Chapter 5

Theory of Angular Momentum and Spin

Rotational symmetry transformations, the group SO(3) of the associated rotation matrices and the corresponding transformation matrices of spin$-\frac{1}{2}$ states forming the group SU(2) occupy a very important position in physics. The reason is that these transformations and groups are closely tied to the properties of elementary particles, the building blocks of matter, but also to the properties of composite systems. Examples of the latter with particularly simple transformation properties are closed shell atoms, e.g., helium, neon, argon, the magic number nuclei like carbon, or the proton and the neutron made up of three quarks, all composite systems which appear spherical as far as their charge distribution is concerned. In this section we want to investigate how elementary and composite systems are described.

To develop a systematic description of rotational properties of composite quantum systems the consideration of rotational transformations is the best starting point. As an illustration we will consider first rotational transformations acting on vectors $\vec{r}$ in 3-dimensional space, i.e., $\vec{r} \in \mathbb{R}_3$, we will then consider transformations of wavefunctions $\psi(\vec{r})$ of single particles in $\mathbb{R}_{\not k}$, and finally transformations of products of wavefunctions like $\prod_{j=1}^{N} \psi_j(\vec{r}_j)$ which represent a system of N (spin-zero) particles in $\mathbb{R}_{\not k}$.

We will also review below the well-known fact that spin states under rotations behave essentially identical to angular momentum states, i.e., we will find that the algebraic properties of operators governing spatial and spin rotation are identical and that the results derived for products of angular momentum states can be applied to products of spin states or a combination of angular momentum and spin states.

5.1 Matrix Representation of the group SO(3)

In the following we provide a brief introduction to the group of three-dimensional rotation matrices. We will also introduce the generators of this group and their algebra as well as the representation of rotations through exponential operators. The mathematical techniques presented in this section will be used throughout the remainder of these notes.

Properties of Rotations in $\mathbb{R}_{\not\mathbb{K}}$

Rotational transformations of vectors $\vec{r} \in \mathbb{R}_{\not\mathbb{K}}$, in Cartesian coordinates $\vec{r} = (x_1, x_2, x_3)^T$, are linear and, therefore, can be represented by 3×3 matrices $R(\vec{\vartheta})$, where $\vec{\vartheta}$ denotes the rotation, namely around an axis given by the direction of $\vec{\vartheta}$ and by an angle $|\vec{\vartheta}|$. We assume the convention that rotations are right-handed, i.e., if the thumb in your right hand fist points in the direction of $\vec{\vartheta}$, then the fingers of your fist point in the direction of the rotation. $\vec{\vartheta}$ parametrizes the rotations uniquely as long as $|\vec{\vartheta}| < 2\pi$.
Let us define the rotated vector as

$$\vec{r}\,' = R(\vec{\vartheta})\,\vec{r} \quad . \tag{5.1}$$

In Cartesian coordinates this reads

$$x'_k = \sum_{j=1}^{3} [R(\vec{\vartheta})]_{kj}\, x_j \quad k = 1, 2, 3 \quad . \tag{5.2}$$

Rotations conserve the scalar product between any pair of vectors $\vec{a}$ and $\vec{b}$, i.e., they conserve $\vec{a} \cdot \vec{b} = \sum_{j=1}^{3} a_j b_j$. It holds then

$$\vec{a}\,' \cdot \vec{b}\,' = \sum_{j,k,\ell=1}^{3} [R(\vec{\vartheta})]_{jk}\, [R(\vec{\vartheta})]_{j\ell}\, a_k\, b_\ell = \sum_{j=1}^{3} a_j b_j \quad . \tag{5.3}$$

Since this holds for any $\vec{a}$ and $\vec{b}$, it follows

$$\sum_{j=1}^{3} [R(\vec{\vartheta})]_{jk}\, [R(\vec{\vartheta})]_{j\ell} = \delta_{k\ell} \quad . \tag{5.4}$$

With the definition of the transposed matrix R^T

$$[R^T]_{jk} \equiv R_{kj} \tag{5.5}$$

this property can be written

$$R(\vec{\vartheta})\, R^T(\vec{\vartheta}) = R^T(\vec{\vartheta})\, R(\vec{\vartheta}) = 1\!\!1 \quad . \tag{5.6}$$

This equation states the key characteristic of rotation matrices. From (5.6) follows immediatety for the determinant of $R(\vec{\vartheta})$ using $\det A\, B = \det A \det B$ and $\det A^T = \det A$

$$\det R(\vec{\vartheta}) = \pm 1 \quad . \tag{5.7}$$

Let us consider briefly an example to illustrate rotational transformations and to interpret the sign of $\det R(\vec{\vartheta})$. A rotation around the x_3-axis by an angle φ is described by the matrix

$$R(\vec{\vartheta} = (0, 0, \varphi)^T) = \pm \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.8}$$

In case of a prefactor $+1$, the matrix represents a proper rotation, in case of a prefactor -1 a rotation and an inversion at the origin. In the latter case the determinant of $R(\vec{\vartheta} = (0, 0, \varphi)^T)$ is negative, i.e. a minus sign in Eq.(5.7) implies that a rotation is associated with an inversion. In the following we want to exclude inversions and consider only rotation matrices with $\det R = 1$.

Definition of the Group SO(3)

We will consider then the following set

$$SO(3) \;=\; \{\, \text{real}\, 3\times 3 \text{ matrices}\, R;\; R\,R^T \;=\; R^T R \;=\; 1\!\!1,\; \det R \;=\; 1\,\} \tag{5.9}$$

This set of matrices is closed under matrix multiplication and, in fact, forms a group $\mathcal{G}$ satisfying the axioms

(i) For any pair $a,\, b \in \mathcal{G}$ the product $c \;=\; a \circ b$ is also in $\mathcal{G}$.

(ii) There exists an element e in $\mathcal{G}$ with the property $\forall a \in \mathcal{G} \rightarrow e \circ a \;=\; a \circ e \;=\; a$.

(iii) $\forall a,\, a \in \mathcal{G} \rightarrow \exists a^{-1} \in \mathcal{G}\, \text{with}\, a \circ a^{-1} \;=\; a^{-1} \circ a \;=\; e$.

(iv) For products of three elements holds the *associative law*
$a \circ (b \circ c) \;=\; (a \circ b) \circ c$.

We want to prove now that SO(3) as defined in (5.9) forms a group. For this purpose we must demonstrate that the group properties (i–iv) hold. In the following we will assume $R_1, R_2 \in$ SO(3) and do not write out "$\circ$" explicitly since it represents the matrix product.

(i) Obviously, $R_3 \;=\; R_1 R_2$ is a real, 3×3–matrix. It holds

$$R_3^T\, R_3 \;=\; (\, R_1\, R_2\,)^T\, R_1\, R_2 = \; R_2^T\, R_1^T\, R_1\, R_2 \;=\; R_2^T\, R_2 \;=\; 1\!\!1 \,. \tag{5.10}$$

Similarly, one can show $R_3 R_3^T \;=\; 1\!\!1$. Furthermore, it holds

$$\det R_3 \;=\; \det (\, R_1\, R_2\,) \;=\; \det R_1 \det R_2 \;=\; 1 \,. \tag{5.11}$$

It follows that R_3 is also an element of SO(3).

