

# Chapter 16

## Angular Momentum



Apart from the Hamiltonian, the angular momentum operator is one of the most important Hermitian operators in quantum mechanics. In this chapter we consider its eigenvalues and eigenfunctions in more detail.

We begin this chapter with the consideration of the orbital angular momentum. This gives rise to a general definition of angular momenta. We derive the eigenvalue spectrum of the orbital angular momentum with an algebraic method. After a brief presentation of the eigenfunctions of the orbital angular momentum in the position representation, we outline some concepts for the addition of angular momenta.

### 16.1 Orbital Angular Momentum Operator

The orbital angular momentum is given by

$$\mathbf{l} = \mathbf{r} \times \mathbf{p}. \quad (16.1)$$

As we have seen in Chap. 3, Vol. 1, it is not necessary to symmetrize for the translation into quantum mechanics (spatial representation). It follows directly that

$$\mathbf{l} = \frac{\hbar}{i} \mathbf{r} \times \nabla, \quad (16.2)$$

or, in components,

$$l_x = \frac{\hbar}{i} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \quad (16.3)$$

plus cyclic permutations ( $x \rightarrow y \rightarrow z \rightarrow x \rightarrow \dots$ ). All the components of  $\mathbf{l}$  are observables.

We know that one can measure two variables simultaneously if the corresponding operators commute. What about the components of the orbital angular momentum? A short calculation (see the exercises) yields

$$[l_x, l_y] = i\hbar l_z; \quad [l_y, l_z] = i\hbar l_x; \quad [l_z, l_x] = i\hbar l_y, \quad (16.4)$$

or, compactly,  $[l_x, l_y] = i\hbar l_z$  and cyclic permutations. This term can be written still more compactly with the Levi-Civita symbol (permutation symbol, epsilon tensor)  $\varepsilon_{ijk}$  (see also Appendix F, Vol. 1):

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{if } ijk \text{ is an even permutation of } 123 \\ -1 & \text{if } ijk \text{ is an odd permutation of } 123 \\ 0 & \text{otherwise} \end{cases} \quad (16.5)$$

namely as

$$[l_i, l_j] = i\hbar \sum_k l_k \varepsilon_{ijk}. \quad (16.6)$$

Each component of the orbital angular momentum commutes with  $\mathbf{l}^2 = l_x^2 + l_y^2 + l_z^2$  (see the exercises):

$$[l_x, \mathbf{l}^2] = [l_y, \mathbf{l}^2] = [l_z, \mathbf{l}^2] = 0. \quad (16.7)$$

## 16.2 Generalized Angular Momentum, Spectrum

We now generalize these facts by the following definition: A vector operator<sup>1</sup>  $\mathbf{J}$  is a (generalized) angular momentum operator, if its components are observables and satisfy the commutation relation

$$[J_x, J_y] = i\hbar J_z. \quad (16.8)$$

and its cyclic permutations.<sup>2</sup> It follows that  $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$  commutes with all the components:

$$[J_x, \mathbf{J}^2] = 0; \quad [J_y, \mathbf{J}^2] = 0; \quad [J_z, \mathbf{J}^2] = 0. \quad (16.9)$$

The task that we address now is the calculation of the angular momentum spectrum. We will deduce that the angular momentum can assume only half-integer and integer values. To this end, we need only (16.8) and (16.9) and the fact that the  $J_i$

<sup>1</sup>Instead of  $\mathbf{J}$ , one often finds  $\mathbf{j}$  (whereby this is of course not to be confused with the probability current density). In this section, we denote the operator by  $\mathbf{J}$  and the eigenvalue by  $j$ .

<sup>2</sup>The factor  $\hbar$  is due to the choice of units, and would be replaced by a different constant if one were to choose different units. The essential factor is  $i$ .

are Hermitian operators,  $J_i^\dagger = J_i$  (whereby it is actually quite amazing that one can extract so much information from such sparse initial data).

We note first that the squares of the components of the angular momentum are positive operators. Thus, we have for an arbitrary state  $|\varphi\rangle$ :

$$\langle \varphi | \mathbf{J}_x^2 | \varphi \rangle = \| J_x | \varphi \rangle \|^2 \geq 0. \quad (16.10)$$

Consequently,  $\mathbf{J}^2$  as a sum of positive Hermitian operators is also positive, so it can have only non-negative eigenvalues. For reasons which will become clear later, these eigenvalues are written in the special form  $j(j+1)$  with  $j \geq 0$  (and not just simply  $j^2$  or something similar).

