### Lecture notes 13

# 13 Addition of angular momenta

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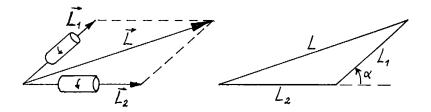
Addition of angular momenta enters the picture when we consider a system in which there is more than one contribution to the total angular momentum. If we consider e.g. a hydrogen atom there are contributions both from the spin of the electron and the orbital motion. Even in the case when the latter is zero there are two contributions to the total angular momentum, because the proton spin can of course not be neglected. We shall now see *how* these contributions to the total angular momentum "add", that is, we shall derive the rules for the "addition" of angular momenta. It turns out that the sum of several angular momenta is quantized according to the same rules that were derived in Lecture notes 11.

(8.4 in Hemmer, 6.10 in B&J, 4.4 in Griffiths)

### 12.1 Introduction

#### Classical addition of angular momenta

In classical mechanics the *total* angular momentum of two systems with angular momenta  $\mathbf{L}_1$  and  $\mathbf{L}_2$  is given by the vector sum  $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ :



Here the size  $L = |\mathbf{L}|$  of the total angular momentum can vary between  $L_1 + L_2$  and  $|L_1 - L_2|$ , depending on the angle  $(\alpha)$  between the two vectors  $\mathbf{L}_1$  and  $\mathbf{L}_2$ . Thus in classical mechanics  $L = |\mathbf{L}|$  satisfies the "triangle inequality"

$$|L_1 - L_2| \le L \le L_1 + L_2. \tag{T13.1}$$

We shall now see that the **total angular momentum** is a meaningful quantity also in quantum mechanics.

Small update October 2022 by H.G. Hugdal.

#### Quantum-mechanical addition of angular momenta

The spins of the electron and the proton in a hydrogen atom have the same size,  $|\mathbf{S}_e| = |\mathbf{S}_p| = \hbar \sqrt{3/4}$ . If we consider a hydrogen atom in the ground state, in which the orbital angular momentum iz zero, what is then the total angular momentum due to the two spins,  $|\mathbf{S}| = |\mathbf{S}_e + \mathbf{S}_p|$ ? Will this quantity vary continuously between 0 and  $2\hbar \sqrt{3/4}$ , as one would expect from the classical triangle inequality above?

The key to the *quantum-mechanical* answer to this question (which definitely is no) lies in the fact that the two spins that we want to add are compatible observables. Therefore the corresponding operators, which we may denote by  $\hat{\mathbf{S}}_1$  and  $\hat{\mathbf{S}}_2$ , commute:

$$[\hat{S}_{1i}, \hat{S}_{2j}] = 0, \quad i, j = x, y, z.$$
 (T13.2)

Since each of the operators  $\hat{\mathbf{S}}_1$  and  $\hat{\mathbf{S}}_2$  are angular-momentum operators, i.e. satisfy the angular-momentum algebra, it is then easy to see that also the operator  $\hat{\mathbf{S}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2$  is an angular-momentum operator (i.e. satisfies the angular-momentum algebra). We have e.g.

$$[\hat{S}_{x}, \hat{S}_{y}] = [\hat{S}_{1x} + \hat{S}_{2x}, \hat{S}_{1y} + \hat{S}_{2y}]$$

$$= [\hat{S}_{1x}, \hat{S}_{1y}] + [\hat{S}_{2x}, \hat{S}_{2y}] + 0 + 0$$

$$= i\hbar \hat{S}_{1z} + i\hbar \hat{S}_{2z} = i\hbar \hat{S}_{z}.$$
(T13.3)

But then our "theory of angular momenta" enters with full force. According to this theory, the possible eigenvalues of  $\hat{\mathbf{S}}^2 = (\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2$  are  $\hbar^2 s(s+1)$ , where anything but integer or half-integer quantum numbers s is excluded. In the case at hand we shall see that the possible values are s=0 and s=1. According to the measurement postulate a measurement of  $|\mathbf{S}_e + \mathbf{S}_p|$  for the hydrogen ground state must then give either 0 or  $\hbar\sqrt{2}$ , in sharp contrast to the classical triangle inequality. In the next section, we shall show why the "addition" of the two spins  $\frac{1}{2}$  must give either s=0 or s=1.

# 13.2 Addition of two spins $\frac{1}{2}$

Instead of measuring the total spin  $|\mathbf{S}_1 + \mathbf{S}_2|$  and its z-component  $S_z$ , we can choose to measure the z-components of the two spins separately. (The two spins are compatible; the four operators  $\hat{S}_{1z}$ ,  $\hat{S}_{2z}$ ,  $\hat{\mathbf{S}}_1^2$  and  $\hat{\mathbf{S}}_2^2$  all commute with each other.) Such a measurement will leave the system in one out of four states which can be represented by abstract vectors in the following way:

Here,  $|\uparrow\downarrow\rangle \equiv |\uparrow\rangle|\downarrow\rangle \equiv |\uparrow_1\rangle|\downarrow_2\rangle$  e.g. stands for a state in which spin no 1 is **up** and spinn no 2 is **down**. We then have

$$\widehat{S}_{1z}|\uparrow\downarrow\rangle = \left(\widehat{S}_{1z}|\uparrow_1\rangle\right)|\downarrow_2\rangle = \frac{1}{2}\hbar|\uparrow\downarrow\rangle, \qquad (m_1 = \frac{1}{2})$$

$$\hat{S}_{2z}|\uparrow\downarrow\rangle = |\uparrow_1\rangle \left(\hat{S}_{2z}|\downarrow_2\rangle\right) = -\frac{1}{2}\hbar |\uparrow\downarrow\rangle \qquad (m_2 = -\frac{1}{2}).$$

We also note that for this state

$$|\hat{S}_z|\uparrow\downarrow\rangle = (\hat{S}_{1z} + \hat{S}_{2z})|\uparrow\downarrow\rangle = 0 \qquad (m = m_1 + m_2 = 0).$$

Thus the four states are eigenstates also of  $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$ , with quantum numbers  $m = m_1 + m_2 = 1, 0, 0$  and -1, as indicated in the figure above.

The four above states together constitute a complete set of states for this two-spin system. Therefore they can be used as a four-dimensional basis, in terms of which any state for this system can be described. This means e.g. that the possible eigenstates  $|s,m\rangle$  of the operators  $\hat{\mathbf{S}}^2$  and  $\hat{S}_z$  for the total spin can be expanded in terms of the four basis states above, which we from now on may call the "old" states. We must expect to find altogether four such "new" states  $|s,m\rangle$ , which can be expressed as linear combinations of the old states  $|\uparrow\uparrow\rangle$ ,  $|\uparrow\downarrow\rangle$ ,  $|\downarrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$ .

The quantum numbers m found above bring us a long way towards the solution of this "mystery", telling us that it is possible to find one new state with m=1, one with m=-1 and two with m=0. Then we don't need much fantasy to guess that the "new" states are a **triplet** of states with s=1:  $|1,1\rangle$ ,  $|1,0\rangle$  and  $|1,-1\rangle$ , together with a **singlet** with s=0:  $|0,0\rangle$ .

These guesses are easily verified. Because the "old" state  $|\uparrow\uparrow\rangle$  is the only one with m=1, we must expect that this state is the upper rung in a triplet ladder, with s=1, that is, an eigenstate of  $\hat{\mathbf{S}}^2$  with eigenvalue  $2\hbar^2$ . This is verified by using equation (T11.37) from Lecture notes 11, on the form

$$\hat{\mathbf{S}}^2 = \hat{S}_z^2 + \hbar \hat{S}_z + \hat{S}_- \hat{S}_+ = \hat{S}_z^2 - \hbar \hat{S}_z + \hat{S}_+ \hat{S}_-.$$
 (T13.4)

The first of these equations gives

$$\widehat{\mathbf{S}}^{2}|\uparrow\uparrow\rangle = (\widehat{S}_{z}^{2} + \hbar\widehat{S}_{z} + \widehat{S}_{-}\widehat{S}_{+})|\uparrow\uparrow\rangle 
= (\hbar^{2} + \hbar\hbar)|\uparrow\uparrow\rangle + \widehat{S}_{-}(\widehat{S}_{1+} + \widehat{S}_{2+})|\uparrow_{1}\rangle|\uparrow_{2}\rangle 
= 2\hbar^{2}|\uparrow\uparrow\rangle, \text{ q.e.d.,}$$
(T13.5)

since  $\hat{S}_{1+}|\uparrow_1\rangle = 0$  and  $\hat{S}_{2+}|\uparrow_2\rangle = 0$ . (See the figure on page 11 in Lecture notes 12.) Thus, if we prepare the state  $|\uparrow\uparrow\rangle$  by measuring  $S_{1z}$  and  $S_{2z}$ , we have in fact at the same time prepared a state with s=1 and m=1; the upper rung in the triplet ladder is  $|1,1\rangle = |\uparrow\uparrow\rangle$ .

In the same manner we have that

$$\widehat{\mathbf{S}}^{2}|\downarrow\downarrow\rangle = (\widehat{S}_{z}^{2} - \hbar\widehat{S}_{z} + \widehat{S}_{+}\widehat{S}_{-})|\downarrow\downarrow\rangle 
= [\hbar^{2} - \hbar(-\hbar)]|\downarrow\downarrow\rangle + \widehat{S}_{+}(\widehat{S}_{1-} + \widehat{S}_{2-})|\downarrow\downarrow\rangle|\downarrow\downarrow\rangle 
= 2\hbar^{2}|\downarrow\downarrow\rangle.$$
(T13.6)

So the lower rung in the triplet ladder is  $|1,-1\rangle = |\downarrow\downarrow\rangle$ .

The "moral" so far is that the two states  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$  with "extreme" m-values (m=1 and m=-1) are also eigenstates of  $\hat{\mathbf{S}}^2$  and  $\hat{S}_z$  (in addition to being eigenstates of  $\hat{\mathbf{S}}^2$ ,  $\hat{\mathbf{S}}^2_2$ ,  $\hat{S}_{1z}$  and  $\hat{S}_{2z}$ ), and are the upper and lower rungs in a triplet ladder.

