result form the Lorentz force, and heavy so we can construct localized wave packets and treat the motion in terms of classical particle trajectories.

How to determine the atomic spin: all the inner electrons of the atom are paired, in such a way that their spin and orbital momenta cancel and the net spin is simply that of the outermost—unpaired—electron. if we use silver atoms, for example, there is only one outmost unpaired electron there, so in this case $s=1/2$, and hence the beam splits in two ($2s+1=2$).

(2) Inhomogeneous magnetic field

In a inhomogeneous magnetic field, there is not only a torque which reduces the precession of the spin, but also a net force which can reduce the separation of the atoms, operating on a magnetic dipole.



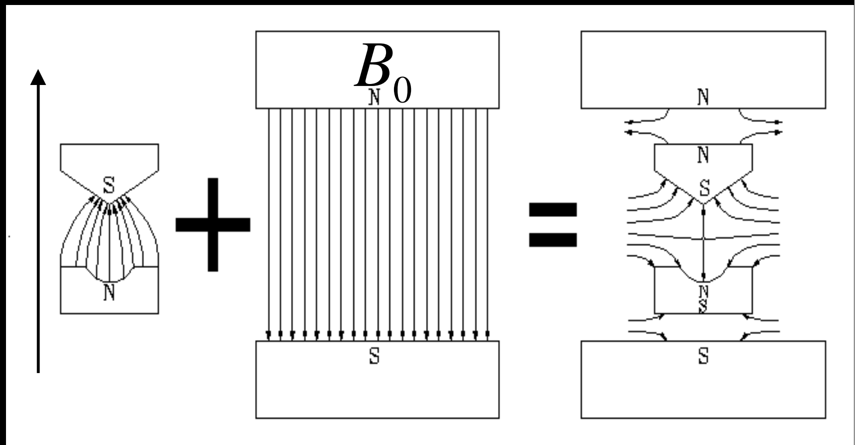
1). Classical picture theory:

In a inhomogeneous magnetic field, there is not only a torque, but also a force, on a magnetic dipole:

This force can be used to separate out particles with a particular spin orientation, as follows.

Imagine a beam of relatively heavy neutral atoms, traveling in the y direction, which passes through a region of inhomogeneous magnetic field—say,

where B_0 is a strong uniform field and the constant α describes a small deviation from homogeneity. Only the z-component of $\boldsymbol{B}$ is important, while x-component of $\boldsymbol{B}$ here is for

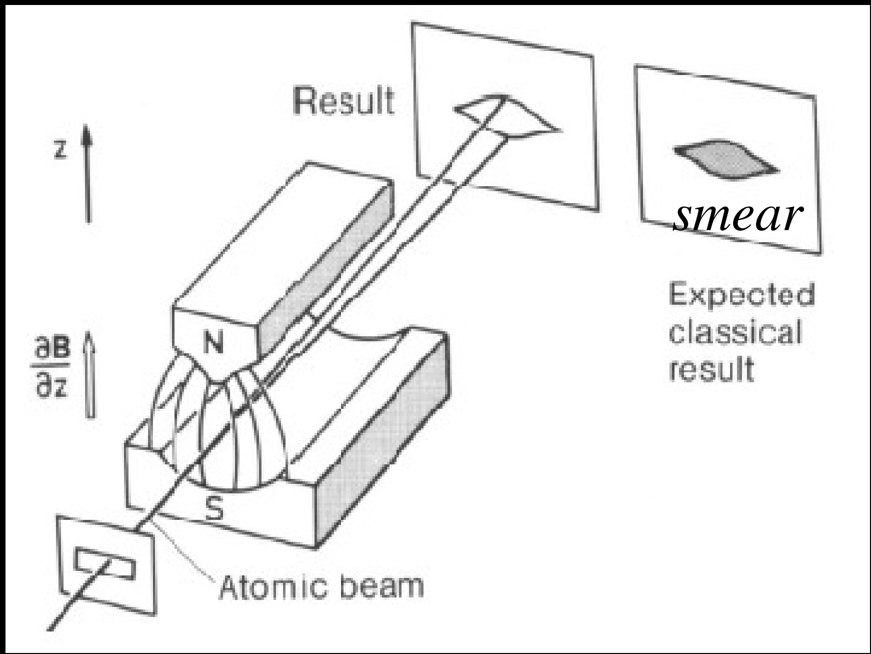


Then the force on these atoms is

But because of the Larmor precession about B_0, S_x oscillates rapidly, and *averages* to zero; the net force is in the z direction:

[4.170]

and the beam is deflected up and down, in proportion to the z component of the spin angular momentum. *Classically*, we'd expect a *smear*, but in fact the beam splits into $2s+1$ separate streams, beautifully demonstrating the quantization of angular momentum.