Equations (16.8) and (16.9) show that  $\mathbf{J}^2$  and one of its components can be measured simultaneously. Traditionally, one chooses the  $z$ -component  $J_z$  and denotes the eigenvalue associated with  $J_z$  by  $m$ .<sup>3</sup>

We are looking for eigenvectors  $|j, m\rangle$  of  $\mathbf{J}^2$  and  $J_z$  with

$$\mathbf{J}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle; \quad J_z |j, m\rangle = \hbar m |j, m\rangle. \quad (16.11)$$

To continue, we must now use the commutation relations (16.8). It turns out that it is convenient to use two new operators instead of  $J_x$  and  $J_y$ , namely

$$J_\pm = J_x \pm iJ_y. \quad (16.12)$$

For reasons that will become apparent immediately, these two operators are called *ladder operators*;  $J_+$  is the *raising operator* and  $J_-$  the *lowering operator*. The operators are adjoint to each other, since  $J_x$  and  $J_y$  are Hermitian:

$$J_\pm^\dagger = J_\mp. \quad (16.13)$$

With  $J_+$  and  $J_-$ , the commutation relations (16.8) are written as

$$[J_z, J_+] = \hbar J_+; \quad [J_z, J_-] = -\hbar J_-; \quad [J_+, J_-] = 2\hbar J_z, \quad (16.14)$$

and for  $\mathbf{J}^2$ , we have

$$\mathbf{J}^2 = \frac{1}{2} (J_+ J_- + J_- J_+) + J_z^2. \quad (16.15)$$

Together with  $[J_+, J_-] = 2\hbar J_z$ , this equation leads to the expressions

$$J_+ J_- = \mathbf{J}^2 - J_z (J_z - \hbar); \quad J_- J_+ = \mathbf{J}^2 - J_z (J_z + \hbar). \quad (16.16)$$

Furthermore,  $\mathbf{J}^2$  commutes with  $J_+$  and  $J_-$  (see the exercises).

---

<sup>3</sup>  $j$  is also called the *angular momentum quantum number* and  $m$  the *magnetic* or *directional quantum number*.

Our interest in the expressions  $J_+J_-$  and  $J_-J_+$  is essentially due to the fact that they are positive operators. This can be easily seen since, because of (16.13), the matrix element  $\langle \varphi | J_+J_- | \varphi \rangle$  is a norm and it follows that  $\langle \varphi | J_+J_- | \varphi \rangle = \|J_- | \varphi \rangle\|^2 \geq 0$ .

We apply  $J_+J_-$  and  $J_-J_+$  to the angular momentum states. With (16.16), it follows that

$$\begin{aligned} J_+J_- |j, m\rangle &= \hbar^2 [j(j+1) - m(m-1)] |j, m\rangle \quad \text{and} \\ J_-J_+ |j, m\rangle &= \hbar^2 [j(j+1) - m(m+1)] |j, m\rangle. \end{aligned} \quad (16.17)$$

Since the operators are positive, we obtain immediately the inequalities

$$\begin{aligned} j(j+1) - m(m-1) &= (j-m)(j+m+1) \geq 0 \quad \text{and} \\ j(j+1) - m(m+1) &= (j+m)(j-m+1) \geq 0 \end{aligned} \quad (16.18)$$

which must be fulfilled simultaneously. This means that e.g. in the first inequality, the brackets  $(j-m)$  and  $(j+m+1)$  must both be positive or both negative. If they were negative, we would have  $j \leq m$  and  $m \leq -j-1$ . But this is a contradiction since  $j$  is positive. Hence we have  $j \geq m$  and  $m \geq -j-1$ . If we consider in addition the second inequality, it follows that

$$-j \leq m \leq j. \quad (16.19)$$

In this way, the range of  $m$  is fixed.

Now we have to determine the possible values of  $j$ . Let us consider the effect of  $J_{\pm}$  on the states  $|j, m\rangle$ . We have

$$\begin{aligned} \mathbf{J}^2 [J_{\pm} |j, m\rangle] &= \hbar^2 j(j+1) [J_{\pm} |j, m\rangle] \quad \text{and} \\ J_z [J_{\pm} |j, m\rangle] &= \hbar (m \pm 1) [J_{\pm} |j, m\rangle]. \end{aligned} \quad (16.20)$$

On the right-hand sides, we have the numbers  $j(j+1)$  and  $(m \pm 1)$ . This means that  $J_{\pm} |j, m\rangle$  is an eigenvector of  $\mathbf{J}^2$  with the eigenvalue  $\hbar^2 j(j+1)$  as well as of  $J_z$  with the eigenvalue  $\hbar (m \pm 1)$ . It follows that

$$J_{\pm} |j, m\rangle = c_{j,m}^{\pm} |j, m \pm 1\rangle. \quad (16.21)$$

The proportionality constant  $c_{j,m}^{\pm}$  can be fixed by using (16.17) (see the exercises). The simplest choice is

$$J_{\pm} |j, m\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)} |j, m \pm 1\rangle. \quad (16.22)$$

Here, we see clearly the reason why  $J_+$  and  $J_-$  are called ladder operators or raising and lowering operators; for if we apply  $J_+$  or  $J_-$  several times to  $|j, m\rangle$ , the magnetic

quantum number is increased or decreased by 1 each time. Hence, with the help of these operators, we can climb down or up step by step, as on a ladder.

