Chapter 5
Motion in Angular Subspace

This chapter deals with the angular degrees of freedom and, therefore, the crucial role is played by the spherical symmetry. The quantum angular momenta are treated from both matrix and differential equation points of view. The difference in the corresponding results reveals the existence of the most important quantum observable: the spin. Addition of angular momenta, quantum rotations and the Wigner–Eckart theorem are also discussed.

The commutation relation (2.15) is straightforwardly generalized to the three-dimensional case

$$[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}. \tag{5.1}$$

In classical physics, angular momentum is a physical, observable vector $\boldsymbol{L}$ that plays an important role, since it is a conserved quantity in the absence of external torques $\boldsymbol{\tau}$:

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}, \qquad \frac{\mathrm{d}\boldsymbol{L}}{\mathrm{d}t} = \boldsymbol{\tau}. \tag{5.2}$$

As in the case of the Schrödinger equation, we quantize the problem by substituting

$$\hat{p}_i \to -\mathrm{i}\hbar\frac{\partial}{\partial x_i} \tag{5.3}$$

into the classical expression (5.2). One obtains the commutation relations

$$[\hat{L}_x, \hat{L}_y] = \mathrm{i}\hbar\hat{L}_z, \qquad [\hat{L}_y, \hat{L}_z] = \mathrm{i}\hbar\hat{L}_x, \qquad [\hat{L}_z, \hat{L}_x] = \mathrm{i}\hbar\hat{L}_y, \tag{5.4}$$

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0. \tag{5.5}$$

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5.1 Eigenvalues and Eigenstates

5.1.1 Matrix Treatment

In the following, we take the commutation relations (5.4) as the definition of quantum angular momentum. Therefore, this definition also takes care of the quantum version of orbital angular momentum (5.2). However, as we shall see, definition (5.4) also includes other types of angular momenta of a purely quantum mechanical origin. From here on we let $\hat{J}_i$ denote operator components that satisfy the relations

$$[\hat{J}_i, \hat{J}_j] = \mathrm{i}\hbar\epsilon_{ijk}\hat{J}_k, \tag{5.6}$$

where ϵ_{ijk} is the Levi–Civita tensor,[1] whatever their origin may be. We use the notation $\hat{L}_i$ for angular momentum operators associated with orbital motion (5.2).

The commutation relations ensure that one can precisely determine the modulus squared simultaneously with one projection of the angular momentum, but not two projections at the same time. Consequently, one may construct eigenfunctions that are common to the operators $\hat{J}^2$ and $\hat{J}_z$. The choice of the z-component is arbitrary, since the space is isotropic and, consequently, there are no preferred directions.

The procedure for solving this problem closely follows the matrix treatment of the harmonic oscillator (Sect. 3.3.1). It is given in detail in Sect. 5.4*. The following results are obtained:

- The two-dimensional angular subspace displays two more symmetries and thus provides two additional quantum numbers. The eigenvalue equations for the operators $\hat{\boldsymbol{J}}^2$ and $\hat{J}_z$ can be written as

$$\hat{\boldsymbol{J}}^2\varphi_{jm} = \hbar^2 j(j+1)\varphi_{jm}, \qquad \hat{J}_z\varphi_{jm} = \hbar m\varphi_{jm}, \tag{5.7}$$

  where the possible values of the quantum numbers j, m are

$$-j \le m \le j, \qquad j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots, \tag{5.8}$$

  with m increasing in units of 1.
- Since the maximum value of m is j, and $j^2 < j(j+1)$, the maximum projection of the angular momentum is always smaller than the modulus (except for $j = 0$). Thus, the angular momentum vector can never be completely aligned with the z-axis. This fact is consistent with the lack of commutativity in (5.6): a complete alignment would imply the vanishing of the components $\hat{J}_x, \hat{J}_y$ and thus the simultaneous determination of the corresponding physical quantities and of J_z (see Problem 3).

[1] $\epsilon_{ijk} = 1$ if i, j, k are cyclical (as for $i = z$, $j = x$, $k = y$); otherwise $\epsilon_{ijk} = -1$ (as for $i = z$, $j = y, k = x$).

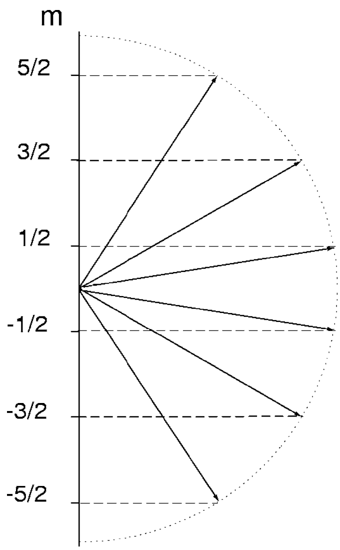

Fig. 5.1 Possible orientations of a $j = 5/2$ angular momentum vector

Figure 5.1 represents the possible orientations of the angular momentum vector for the case $j = 5/2$. It looks as if the angular momentum precesses around the z-axis. However, this picture is incorrect, since it implies that the end point of the angular momentum vector goes through a circular trajectory, something that does not make sense from the point of view of quantum uncertainty relations.

- The operators $\hat{J}_x$ and $\hat{J}_y$ display non-diagonal matrix elements within the basis (5.7), namely

$$\langle j'm'|J_x|jm\rangle = \delta_{j'j}\delta_{m'(m\pm 1)}\frac{\hbar}{2}\sqrt{(j \mp m)(j \pm m + 1)},$$
$$\langle j'm'|J_y|jm\rangle = \mp\delta_{j'j}\delta_{m'(m\pm 1)}\frac{\mathrm{i}\hbar}{2}\sqrt{(j \mp m)(j \pm m + 1)}. \qquad (5.9)$$

- None of the operators $\hat{J}_x, \hat{J}_y, \hat{J}_z, \hat{J}^2$ connects states with different values of the quantum number j.
- Properties of the unitary operator associated with rotations are discussed in Sect. 5.3.2†.