(ii) The group element 'e' is played by the 3×3 identity matrix $1\!\!1$.

(iii) From $\det R_1 \;\neq\; 0$ follows that R_1 is non-singular and, hence, there exists a real 3×3–matrix R_1^{-1} which is the inverse of R_1. We need to demonstrate that this inverse belongs also to SO(3). Since $(R_1^{-1})^T \;=\; (R_1^T)^{-1}$ it follows

$$(R_1^{-1})^T\, R_1^{-1} \;=\; (R_1^T)^{-1}\, R_1^{-1} \;=\; \left(\, R_1\, R_1^T\,\right)^{-1} \;=\; 1\!\!1^{-1} \;=\; 1\!\!1 \tag{5.12}$$

which implies $R_1^{-1} \;\in\;$ SO(3).

(iv) Since the associative law holds for multiplication of any square matrices this property holds for the elements of SO(3).

We have shown altogether that the elements of SO(3) form a group.
We would like to point out the obvious property that for all elements R of SO(3) holds

$$R^{-1} \;=\; R^T \tag{5.13}$$

Exercise 5.1.1: Test if the following sets together with the stated binary operation '$\circ$' form groups; identify subgroups; establish if 1-1 homomorphic mappings exist, i.e. mappings between the sets which conserve the group properties:
(a) the set of real and imaginary numbers $\{1, i, -1, -i\}$ together with multiplication as the binary operation '$\circ$';
(b) the set of matrices $\{M_1,\, M_2,\, M_3,\, M_4\}$

$$= \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right\} \tag{5.14}$$

together with matrix multiplication as the binary operation '$\circ$';
(c) the set of four rotations in the x_1, x_2–plane {rotation by O^o, rotation by 90^o, rotation by 180^o, rotation by 270^o} and consecutive execution of rotation as the binary operation '$\circ$'.

Generators, Lie Group, Lie Algebra

We want to consider now a most convenient, compact representation of $R(\vec{\vartheta})$ which will be of general use and, in fact, will play a central role in the representation of many other symmetry transformations in Physics. This representation expresses rotation matrices in terms of three 3×3–matrices $J_1,\, J_2,\, J_3$ as follows

$$R(\vec{\vartheta}) \;=\; \exp\left(-\frac{i}{\hbar} \vec{\vartheta} \cdot \vec{J} \right) \tag{5.15}$$

Below we will construct appropriate matrices J_k, presently, we want to assume that they exist. We want to show that for the property $R\,R^T \;=\; 1$ to hold, the matrices

$$L_k \;=\; -\frac{i}{\hbar} J_k \tag{5.16}$$

must be antisymmetric. To demonstrate this property consider rotations with $\vec{\vartheta} \;=\; \vartheta_k \hat{e}_k$ where $\hat{e}_k$ is a unit vector in the direction of the Cartesian k–axis. Geometric intuition tells us

$$R(\vartheta_k \hat{e}_k)^{-1} \;=\; R(-\vartheta_k \hat{e}_k) \;=\; \exp\left(-\vartheta_k\, L_k \right) \tag{5.17}$$

Using the property which holds for matrix functions

$$[f(R)]^T \;=\; f(R^T) \tag{5.18}$$

we can employ (5.13)

$$R(\vartheta_k \hat{e}_k)^{-1} \;=\; R(\vartheta_k \hat{e}_k)^T \;=\; [\exp\left(\vartheta_k\, L_k \right)]^T \;=\; \exp\left(\vartheta_k\, L_k^T \right) \tag{5.19}$$

and, due to the uniqueness of the inverse, we arrive at the property

$$\exp\left(\vartheta_k\, L_k^T \right) \;=\; \exp\left(-\vartheta_k\, L_k \right) \tag{5.20}$$

from which follows $L_k^T \;=\; -L_k$.

We can conclude then that if elements of SO(3) can be expressed as $R = e^A$, the real matrix A is anti-symmetric. This property gives A then only three independent matrix elements, i.e., A must have the form

$$A = \begin{pmatrix} 0 & a & b \\ -a & 0 & c \\ -b & -c & 0 \end{pmatrix} . \tag{5.21}$$

It is this the reason why one can expect that three-dimensional rotation matrices can be expressed through (5.15) with three real parameters $\vartheta_1, \vartheta_2, \vartheta_3$ and three matrices L_1, L_2, L_3 which are independent of the rotation angles.

We assume now that we parameterize rotations through a three-dimensional rotation vector $\vec{\vartheta} = (\vartheta_1, \vartheta_2, \vartheta_3)^T$ such that for $\vec{\vartheta} = (0,0,0)^T$ the rotation is the identity. One can determine then the matrices L_k defined in (5.15) as the derivatives of $R(\vec{\vartheta})$ with respect to the Cartesian components ϑ_k taken at $\vec{\vartheta} = (0,0,0)^T$. Using the definition of partial derivatives we can state

$$L_1 = \lim_{\vartheta_1 \to 0} \vartheta_1^{-1} \left(R(\vec{\vartheta} = (\vartheta_1, 0, 0)^T) - \mathbb{1} \right) \tag{5.22}$$

and similar for L_2 and L_3.

Let us use this definition to evaluate L_3. Using (5.8) we can state

$$\lim_{\vartheta_3 \to 0} R[(0,0,\vartheta_3)^T] = \lim_{\vartheta_3 \to 0} \begin{pmatrix} \cos\vartheta_3 & -\sin\vartheta_3 & 0 \\ \sin\vartheta_3 & \cos\vartheta_3 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -\vartheta_3 & 0 \\ \vartheta_3 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{5.23}$$

Insertion into (5.22) for $k = 3$ yields

$$L_3 = \vartheta_3^{-1} \begin{pmatrix} 0 & -\vartheta_3 & 0 \\ \vartheta_3 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} . \tag{5.24}$$

One obtains in this way

$$-\frac{i}{\hbar} J_1 = L_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \tag{5.25}$$

$$-\frac{i}{\hbar} J_2 = L_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \tag{5.26}$$

$$-\frac{i}{\hbar} J_3 = L_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5.27}$$

The matrices L_k are called the *generators* of the group SO(3).

Exercise 5.1.2: Determine the generator L_1 according to Eq.(5.22).