We can find the "central" rung in the triplet ladder by using the ladder operator  $\hat{S}_{-}$ . From (T11.52) we have the relations

$$\widehat{S}_{\pm}|s,m\rangle = \hbar\sqrt{(s\mp m)(s+1\pm m)}|s,m\pm 1\rangle, \tag{T13.7}$$

which provide us with the following useful formulae:

$$\widehat{S}_{-}|1,1\rangle = \hbar\sqrt{2}|1,0\rangle \tag{T13.8}$$

and [cf (T12.21)]

$$\widehat{S}_{1-}|\uparrow_1\rangle \equiv \widehat{S}_{1-}|\frac{1}{2},\frac{1}{2}\rangle = \hbar |\downarrow_1\rangle$$
 and  $\widehat{S}_{2-}|\uparrow_2\rangle = \hbar |\downarrow_2\rangle$ . (T13.9)

This gives for the central rung:

$$|1,0\rangle \stackrel{(8)}{=} \frac{1}{\hbar\sqrt{2}} \widehat{S}_{-} |1,1\rangle = \frac{1}{\hbar\sqrt{2}} (\widehat{S}_{1-} + \widehat{S}_{2-}) |\uparrow_{1}\rangle |\uparrow_{2}\rangle$$

$$= \frac{1}{\hbar\sqrt{2}} \left[ (\widehat{S}_{1-} |\uparrow_{1}\rangle) |\uparrow_{2}\rangle + |\uparrow_{1}\rangle (\widehat{S}_{2-} |\uparrow_{2}\rangle) \right]$$

$$\stackrel{(9)}{=} \frac{1}{\sqrt{2}} \left[ |\downarrow_{1}\rangle |\uparrow_{2}\rangle + |\uparrow_{1}\rangle |\downarrow_{2}\rangle \right]$$

$$\equiv \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle).$$
(T13.10)

We observe that this is a 50/50 linear combination of the "old" states with m = 0. This completes the triplet ladder.

$$\begin{array}{c|c} \hat{S}' & & \\ \hline 11,0> = \frac{1}{\sqrt{2}}(1+1>+1+1>) \\ \hline 11,-1> = 1+1> \end{array}$$

**A small exercise:** (1) Check that  $|1,0\rangle$  is normalized. (2) According to equation (T13.7),  $|1,-1\rangle = \hat{S}_{-}|1,0\rangle/(\hbar\sqrt{2})$ . Check that this formula gives the correct result. (3) If the state  $|1,0\rangle$  is prepared by a measurement of  $\mathbf{S}^2$  and  $S_z$ , what is then the probability that a new measurement of  $S_{1z}$  gives  $+\frac{1}{2}\hbar$ ?

Now it only remains to find the singlet, the state with s = m = 0 (a "ladder" with only one rung). This state too must be a linear combination of the two states  $|\uparrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$  with m = 0, while it is orthogonal to  $|1,0\rangle$  (because the quantum numbers s are different). Orthogonality is achieved simply by replacing the plus sign between the two terms by a minus sign:

$$|0,0\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\rangle|\downarrow_2\rangle - |\downarrow_1\rangle|\uparrow_2\rangle) \equiv \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).$$
 (T13.12)

**A small exercise**: Check that this state is an eigenstate of  $\hat{\mathbf{S}}^2 = \hat{S}_z^2 + \hbar \hat{S}_z + \hat{S}_- \hat{S}_+$  with eigenvalue equal to zero. [Hint:  $\hat{S}_+ = \hat{S}_{1+} + \hat{S}_{2+}$ .]

#### Conclusion and comments

- (i) By measuring both  $S_{1z}$  and  $S_{2z}$  we can prepare the two-spin system in one of the "old" states,  $|\uparrow_1\uparrow_2\rangle$ ,  $|\uparrow_1\downarrow_2\rangle$ ,  $|\downarrow_1\uparrow_2\rangle$ ,  $|\downarrow_1\downarrow_2\rangle$ . In these states  $S_{1z}$  and  $S_{2z}$  have sharp values, and so does  $S_z$ .
- (ii) For these "old" states  $\mathbf{S}^2$  is not sharp, except for  $|\uparrow_1\uparrow_2\rangle$  and  $|\downarrow_1\downarrow_2\rangle$ , which happen to be the upper and lower rungs in the triplet ladder. The reason that  $\mathbf{S}^2$  is not sharp for the other "old" states  $(|\uparrow_1\downarrow_2\rangle)$  and  $|\downarrow_1\uparrow_2\rangle)$  is that  $\hat{\mathbf{S}}^2$  does not commute with  $\hat{S}_{1z}$  and  $\hat{S}_{2z}$ .
- (iii) If we choose instead to measure  $S_z$  and  $|\mathbf{S}|$ , this spin system is prepared in one of the "new" states, either in one of the triplet states

$$|1,1\rangle = |\uparrow_1\uparrow_2\rangle,$$

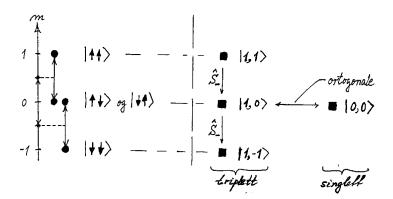
$$|1,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow_1\downarrow_2\rangle + |\downarrow_1\uparrow_2\rangle), \qquad \text{(triplet)}$$

$$|1,-1\rangle = |\downarrow_1\downarrow_2\rangle,$$

or in the singlet,

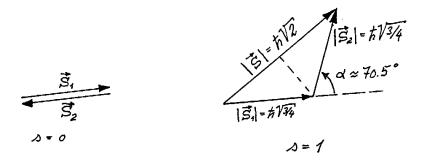
$$|0,0\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow_1 \downarrow_2 \rangle - |\downarrow_1 \uparrow_2 \rangle \right).$$
 (singlet) (T13.14)

Here  $S_{1z}$  and  $S_{2z}$  are unsharp, except in the two states  $|\uparrow_1\uparrow_2\rangle$  and  $|\downarrow_1\downarrow_2\rangle$ . The figure below gives an illustration of both the old and the new states.