5.1.2 Treatment Using Position Wave Functions

The concept of orbital angular momentum is especially useful in problems with spherical symmetry (like those involving atoms, nuclei, etc.), for which it is convenient to use the spherical coordinates

$$x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi, \qquad z = r\cos\theta,$$
$$\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi, \tag{5.10}$$
$$0 \le \theta \le \pi, \qquad 0 \le \phi \le 2\pi, \qquad 0 \le r \le \infty.$$

In these coordinates, the orbital angular momentum operators read

$$\begin{aligned}
\hat{L}_x &= \mathrm{i}\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right),\\
\hat{L}_y &= \mathrm{i}\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right),\\
\hat{L}_z &= -\mathrm{i}\hbar\frac{\partial}{\partial\phi},\\
\hat{L}^2 &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).
\end{aligned} \tag{5.11}$$

The detailed treatment of the orbital angular momentum operator is given in Sect. 5.5*. The results of such an approach are as follows:

- The simultaneous eigenfunctions of the operators $\hat{L}^2, \hat{L}_z$ are called spherical harmonics and denoted by $Y_{lm_l}(\theta,\phi)$. They satisfy the eigenvalue equations

$$\begin{aligned}
\hat{L}_z Y_{lm_l} &= \hbar m_l Y_{lm_l},\\
\hat{L}^2 Y_{lm_l} &= \hbar^2 l(l+1) Y_{lm_l},\\
\hat{\Pi} Y_{lm_l} &= (-1)^l Y_{lm_l},
\end{aligned} \tag{5.12}$$

  where
$$-l \le m_l \le l, \qquad l = 0, 1, 2, \ldots. \tag{5.13}$$
  and $\hat{\Pi}$ is the parity operator[2] (3.49).
- Using the expressions (5.11), one may construct the matrix elements of the operators $\hat{L}_x, \hat{L}_y$. One obtains the same form as the matrix elements in (5.9), with the replacement $j \to l$, $m \to m_l$.
- The spherical harmonics constitute a complete set of single-valued basis states on the surface of a sphere of unit radius:

$$\Psi(\theta,\phi) = \sum_{lm_l} c_{lm_l} Y_{lm_l}. \tag{5.14}$$

[2]For the three-dimensional case, the parity operation is written as $\boldsymbol{r} \to -\boldsymbol{r}$ or equivalently, $r \to r$, $\theta \to \pi - \theta$, $\phi \to \pi + \phi$.

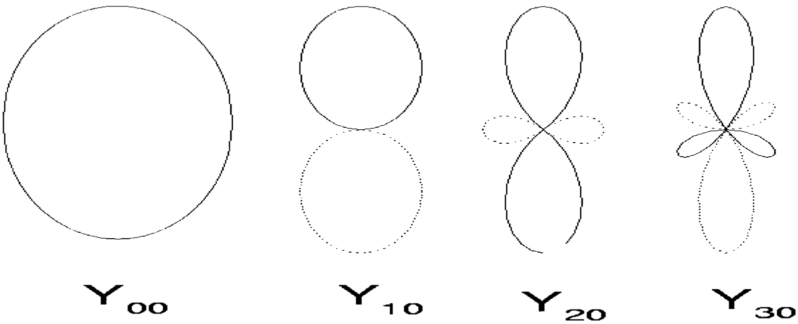

Fig. 5.2 Projection of the spherical harmonics Y_{l0} on the (x, z) plane, for the values $l = 0$–3. While all the Y_{l0} are axially symmetric wave functions, $l = 0$ implies full spherical symmetry. The distance from the *center* to the *top* of the figures is $\sqrt{(2l+1)/4\pi}$. *Solid lines* denote positive lobules; *dotted lines*, negative ones

They can be visualized as vibrational modes of a soap bubble.
- Figure 5.2 displays the projection of some spherical harmonics on the (x, z) plane. The protruding shapes have important consequences in the construction of chemical bonds.
- The rotational Hamiltonian of a molecule is proportional to the operator $\hat{\boldsymbol{L}}^2$. The corresponding energy eigenvalues therefore follow the rule $l(l+1)$ (see Sect. 8.4.2).

By taking the commutation relations as the definition of the angular momentum operators, we have obtained operators that are not derived from the classical orbital angular momentum (see Sects. 5.1.1 and 5.1.2). This statement is supported by the fact that the quantum numbers j, m associated with these quantum mechanical angular momenta may take either integer or half-integer values, in contrast with those labeling the orbital angular momentum, which can only take integer values. Otherwise we obtain the same matrix elements for the projections $\hat{J}_i$ (5.9) as for the orbital angular momentum projections $\hat{L}_i$. On the other hand, the probability densities associated with the orbital angular momentum display interesting and useful features that are lacking in the more general derivation (Fig. 5.2).

5.2 Spin

5.2.1 Stern–Gerlach Experiment

A particle with a magnetic moment $\boldsymbol{\mu}$ and subject to a magnetic field $\boldsymbol{B}$ experiences a torque $\boldsymbol{\tau}$. When the particle is rotated through an angle $\mathrm{d}\theta$ about the direction of $\boldsymbol{\tau}$, the potential energy U increases:

$$\boldsymbol{\tau} = \boldsymbol{\mu} \times \boldsymbol{B}, \qquad \mathrm{d}U = \mu B \sin\theta \mathrm{d}\theta, \qquad U(\theta) = -\mu B \cos\theta = -\boldsymbol{\mu} \cdot \boldsymbol{B}. \quad (5.15)$$

According to classical electromagnetism, an electric current i produces a magnetic moment proportional to the area subtended by the current. If this current is due to a particle with charge e and velocity v moving along a circumference of radius r, then

$$\mu_l = i\mathcal{A} = \frac{ev}{2\pi r}\pi r^2 = \frac{e}{2M}L = \frac{e}{|e|}\frac{g_l \mu_{\mathrm{B}}}{\hbar}L. \tag{5.16}$$

Thus, the magnetic moment due to the orbital motion is proportional to the orbital angular momentum. In vector and operator notation,

$$\hat{\boldsymbol{\mu}}_l = \frac{e}{|e|}\frac{g_l \mu_{\mathrm{B}}}{\hbar}\hat{\boldsymbol{L}}, \tag{5.17}$$

where $\mu_{\mathrm{B}} \equiv |e|\hbar/2M$ is called the Bohr magneton (Table A.1) and $g_l = 1$ is the orbital gyromagnetic ratio.