Sofar it is by no means obvious that the generators L_k allow one to represent the rotation matrices for any finite rotation, i.e., that the operators (5.15) obey the group property. The latter property implies that for any $\vec{\vartheta}_1$ and $\vec{\vartheta}_2$ there exists a $\vec{\vartheta}_3$ such that

$$\exp\left(-\frac{i}{\hbar}\vec{\vartheta}_1 \cdot \vec{J}\right) \exp\left(-\frac{i}{\hbar}\vec{\vartheta}_2 \cdot \vec{J}\right) \;=\; \exp\left(-\frac{i}{\hbar}\vec{\vartheta}_3 \cdot \vec{J}\right) \tag{5.28}$$

The construction of the generators through the limit taken in Eq. (5.22) implies, however, that the generators represent infinitesimal rotations with $1 >> |\vec{\vartheta}|$ around the x_1-, x_2-, and x_3-axes. Finite rotations can be obtained by applications of many infinitesimal rotations of the type $R(\vec{\vartheta} = (\epsilon_1, 0, 0)^T) \;=\; \exp(\epsilon_1 L_1)$, $R(\vec{\vartheta} = (0, \epsilon_2, 0)^T) \;=\; \exp(\epsilon_2 L_2)$ and $R(\vec{\vartheta} = (0, 0, \epsilon_3)^T) \;=\; \exp(\epsilon_3 L_3)$. The question is then, however, if the resulting products of exponential operators can be expressed in the form (5.15). An answer can be found considering the Baker-Campbell-Hausdorf expansion

$$\exp(\,\lambda A\,)\exp(\,\lambda B\,) \;=\; \exp(\sum_{n=1}^{\infty} \lambda^n\, Z_n\,) \tag{5.29}$$

where $Z_1 \;=\; A \,+\, B$ and where the remaining operators Z_n are commutators of A and B, commutators of commutators of A and B, etc. The expression for Z_n are actually rather complicated, e.g. $Z_2 \;=\; \frac{1}{2}[A,\, B]$, $Z_3 \;=\; \frac{1}{12}(\,[A,\,[A,\,B]] \,+\, [[A,\,B],\,B]\,)$. From this result one can conclude that expressions of the type (5.15) will be closed under matrix multiplication only in the case that commutators of L_k can be expressed in terms of linear combinations of generators, i.e., it must hold

$$[L_k,\, L_\ell] \;=\; \sum_{m=1}^{3} f_{k\ell m}\, L_m \quad . \tag{5.30}$$

Groups with the property that their elements can be expressed like (5.15) and their generators obey the property (5.30) are called *Lie groups*, the property (5.30) is called the *Lie algebra*, and the constants $f_{k\ell m}$ are called the *structure constants*. Of course, Lie groups can have any number of generators, three being a special case.

In case of the group SO(3) the structure constants are particularly simple. In fact, the Lie algebra of SO(3) can be written

$$[L_k,\, L_\ell] \;=\; \epsilon_{k\ell m}\, L_m \tag{5.31}$$

where $\epsilon_{k\ell m}$ are the elements of the totally antisymmetric 3-dimensional tensor, the elements of which are

$$\epsilon_{k\ell m} \;=\; \begin{cases} 0 & \text{if any two indices are identical} \\ 1 & \text{for } k=1, \ell=2, m=3 \\ 1 & \text{for any even permutation of } k=1, \ell=2, m=3 \\ -1 & \text{for any odd permutation of } k=1, \ell=2, m=3 \end{cases} \quad . \tag{5.32}$$

For the matrices $J_k \;=\; i\hbar L_k$ which, as we see later, are related to angular momentum operators, holds the algebra

$$[J_k,\, J_\ell] \;=\; i\,\hbar\,\epsilon_{k\ell m}\, J_m \quad . \tag{5.33}$$

We want to demonstrate now that $\exp(\vec{\vartheta} \cdot \vec{L})$ yields the known rotational transformations, e.g., the matrix (5.8) in case of $\vartheta \;=\; (0, 0, \varphi)^T$. We want to consider, in fact, only the latter example and determine $\exp(\varphi L_3)$. We note, that the matrix φL_3, according to (5.27), can be written

$$\varphi L_3 = \begin{pmatrix} A & & 0 \\ & & 0 \\ 0 & 0 & 0 \end{pmatrix} , \quad A = \varphi \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} . \tag{5.34}$$

One obtains then for the rotational transformation

$$\begin{aligned} \exp\left[\begin{matrix} A & & 0 \\ & & 0 \\ 0 & 0 & 0 \end{matrix} \right] &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \sum_{\nu=1}^{\infty} \frac{1}{\nu!} \begin{pmatrix} A & & 0 \\ & & 0 \\ 0 & 0 & 0 \end{pmatrix}^{\nu} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \sum_{\nu=1}^{\infty} \frac{1}{\nu!} \begin{pmatrix} A^{\nu} & & 0 \\ & & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \sum_{\nu=0}^{\infty} \frac{1}{\nu!} A^{\nu} & & 0 \\ & & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} e^{A} & & 0 \\ & & 0 \\ 0 & 0 & 1 \end{pmatrix} . \end{aligned} \tag{5.35}$$

To determine $expA = \sum_{\nu=1}^{\infty} A^{\nu}/\nu!$ we split its Taylor expansion into even and odd powers

$$e^{A} = \sum_{n=0}^{\infty} \frac{1}{(2n)!} A^{2n} + \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} A^{2n+1} . \tag{5.36}$$

The property

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^{2} = - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.37}$$

allows one to write

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^{2n} = (-1)^{n} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \quad \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}^{2n+1} = (-1)^{n} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{5.38}$$

and, accordingly,

$$e^{A} = \sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2n)!} \varphi^{2n} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2n+1)!} \varphi^{2n+1} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} . \tag{5.39}$$

Recognizing the Taylor expansions of $\cos\varphi$ and $\sin\varphi$ one obtains

$$e^{A} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \tag{5.40}$$

and, using (5.34, 5.35),

$$e^{\varphi L_3} = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.41}$$

which agrees with (5.8).

Exercise 5.1.3: Show that the generators L_k of SO(3) obey the commutation relationship (5.31).

5.2 Function space representation of the group SO(3)

In this section we will investigate how rotational transformations act on single particle wavefunctions $\psi(\vec{r})$. In particular, we will learn that transformation patterns and invariances are connected with the angular momentum states of quantum mechanics.

Definition

We first define how a rotational transformation acts on a wavefunction $\psi(\vec{r}\,)$. For this purpose we require stringent continuity properties of the wavefunction: the wavefunctions under consideration must be elements of the set $\mathbb{C}_\infty(\nvDash)$, i.e., complex-valued functions over the 3-dimensional space $\mathbb{R}_\nvDash$ which can be differentiated infinitely often. In analogy to $R(\vec{\vartheta})$ being a linear map $\mathbb{R}_\nvDash \to \mathbb{R}_\nvDash$, we define rotations $\mathcal{R}(\vec{\vartheta})$ as linear maps $\mathbb{C}_\infty(\nvDash) \to \mathbb{C}_\infty(\nvDash)$, namely

$$\mathcal{R}(\vec{\vartheta})\psi(\vec{r}\,) \;=\; \psi(R^{-1}(\vec{\vartheta})\,\vec{r}\,) \quad . \tag{5.42}$$

Obviously, the transformation $\mathcal{R}(\vec{\vartheta})$: $\mathbb{C}_\infty(\nvDash) \to \mathbb{C}_\infty(\nvDash)$ is related to the transformation $R(\vec{\vartheta})$: $\mathbb{R}_\nvDash \to \mathbb{R}_\nvDash$, a relationship which we like to express as follows

$$\mathcal{R}(\vec{\vartheta}) \;=\; \rho\left(R(\vec{\vartheta})\right) \quad . \tag{5.43}$$