Especially for  $m = j$  or  $m = -j$ , we have  $\|J_+ |j, j\rangle\|^2 = 0$  or  $\|J_- |j, -m\rangle\|^2 = 0$ . Since the norm of a vector vanishes iff it is the zero vector, it follows that

$$J_+ |j, j\rangle = 0; \quad J_- |j, -j\rangle = 0. \quad (16.23)$$

We now apply the ladder operators repeatedly and can conclude that  $J_\pm^N |j, m\rangle$  is an eigenvector of  $J_z$  with the eigenvalue  $\hbar(m \pm N)$  (see the exercises), i.e. that it is proportional to  $|j, m \pm N\rangle$  with  $N \in \mathbb{N}$ . In other words, if we start from any state  $|j, m\rangle$  with  $-j < m < j$ , then after a few steps<sup>4</sup> we obtain states whose norm is negative (or rather would obtain them), or whose magnetic quantum number  $m \pm N$  violates the inequality (16.19). This can be avoided only if the following conditions are fulfilled, ‘going up’ for  $J_+$  and ‘going down’ for  $J_-$ :

$$m + N_1 = j \quad \text{and} \quad m - N_2 = -j; \quad N_1, N_2 \in \mathbb{N}. \quad (16.24)$$

For as we know from (16.23),  $J_+ |j, j\rangle = 0$ , and further applications of  $J_+$  yield just zero again; and similarly for  $J_-$ .

The addition of the two last equations (16.24) leads to  $2j = N_1 + N_2$ . It follows with  $j \geq 0$  that the allowed values for  $j$  are given by

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots \quad (16.25)$$

and for  $m$  by

$$m = -j, -j + 1, -j + 2, \dots, j - 2, j - 1, j \quad (16.26)$$

In this way, we have determined the possible eigenvalues of the general angular momentum operators  $\mathbf{J}^2$  and  $J_z$ .

We remark that there are operators with only integer eigenvalues (e.g. the orbital angular momentum operator), or only half-integer eigenvalues (e.g. the spin- $\frac{1}{2}$  operator), but also those which have half-integer and integer eigenvalues. One of the latter operators, for example, occurs in connection with the Lenz vector; see Appendix G, Vol. 2.

As for elementary particles, nature has apparently set up two classes, which differ by their spins: those with half-integer spin are called *fermions*, those with integer spin *bosons*. General quantum objects can, however, have half-integer or integer spin, as we see in the example of helium, occurring as  ${}^3\text{He}$  (fermion) and as  ${}^4\text{He}$  (boson). We point out that a very general theorem (the *spin-statistics theorem*) shows the connection between the spin and quantum statistics, proving that all fermions obey Fermi-Dirac statistics and all bosons obey Bose-Einstein statistics.

---

<sup>4</sup>For e.g.  $J_+, |j, m\rangle \rightarrow |j, m + 1\rangle \rightarrow |j, m + 2\rangle \rightarrow \dots$

We note that in the derivation of the angular-momentum eigenvalues, we have obtained little information about the eigenvectors—but we do not need it in order to derive the spectrum. It is understandable if this leaves feelings of uncertainty at first sight; but on the other hand, it is simply superb that there is such an elegant technique!

### 16.3 Matrix Representation of Angular Momentum Operators

With (16.22), it follows that

$$\langle j, m' | J_{\pm} | j, m \rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)} \delta_{m', m \pm 1}. \quad (16.27)$$

By means of this equation, we can represent the angular momentum operators as matrices. We assume that the eigenstates are given as column vectors.

We consider the case of spin  $\frac{1}{2}$ , where one usually writes  $s$  instead of  $J$ . We can represent the two possible states as<sup>5</sup>

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (16.28)$$

Only two matrix elements do not vanish, namely

$$\left\langle \frac{1}{2}, \frac{1}{2} \right| s_+ \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \hbar \quad \text{and} \quad \left\langle \frac{1}{2}, -\frac{1}{2} \right| s_- \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \hbar \quad (16.29)$$

or

$$s_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad s_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (16.30)$$

With the definition of the ladder operators,  $s_{\pm} = s_x \pm i s_y$  or  $s_x = (s_+ + s_-)/2$  and  $s_y = (s_+ - s_-)/2i$ , it follows that

$$s_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2} \sigma_x \quad \text{and} \quad s_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2} \sigma_y \quad (16.31)$$

i.e. two of the well-known spin matrices ( $s$ ) or Pauli matrices ( $\sigma$ ). We obtain the third one by using the equation  $s_z |1/2, m\rangle = \hbar m |1/2, m\rangle$  directly as

---

<sup>5</sup>We omit here the distinction between = and  $\cong$ .

$$s_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2} \sigma_z. \quad (16.32)$$

In the same way, we can obtain e.g. the matrix representation of the orbital angular momentum operator for  $l = 1$ ; see the exercises.