Therefore, the presence of a magnetic field displaces the energy of a particle by an amount proportional to the component of the angular momentum along the magnetic field (Zeeman effect). Classically, this change is a continuous function of the orientation of the angular momentum but, according to quantum mechanics, the projections of the angular momentum are discretized (5.12):

$$\Delta E_{m_l} = g_l \mu_{\mathrm{B}} B m_l. \tag{5.18}$$

Therefore, an orbital angular momentum should give rise to an odd number $(2l+1)$ of energy eigenstates.

For a uniform magnetic field, there is no net force acting on the magnetic dipole. However, if the field has a gradient in the z-direction, the net force is

$$F_z = \frac{\partial}{\partial z}(\boldsymbol{\mu} \cdot \boldsymbol{B}) = \mu_z \frac{\partial B}{\partial z}. \tag{5.19}$$

Figure 5.3 is a sketch of the experimental set-up used by Stern and Gerlach [17]. Silver atoms are heated in an oven and escape through a hole. The beam is collimated and subsequently deflected by a nonuniform magnetic field perpendicular to its direction. Finally, a visible deposit is allowed to build up on a glass plate located far from the region of deflection.

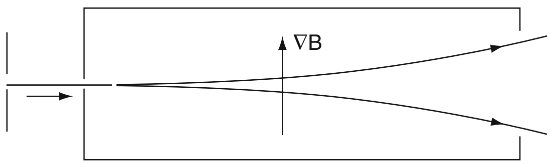

Fig. 5.3 Sketch of the Stern–Gerlach experimental arrangement

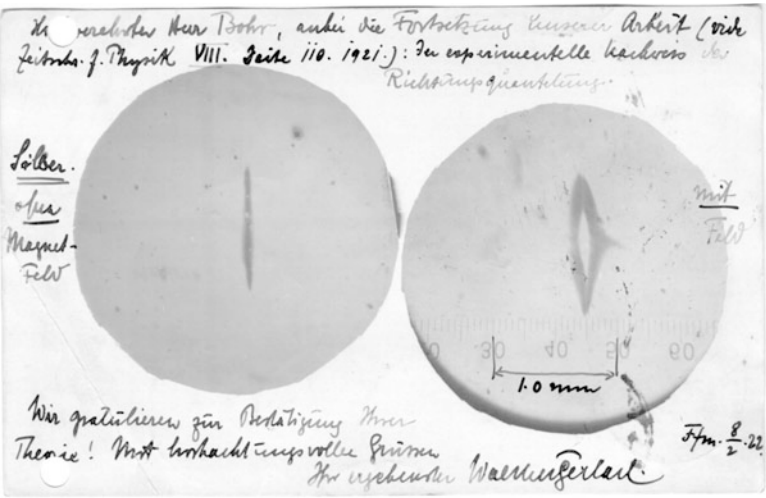

Fig. 5.4 Two figures contained in a letter to Bohr from Stern, communicating his experimental results. Stern explains that the magnetic field was too weak at the extremes of the beam. The figure to the left was obtained, for comparison, in the absence of magnetic field. (Reproduced with permission from Niels Bohr Archive, Copenhagen)

We may ignore the nuclear contributions to the magnetic moment on the grounds that the nuclear magneton is about 2,000 times smaller than the Bohr magneton. (It includes the proton mass in the denominator, instead of the electron mass.) Moreover, 46 of the 47 electrons form a spherically symmetric electron cloud with no net angular momentum (see Sect. 7.3). Therefore, the total spin of the Ag atom may be ascribed to the last electron.

The Stern–Gerlach result is reproduced in Fig. 5.4. Neither the classical continuous pattern nor the orbital quantum mechanical results displaying the separation into an odd number of terms were obtained: the beam was split into only two other beams, as would befit an angular momentum with $j = s = 1/2$.

Spin has become the most important quantum observable, both due to its conceptual importance and because quantum information is based on two-state systems (Chap. 13). Consistently with this relevance, modern techniques for spin detection and manipulation have greatly improved since Stern and Gerlach's times. It is now possible to deal with individual spins, rising the hopes for spintronics – exploiting the spin degree of freedom in electronic circuits, playing a similar role as the charge degree of freedom (Sect. 7.4.5†).

5.2.2 Spin Formalism

Three years after the publication of the Stern–Gerlach experiment, George Uhlenbeck and Samuel Goudsmit proposed another quantum number to specify the state of electrons (and of many other fundamental particles) [35]. It labels the two projections of the spin, by then a new physical entity representing an intrinsic angular momentum.

Since the spin is a pure quantum observable, only the matrix treatment formalism is possible. If $s = 1/2$, then the basis set of states is given by the two-component vectors (3.15) [36]

$$\varphi_{\uparrow}^{(z)} \equiv \varphi_{\frac{1}{2}\frac{1}{2}} \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \varphi_{\downarrow}^{(z)} \equiv \varphi_{\frac{1}{2}(-\frac{1}{2})} \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{5.20}$$

The following representation of the spin operators reproduces (5.7) and (5.9) for $j = 1/2$

$$\hat{S}_i = \frac{\hbar}{2}\sigma_i, \qquad (\hat{S}_i)^2 = \frac{\hbar^2}{4}\mathcal{I}, \qquad i = x, y, z, \tag{5.21}$$

where the σ_i are the Pauli matrices (3.16). Therefore the algebra suited for the spin case has been developed in Sect. 3.2.