$\rho(\;)$ conserves the group property of SO(3), i.e. for A, $B \in$ SO(3) holds

$$\rho(A\,B) \;=\; \rho(A)\,\rho(B) \quad . \tag{5.44}$$

This important property which makes $\rho($ SO(3) $)$ also into a group can be proven by considering

$$\rho\left(R(\vec{\vartheta}_1)\,R(\vec{\vartheta}_2)\right)\,\psi(\vec{r}) \qquad = \;\psi([\,R(\vec{\vartheta}_1)\,R(\vec{\vartheta}_2)\,]^{-1}\vec{r}) \tag{5.45}$$

$$= \;\psi([R(\vec{\vartheta}_2)]^{-1}\,[R(\vec{\vartheta}_1)]^{-1}\vec{r}) \quad = \;\rho\left(\,R(\vec{\vartheta}_2)\right)\,\psi([R(\vec{\vartheta}_1)]^{-1}\vec{r}) \tag{5.46}$$

$$= \;\rho\left(\,R(\vec{\vartheta}_1)\right)\,\rho\left(\,R(\vec{\vartheta}_2)\right)\,\psi(\vec{r}) \quad . \tag{5.47}$$

Since this holds for any $\psi(\vec{r}\,)$ one can conclude $\rho\left(\,R(\vec{\vartheta}_1)\right)\,\rho\left(\,R(\vec{\vartheta}_2)\right) \;=\; \rho\left(R(\vec{\vartheta}_1)\,R(\vec{\vartheta}_2)\right)$, i.e. the group property (5.44) holds.

Exercise 5.2.1: Assume the definition $\rho'\left(R(\vec{\vartheta})\right)\psi(\vec{r}) \;=\; \psi(R(\vec{\vartheta})\,\vec{r}\,)$. Show that in this case holds $\rho'(A\,B) \;=\; \rho'(B)\,\rho'(A)$.

Generators

One can assume then that $\mathcal{R}(\vec{\vartheta})$ should also form a Lie group, in fact, one isomorphic to SO(3) and, hence, its elements can be represented through an exponential

$$\mathcal{R}(\vec{\vartheta}) \;=\; \exp\left(-\frac{i}{\hbar}\,\vec{\vartheta}\cdot\vec{\mathcal{J}}\right) \tag{5.48}$$

where the generators can be determined in analogy to Eq. (5.22) according to

$$-\frac{i}{\hbar}\mathcal{J}_1 \;=\; \lim_{\vartheta_1\to 0}\vartheta_1^{-1}\left(\mathcal{R}(\vec{\vartheta}\;=\;(-\vartheta_1,0,0)^T)\;-\;1\right) \tag{5.49}$$

(note the minus sign of $-\vartheta_1$ which originates from the inverse of the rotation in Eq.(5.42)) and similarly for $\mathcal{J}_2$ and $\mathcal{J}_3$.
The generators $\mathcal{J}_k$ can be determined by applying (5.49) to a function $f(\vec{r})$, i.e., in case of $\mathcal{J}_3$,

$$\begin{aligned}-\frac{i}{\hbar}\mathcal{J}_3\, f(\vec{r}) \;&=\; \lim_{\vartheta_3\to 0}\vartheta_3^{-1}\left(\mathcal{R}(\vec{\vartheta}\;=\;(0,0,\vartheta_3)^T)\, f(\vec{r})\;-\;f(\vec{r})\right)\\ &=\; \lim_{\vartheta_3\to 0}\vartheta_3^{-1}\;(\;f(\,R(0,0,-\vartheta_3)\,\vec{r}\,)\;-\;f(\vec{r})\;)\;.\end{aligned} \tag{5.50}$$

Using (5.23, 5.24) one can expand

$$R(0,0,-\vartheta_3)\,\vec{r}\;\approx\;\begin{pmatrix}1 & \vartheta_3 & 0\\ -\vartheta_3 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x_1\\ x_2\\ x_3\end{pmatrix}\;=\;\begin{pmatrix}x_1+\vartheta_3 x_2\\ -\vartheta_3 x_1 + x_2\;.\\ x_3\end{pmatrix} \tag{5.51}$$

Inserting this into (5.50) and Taylor expansion yields

$$\begin{aligned}-\frac{i}{\hbar}\mathcal{J}_3\, f(\vec{r}) \;&=\; \lim_{\vartheta_3\to 0}\vartheta_3^{-1}\;(\;f(\vec{r})\;+\;\vartheta_3\, x_2\,\partial_1 f(\vec{r})\;-\;\vartheta_3\, x_1\,\partial_2 f(\vec{r})\;-\;f(\vec{r})\;)\\ &=\;(\,x_2\,\partial_1\;-\;x_1\,\partial_2\,)\;f(\vec{r})\;.\end{aligned} \tag{5.52}$$

Carrying out similar calculations for $\mathcal{J}_1$ and $\mathcal{J}_2$ one can derive

$$-\frac{i}{\hbar}\mathcal{J}_1 \;=\; x_3\partial_2\;-\;x_2\partial_3 \tag{5.53}$$

$$-\frac{i}{\hbar}\mathcal{J}_2 \;=\; x_1\partial_3\;-\;x_3\partial_1 \tag{5.54}$$

$$-\frac{i}{\hbar}\mathcal{J}_3 \;=\; x_2\partial_1\;-\;x_1\partial_2\quad . \tag{5.55}$$

Not only is the group property of SO(3) conserved by $\rho(\;)$, but also the Lie algebra of the generators. In fact, it holds

$$[\mathcal{J}_k,\,\mathcal{J}_\ell]\;=\;i\,\hbar\,\epsilon_{k\ell m}\,\mathcal{J}_m\quad . \tag{5.56}$$

We like to verify this property for $[\mathcal{J}_1,\,\mathcal{J}_2]$. One obtains using (5.53–5.55) and $f(\vec{r})\;=\;f$

$$\begin{aligned}&[\mathcal{J}_1,\mathcal{J}_2]\,f(\vec{r})\;=\;-\hbar^2\,[-\tfrac{i}{\hbar}\mathcal{J}_1,-\tfrac{i}{\hbar}\mathcal{J}_2]\,f(\vec{r})\;=-\hbar^2\times\\ &[\,(x_3\partial_2\,-\,x_2\partial_3)\,(x_1\partial_3 f\,-\,x_3\partial_1 f)\;-\;(x_1\partial_3\,-\,x_3\partial_1)\,(x_3\partial_2 f\,-\,x_2\partial_3 f)\,]\\ &=\;-\hbar^2\,[\,+x_1x_3\partial_2\partial_3 f\;-x_1x_2\partial_3^2 f\;-x_3^2\partial_1\partial_2 f\;+x_2x_3\partial_1\partial_3 f\;+\;x_2\partial_1 f\\ &-x_1\partial_2 f\;-x_1x_3\partial_2\partial_3 f\;+x_3^2\partial_1\partial_2 f\;+x_1x_2\partial_3^2 f\;-x_2x_3\partial_1\partial_3 f\;]\\ &=\;-\hbar^2\,(\,x_2\partial_1\,-\,x_1\partial_2\,)\,f(\vec{r})\;=\;i\hbar\mathcal{J}_3\,f(\vec{r})\;.\end{aligned} \tag{5.57}$$

Exercise 5.2.2: (a) Derive the generators $\mathcal{J}_k,\ k=1,2$ by means of limits as suggested in Eq. (5.49); show that (5.56) holds for $[\mathcal{J}_2,\,\mathcal{J}_3]$ and $[\mathcal{J}_3,\,\mathcal{J}_1]$.