We recall briefly some properties of the Pauli matrices (cf. Chap. 4, Vol. 1). With a view to a more convenient notation, one often writes  $\sigma_1, \sigma_2, \sigma_3$  instead of  $\sigma_x, \sigma_y, \sigma_z$ . In this notation,<sup>6</sup>

$$[\sigma_i, \sigma_j] = 2i \sum_k \varepsilon_{ijk} \sigma_k; \{\sigma_i, \sigma_j\} = 2\delta_{ij}; \sigma_i^2 = 1; \sigma_i \sigma_j = i \sum_k \varepsilon_{ijk} \sigma_k \quad (16.33)$$

holds. Finally, we note that every  $2 \times 2$ -matrix can be represented as a linear combination of the three Pauli matrices and the unit matrix.

## 16.4 Orbital Angular Momentum: Spatial Representation of the Eigenfunctions

The eigenvalues of the orbital angular momentum are integers. For the position representation of the eigenfunctions, it is advantageous to use spherical coordinates. In these coordinates, we find that<sup>7</sup>:

$$l^2 = -\hbar^2 \left[ \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2} \right]; l_z = \frac{\hbar}{i} \frac{\partial}{\partial \varphi}. \quad (16.34)$$

The eigenvalue problem (16.11) is written as

$$\begin{aligned} \left[ \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2} \right] Y_l^m(\vartheta, \varphi) &= -l(l+1) Y_l^m(\vartheta, \varphi) \\ \frac{\partial}{\partial \varphi} Y_l^m(\vartheta, \varphi) &= im Y_l^m(\vartheta, \varphi), \end{aligned} \quad (16.35)$$

or, more compactly, as

$$\begin{aligned} l^2 Y_l^m(\theta, \varphi) &= \hbar^2 l(l+1) Y_l^m(\theta, \varphi) \quad \text{with } l = 0, 1, 2, 3, \dots \\ l_z Y_l^m(\theta, \varphi) &= \hbar m Y_l^m(\theta, \varphi) \quad \text{with } -l \leq m \leq l \end{aligned} \quad (16.36)$$

<sup>6</sup>The anticommutator is defined as usual by  $\{A, B\} = AB + BA$ .

<sup>7</sup>We recall the equality

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{l^2}{\hbar^2 r^2}$$

See also Appendix D, Vol. 1.

where the functions  $Y_l^m(\vartheta, \varphi)$  are the eigenfunctions of the orbital angular momentum in the position representation<sup>8</sup>; they are called *spherical functions* (or spherical harmonics). The number  $l$  is the *orbital angular momentum (quantum) number*,  $m$  the *magnetic* (or *directional*) *(quantum) number*.

With the separation *ansatz*  $Y_l^m(\vartheta, \varphi) = \Theta(\vartheta) \Phi(\varphi)$ , we obtain

$$\begin{aligned} \frac{\partial}{\partial \varphi} \Phi(\varphi) &= im \Phi(\varphi) \\ \left[ \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left( \sin \vartheta \frac{\partial}{\partial \vartheta} \right) - \frac{m^2}{\sin^2 \vartheta} + l(l+1) \right] \Theta(\vartheta) &= 0. \end{aligned} \quad (16.37)$$

The solutions of the first equation are well-known special functions (associated Legendre functions). The solutions of the second equation can immediately be written down as  $\Phi(\varphi) = e^{im\varphi}$ .

We will not deal with the general form of the spherical functions (for details see Appendix B, Vol. 2), but just note here some important features as well as the simplest cases. The spherical harmonics form a CONS. They are orthonormal

$$\int_0^\pi d\vartheta \sin \vartheta \int_0^{2\pi} d\varphi [Y_l^m(\vartheta, \varphi)]^* Y_{l'}^{m'}(\vartheta, \varphi) = \delta_{ll'} \delta_{mm'} \quad (16.38)$$

and complete

$$\sum_{l=0}^{\infty} \sum_{m=-l}^l Y_l^m(\vartheta, \varphi) [Y_l^m(\vartheta', \varphi')]^* = \frac{\delta(\vartheta - \vartheta') \delta(\varphi - \varphi')}{\sin \vartheta}. \quad (16.39)$$