The spin has its own associated magnetic moment

$$\hat{\boldsymbol{\mu}}_s = \frac{g_s \mu_\nu}{\hbar}\hat{\boldsymbol{S}}, \tag{5.22}$$

with a gyromagnetic ratio of $g_s = 2.00$ for electrons,[3] $g_s = 5.58$ for protons and $g_s = -3.82$ for neutrons. The constant μ_ν stands for minus the Bohr magneton μ_{B} in the case of electrons, or for the nuclear magneton $\mu_{\mathrm{p}} = e_{\mathrm{p}}\hbar/2M_{\mathrm{p}}$ in the case of protons and neutrons (Table A.1), where e_{p} and M_{p} are the proton charge and mass, respectively. The total magnetic moment operator is given by

$$\hat{\boldsymbol{\mu}} = \hat{\boldsymbol{\mu}}_s + \hat{\boldsymbol{\mu}}_l = \frac{\mu_\nu}{\hbar}\left(g_s\hat{\boldsymbol{S}} + g_l\hat{\boldsymbol{L}}\right). \tag{5.23}$$

Obviously, $g_l = 0$ for neutrons. The quantal magnetic moment is not always proportional to the angular momentum.

The eigenstates of the operator $\hat{S}_x$ have been obtained by means of a unitary transformation of the eigenvectors of $\hat{S}_z$ (3.21). This is a particular case of the more general transformation aligning the spin $s = 1/2$ operator with a direction of space labeled by the angles β, ϕ. The operator $\hat{S}_{\beta\phi}$ may be written as the scalar product of the spin vector $\hat{\boldsymbol{S}}$ times a unit vector along the chosen direction (see Problem 5 in Chap. 3):

$$\begin{aligned} \hat{S}_{\beta\phi} &= \sin\beta\cos\phi\,\hat{S}_x + \sin\beta\sin\phi\,\hat{S}_y + \cos\beta\,\hat{S}_z \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\beta & \sin\beta\exp(-\mathrm{i}\phi) \\ \sin\beta\exp(\mathrm{i}\phi) & -\cos\beta \end{pmatrix}. \end{aligned} \tag{5.24}$$

[3]The spectroscopy of single trapped electrons has yielded the value of $g_s = 2 \times 1.00159652188$. The theoretical QED calculation agrees within a few parts per billion [37], p. 5.

The same two eigenvalues $\pm\hbar/2$ are obtained upon diagonalization. As explained in Sect. 3.2, this is a consequence of space isotropy. The diagonalization also yields the state vectors

$$\varphi_{\uparrow}^{(\beta\phi)} = \begin{pmatrix} \cos\dfrac{\beta}{2} \\ \sin\dfrac{\beta}{2}\exp(\mathrm{i}\phi) \end{pmatrix}_z, \qquad \varphi_{\downarrow}^{(\beta\phi)} = \begin{pmatrix} \sin\dfrac{\beta}{2}\exp(-\mathrm{i}\phi) \\ -\cos\dfrac{\beta}{2} \end{pmatrix}_z, \tag{5.25}$$

while the rotational unitary transformation acting on states (5.20) is

$$\mathcal{U}_{\beta\phi} = \begin{pmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2}\exp(-\mathrm{i}\phi) \\ \sin\frac{\beta}{2}\exp(\mathrm{i}\phi) & -\cos\frac{\beta}{2} \end{pmatrix}. \tag{5.26}$$

The factor $1/2$ multiplying the angle β is characteristic of the effect of rotations on $j = 1/2$ objects. It may be verified through the value of the amplitudes (3.21) in the case of transformation from the z to the x eigenstates. In that case, $\beta = \pi/2, \phi = 0$.

An arbitrary linear combination of spin up and spin down states such as in (5.25) is called a qubit. The word "qubit" is short for "quantum bit," a concept used in quantum computation (Sect. 13.4†).

5.3 Other Features of the Motion in Angular Subspace

The contents of this section are extracted from [38], Appendix 1A.

5.3.1 Addition of Angular Momenta

Consider two angular momentum vector operators, $\hat{\boldsymbol{J}}_1$ and $\hat{\boldsymbol{J}}_2$. They are independent vectors, i.e. $[\hat{\boldsymbol{J}}_1, \hat{\boldsymbol{J}}_2] = 0$. Therefore, the product states are simultaneous eigenstates of the operators $\hat{J}_1^2,\ \hat{J}_{z1},\ \hat{J}_2^2$ and $\hat{J}_{z2}$:

$$\varphi_{j_1 m_1 j_2 m_2} = \varphi_{j_1 m_1}\varphi_{j_2 m_2}. \tag{5.27}$$

These $(2j_1+1)(2j_2+1)$ eigenstates constitute a complete basis for states carrying the quantum numbers j_1, m_1, j_2, m_2. However, it may not be the most useful one. We may prefer a basis labeled by the quantum numbers associated with the total angular momentum $\hat{\boldsymbol{J}}$ (see Fig. 5.5):

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{J}}_1 + \hat{\boldsymbol{J}}_2. \tag{5.28}$$

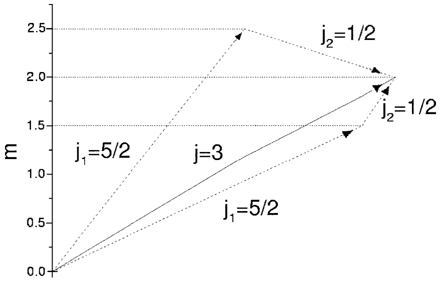

Fig. 5.5 Coupling of two vectors with $j_1 = 5/2$ and $j_2 = 1/2$ (*dotted lines*) may yield a vector with $j = 3$, $m = 2$ (*continuous line*). The superposition (5.31) has two components, with $m_1 = \frac{3}{2}$, $m_2 = \frac{1}{2}$ and $m_1 = \frac{5}{2}$, $m_2 = -\frac{1}{2}$, respectively