Remember: The "old" states on the left are prepared by measuring  $S_{1z}$  and  $S_{2z}$  separately. The "new" states on the right are prepared by measuring the size  $|\mathbf{S}|$  and the z-component  $S_z$  of the total spin.

(iv) The singlet corresponds to  $\mathbf{S} = 0$ , which means that the two spins  $\mathbf{S}_1$  and  $\mathbf{S}_2$  are antiparallel. The triplet corresponds to an angle  $\alpha = 2\arccos\sqrt{2/3} \approx 70.5^{\circ}$  between the two vectors  $\mathbf{S}_1$  and  $\mathbf{S}_2$ . This is the closest the two spins come to being parallel.



(v) The old and the new sets of states are both perfectly applicable as basis sets for this two-spin system. We note, however, that the triplet and singlet states are respectively symmetric and antisymmetric with respect to the interchange of the particle indices 1 and 2. This is important when the two particles (fermions) are identical. Then the total state is required to be antisymmetric with respect to interchange. This can be achieved either by combining a triplet spin state with a spatial wave function that is antisymmetric with respect to interchange, or by combining the antisymmetric singlet state with a symmetric spatial wave function.

A small exercise: Express the "old" states  $|\uparrow_1\downarrow_2\rangle$  and  $|\downarrow_1\uparrow_2\rangle$  in terms of the "new" states  $|0,0\rangle$  and  $|1,0\rangle$ . If we prepare  $|\uparrow_1\downarrow_2\rangle$  by a measurement of  $S_{1z}$  and  $S_{2z}$ , what are then the possible results of a new measurement of  $S_z$  and  $S_z$ , and what are the probabilities for these results?

## 13.3 General addition of angular momenta

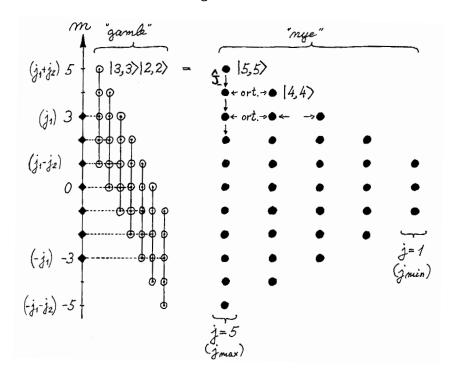
It is easy to generalize the treatment above so that we can combine any two angular momenta. If

$$|j_1, m_1\rangle$$
  $(m_1 = -j_1, -j_1 + 1, ..., j_1)$ 

is a multiplet of eigenstates of the angular-momentum operators  $\hat{\mathbf{J}}_1^2$  and  $\hat{J}_{1z}$ , and

$$|j_2, m_2\rangle$$
  $(m_2 = -j_2, -j_2 + 1, ..., j_2)$ 

is a multiplet of eigenstates of  $\hat{\mathbf{J}}_2^2$  and  $\hat{J}_{2z}$ , then we have a set of  $(2j_1+1)(2j_2+1)$  "old" states of the type  $|j_1, m_1\rangle|j_2, m_2\rangle$ . The quantum numbers  $m_1, m_2$  and  $m=m_1+m_2$  of these states are illustrated on the left in the figure below for the case  $j_1=3, j_2=2$ , which gives  $7\times 5=35$  old states.



The "extreme" values of m here are  $m = j_1 + j_2 = 3 + 2 = 5$  for the state  $|3,3\rangle|2,2\rangle$  and  $m = -j_1 - j_2 = -3 - 2 = -5$  for the state  $|3,-3\rangle|2,-2\rangle$ . It is easy to check that both these states are eigenstates of  $\hat{\mathbf{J}}^2 = (\hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2)^2$  with the quantum number  $j = j_1 + j_2 = 5$ . (In analogy with (T13.5) and (T13.6) one only needs to operate with  $\hat{\mathbf{J}}^2 = \hat{J}_z^2 \pm \hbar \hat{J}_z + \hat{J}_{\mp} \hat{J}_{\pm}$ .) It follows that these two states are respectively the top rung ( $|5,5\rangle$ ), and the bottom rung ( $|5,-5\rangle$ ) in a ladder for  $j = j_1 + j_2 = 5$ . The remaining rungs of this ladder can be found by operating with  $\hat{J}_-$ .