With the notation  $\Omega = (\vartheta, \varphi)$  for the solid angle and  $d\Omega = \sin \vartheta d\vartheta d\varphi$  (also written as  $d^2\hat{r}$  or  $d\hat{r}$ , see Appendix D, Vol. 1) for its differential element, we can write the orthogonality relation as

$$\int [Y_l^m(\vartheta, \varphi)]^* Y_{l'}^{m'}(\vartheta, \varphi) d\Omega = \delta_{ll'} \delta_{mm'}. \quad (16.40)$$

Because of the completeness of the spherical harmonics, we can expand any (sufficiently well-behaved) function  $f(\vartheta, \varphi)$  in terms of them:

$$f(\vartheta, \varphi) = \sum_{l,m} c_{lm} Y_l^m(\vartheta, \varphi) \quad (16.41)$$

with

---

<sup>8</sup>Other notations:  $Y_l^m(\vartheta, \varphi) = Y_l^m(\hat{r}) = \langle \hat{r} | l, m \rangle$ .  $\hat{r}$  is the unit vector and is an abbreviation for the pair  $(\vartheta, \varphi)$ . Moreover, the notation  $Y_{lm}(\vartheta, \varphi)$  is also common.

$$c_{lm} = \int Y_l^{m*}(\vartheta, \varphi) f(\vartheta, \varphi) d\Omega. \quad (16.42)$$

Such an expansion is called a *multipole expansion*; the contribution for  $l = 0$  is called the monopole (term), for  $l = 1$  the dipole, for  $l = 2$  the quadrupole, and generally, that for  $l = n$  the  $2^n$ -pole.

Finally, we write down the first spherical harmonics explicitly (more spherical functions may be found in Appendix B, Vol. 2, where there are also some graphs):

$$\begin{aligned} Y_0^0 &= \frac{1}{\sqrt{4\pi}}; Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \vartheta; Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin \vartheta e^{i\varphi} \\ Y_2^0 &= \sqrt{\frac{5}{16\pi}} (3 \cos^2 \vartheta - 1); Y_2^1 = -\sqrt{\frac{15}{8\pi}} \sin \vartheta \cos \vartheta e^{i\varphi}; Y_2^2 = \sqrt{\frac{15}{32\pi}} \sin^2 \vartheta e^{2i\varphi}. \end{aligned} \quad (16.43)$$

For negative  $m$ , the functions are given by

$$Y_l^{-m}(\vartheta, \varphi) = (-1)^m Y_l^{m*}(\vartheta, \varphi). \quad (16.44)$$

## 16.5 Addition of Angular Momenta

This section is intended to give a brief overview of the topic. Therefore, only some results are given, without derivation. In this section, we denote the angular-momentum operators by lower-case letters  $\mathbf{j}$ .

The addition theorem for angular momentum states that: If one adds two angular momenta  $\mathbf{j}_1$  and  $\mathbf{j}_2$ , then  $j$ , the quantum number of the total angular momentum  $\mathbf{j} = \mathbf{j}_1 + \mathbf{j}_2$  can assume only one of the values<sup>9</sup>:

$$j_1 + j_2, j_1 + j_2 - 1, j_1 + j_2 - 2, \dots, |j_1 - j_2| \quad (16.45)$$

while the projections onto the  $z$ -axis are added directly:

$$m = m_1 + m_2. \quad (16.46)$$

Total angular momentum states  $|jm; j_1 j_2\rangle$  can be obtained from the individual states  $|j_1, m_1\rangle$  and  $|j_2, m_2\rangle$  through the relation:

$$|jm; j_1 j_2\rangle = \sum_{m_1+m_2=m} \langle j_1 j_2 m_1 m_2 | jm \rangle |j_1, m_1\rangle |j_2, m_2\rangle \quad (16.47)$$

<sup>9</sup>Intuitively-clear reason: If the two angular momentum vectors are parallel to each other, then their angular-momentum quantum numbers are added to give  $j = j_1 + j_2$ . For other arrangements,  $j$  is smaller. The smallest value is  $|j_1 - j_2|$ , because of  $j \geq 0$ .

where of course  $|j_1 - j_2| \leq j \leq j_1 + j_2$  has to be satisfied. The numbers  $\langle j_1 j_2 m_1 m_2 | jm \rangle$  are called *Clebsch–Gordan coefficients*<sup>10</sup>; they are real and are tabulated in relevant works on the angular momentum in quantum mechanics.<sup>11</sup> The inverse of the last equation is

$$|j_1, m_1\rangle |j_2, m_2\rangle = \sum_{j=|j_1-j_2|}^{j_1+j_2} \langle j_1 j_2 m_1 m_2 | jm \rangle |jm; j_1 j_2\rangle. \quad (16.48)$$

As an application, we consider the spin-orbit coupling, i.e. the coupling of the orbital angular momentum  $\mathbf{l}$  of electrons with their spins  $\mathbf{s}$ . The total angular momentum of the electron is

$$\mathbf{j} = \mathbf{l} + \mathbf{s} \quad (16.49)$$

and its possible values are  $j = l + \frac{1}{2}$  and  $j = l - \frac{1}{2}$  (except for  $l = 0$  in which case only  $j = \frac{1}{2}$  occurs). Intuitively, this means that orbital angular momentum and spin are either parallel ( $j = l + \frac{1}{2}$ ) or antiparallel ( $j = l - \frac{1}{2}$ ).