Since the components $\hat{J}_x, \hat{J}_y, \hat{J}_z$ also satisfy the commutation relations (5.4) and (5.6), there must exist another basis set made up from eigenstates of the operators $\hat{J}^2$ and $\hat{J}_z$. Since the commutation relations

$$[\hat{J}^2, \hat{J}_1^2] = [\hat{J}^2, \hat{J}_2^2] = [\hat{J}^2, \hat{J}_z] = [\hat{J}_1^2, \hat{J}_z] = [\hat{J}_2^2, \hat{J}_z] = 0 \tag{5.29}$$

vanish, the new set of basis states may be labeled by the quantum numbers j_1, j_2, j, m

$$\varphi_{j_1 j_2 j m} \equiv \left[\varphi_{j_1}\varphi_{j_2}\right]^j_m . \tag{5.30}$$

The two basis sets (5.27) and (5.30) are equally legitimate. According to Sect. 2.7.2*, there is a unitary transformation connecting the two bases

$$\varphi_{j_1 j_2 j m} = \sum_{m_1 m_2} c(j_1 m_1; j_2 m_2; jm)\, \varphi_{j_1 m_1 j_2 m_2}. \tag{5.31}$$

The quantum numbers j_1, j_2 are valid for both sets and they are not therefore summed up in (5.31). The sum over m_1, m_2 is restricted by the addition of projections

$$m = m_1 + m_2 \tag{5.32}$$

For classical vectors, the modulus of the sum of two vectors lies between the sum of their moduli and the absolute value of their difference. Something similar takes place in quantum mechanics:

$$j_1 + j_2 \geq j \geq |j_1 - j_2|. \tag{5.33}$$

The quantum number j is an integer if both j_1, j_2 are integers or half-integers; j is a half-integer if only one of the constituents is an integer. The amplitudes $c(j_1 m_1; j_2 m_2; jm)$ are called Wigner or Clebsch–Gordan coefficients. They are real numbers satisfying the symmetry relations

$$\begin{aligned} c(j_1m_1; j_2m_2; jm) &= (-1)^{j_1+j_2-j} c\big(j_1(-m_1); j_2(-m_2); j(-m)\big) \\ &= (-1)^{j_1+j_2-j} c\big(j_2m_2; j_1m_1; jm\big) \\ &= (-1)^{j_1-m_1}\sqrt{\frac{2j+1}{2j_2+1}} c\big(j_1m_1; j(-m); j_2(-m_2)\big) \\ &= (-1)^{j_2+m_2}\sqrt{\frac{2j+1}{2j_1+1}} c\big(j(-m); j_2m_2; j_1(-m_1)\big)\,. \end{aligned} \tag{5.34}$$

The inverse transformation is

$$\varphi_{j_1m_1}\varphi_{j_2m_2} = \sum_{j=|j_1-j_2|}^{j=j_1+j_2} c(j_1m_1; j_2m_2; jm)\left[\varphi_{j_1}\varphi_{j_2}\right]^j_{m=m_1+m_2}\,. \tag{5.35}$$

Replacement of (5.35) into the r.h.s. of (5.31) (and vice versa) yield the orthogonality relations

$$\begin{aligned} \sum_{m_1m_2} c(j_1m_1; j_2m_2; jm)\, c(j_1m_1; j_2m_2; j'm') &= \delta_{j'j}\delta_{m'm}\,, \\ \sum_{jm} c(j_1m_1; j_2m_2; jm)\, c(j_1m_1'; j_2m_2'; jm) &= \delta_{m_1'm_1}\delta_{m_2'm_2}\,. \end{aligned} \tag{5.36}$$

The example of the summation of an angular momentum j_1 with the spin $j_2 = s_2 = 1/2$ is given in Sect. 5.6* (See also Fig. 5.5).

5.3.2† *Rotations*

In analogy with (4.7), the unitary operator associated with rotations is

$$\mathcal{U}(\boldsymbol{\alpha}) = \exp\left(\frac{\mathrm{i}}{\hbar}\boldsymbol{\alpha}\cdot\hat{\boldsymbol{J}}\right). \tag{5.37}$$

The rotation is specified by the axis of rotation (direction of the vector $\boldsymbol{\alpha}$) and the magnitude of the rotation angle α. The operator $\hat{J}_i$ is referred to as the generator of rotations around the i-axis. The following properties stem from the commutators (5.4):

- The rotated state may be expressed as linear combinations of states carrying the same value of J.

$$\varphi_{JM} = \sum_K D^J_{MK}(\boldsymbol{\alpha})\,\varphi_{JK}\,. \tag{5.38}$$

- The operator (5.37) cannot be straightforwardly written as a product of three successive rotations along orthogonal coordinate axes. Instead, the transformation may be decomposed into the following three rotations, using the Euler parametrization ($\boldsymbol{\alpha} \rightarrow (\phi, \theta, \omega)$)

$$\begin{aligned}\mathcal{U}(\phi,\theta,\omega) &= \exp\left(\frac{\mathrm{i}}{\hbar}\hat{J}_z\phi\right)\exp\left(\frac{\mathrm{i}}{\hbar}\hat{J}_y\theta\right)\exp\left(\frac{\mathrm{i}}{\hbar}\hat{J}_z\omega\right)\\ D^J_{MK}(\phi,\theta,\omega) &= \langle JM|\mathcal{U}(\phi,\theta,\omega)|JK\rangle\\ &= \exp(\mathrm{i}M\phi)\; d^J_{MK}(\theta)\;\exp(\mathrm{i}K\omega)\,,\end{aligned} \tag{5.39}$$

  where

$$0 \le \phi \le 2\pi\,,\qquad 0 \le \theta \le \pi\,,\qquad 0 \le \omega \le 2\pi. \tag{5.40}$$

The unitary character of the rotational transformation is expressed by the relations

$$\sum_M D^{J*}_{MK_1}\,D^J_{MK_2} = \delta_{K_1K_2},\qquad \sum_K D^{J*}_{M_1K}\,D^J_{M_2K} = \delta_{M_1M_2}. \tag{5.41}$$