Exercise 5.2.3: Consider a wave function $\psi(\phi)$ which depends only on the azimutal angle ϕ of the spherical coordinate system (r, θ, ϕ), i.e. the system related to the Cartesian coordinates through $x_1 = r\sin\theta\cos\phi$, $x_2 = r\sin\theta\sin\phi$, and $x_3 = r\cos\theta$. Show that for $\mathcal{J}_3$ as defined above holds $\exp(\frac{i\alpha}{\hbar}\mathcal{J}_3)\,\psi(\phi) = \psi(\phi + \alpha)$.

5.3 Angular Momentum Operators

The generators $\mathcal{J}_k$ can be readily recognized as the angular momentum operators of quantum mechanics. To show this we first note that (5.53–5.55) can be written as a vector product of $\vec{r}$ and ∇

$$-\frac{i}{\hbar}\vec{\mathcal{J}} = -\vec{r} \times \nabla\,. \tag{5.58}$$

From this follows, using the momentum operator $\vec{p} = \frac{\hbar}{i}\nabla$,

$$\vec{\mathcal{J}} = \vec{r} \times \frac{\hbar}{i}\nabla = \vec{r} \times \vec{p} \tag{5.59}$$

which, according to the correspondence principle between classical and quantum mechanics, identifies $\vec{\mathcal{J}}$ as the quantum mechanical angular momentum operator.
Equation (5.56) are the famous commutation relationships of the quantium mechanical angular momentum operators. The commutation relationships imply that no simultaneous eigenstates of all three $\mathcal{J}_k$ exist. However, the operator

$$\mathcal{J}^2 = \mathcal{J}_1^2 + \mathcal{J}_2^2 + \mathcal{J}_3^2 \tag{5.60}$$

commutes with all three $\mathcal{J}_k$, $k = 1, 2, 3$, i.e.,

$$[\mathcal{J}^2, \mathcal{J}_k] = 0\,, \quad k = 1, 2, 3\,. \tag{5.61}$$

We demonstrate this property for $k = 3$. Using $[AB, C] = A[B, C] + [A, C]B$ and (5.56) one obtains

$$\begin{aligned}
[\mathcal{J}^2, \mathcal{J}_3] &= [\mathcal{J}_1^2 + \mathcal{J}_2^2, \mathcal{J}_3] \qquad (5.62)\\
&= \mathcal{J}_1\,[\mathcal{J}_1, \mathcal{J}_3] + [\mathcal{J}_1, \mathcal{J}_3]\,\mathcal{J}_1 + \mathcal{J}_2\,[\mathcal{J}_2, \mathcal{J}_3] + [\mathcal{J}_2, \mathcal{J}_3]\,\mathcal{J}_2 \\
&= -i\hbar\,\mathcal{J}_1\,\mathcal{J}_2 - i\hbar\,\mathcal{J}_2\,\mathcal{J}_1 + i\hbar\,\mathcal{J}_2\,\mathcal{J}_1 + i\hbar\,\mathcal{J}_1\,\mathcal{J}_2 = 0
\end{aligned}$$

According to (5.61) simultaneous eigenstates of $\mathcal{J}^2$ and of one of the $\mathcal{J}_k$, usually chosen as $\mathcal{J}_3$, can be found. These eigenstates are the well-known spherical harmonics $Y_{\ell m}(\theta, \phi)$. We will show now that the properties of spherical harmonics

$$\mathcal{J}^2\,Y_{\ell m}(\theta, \phi) = \hbar^2\ell(\ell + 1)\,Y_{\ell m}(\theta, \phi) \tag{5.63}$$

$$\mathcal{J}_3\,Y_{\ell m}(\theta, \phi) = \hbar\,m\,Y_{\ell m}(\theta, \phi) \tag{5.64}$$

as well as the effect of the so-called raising and lowering operators

$$\mathcal{J}_\pm = \mathcal{J}_1 \pm i\,\mathcal{J}_2 \tag{5.65}$$

on the spherical harmonics, namely,

$$\mathcal{J}_+ \, Y_{\ell m}(\theta,\phi) \;=\; \hbar \sqrt{(\ell+m+1)(\ell-m)}\, Y_{\ell m+1}(\theta,\phi) \tag{5.66}$$

$$\mathcal{J}_+ \, Y_{\ell\ell}(\theta,\phi) \;=\; 0 \tag{5.67}$$

$$\mathcal{J}_- \, Y_{\ell m+1}(\theta,\phi) \;=\; \hbar \sqrt{(\ell+m+1)(\ell-m)}\, Y_{\ell m}(\theta,\phi) \tag{5.68}$$

$$\mathcal{J}_- \, Y_{\ell\, -\ell}(\theta,\phi) \;=\; 0 \tag{5.69}$$

are a consequence of the Lie algebra (5.56). For this purpose we prove the following theorem.

An Important Theorem

Theorem 1.1 *Let L_k, $k = 1,2,3$ be operators acting on a Hilbert space $\mathbb{H}$ which obey the algebra $[L_k, L_\ell] = \epsilon_{k\ell m}\, L_m$ and let $L_\pm = L_1 \pm i\, L_2$, $L^2 = L_1^2 + L_2^2 + L_3^2$. Let there exist states $|\ell\,\ell\rangle$ in $\mathbb{H}$ with the property*

$$L_+ \, |\ell\,\ell\rangle \;=\; 0 \tag{5.70}$$

$$L_3 \, |\ell\,\ell\rangle \;=\; -i\,\ell\, |\ell\,\ell\rangle \tag{5.71}$$

then the states defined through

$$L_- \, |\ell\, m+1\rangle \;=\; -i\,\beta_m \, |\ell\, m\rangle \tag{5.72}$$

have the following properties

$$(i) \quad L_+ \, |\ell\, m\rangle \;=\; -i\,\alpha_m \, |\ell\, m+1\rangle \tag{5.73}$$

$$(ii) \quad L_3 \, |\ell\, m\rangle \;=\; -i\, m\, |\ell\, m\rangle \tag{5.74}$$

$$(iii) \quad L^2 \, |\ell\, m\rangle \;=\; -\,\ell(\ell+1)\, |\ell\, m\rangle \tag{5.75}$$

To prove this theorem we first show by induction that (i) holds. For this purpose we first demonstrate that the property holds for $m = \ell - 1$ by considering (i) for the state $L_-|\ell\ell\rangle \sim |\ell\ell-1\rangle$. It holds $L_+L_-|\ell\ell\rangle = (L_+L_- - L_-L_+ + L_-L_+)|\ell\,\ell\rangle = ([L_+,L_-] + L_-L_+)|\ell\,\ell\rangle$. Noting $[L_+,L_-] = [L_1 + iL_2, L_1 - iL_2] = -2iL_3$ and $L_+|\ell\,\ell\rangle = 0$ one obtains $L_+L_-|\ell\ell\rangle = -2iL_3|\ell\ell\rangle = -2\ell|\ell\ell\rangle$, i.e., in fact, L_+ raises the m-value of $|\ell\ell-1\rangle$ from $m = \ell - 1$ to $m = \ell$. The definitions of the coefficients $\alpha_{\ell-1}$ and $\beta_{\ell-1}$ yield $L_+L_-|\ell\ell\rangle = L_+(\,i\beta_{\ell-1}|\ell\ell-1\rangle = -\,\alpha_{\ell-1}\beta_{\ell-1}\,|\ell\ell\rangle$, i.e.