The next-highest rung of this ladder,  $|5,4\rangle$ , must be a linear combination of the two old states with m=4, which are  $|3,3\rangle|2,1\rangle$  and  $|3,2\rangle|2,2\rangle$ . The other linear combination of these two — orthogonal to the first one — turns out to be the top rung of a ladder for  $j=j_1+j_2-1=4$ , that is  $|4,4\rangle$ . This can be checked by operating with  $\hat{\mathbf{J}}^2$ . Then one only has to operate with  $\hat{J}_-$  to find the remaining rungs of this ladder.

We have now "spent" the old states with  $|m| \ge 4$ . For m = 3, we have three old states. The new states  $|5,3\rangle$  and  $|4,3\rangle$  are linear combinations of these three old states. The third linear combination of these three old states — orthogonal to  $|5,3\rangle$  and  $|4,3\rangle$  — is the top rung of a ladder with  $j = j_1 + j_2 - 2 = 3$ .

For m=2, there are four old states, allowing for four linear combinations. Three of these enter the ladders for j=5, 4 and 3. The fourth linear combination becomes the top rung of a ladder with j=2.

As shown in the figure, the number of old states increases to 5 for  $m = j_1 - j_2 = 1$ , meaning that also in this case a new ladder enters the picture, with  $j = j_1 - j_2$ . But this is the last time a new ladder appears; for  $m = j_2 - j_1 - 1 = 0$  the number of old states is still only five, and no new ladder enters. This way all the old states are "spent". Thus, in this example we end up with 5 multiplets with respectively 11, 9, 7, 5 and 3 new states, which are all eigenstates of  $\hat{\mathbf{J}}^2$  and  $\hat{J}_z$ . As illustrated in the figure, the number of new states equals the number of old ones.

It important to note that the use of the ladder operator  $\hat{J}_{-}$  determines the coefficients in the linear combinations, where the new states are expressed in terms of the old ones.

We saw an example of this in the addition of two spins  $\frac{1}{2}$ . These coefficients are called Clebsch–Gordan coefficients.

This example illustrates the general rules for the addition of two angular momenta, which are: When  $j_1$  and  $j_2$ " are "added", the maximal and minimal values of j are

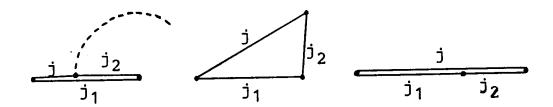
$$j_{\text{max}} = j_1 + j_2,$$
 $j_{\text{min}} = |j_1 - j_2|,$ 
(T13.15)

and the allowed j-values in this interval are

$$j = |j_1 - j_2|, |j_1 - j_2| + 1, \dots, j_1 + j_2.$$
 (T13.16)

We note that if both  $j_1$  and  $j_2$  are half-integral, or if both are integers, then the possible quantum numbers j are integers. In the opposite case, when when either  $j_1$  or  $j_2$  is half-integral while the other one is an integer, the resulting j-values become half-integral. Note also that it is the *quantum numbers* that enter the triangular inequality this time (not the sizes  $|\hat{\mathbf{J}}_1|$  and  $|\hat{\mathbf{J}}_2|$ , as we had in the classical case):

$$|j_1 - j_2| \le j \le j_1 + j_2.$$
 (triangular inequality) (T13.17)



This method can easily be generalized to more than two angular momenta. One starts with combining  $J_1$  and  $J_2$ . Then the sum  $J_{12}$  of these is combined with  $J_3$ , etc.

### 13.4 Commutation rules

Let us summarize the commutation rules for the two angular momenta that were added. In analogy with (T13.2), the two operators  $\hat{\mathbf{J}}_1$  and  $\hat{\mathbf{J}}_2$  commute. Since the three operators  $\hat{\mathbf{J}}_1$ ,  $\hat{\mathbf{J}}_2$  and  $\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$  all satisfy the angular-momentum algebra, it follows in the usual way that

$$[\widehat{\mathbf{J}}_1^2, \widehat{\mathbf{J}}_1] = 0, \qquad [\widehat{\mathbf{J}}_2^2, \widehat{\mathbf{J}}_2] = 0 \quad \text{and} \quad [\widehat{\mathbf{J}}^2, \widehat{\mathbf{J}}] = 0.$$

It should be noted that also  $\hat{\mathbf{J}}_1^2$  and  $\hat{\mathbf{J}}_2^2$  commute with  $\hat{\mathbf{J}}^2$  and  $\hat{J}_z$ :

$$[\hat{\mathbf{J}}^2, \hat{\mathbf{J}}_1^2] = [\hat{\mathbf{J}}^2, \hat{\mathbf{J}}_2^2] = 0, \qquad [\hat{J}_z, \hat{\mathbf{J}}_1^2] = [\hat{J}_z, \hat{\mathbf{J}}_2^2] = 0.$$

[Show this by using that  $\hat{\mathbf{J}}^2 = \hat{\mathbf{J}}_1^2 + \hat{\mathbf{J}}_2^2 + 2\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2$ .] Thus, in the "new" states  $|j,m\rangle$ , not only  $\mathbf{J}^2 = \hbar^2 j(j+1)$  and  $J_z = \hbar m$  are sharp, but also  $\mathbf{J}_1^2 = \hbar^2 j_1(j_1+1)$  and

 $J_2^2 = \hbar^2 j_2(j_2 + 1)$ . It is customary to state that  $j_1$  and  $j_2$  are "good quantum numbers" in the new states, in addition to j and m.