For the inverse rotation $(\phi,\theta,\omega)^{-1} = (\pi-\omega,\theta,-\pi-\phi)$

$$D^J_{MK}((\phi,\theta,\omega)^{-1}) = D^{J*}_{KM}(\phi,\theta,\omega). \tag{5.42}$$

The D functions constitute a complete orthogonal set of basis functions in the ϕ,θ,ω space.[4] Their normalization is obtained from the integral

$$\int_0^\pi \sin\theta d\theta\int_0^{2\pi}d\phi\int_0^{2\pi}d\omega\, D^{J*}_{MK}D^{J'}_{M'K'} = \frac{8\pi^2}{2J+1}\delta_{J'J}\delta_{M'M}\delta_{K'K}. \tag{5.43}$$

They represent generalizations of spherical harmonics, which are the complete orthogonal set in θ,ϕ space (Sect. 5.5*)

$$D^J_{M0}(\phi,\theta,\omega) = \left(\frac{4\pi}{2J+1}\right)^{1/2} Y_{JM}(\theta,\phi). \tag{5.44}$$

5.3.3† The Wigner–Eckart Theorem

One may also characterize operators $\hat{Q}_{\lambda\mu}$ by their transformation properties under rotations

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[4]In fact, they are the eigenstates of the axially symmetric top, K being the projection over the symmetry axis.

$$\hat{Q}_{\lambda\mu} = \sum_{\nu} D^{\lambda}_{\mu\nu}\, \hat{Q}_{\lambda\nu}. \tag{5.45}$$

An operator carrying $\lambda = 0$ is a scalar. A vector corresponds to a tensor of rank λ=1. Any operator can be expanded in a series of spherical tensors.

Since the expansions (5.31) and (5.35) have a pure geometrical origin, they are valid even if one or both of the state vectors are replaced by operators carrying angular momentum quantum numbers:

$$\varphi_{J_2 M_2} = \sum_{\mu M_1} c(J_1 M_1; \lambda\mu; J_2 M_2)\, \hat{Q}_{\lambda\mu}\, \varphi_{J_1 M_1}. \tag{5.46}$$

The scalar product of both sides with a state carrying the quantum numbers J_2', M_2' is given by

$$\sum_{\mu M_1} c(J_1 M_1; \lambda\mu | J_2 M_2)\, \langle J_2' M_2' | Q_{\lambda\mu} | J_1 M_1 \rangle = \mathcal{N}\, \delta_{J_2' J_2} \delta_{M_2' M_2}, \tag{5.47}$$

where $\mathcal{N}$ is independent of the magnetic quantum numbers. The Wigner–Eckart theorem is obtained multiplying both sides by the coefficient $c(J_1 M_1'; \lambda\mu'; J_2 M_2)$ and applying the orthogonality properties (5.36) (i.e. summing over J_2, M_2)

$$\langle J_2 M_2 | Q_{\lambda\mu} | J_1 M_1 \rangle = \mathcal{N}\, c(J_1 M_1; \lambda\mu; J_2 M_2). \tag{5.48}$$

All the dependence of the matrix element on the magnetic quantum numbers is expressed by means of a Clebsch–Gordan coefficient. Let us remark that this result holds whatever the nature of the initial and final states. The constant $\mathcal{N}$ is usually expressed through the reduced matrix element,[5] which is defined as

$$\langle J_2 || Q_{\lambda} || J_1 \rangle = \mathcal{N}\, (2J_2 + 1). \tag{5.49}$$

As a consequence of (5.48), we obtain selection rules analogous to (5.32) and (5.33) for the matrix elements $\langle J_2 M_2 | Q_{\lambda\mu} | J_1 M_1 \rangle$. For instance, matrix elements of a spherically symmetric operator vanish unless initial and final states are characterized by the same angular momentum quantum numbers. This is frequently the case of the Hamiltonian. In addition, the product of parities should be $\pi_f\, \pi_Q\, \pi_i = +1$. See also Problem 5.

5.4* Details of the Matrix Treatment

We define the operators

[5]The concept of reduced matrix element is applied in Sect. 9.8.5†.

$$\hat{J}_{\pm} = \hat{J}_x \pm \mathrm{i}\hat{J}_y. \tag{5.50}$$

They play a role similar to the creation and destruction operators a^+, a in the harmonic oscillator case (Sect. 3.3.1). Since the operator $\hat{J}_-$ is Hermitian conjugate to $\hat{J}_+$ (Sect. 2.7.1*),

$$\langle jm|J_+|jm'\rangle = \langle jm'|J_-|jm\rangle^*. \tag{5.51}$$

Applying the commutation relations (5.6), we obtain the relations

$$[\hat{J}_z, \hat{J}_+] = \hbar\hat{J}_+, \tag{5.52}$$
$$[\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z. \tag{5.53}$$

The matrix elements of (5.52) read

$$\langle jm'|[J_z, J_+]|jm\rangle = \hbar(m' - m)\langle jm'|J_+|jm\rangle = \hbar\langle jm'|J_+|jm\rangle, \tag{5.54}$$

which implies that $\langle jm'|J_+|jm\rangle$ is only different from zero if $m' = m + 1$. Therefore the operator $\hat{J}_+$ raises the projection of the angular momentum by one unit of $\hbar$ (and $\hat{J}_-$ does the opposite).

The expectation value of (5.53) yields

$$\begin{aligned}\langle jm|[J_+, J_-]|jm\rangle &= \langle jm|J_+|j(m-1)\rangle\langle j(m-1)|J_-|jm\rangle \\ &\quad -\langle jm|J_-|j(m+1)\rangle\langle j(m+1)|J_+|jm\rangle \\ &= |\langle jm|J_+|j(m-1)\rangle|^2 - |\langle j(m+1)|J_+|jm\rangle|^2 \\ &= 2\hbar^2 m,\end{aligned} \tag{5.55}$$

where (5.51) has been used. The solution to this first-order difference equation in $|\langle j(m+1)|J_+|jm)\rangle|^2$ is

$$|\langle j(m+1)|J_+|jm)\rangle|^2 = \hbar^2\big[c - m(m+1)\big]. \tag{5.56}$$

Since the left-hand side is positive, only the values of m that make the right-hand side positive are allowed and the matrix element between the last allowed eigenstate $\varphi_{jm_{\max}}$ and the first rejected eigenstate $\varphi_{j(m_{\max}+1)}$ should therefore vanish. Here $m_{\max}$ is the positive root of the equation $c = m(m+1)$. The assignment of the quantum number $j = m_{\max}$ determines the value of the constant $c = j(j+1)$. Therefore,

$$\langle j(m+1)|J_+|jm)\rangle = \hbar\sqrt{(j-m)(j+m+1)}, \tag{5.57}$$

where the positive value for the square root is chosen by convention. The relative phases of states with different values of m are also fixed by this convention.