$$\alpha_{\ell-1}\beta_{\ell-1} \;=\; 2\ell \quad . \qquad (*) \tag{5.76}$$

We now show that property (ii) also holds for $m = \ell - 1$ proceeding in a similar way. We note $L_3L_-|\ell\ell\rangle = (\,[L_3,L_-] + L_-L_3\,)\,|\ell\ell\rangle$. Using $[L_3,L_-] = [L_3, L_1 - iL_2] = L_2 + iL_1 = i\,(L_1 - iL_2) = iL_-$ and $L_3|\ell\ell\rangle = -i\ell|\ell\ell\rangle$ we obtain $L_3L_-|\ell\ell\rangle = (\,iL_- + L_-L_3\,)|\ell\ell\rangle = i(-\ell+1)\,L_-|\ell\ell\rangle$. From this follows that $L_-|\ell\ell\rangle$ is an eigenstate of L_3, and since we have already shown $|\ell\ell-1\rangle = (i\beta_{\ell-1})^{-1}L_-|\ell\ell\rangle$ we can state $L_3|\ell\ell-1\rangle = -i(\ell-1)|\ell\ell-1\rangle$.

Continuing our proof through induction we assume now that property (i) holds for m. We will show that this property holds then also for $m-1$. The arguments are very similar to the ones used above and we can be brief. We consider $L_+L_-|\ell m\rangle = (\,[L_+,L_-] + L_-L_+\,)|\ell m\rangle = (\,-2iL_3 +$

$L_-L_+)|\ell m\rangle = (-2m - \alpha_m\beta_m)|\ell m\rangle$. This implies that (i) holds for $m-1$, in particular, from $L_+L_-|\ell m\rangle = -\alpha_{m-1}\beta_{m-1}|\ell m\rangle$ follows the recursion relationship

$$\alpha_{m-1}\beta_{m-1} = 2m + \alpha_m\beta_m \quad . \qquad (**) \tag{5.77}$$

We will show now that if (ii) holds for m, it also holds for $m-1$. Again the argumemts are similar to the ones used above. We note $L_3L_-|\ell m\rangle = ([L_3, L_-] + L_-L_3)|\ell m\rangle = (iL_- - i\,m\,L_-)|\ell m\rangle = -i\,(m-1)\,L_-|\ell m\rangle$ from which we can deduce $L_3|\ell m-1\rangle = -i(m-1)|\ell m-1\rangle$.
Before we can finally show that property (iii) holds as well for all $-\ell \leq m \leq \ell$ we need to determine the coefficients α_m and β_m. We can deduce from $(*)$ and $(**)$

$$\begin{aligned}
\alpha_{\ell-1}\beta_{\ell-1} &= 2\ell \\
\alpha_{\ell-2}\beta_{\ell-2} &= 2\,(\ell - 1 + \ell) \\
\alpha_{\ell-3}\beta_{\ell-3} &= 2\,(\ell - 2 + \ell - 1 + \ell) \\
&\;\;\vdots
\end{aligned}$$

Obviously, it holds $\alpha_m\beta_m = 2\left(\sum_{k=m+1}^{\ell} k\right)$. Using the familiar formula $\sum_{k=0}^{n} k = n\,(n+1)/2$ one obtains

$$\begin{aligned}
\alpha_m\beta_m &= (\ell+1)\,\ell - (m+1)\,m = (\ell+1)\,\ell + m\,\ell - \ell\,m - (m+1)\,m \\
&= (\ell + m + 1)(\ell - m)
\end{aligned} \tag{5.78}$$

One can normalize the states $|\ell m\rangle$ such that $\alpha_m = \beta_m$, i.e., finally

$$\alpha_m = \beta_m = \sqrt{(\ell + m + 1)(\ell - m)}\,. \tag{5.79}$$

We can now show that (iii) holds for all proper m–values. We note that we can write $L^2 = \frac{1}{2}L_+L_- + \frac{1}{2}L_-L_+ + L_3^2$. It follows then $L^2|\ell m\rangle = -\left(\frac{1}{2}\alpha_{m-1}\beta_{m-1} + \frac{1}{2}\alpha_m\beta_m + m^2\right)|\ell m\rangle = -\left(\frac{1}{2}(\ell+m+1)(\ell-m)\right.$
$\left.+\frac{1}{2}(\ell+m)(\ell-m+1) + m^2\right) = -\ell(\ell+1)|\ell m\rangle$. This completes the proof of the theorem.
We note that Eqs. (5.70, 5.72, 5.73, 5.79) read

$$L_+|\ell m\rangle = -i\sqrt{(\ell+m+1)(\ell-m)}\,|\ell m+1\rangle \tag{5.80}$$

$$L_-|\ell m+1\rangle = -i\sqrt{(\ell+m+1)(\ell-m)}\,|\ell m\rangle\,, \tag{5.81}$$

i.e., yield properties (5.66, 5.69).
We will have various opportunities to employ the Theorem just derived. A first application will involve the construction of the eigenstates of the angular momentum operators as defined in (5.63, 5.64). For this purpose we need to express the angular momentum operators in terms of spherical coordinates (r, θ, ϕ.

Angular Momentum Operators in Spherical Coordinates

We want to express now the generators $\mathcal{J}_k$, given in (5.53–5.55), in terms of spherical coordinates defined through

$$x_1 = r\sin\theta\cos\phi \tag{5.82}$$

$$x_2 = r\sin\theta\sin\phi \tag{5.83}$$

$$x_3 = r\cos\theta \tag{5.84}$$

We first like to demonstrate that the generators $\mathcal{J}_k$, actually, involve only the angular variables θ and ϕ and not the radius r. In fact, we will prove

$$-\frac{i}{\hbar}\mathcal{J}_1 = \mathcal{L}_1 = \sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi} \tag{5.85}$$

$$-\frac{i}{\hbar}\mathcal{J}_2 = \mathcal{L}_2 = -\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi} \tag{5.86}$$

$$-\frac{i}{\hbar}\mathcal{J}_3 = \mathcal{L}_3 = -\frac{\partial}{\partial\phi} \quad . \tag{5.87}$$