We should also note that the "coupling term"  $\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2$  has sharp values in the "new" states. Using the relation  $\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2 = \frac{1}{2}(\hat{\mathbf{J}}^2 - \hat{\mathbf{J}}_1^2 - \hat{\mathbf{J}}_2^2)$ , we find that this coupling term commutes with all the operators  $\hat{\mathbf{J}}_1^2$ ,  $\hat{\mathbf{J}}_2^2$ ,  $\hat{\mathbf{J}}_2^2$  and  $\hat{\mathbf{J}}_2$ :

$$[\widehat{\mathbf{J}}_1 \cdot \widehat{\mathbf{J}}_2, \widehat{\mathbf{J}}_1^2] = [\widehat{\mathbf{J}}_1 \cdot \widehat{\mathbf{J}}_2, \widehat{\mathbf{J}}_2^2] = [\widehat{\mathbf{J}}_1 \cdot \widehat{\mathbf{J}}_2, \widehat{\mathbf{J}}^2] = [\widehat{\mathbf{J}}_1 \cdot \widehat{\mathbf{J}}_2, \widehat{\mathbf{J}}_z] = 0.$$
 (T13.18)

And for a state with quantum numbers  $j, m, j_1$  and  $j_2$  we then have that

$$\mathbf{J}_1 \cdot \mathbf{J}_2 = \frac{1}{2} (\mathbf{J}^2 - \mathbf{J}_1^2 - \mathbf{J}_2^2) = \frac{1}{2} \hbar^2 [j(j+1) - j_1(j_1+1) - j_2(j_2+1)]$$
 (T13.19)

is sharp.

On page 4 we stressed that  $\hat{\mathbf{S}}^2$  does not commute with  $\hat{S}_{1z}$  and  $\hat{S}_{2z}$ . This is shown as follows:

$$[\hat{\mathbf{J}}^{2}, \hat{J}_{1z}] = [\hat{\mathbf{J}}_{1}^{2} + \hat{\mathbf{J}}_{2}^{2} + 2(\hat{J}_{1x}\hat{J}_{2x} + \hat{J}_{1y}\hat{J}_{2y} + \hat{J}_{1z}\hat{J}_{2z}), \hat{J}_{1z}]$$

$$= 0 + 0 + 2[\hat{J}_{1x}, \hat{J}_{1z}]\hat{J}_{2x} + 2[\hat{J}_{1y}, \hat{J}_{1z}]\hat{J}_{2y} + 0$$

$$= -2i\hbar \hat{J}_{1y}\hat{J}_{2x} + 2i\hbar \hat{J}_{1x}\hat{J}_{2y} = 2i\hbar (\hat{\mathbf{J}}_{1} \times \hat{\mathbf{J}}_{2})_{z}.$$
(T13.20)

This can be generalized to

$$[\hat{\mathbf{J}}^2, \hat{\mathbf{J}}_1] = 2i\hbar(\hat{\mathbf{J}}_1 \times \hat{\mathbf{J}}_2), \tag{T13.21}$$

and then you will probably be able to argue that

$$[\hat{\mathbf{J}}^2, \hat{\mathbf{J}}_2] = -2i\hbar(\hat{\mathbf{J}}_1 \times \hat{\mathbf{J}}_2). \tag{T13.22}$$

From  $\hat{\mathbf{J}}^2 = \hat{\mathbf{J}}_1^2 + \hat{\mathbf{J}}_2^2 + 2\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2$  it then follows that

$$[\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2, \hat{\mathbf{J}}_1] = i\hbar(\hat{\mathbf{J}}_1 \times \hat{\mathbf{J}}_2)$$
 and  $[\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2, \hat{\mathbf{J}}_2] = -i\hbar(\hat{\mathbf{J}}_1 \times \hat{\mathbf{J}}_2),$  (T13.23)

so that

$$[\widehat{\mathbf{J}}_1 \cdot \widehat{\mathbf{J}}_2, \widehat{\mathbf{J}}] = 0. \tag{T13.24}$$

Well, this was quite a few formulae, but it may be practical to have them collected this way, for possible future reference.

## 13.5 Addition of orbital angular momentum and spin

An important example (e.g. if we want to study the hydrogen atom more closely) is the addition of the orbital angular momentum L and the spin S of the electron:

$$\mathbf{J} = \mathbf{L} + \mathbf{S}.\tag{T13.25}$$

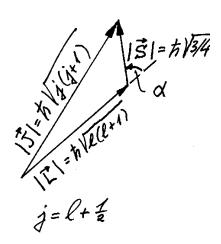
The triangular inequality (T13.17) then gives half-integral values for the quantum number j for the total angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ :

$$|l - \frac{1}{2}| \le j \le l + \frac{1}{2}.$$

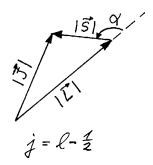
For l=0, we have  $\mathbf{J}=\mathbf{S}$  and  $j=s=\frac{1}{2}$ , so that we have two states, with  $J_z=\hbar m=\pm\frac{1}{2}\hbar$ . (Here, the magnetic quantum number m denotes the z-component of the total angular momentum.)