The spin is a relativistic phenomenon and can, if one argues from the nonrelativistic SEq, at best be introduced heuristically. A clear-cut approach starts e.g. from the relativistically correct *Dirac equation*  $i\hbar \frac{\partial}{\partial t} \psi = (c\boldsymbol{\alpha}\mathbf{p} + \beta mc^2 + e\phi) \psi = H_{Dirac} \psi$ . Here,  $\mathbf{p}$  is the three-dimensional momentum operator  $\mathbf{p} = \frac{\hbar}{i} \nabla$ , while  $\beta$  and the three components of the vector  $\boldsymbol{\alpha}$  are certain  $4 \times 4$  matrices, the *Dirac matrices*.

<sup>10</sup>There are several different notations for these coefficients, e.g.  $C_{m_1 m_2; j m}^{j_1 j_2}$ . The so-called *3j-symbols* are related coefficients:

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = (-1)^{j_1 - j_2 - m} \frac{1}{\sqrt{2j+1}} \langle j_1 j_2 m_1 m_2 | j - m \rangle.$$

The 3j-symbols are invariant against cyclic permutation:

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \begin{pmatrix} j & j_1 & j_2 \\ m & m_1 & m_2 \end{pmatrix}, \text{ etc.}$$

<sup>11</sup>The two conditions  $|j_1 - j_2| \leq j \leq j_1 + j_2$  and  $m = m_1 + m_2$  must be met in order that a Clebsch-Gordan coefficient is nonzero. The CGC satisfy the orthogonality relations

$$\begin{aligned} \sum_{m_1, m_2} \langle j_1 j_2 m_1 m_2 | jm \rangle \langle j_1 j_2 m_1 m_2 | j' m' \rangle &= \delta_{j j'} \delta_{m m'} \\ \sum_{j, m} \langle j_1 j_2 m_1 m_2 | jm \rangle \langle j_1 j_2 m'_1 m'_2 | j m \rangle &= \delta_{m_1 m'_1} \delta_{m_2 m'_2}. \end{aligned}$$

A particular CGC can in principle be calculated using the ladder operators  $j_{1\pm} + j_{2\pm}$ , whereby one starts e.g. from  $\langle j_1 j_2 j_1 j_2 | j_1 + j_2 j_1 + j_2 \rangle = 1$ . In this way, one obtains for example

$$\begin{pmatrix} A & B & A+B \\ a & b & c \end{pmatrix} = (-1)^{A-B-c} \left[ \frac{(2A)! (2B)! (A+B+c)! (A+B-c)!}{(2A+2B+1)! (A+a)! (A-a)! (B+b)! (B-b)!} \right]^{\frac{1}{2}}.$$

Essentially, one performs an expansion of this equation in powers of  $(\frac{v}{c})^2$  and retains only the lowest term for the nonrelativistic description. Then it turns out that in the SEq, a spin-orbit term  $F(r) \mathbf{l} \cdot \mathbf{s}$  appears (see also Chap. 19), with  $F(r)$  a radially-symmetric function. Because of

$$(\mathbf{l} + \mathbf{s})^2 = \mathbf{j}^2 = \mathbf{l}^2 + 2\mathbf{l}\mathbf{s} + \mathbf{s}^2, \quad (16.50)$$

$\mathbf{l} \cdot \mathbf{s}$  has the values

$$\mathbf{l} \cdot \mathbf{s} = \frac{1}{2} \hbar^2 [j(j+1) - l(l+1) - s(s+1)]. \quad (16.51)$$

It follows for the spin-orbit term in the SEq:

$$F(r) \mathbf{l} \cdot \mathbf{s} = \begin{cases} \frac{1}{2} \hbar^2 l F(r) & \text{for } j = l + \frac{1}{2} \\ -\frac{1}{2} \hbar^2 (l+1) F(r) & \text{for } j = l - \frac{1}{2}. \end{cases} \quad (16.52)$$