To derive these properties we consider, for example, $\mathcal{L}_1 f(\theta,\phi) = (x_3\partial_2 - x_2\partial_3)f(\theta,\phi)$. Using (5.82–5.84) one obtains, applying repeatedly the chain rule,

$$\mathcal{L}_1 f(\theta,\phi) = (x_3\partial_2 - x_2\partial_3)\, f(\theta,\phi) \tag{5.88}$$

$$= \Big(x_3 \frac{\partial x_2/x_1}{\partial x_2}\frac{\partial}{\partial\tan\phi} + x_3\frac{\partial x_3/r}{\partial x_2}\frac{\partial}{\partial\cos\theta} \tag{5.89}$$

$$- x_2 \underbrace{\frac{\partial x_2/x_1}{\partial x_3}}_{=0} \frac{\partial}{\partial\tan\phi} - x_2\frac{\partial x_3/r}{\partial x_3}\frac{\partial}{\partial\cos\theta}\Big) f(\theta,\phi)$$

$$= \left(\frac{x_3}{x_1}\frac{\partial}{\partial\tan\phi} - \frac{x_3^2 x_2}{r^3}\frac{\partial}{\partial\cos\theta} - x_2\frac{x_1^2 + x_2^2}{r^3}\frac{\partial}{\partial\cos\theta}\right) f(\theta,\phi) \tag{5.90}$$

This yields, using $\partial/\partial\tan\phi = \cos^2\phi\,\partial/\partial\phi$ and $\partial/\partial\cos\theta = -(1/\sin\theta)\,\partial/\partial\theta$,

$$\mathcal{L}_1 f(\theta,\phi) = \Big(\frac{\cos\theta}{\sin\theta\cos\phi}\cos^2\phi\frac{\partial}{\partial\phi} + \tag{5.91}$$

$$+ \frac{\cos^2\theta\sin\theta\sin\phi}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{\sin\theta\sin\phi}{\sin\theta}\sin^2\theta\frac{\partial}{\partial\theta}\Big) f(\theta,\phi)$$

which agrees with expression (5.85).
We like to express now the operators $\mathcal{J}_3$ and $\mathcal{J}^2$, the latter defined in (5.60), in terms of spherical coordinates. According to (5.87) holds

$$\mathcal{J}_3 = \frac{\hbar}{i}\,\partial_\phi \,. \tag{5.92}$$

To determine $\mathcal{J}^2$ we note, using (5.85),

$$\begin{aligned}(\mathcal{L}_1)^2 &= \left(\sin\phi\,\frac{\partial}{\partial\theta} + \cot\theta\,\cos\phi\,\frac{\partial}{\partial\phi}\right)^2 \\ &= \sin^2\!\phi\,\frac{\partial^2}{\partial\theta^2} - \frac{1}{\sin^2\!\theta}\sin\!\phi\cos\!\phi\,\frac{\partial}{\partial\phi} + 2\cot\!\theta\sin\!\phi\cos\!\phi\,\frac{\partial^2}{\partial\theta\partial\phi} \\ &\quad + \cot\!\theta\cos^2\!\phi\,\frac{\partial}{\partial\theta} + \cot^2\!\theta\cos^2\!\phi\,\frac{\partial^2}{\partial\phi^2}\end{aligned} \tag{5.93}$$

and similarly, using (5.86),

$$(\mathcal{L}_2)^2 = \left(-\cos\phi\,\frac{\partial}{\partial\theta} + \cot\theta\,\sin\phi\,\frac{\partial}{\partial\phi}\right)^2$$

$$= \cos^2\phi \frac{\partial^2}{\partial\theta^2} + \frac{1}{\sin^2\theta}\sin\phi\cos\phi\frac{\partial}{\partial\phi} - 2\cot\theta\sin\phi\cos\phi\frac{\partial^2}{\partial\theta\partial\phi} + \cot\theta\sin^2\phi\frac{\partial}{\partial\theta} + \cot^2\theta\sin^2\phi\frac{\partial^2}{\partial\phi^2} . \tag{5.94}$$

It follows

$$(\mathcal{L}_1)^2 + (\mathcal{L}_2)^2 + (\mathcal{L}_3)^2 = \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + (\cot^2\theta + 1)\frac{\partial^2}{\partial\phi^2} . \tag{5.95}$$

With $\cot^2\theta + 1 = 1/\sin^2\theta$,

$$\frac{1}{\sin^2\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\left(\sin\theta\frac{\partial}{\partial\theta}\right) = \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} , \tag{5.96}$$

and the relationship between $\mathcal{L}_k$ and $\mathcal{J}_k$ as given in (5.85, 5.86, 5.87), one can conclude

$$\mathcal{J}^2 = -\frac{\hbar^2}{\sin^2\theta}\left[\left(\sin\theta\frac{\partial}{\partial\theta}\right)^2 + \frac{\partial^2}{\partial\phi^2}\right] . \tag{5.97}$$

Kinetic Energy Operator The kinetic energy of a classical particle can be expressed

$$\frac{\vec{p}^2}{2m} = \frac{p_r^2}{2m} + \frac{J^2_{\text{class}}}{2m\,r^2} \tag{5.98}$$

where $\vec{J}_{\text{class}} = \vec{r}\times m\vec{v}$ is the angular momentum and $p_r = m\dot{r}$ is the radial momentum. The corresponding expression for the quantum mechanical kinetic energy operator is

$$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\mathcal{J}^2}{2m\,r^2} , \tag{5.99}$$

which follows from the identity

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2\sin^2\theta}\left[\left(\sin\theta\frac{\partial}{\partial\theta}\right)^2 + \frac{\partial^2}{\partial\phi^2}\right] \tag{5.100}$$

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}r = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \tag{5.101}$$

and comparision with (5.97).

5.4 Angular Momentum Eigenstates

According to the theorem on page 107 above the eigenfunctions (5.63, 5.64) can be constructed as follows. One first identifies the Hilbert space $\mathbb{H}$ on which the generators $\mathcal{L}_k$ operate. The operators in the present case are $\mathcal{L}_k = -\frac{i}{\hbar}\mathcal{J}_k$ where the $\mathcal{J}_k$ are differential operators in θ and ϕ given in (5.85, 5.86, 5.87). These generators act on a subspace of $\mathbb{C}_\infty(\not{\mathbb{R}})$, namely on the space of complex-valued functions on the unit 3-dim. sphere S_2, i.e. $\mathbb{C}_\infty(\mathbb{S}_{\not{\in}})$. The functions in $\mathbb{C}_\infty(\mathbb{S}_{\not{\in}})$ have real variables

θ, ϕ, $0 \le \theta < \pi$, $0 \le \phi < 2\pi$, and to be admissable for description of quantum states, must be cyclic in ϕ with period 2π. The norm in $\mathbb{H}$ is defined through

$$|f|^2 = \int_{S_2} d\Omega\, f^*(\theta,\phi) f(\theta,\phi) \tag{5.102}$$

where $d\Omega = \sin\theta\, d\theta\, d\phi$ is the volume element of S_2. The function space endowed with this norm and including only functions for which the integral (5.102) exists, is indeed a Hilbert space.
The eigenfunctions (5.63, 5.64) can be constructed then by seeking first functions $Y_{\ell\ell}(\theta,\phi)$ in $\mathbb{H}$ which satisfy $\mathcal{L}_+ Y_{\ell\ell}(\theta,\phi) = 0$ as well as $\mathcal{L}_3 Y_{\ell\ell}(\theta,\phi) = -i\ell\, Y_{\ell\ell}(\theta,\phi)$, normalizing these functions, and then determining the family $\{Y_{\ell m}(\theta,\phi), m = -\ell, -\ell+1, \dots, \ell\}$ applying

$$\mathcal{L}_- Y_{\ell m+1}(\theta,\phi) = -i\sqrt{(\ell+m+1)(\ell-m)}\, Y_{\ell m}(\theta,\phi) \tag{5.103}$$

iteratively for $m = \ell-1, \ell-2, \dots, -\ell$. One obtains in this way

$$Y_{\ell m}(\theta,\phi) = \Delta(\ell,m) \left(\frac{1}{\hbar}\mathcal{J}_-\right)^{\ell-m} Y_{\ell\ell}(\theta,\phi) \tag{5.104}$$

$$\Delta(\ell,m) = \left[\frac{(\ell+m)!}{(2\ell)!\,(\ell-m)!}\right]^{\frac{1}{2}} \tag{5.105}$$