For  $l \ge 1$  we have two possible values for j, namely  $j = l + \frac{1}{2}$  and  $j = l - \frac{1}{2}$ .

 $\underline{j = l + \frac{1}{2}}$ : In this case **L** and **S** are as "parallel" as they can possibly be (for a given  $\underline{l}$ ). As illustrated in the figure, the angle  $\alpha$  between **L** and **S** then is not equal to zero:



 $\underline{j} = l - \frac{1}{2}$ : In this case **L** and **S** are as "antiparallel" as they can possibly be (for a given l):



In both these cases, j and l are good quantum numbers. This means that the angle  $\alpha$  between  $\mathbf{L}$  and  $\mathbf{S}$  can be calculated by means of the relation  $\mathbf{J}^2 = \mathbf{L}^2 + 2\mathbf{L}\cdot\mathbf{S} + \mathbf{S}^2$ , which gives

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2} (\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) = \frac{1}{2} \hbar^2 [j(j+1) - l(l+1) - 3/4].$$
 (T13.26)

This relation is a special case of (T13.19).

### 13.6 Addition of several angular momenta

The rules given above can also be used when there are more than two contributions to the total angular momentum of a system:

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3 + \cdots.$$

We may then start by combining  $J_1$  and  $J_2$  to  $J_{12} = J_1 + J_2$ . The possible quantum numbers  $j_{12}$  are then limited by the triangular inequality:

$$|j_1 - j_2| \le j_{12} \le j_1 + j_2.$$

We continue by combining  $J_{12}$  with  $J_3$ , and again use the triangular inequality. Continuing this process, we end up finding all possible values of the resulting quantum number j. An example is

#### Nuclear spin

With the exception of ordinary hydrogen, all atomic nuclei consist of Z protons and N = A - Z neutrons, where A is the nucleon number. The total angular momentum of a nucleus  ${}_{Z}^{A}X$  is called the nuclear spin and is denoted by an angular-momentum (spin) quantum number I. Thus, a single proton or a single neutron has  $I = \frac{1}{2}$ .

Let us now see what the rules for the addition of angular momenta have to say about the spin quantum number I of the "next" nucleus, the **deuteron** — the stable nucleus of **deuterium**,  ${}_{1}^{2}H$ , "heavy" hydrogen.

There are in principle three contributions to the total angular momentum  $\mathbf{I}$  (the spin) of the deuteron. These are the spins  $\mathbf{S}_p$  and  $\mathbf{S}_n$  of the proton and the neutron and a possible orbital angular momentum  $\mathbf{L}$  of the proton-neutron system:

$$\mathbf{I} = \mathbf{S}_n + \mathbf{S}_n + \mathbf{L}.$$

If we first imagine the two spins combined to  $\mathbf{S} = \mathbf{S}_p + \mathbf{S}_n$ , then this can result either in a triplet, characterized by the quantum number S=1, or a singlet with S=0. Thus we have two possibilities for the spin. Furthermore, from the addition rules for angular momenta we can not rule out the possibility that the neutron-proton system in its ground state has a non-zero orbital angular momentum, characterized by an integer quantum number L. When this is combined either with S=0 or S=1, it follows that the deuteron must have an integer quantum number L. This is as far as the addition rules can take us.

Experimentally it turns out that the spins of the proton and the neutron together form a triplet, S=1, while the resulting angular-momentum quantum number of the deuteron is I=1 (spin 1). The addition rules then limit the orbital angular-momentum quantum number to the values L=0,1,2. (All these can be combined with S=1 to the resultant I=1.) Here it turns out that L=1 is excluded (for reasons that we cannot enter into here). Then two possibilities remain, one with L=0 and one with L=2. Experimentally it turns out that the deuteron is in a superposition of these two states; L=0 is the dominating contribution, but there is also a small admixture of L=2, which results in a ground state for the deuteron deviating slightly from being spherically symmetric. This deviation is an experimental fact. <sup>2</sup>

From the discussion above, we understand that the spin quantum number (I) for a heavier nucleus must be an integer for a nucleus with even nucleon number A and half-integral for a nucleus with odd A.

Of the nuclei with even A it turns out that almost all have I = 0. The exceptions are nuclei for which both N and Z are odd. In addition to the deuteron  ${}_{1}^{2}$ H (I = 1), there are only a few such nuclei which are stable, two of which are  ${}_{3}^{6}$ Li (I = 1) and  ${}_{7}^{14}$ N (I = 1). But

$$|\mathbf{S}| = \hbar \sqrt{S(S+1)}, \qquad |\mathbf{L}| = \hbar \sqrt{L(L+1)}.$$

It is also usual to use the capital letters S,P,D,F,G,H for states with L = 0, 1, 2, 3, 4, 5, in analogy with the symbols s,p,d,f,g,h used for one-particle states with l = 0, 1, 2, 3, 4, 5.

<sup>2</sup>It may perhaps be somewhat confusing to learn that the ground state does not have a sharply defined orbital angular momentum. This has to do with the fact that the strong nuclear force, which provides the binding, is described by a model with a non-central potential. Then  $\hat{\mathbf{L}}$  does not commute with the Hamiltonian operator, and L is not a so-called "good quantum number".