We verify the vanishing of the matrix elements connecting admitted and rejected states:

$$\langle j(j+1)|J_+|jj\rangle = \langle j(-j)|J_+|j(-j-1)\rangle = 0. \tag{5.58}$$

Since m increases in steps of one unit between $-j$ and j [see (5.54)], the possible values of the quantum numbers j, m are those given in (5.8).

The matrix elements (5.9) corresponding to the operators $\hat{J}_x$ and $\hat{J}_y$ can be obtained from (5.51) and from (5.57). Addition of the squares of these matrices yields the (diagonal) matrix elements of $\hat{J}^2$ (5.7).

5.5* Details of the Treatment of Orbital Angular Momentum

Eigenvalue Equation for the Operator $\hat{L}_z$

The eigenvalue equation for the operator $\hat{L}_z$ is

$$-\mathrm{i}\hbar\frac{\mathrm{d}\Psi(\phi)}{\mathrm{d}\phi} = l_z\Psi(\phi). \tag{5.59}$$

The solution is proportional to $\exp(\mathrm{i}l_z\phi/\hbar)$. We may require $\Psi(\phi+2\pi) = \Psi(\phi)$, which implies the existence of discrete values for the eigenvalue $l_z = \hbar m_l$ ($m_l = 0, \pm 1, \pm 2, \ldots$). Thus the orthonormal set of eigenfunctions[6] of the operator $\hat{L}_z$ is given by

$$\varphi_{m_l}(\phi) = \frac{1}{\sqrt{2\pi}}\exp(\mathrm{i}m_l\phi). \tag{5.60}$$

Eigenvalue Equation for the Operators $\hat{L}^2$, $\hat{L}_z$

We try a function of the form $\Psi(\theta,\phi) = P_{lm_l}(\theta)\exp(\mathrm{i}m_l\phi)$. It follows that, in the eigenvalue equation for the operator $\hat{L}^2$:

- We can make the replacement $\mathrm{d}^2/\mathrm{d}\phi^2 \to -m_l^2$
- We may drop the exponential $\exp(\mathrm{i}m_l\phi)$ from both sides of the equation

We obtain a differential equation depending on the single variable θ :

$$-\hbar^2\left(\frac{\mathrm{d}^2}{\mathrm{d}\theta^2} + \cot\theta\frac{\mathrm{d}}{\mathrm{d}\theta} - \frac{m_l^2}{\sin^2\theta}\right)P_{lm_l}(\theta) = \zeta P_{lm_l}(\theta). \tag{5.61}$$

[6] This is also the complete set in the angular subspace of a two-dimensional space.

The solutions to this equation for $m_l = 0$ may be expressed as polynomials $P_l(\cos\theta)$ of order l in $\cos\theta$, called Legendre polynomials ($l = 0, 1, 2, \dots$). Each P_l gives rise to the $2l + 1$ associated Legendre functions $P_{lm_l}(\theta)$ with $|m_l| \le l$. All of them are eigenfunctions of the operator $\hat{\boldsymbol{L}}^2$ with eigenvalue $\zeta = l(l+1)\hbar^2$.

The simultaneous eigenfunctions of the operators $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$ are called spherical harmonics:

$$Y_{lm_l}(\theta, \phi) = N_{lm_l} P_{lm_l}(\theta) \exp(\mathrm{i} m_l \phi), \tag{5.62}$$

where N_{lm_l} are constants chosen to satisfy the orthonormalization equation

$$\langle l' m_l' | l m_l \rangle = \int_0^{\pi} \sin\theta \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \, Y^*_{l'm_l'} Y_{lm_l} = \delta_{ll'} \delta_{m_l m_l'}. \tag{5.63}$$

Here

$$Y^*_{lm_l} = (-1)^{m_l} Y_{l(-m_l)}. \tag{5.64}$$

The spherical harmonics corresponding to the lower values of l are given in Table 5.1.

In particular, the vector $\mathbf{r}$ can be written in terms of the spherical harmonics $Y_{1\mu}$:

$$x = \sqrt{\frac{2\pi}{3}} r\,(-Y_{11} + Y_{1(-1)}), \qquad y = \mathrm{i}\sqrt{\frac{2\pi}{3}} r\,(Y_{11} + Y_{1(-1)}), \qquad z = \sqrt{\frac{4\pi}{3}} r\, Y_{10}. \tag{5.65}$$

The l values (5.13) are traditionally replaced by symbolic letters in the literature (Table 5.2). This correspondence has only historical support.