2). Quantum picture theory:

We examine the process from the perspective of a reference frame that moves along with the beam. In this frame the Hamiltonian starts out zero, turns on for a time *T*, and then turns off again:

Suppose the atom has spin 1/2, and starts out in the state

for

While the Hamiltonian acts, evolves in the usual way:

for

where we know

and hence it emerges in the sense

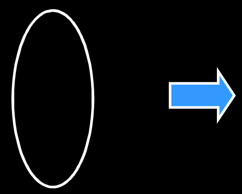
for

As the eigenfunction of momentum

corresponds to a momentum in z-direction of p, the two terms above carry momentum in the z direction; the spin up component has momentum

and it moves in the plus-z direction; the spin-down component has the opposite momentum, and it moves in the minus-z direction. Thus the beam splits in two.

Comparison: in classical point of view,



The significance of Stern-Gerlach experiment:

(1) The experiment demonstrated the spatial quantization of the quantum theory. However, this experiment was performed before the notion of *spin* was proposed; and later it turned out that the two split lines are due to the *spin* of the outermost electron of silver.

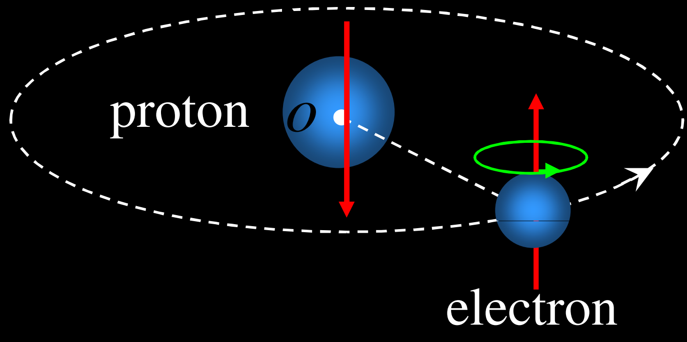
(2) Measurement of the state——spin-up state or spin-down state.

(3) Preparation of state——spin-up state or spin-down state.

4.4.3 Addition of Angular Momenta

1. Simplest example:

Suppose now that we have *two* spin-1/2 particle, the electron and the proton in the ground state of hydrogen. Each can have spin up or spin down, so there are four possibilities in all:



The first arrow refers to the electron and the second to the proton.

Question: What is the total angular momentum of the atom?

Let total angular momenta of the system is

Above composite states of the system can be represented by Applying

$S_z = S_z^{(1)} +$ on

Note that $\boldsymbol{S}^{(1)}$ acts only on χ_1, and $\boldsymbol{S}^{(2)}$ acts only on χ_2. That is

So m (the quantum number for the composite system) is just m_1+m_2:

Note that above four states are orthogonal each other (independent states).

But we get two states with m=0 ? According to general theory of angular momentum, the state can be generated by

So if we apply the lowering operator, to the state

if we apply the lowering operator, to the state

$S_{-}($

Evidently the three states are in the same set with s=1, which are:

The total s=1 and m=-1,0,1 and there have three states as

This is called the ***triplet*** combination.

Meanwhile, the other orthogonal state with m=0 carries s=0:

This is called the ***singlet*** combination.

Conclusion: *the combination of two spin-1/2 particles can carry a total spin of 1 or 0*, depending on whether they occupy the triplet or the singlet configuration. Now we prove it by getting the eigenvalue of $\boldsymbol{S}^2$.

As

Applying it on the triplet, we have

Similarly,

Then

Similarly,

The eigenvalue of S^2 on triplet is

2. General theory of addition of angular momenta:

If you combine spin s_1 with spin s_2, what total spins s can you get ? The answer is that you get every spin from $(s_1 + s_2)$ down to $(s_1 - s_2)$——or $(s_2 - s_1)$, if $s_2 > s_1$——in integer steps:

Some examples: book

The spin states for s_1 is: $|s_1\ m_1>$; The spin states for s_2 is: $|s_2\ m_2>$.

The **direct product** states for composite state is: $|s_1\ m_1> |s_2\ m_2>$.

The **combined state** for the total spin s of the system is $|s\ m>$.