<sup>&</sup>lt;sup>1</sup>When the spins or orbital angular momenta of several particles are added, it is customary to use capital letters for the quantum numbers,

there are of course many *unstable* "odd-odd" nuclei. An example is the cobalt isotope  $^{60}_{27}$ Co with a life-time of around five years, which has I=5.

Examples of nuclei with odd nucleon numbers are the iron isotopes  ${}_{26}^{55}$ Fe (I=3/2,  $\tau=2.7$  years) and  ${}_{26}^{57}$ Fe ( $I=\frac{1}{2}$ , stable), and the stable cobalt isotope  ${}_{27}^{59}$ Co, which has I=7/2. Another example is the relatively rare helium isotope  ${}_{2}^{3}$ He (helium-3) which has  $I=\frac{1}{2}$ .

From what was stated above it follows that all nuclei for which both Z and N are even have spin zero (I=0). An example is the  $\alpha$  particle, the nucleus of  ${}_{2}^{4}$ He.

### Resulting spin, orbital angular momentum and total angular momentum for atomic electrons

As an example we may consider carbon, with the electron configuration  $1s^22s^22p^2$  in the ground state. The spins and the orbital angular momenta in the closed 1s and 2s shells both add up to zero. Therefore, the quantum numbers S, P and J for the total spin, the total orbital angular momentum and the total angular momentum of the six electrons in carbon are determined by the two 2p electrons.

For the two spins there are two possibilities: They can either form a singlet (S=0) or a triplet (S=1). If they are in the singlet state, we remember from the explicit construction of this state that it it is antisymmetric with respect to interchange of the two electrons. The Pauli principle then requires that the spatial state of the two electrons is symmetric. (We remember that the "total" state of the two identical electrons must be antisymmetric with respect to interchange of the particle indices, according to Pauli's exclusion principle.) Carrying through the coupling of the spatial states with  $l_1=1$  and  $l_2=1$  explicitly, one finds (cf exercise) that the resulting spatial states for L=1 are antisymmetric, while the states for L=0 and L=2 are symmetric with respect to interchange. Thus the states with L=0 and L=2 can be combined with the singlet spin state. The resulting total states are denoted respectively by

$$^{1}S_{0}$$
 and  $^{1}D_{2}$ .

Here the upper index gives the spin multiplicity 2S + 1. The letters S and D signify that the total orbital angular momentum quantum number L is respectively zero and 2. The lower index is the quantum number J, which here equals L, since S = 0. Thus the notation is

$$^{2S+1}(L-\text{letter})_J$$
.

The other possibility is that the spins form a triplet (S=1) (which is symmetric with respect to interchange). The only possibility for the orbital quantum number L then is L=1, so that the state is characterized by  ${}^3\mathrm{P}_J$ . On combining S=1 and L=1 we have three possibilities for the quantum number J of the total angular momentum: J=0,1,2. Experiments show that the lowest energy for the carbon atom (and hence the ground state) is obtained when S=1, L=1 and J=0. So, the ground state for carbon can be denoted by  ${}^3\mathrm{P}_0$ .

The table below shows the configuration and the resulting quantum numbers L, S and J for a selection of elements. Here we see that helium, neon and all the other noble gases have  ${}^{1}S_{0}$ , that is a total spin S=0, total orbital angular momentum L=0 and hence also total angular momentum J=0. In view of this, it is perhaps not very strange to find that the alkali metals sodium and potassium etc, with one electron in an s-state outside filled shells, get the same quantum numbers as hydrogen, namely  ${}^{2}S_{1/2}$ .

# ${\bf Ground\text{-}state}\ {\bf configuration}\ {\bf for}\ {\bf some}\ {\bf elements}$

| Z  | Element | Configuration                                 | Symbol                   |
|----|---------|---|--------------------------|
| 1  | Н       | 1s  | $^{2}S_{1/2}$            |
| 2  | Не      | $(1s)^2$                                      | $^{1}\mathrm{S}_{0}$     |
| 3  | Li      | [He](2s)                                      | ${}^{2}\mathrm{S}_{1/2}$ |
| 4  | Be      | $[\mathrm{He}](2\mathrm{s})^2$                | $^{1}\mathrm{S}_{0}$     |
| 5  | В       | $[\mathrm{He}](2\mathrm{s})^2(2\mathrm{p})$   | ${}^{2}\mathrm{P}_{1/2}$ |
| 6  | С       | $[\mathrm{He}](2\mathrm{s})^2(2\mathrm{p})^2$ | $^{3}P_{0}$              |
| 7  | N       | $[\mathrm{He}](2\mathrm{s})^2(2\mathrm{p})^3$ | $^4\mathrm{S}_{3/2}$     |
| 8  | О       | $[\mathrm{He}](2\mathrm{s})^2(2\mathrm{p})^4$ | $^3\mathrm{P}_2$         |
| 9  | F       | $[\mathrm{He}](2\mathrm{s})^2(2\mathrm{p})^5$ | ${}^{2}\mathrm{P}_{3/2}$ |
| 10 | Ne      | $[\mathrm{He}](2\mathrm{s})^2(2\mathrm{p})^6$ | $^{1}\mathrm{S}_{0}$     |
| 11 | Na      | [Ne](3s)                                      | $^{2}S_{1/2}$            |
|    |         |   |                          |