Next, we briefly discuss the corresponding eigenfunctions and write down their explicit form. We start from the states for the spin  $|sm_s\rangle$  and the orbital angular momentum  $|Q; lm_l\rangle$ , where  $Q$  stands for possible additional quantum numbers (e.g. the principal quantum number of the hydrogen atom). The total angular momentum state is then described by

$$|Q; j, m_j; l\rangle; \quad j = l \pm \frac{1}{2} \text{ for } l \geq 1; \quad j = \frac{1}{2} \text{ for } l = 0 \quad (16.53)$$

and is composed of spin and orbital angular momentum states:

$$|Q; j, m_j; l\rangle = \sum_{m_l+m_s=m_j} \langle lsm_l m_s | jm_j \rangle |Q; lm_l\rangle |sm_s\rangle \quad (16.54)$$

Calculating the Clebsch-Gordan coefficients yields

$$\begin{aligned} & |Q; j = l + 1/2, m_j; l\rangle \\ &= \sqrt{\frac{l+m_j+1/2}{2l+1}} |Q; l, m_j - 1/2\rangle |s, 1/2\rangle + \sqrt{\frac{l-m_j+1/2}{2l+1}} |Q; l, m_j + 1/2\rangle |s, -1/2\rangle \\ & |Q; j = l - 1/2, m_j; l\rangle \\ &= \sqrt{\frac{l-m_j+1/2}{2l+1}} |Q; l, m_j - 1/2\rangle |s, 1/2\rangle + \sqrt{\frac{l+m_j+1/2}{2l+1}} |Q; l, m_j + 1/2\rangle |s, -1/2\rangle \end{aligned} \quad (16.55)$$

with  $m_j = l + 1/2, \dots, -(l + 1/2)$  in the upper line and  $m_j = l - 1/2, \dots, -(l - 1/2)$  in the lower line. With the notation as column vectors, we obtain using

$$|s, 1/2\rangle \equiv |1/2, 1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |s, -1/2\rangle \equiv |1/2, -1/2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (16.56)$$

the explicit formulations

$$|Q; j = l + 1/2, m_j; l\rangle = \begin{pmatrix} \sqrt{\frac{l+m_j+1/2}{2l+1}} |Q; l, m_j - 1/2\rangle \\ \sqrt{\frac{l-m_j+1/2}{2l+1}} |Q; l, m_j + 1/2\rangle \end{pmatrix}$$

with  $m_j = l + 1/2, \dots, -(l + 1/2)$  (16.57)

and

$$|Q; j = l - 1/2, m_j; l\rangle = \begin{pmatrix} -\sqrt{\frac{l-m_j+1/2}{2l+1}} |Q; l, m_j - 1/2\rangle \\ \sqrt{\frac{l+m_j+1/2}{2l+1}} |Q; l, m_j + 1/2\rangle \end{pmatrix}$$

with  $m_j = l - 1/2, \dots, -(l - 1/2)$ . (16.58)

## 16.6 Exercises

1. For which  $K, N, M$  are the spherical harmonics (in spherical coordinates)

$$f(\vartheta, \varphi) = \cos^K \vartheta \cdot \sin^M \vartheta \cdot e^{iN\varphi} \quad (16.59)$$

eigenfunctions of  $\mathbf{I}^2$ ?

2. Write out the spherical harmonics for  $l = 1$  using Cartesian coordinates,  $x, y, z$ .
3. Show that:

$$\mathbf{l} \cdot \hat{\mathbf{r}} = \hat{\mathbf{r}} \cdot \mathbf{l} = 0 \quad (16.60)$$

4. Show that the components of  $\mathbf{l}$  are Hermitian.
5. Show that for the orbital angular momentum, it holds that

$$[l_x, l_y] = i\hbar l_z; [l_y, l_z] = i\hbar l_x; [l_z, l_x] = i\hbar l_y. \quad (16.61)$$

6. Show that  $[A, BC] = B[A, C] + [A, B]C$  holds. Using this identity and the commutators  $[l_x, l_y] = i\hbar l_z$  plus cyclic permutations, prove that  $[l_x, \mathbf{l}^2] = 0$ .
7. Show that:

$$[\mathbf{J}^2, J_{\pm}] = 0. \quad (16.62)$$

8. We have seen in the text that

$$J_{\pm} |j, m\rangle = c_{j,m}^{\pm} |j, m \pm 1\rangle. \quad (16.63)$$

Using

$$\begin{aligned} J_+ J_- |j, m\rangle &= \hbar^2 [j(j+1) - m(m-1)] |j, m\rangle \\ J_- J_+ |j, m\rangle &= \hbar^2 [j(j+1) - m(m+1)] |j, m\rangle, \end{aligned} \quad (16.64)$$

show that for the coefficients  $c_{j,m}^\pm$ ,

$$c_{j,m}^\pm = \hbar \sqrt{j(j+1) - m(m \pm 1)} \quad (16.65)$$

holds.