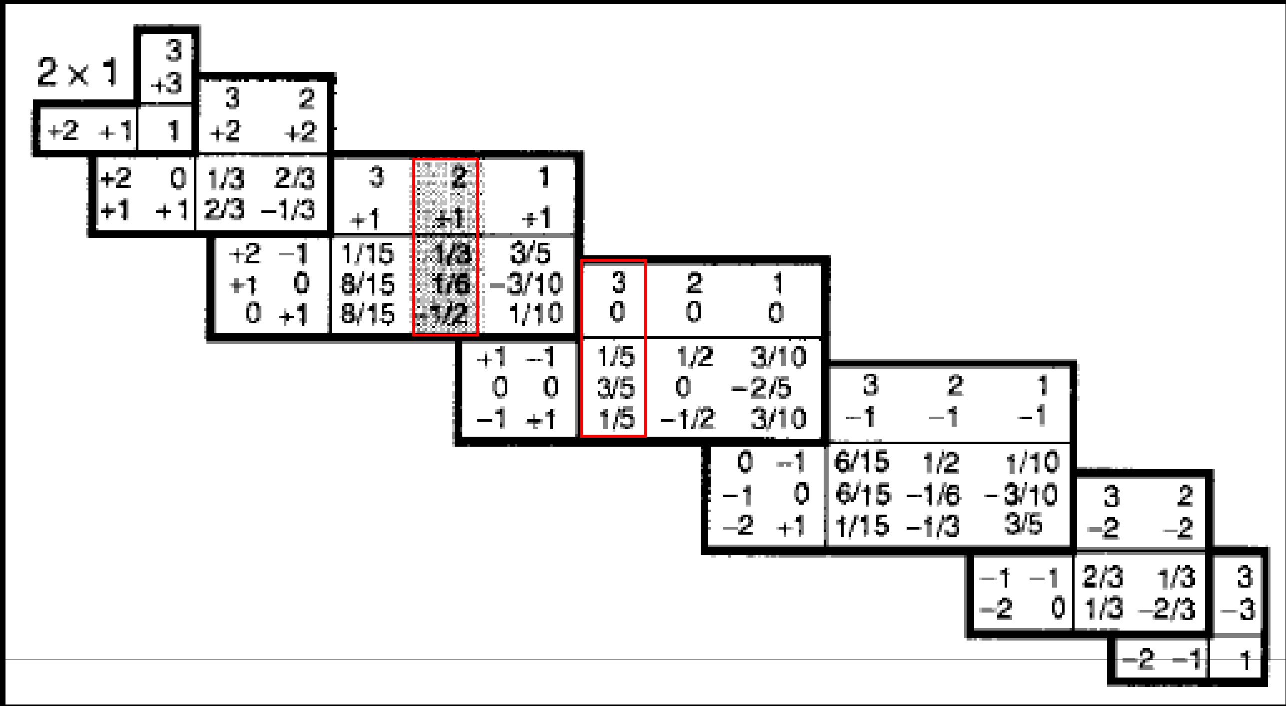
Then the combined state $|s\ m>$ with total spin s and z-component m will be some linear combination of composite states $|s_1\ m_1> |s_2\ m_2>$:

The constants are called ***Clebsch-Gordan*** coefficients.

Or reversely

See the table:

1/2 × 1/2		1			
		+1	1	0	
+1/2	+1/2	1	0	0	
+1/2	−1/2		1/2	1/2	1
−1/2	+1/2		1/2	−1/2	−1
−1/2	−1/2				1



2 × 1
3
+3
+2 +1 | 1
3 2
+2 +2
+2 0 | 1/3 2/3
+1 +1 | 2/3 −1/3
3 2 1
+1 +1 +1
+2 −1 | 1/15 1/3 3/5
+1 0 | 8/15 1/6 −3/10
0 +1 | 8/15 −1/2 1/10
3 2 1
0 0 0
+1 −1 | 1/5 1/2 3/10
0 0 | 3/5 0 −2/5
−1 +1 | 1/5 −1/2 3/10
3 2 1
−1 −1 −1
0 −1 | 6/15 1/2 1/10
−1 0 | 6/15 −1/6 −3/10
−2 +1 | 1/15 −1/3 3/5
3 2
−2 −2
−1 −1 | 2/3 1/3
−2 0 | 1/3 −2/3
3
−3
−2 −1 | 1

3/2 × 1

m_1	m_2	J = 5/2, M = +5/2
+3/2	+1	1

m_1	m_2	J = 5/2, M = +3/2	J = 3/2, M = +3/2
+3/2	0	2/5	3/5
+1/2	+1	3/5	−2/5

m_1	m_2	J = 5/2, M = +1/2	J = 3/2, M = +1/2	J = 1/2, M = +1/2
+3/2	−1	1/10	2/5	1/2
+1/2	0	3/5	1/15	−1/3
−1/2	+1	3/10	−8/15	1/6

m_1	m_2	J = 5/2, M = −1/2	J = 3/2, M = −1/2	J = 1/2, M = −1/2
+1/2	−1	3/10	8/15	1/6
−1/2	0	3/5	−1/15	−1/3
−3/2	+1	1/10	−2/5	1/2

m_1	m_2	J = 5/2, M = −3/2	J = 3/2, M = −3/2
−1/2	−1	3/5	2/5
−3/2	0	2/5	−3/5

m_1	m_2	J = 5/2, M = −5/2
−3/2	−1	1

Group theory

The composition of the direct product of two irreducible representations of the rotation group into a direct sum of irreducible representation.