The coupling to angular momentum zero of two spherical harmonics depending on different orientations in space depends on the angle α_{12} subtended by the two orientations through the equation

Table 5.1 Spherical harmonics corresponding to the lowest values of l

$Y_{00} = \dfrac{1}{\sqrt{4\pi}}$	$Y_{1(\pm 1)} = \mp\sqrt{\dfrac{3}{8\pi}} \sin\theta \exp(\pm \mathrm{i}\phi)$
$Y_{10} = \sqrt{\dfrac{3}{4\pi}} \cos\theta$	$Y_{2(\pm 1)} = \mp\sqrt{\dfrac{15}{32\pi}} \sin(2\theta) \exp(\pm \mathrm{i}\phi)$
$Y_{20} = \sqrt{\dfrac{5}{16\pi}} (3\cos^2\theta - 1)$	$Y_{2(\pm 2)} = \sqrt{\dfrac{15}{32\pi}} \sin^2\theta \exp(\pm \mathrm{i}2\phi)$

Table 5.2 Equivalence between quantum number l and symbolic letters

l	Symbol
0	s
1	p
2	d
3	f
4	g

$$\left[Y_l(\theta_1,\phi_1)Y_l(\theta_2\phi_2)\right]_0^0 = \frac{1}{\sqrt{2l+1}}\sum_{m_l=-l}^{m_l=l}(-1)^{l-m_l}Y_{lm_l}(\theta_1,\phi_1)Y_{l(-m_l)}(\theta_2,\phi_2)$$
$$= (-1)^l\frac{\sqrt{2l+1}}{4\pi}P_l(\cos\alpha_{12}). \qquad (5.66)$$

5.6* Coupling with Spin $s = 1/2$

The use of (5.31) is exemplified in the case where the second angular momentum is the spin $j_2 = s = 1/2$ (Fig. 5.5). Here the summation consists of two terms, corresponding to the two values of the spin projection $m_s = \pm 1/2$. According to (5.33), there are also two values for the total angular momentum $j = j_1 \pm 1/2$. However, if $j_1 = 0$, only the value $j = 1/2$ is allowed:

$$\varphi_{(j_1=j+\frac{1}{2})sjm} = -\sqrt{\frac{j-m+1}{2j+2}}\varphi_{j_1(m-\frac{1}{2})_1}\begin{pmatrix}1\\0\end{pmatrix}_2 + \sqrt{\frac{j+m+1}{2j+2}}\varphi_{j_1(m+\frac{1}{2})_1}\begin{pmatrix}0\\1\end{pmatrix}_2, \qquad (5.67)$$
$$\varphi_{(j_1=j-\frac{1}{2})sjm} = \sqrt{\frac{j+m}{2j}}\varphi_{j_1(m-\frac{1}{2})_1}\begin{pmatrix}1\\0\end{pmatrix}_2 + \sqrt{\frac{j-m}{2j}}\varphi_{j_1(m+\frac{1}{2})_1}\begin{pmatrix}0\\1\end{pmatrix}_2.$$

A particular application of this example is the coupling of orbital motion with the spin of an electron (Sect. 6.2). In this case, the eigenstates $\varphi_{j_1m_1}$ are the spherical harmonics $Y_{l_1m_{l1}}$ (5.62). However, (5.67) is valid whatever the nature of the angular momentum j_1 may be.

If $j = j_1 + \frac{1}{2}$ and $|m| = j$, there is a single term in (5.67). For the particular case $j_1 = 0$, this is a physical consequence of the fact that a spherical object should be uncoupled from the total angular momentum (Fig. 5.2).

Problems

Problem 1. A plastic disk rotates with angular velocity 100 rad/s. Estimate, in units of $\hbar$, the order of magnitude of the angular momentum.

Problem 2. 1. Construct the matrix for the operator $\hat{L}_x$ (5.11) in the basis of spherical harmonics Y_{1m_l} (Table 5.1).

2. Diagonalize the matrix and compare its eigenvalues with those of the operator $\hat{L}_z$.

Problem 3. Verify that the product of the uncertainties $\Delta_{J_x}\Delta_{J_y}$ satisfies the inequality (2.36).

Problem 4. Calculate $\hat{\boldsymbol{J}} \times \hat{\boldsymbol{J}}$.

Problem 5. Consider the following matrix elements between spherical harmonic states:

$$\langle 00|Y_{20}|00\rangle, \quad \langle 10|Y_{20}|10\rangle, \quad \langle 11|Y_{21}|21\rangle, \quad \langle 00|Y_{11}|11\rangle, \quad \langle 00|Y_{11}|1(-1)\rangle,$$

$$\langle 00|\Pi|00\rangle, \quad \langle 11|\Pi|11\rangle, \quad \langle 00|\Pi|10\rangle.$$

1. Find out which of the above matrix elements vanishes due to conservation of orbital angular momentum and/or parity.
2. Calculate those that remain.

Problem 6. Calculate $[\hat{S}_x^2, \hat{S}_z]$ for spin $s = 1/2$ particles.

Problem 7. 1. Construct the eigenstates of $\hat{S}_x$ and $\hat{S}_y$ using the eigenstates of $\hat{S}_z$ as basis states.
2. If the spin S_x is measured when the particle is in an eigenstate of the operator $\hat{S}_y$, what are the possible results and their probabilities?
3. Construct the matrix corresponding to $\hat{S}_x$ using the eigenstates of $\hat{S}_y$ obtained in the first part as basis states.
4. Express the eigenstates $\varphi^{(s_x)}$ using the eigenstates $\varphi^{(s_y)}$ as basis states.

Problem 8. A particle is in the spin state $\begin{pmatrix} a \\ b \end{pmatrix}$, with a, b real. Calculate the probability of obtaining the eigenvalue $\hbar/2$ if:

1. S_x is measured
2. S_y is measured
3. S_z is measured

Problem 9. A particle is in the spin state $\Psi = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}$.

1. What are the values of S_z that would appear as a result of a measurement of this observable? What are the associated probabilities?
2. What is the mean value of S_z in this state?

Problem 10. 1. Construct the possible states with $m = 1/2$ that are obtained by coupling an orbital angular momentum $l = 2$ with a spin $s = 1/2$.
2. Verify the orthonormality of the coupled states.
3. Construct the wave vector corresponding to the state with $j = m = l + 1/2$. What is the probability that the spin points up?

Problem 11. Write the two-spin state vectors with $s = \frac{1}{2}$ that have a definite total angular momentum.

Problem 12. Apply the closure property as in (2.59) to the transformations (5.31) and (5.35).

Problem 13. Relate the coupling between an orbital angular momentum l and a spin $s = \frac{1}{2}$ to the coupling of the spin to the same orbital angular momentum.