9. Given the Pauli matrices  $\sigma_k$ ,

(a) Show (once more) that

$$[\sigma_i, \sigma_j] = 2i \varepsilon_{ijk} \sigma_k; \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij}; \quad \sigma_i^2 = 1; \quad \sigma_i \sigma_j = i \varepsilon_{ijk} \sigma_k; \quad (16.66)$$

(b) Prove that

$$(\boldsymbol{\sigma} \mathbf{A})(\boldsymbol{\sigma} \mathbf{B}) = \mathbf{A} \mathbf{B} + i \boldsymbol{\sigma} (\mathbf{A} \times \mathbf{B}) \quad (16.67)$$

where  $\boldsymbol{\sigma}$  is the vector  $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$  and  $\mathbf{A}, \mathbf{B}$  are three-dimensional vectors;

(c) Show that every  $2 \times 2$  matrix can be expressed as a linear combination of the three Pauli matrices and the unit matrix.

10. Given the orbital angular momentum operator  $\mathbf{l}$  and the spin operator  $\mathbf{s}$ , show that  $[\mathbf{l}_z, \mathbf{s} \cdot \mathbf{l}] \neq 0$ ;  $[\mathbf{s}_z, \mathbf{s} \cdot \mathbf{l}] \neq 0$ ;  $[\mathbf{l}_z + \mathbf{s}_z, \mathbf{s} \cdot \mathbf{l}] = 0$ .

11. The ladder operators for a generalized angular momentum are given as  $J_\pm = J_x \pm i J_y$ .

(a) Show that  $[J_z, J_+] = \hbar J_+$ ,  $[J_z, J_-] = -\hbar J_-$ ,  $[J_+, J_-] = 2\hbar J_z$ , as well as  $\mathbf{J}^2 = \frac{1}{2}(J_+ J_- + J_- J_+) + J_z^2$ .

(b) Show that it follows from the last equation that:

$$J_+ J_- = \mathbf{J}^2 - J_z (J_z - \hbar); \quad J_- J_+ = \mathbf{J}^2 - J_z (J_z + \hbar) \quad (16.68)$$

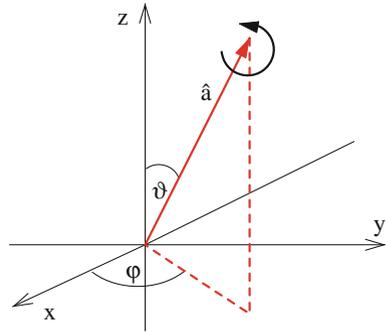
and hence

$$\begin{aligned} J_+ J_- |j, m\rangle &= \hbar^2 [j(j+1) - m(m-1)] |j, m\rangle \\ J_- J_+ |j, m\rangle &= \hbar^2 [j(j+1) - m(m+1)] |j, m\rangle. \end{aligned} \quad (16.69)$$

(c) Show that from the last two equations, it follows that:

$$\begin{aligned} j(j+1) - m(m-1) &= (j-m)(j+m+1) \geq 0 \\ j(j+1) - m(m+1) &= (j+m)(j-m+1) \geq 0 \end{aligned} \quad (16.70)$$

**Fig. 16.1** Rotation about an axis  $\hat{a}$



and hence

$$-j \leq m \leq j. \tag{16.71}$$

- 12. What is the matrix representation of the orbital angular momentum for  $l = 1$ ?
- 13. Consider the orbital angular momentum  $l = 1$ . Express the operator  $e^{-i\alpha L_z/\hbar}$  as sum over dyadic products (representation-free). Specify this for the bases

$$|1, 1\rangle \cong \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; |1, 0\rangle \cong \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}; |1, -1\rangle \cong \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{16.72}$$

and

$$|1, 1\rangle \cong \pm \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}; |1, 0\rangle \cong \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}; |1, -1\rangle \cong \mp \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}. \tag{16.73}$$

- 14. Calculate the term

$$e^{-i \frac{\gamma \hat{\mathbf{a}} \cdot \mathbf{L}}{\hbar}} = e^{-i\gamma \hat{\mathbf{a}} \cdot \mathbf{l}} \tag{16.74}$$

for the orbital angular momentum  $l = 1$  and the basis (16.73).<sup>12</sup>  $\hat{\mathbf{a}}$  is the rotation axis (a unit vector),  $\gamma$  the rotation angle. For reasons of economy, use the ‘simplified’ angular momentum  $\mathbf{l} = \mathbf{L}/\hbar$ , i.e. the theoretical units system.

- (a) Express the rotations around the  $x$ -,  $y$ - and  $z$ -axis as matrices.
- (b) Express the rotations about an axis  $\hat{a}$  with rotation angle  $\gamma$  as matrices (the angles in spherical coordinates are  $\vartheta$  and  $\varphi$ ; see Fig. 16.1).

---

<sup>12</sup>Of course, all the calculations may also be performed representation-free.