Constructing $Y_{\ell\ell} \to Y_{\ell\ell-1} \to\to \cdots Y_{\ell-\ell}$

We like to characterize the resulting eigenfunctions $Y_{\ell m}(\theta,\phi)$, the so-called *spherical harmonics*, by carrying out the construction according to (5.104, 5.105) explicitly. For this purpose we split off a suitable normalization factor as well as introduce the assumption that the dependence on ϕ is described by a factor $\exp(im\phi)$

$$Y_{\ell m}(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_{\ell m}(\cos\theta)\, e^{im\phi} . \tag{5.106}$$

It must hold

$$\mathcal{L}_+ Y_{\ell\ell}(\theta,\phi) = 0 \tag{5.107}$$

$$\mathcal{L}_3 Y_{\ell\ell}(\theta,\phi) = -i\,\ell\, Y_{\ell\ell}(\theta,\phi) . \tag{5.108}$$

The latter property is obviously satisfied for the chosen ϕ-dependence. The raising and lowering operators

$$\mathcal{L}_\pm = \mathcal{L}_1 \pm i\,\mathcal{L}_2 , \tag{5.109}$$

using (5.85–5.87), can be expressed

$$\mathcal{L}_\pm = \mp i\, e^{\pm i\phi} \left(\frac{\partial}{\partial\theta} \pm i\cot\theta \frac{\partial}{\partial\phi}\right) . \tag{5.110}$$

Accordingly, (5.107) reads

$$\left(\frac{\partial}{\partial\theta} + i\cot\theta \frac{\partial}{\partial\phi}\right) P_{\ell\ell}(\cos\theta)\, e^{i\ell\phi} = 0 \tag{5.111}$$

or

$$\left(\frac{\partial}{\partial\theta} \,-\, \ell\cot\theta \right) P_{\ell\ell}(\cos\theta) \;=\; 0 \tag{5.112}$$

where we employed the definition of $P_{\ell\ell}(\cos\theta)$ in (5.107). A proper solution of this equation, i.e., one for which

$$\int_0^\pi d\theta \sin\theta \, |P_{\ell\ell}(\cos\theta)|^2 \tag{5.113}$$

is finite, is

$$P_{\ell\ell}(\cos\theta) \;=\; N_\ell \sin^\ell\theta \tag{5.114}$$

as one can readily verify. The normalization factor N_ℓ is chosen such that

$$\int_0^\pi d\theta \sin\theta \, |Y_{\ell\ell}(\cos\theta)|^2 \;=\; 1 \tag{5.115}$$

holds. (5.106, 5.114) yield

$$|N_\ell|^2 \, \frac{2\ell+1}{4\pi} \, \frac{1}{(2\ell)!} \, 2\pi \int_0^\pi d\theta \sin^{2\ell+1}\theta \;=\; 1 \,. \tag{5.116}$$

The integral appearing in the last expression can be evaluated by repeated integration by parts. One obtains, using the new integration variable $x \,=\, \cos\theta$,

$$\begin{aligned}
\int_0^\pi d\theta \sin^{2\ell+1}\theta \;&=\; \int_{-1}^{+1} dx \, (1 \,-\, x^2)^\ell \\
&=\; \Big[x\,(1 \,-\, x^2)^\ell \Big]_{-1}^{+1} \,+\, 2\ell \int_{-1}^{+1} dx \, x^2 \, (1 \,-\, x^2)^{\ell-1} \\
&=\; 2\ell \left[\frac{x^3}{3} \, (1 \,-\, x^2)^{\ell-1} \right]_{-1}^{+1} \,+\, \frac{2\ell\cdot(2\ell-2)}{1\cdot 3} \int_{-1}^{+1} dx \, x^4 \, (1 \,-\, x^2)^{\ell-2} \\
&\;\;\vdots \\
&=\; \frac{2\ell\cdot(2\ell-2)\cdots 2}{1\cdot 3\cdot 5\cdots(2\ell-1)} \int_{-1}^{+1} dx \, x^{2\ell} \\
&=\; \frac{2\ell\cdot(2\ell-2)\cdots 2}{1\cdot 3\cdot 5\cdots(2\ell-1)} \, \frac{2}{2\ell+1} \;=\; \frac{(2\ell)!}{[1\cdot 3\cdot 5\cdots(2\ell-1)]^2} \, \frac{2}{2\ell+1}
\end{aligned} \tag{5.117}$$

Accordingly, (5.116) implies

$$|N_\ell|^2 \, \frac{1}{[1\cdot 3\cdot 5\cdots(2\ell-1)]^2} \;=\; 1 \tag{5.118}$$

from which we conclude

$$N_\ell \;=\; (-1)^\ell \, 1\cdot 3\cdot 5\cdots(2\ell-1) \tag{5.119}$$

where the factor $(-1)^\ell$ has been included to agree with convention[1]. We note that (5.106, 5.114, 5.119) provide the following expression for $Y_{\ell\ell}$

$$Y_{\ell\ell}(\theta,\phi) \;=\; (-1)^\ell \sqrt{\frac{2\ell+1}{4\pi} \, \frac{1}{(2\ell)!}} \, \frac{1}{2^\ell \ell!} \, \sin^\ell\theta \, e^{i\ell\phi} \,. \tag{5.120}$$

[1]See, for example, "Classical Electrodynamics, 2nd Ed." by J.D. Jackson (John Wiley, New York, 1975)

We have constructed a normalized solution of (5.106), namely $Y_{\ell\ell}(\theta,\phi)$, and can obtain now, through repeated application of (5.103, 5.110), the eigenfunctions $Y_{\ell m}(\theta,\phi)$, $m = \ell-1, \ell-2, \ldots -\ell$ defined in (5.63, 5.64). Actually, we seek to determine the functions $P_{\ell m}(\cos\theta)$ and, therefore, use (5.103, 5.110) together with (5.106)

$$\begin{aligned} & i\, e^{-i\phi} \left(\frac{\partial}{\partial\theta} - i\cot\theta \, \frac{\partial}{\partial\phi} \right) \sqrt{ \frac{2\ell+1}{4\pi} \frac{(\ell-m-1)!}{(\ell+m+1)!} }\, P_{\ell m+1}(\cos\theta)\, e^{i(m+1)\phi} \\ = & -i\sqrt{(\ell+m+1)(\ell-m)} \sqrt{ \frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!} }\, P_{\ell m}(\cos\theta)\, e^{im\phi} . \end{aligned} \quad (5.121)$$

This expressions shows that the factor $e^{im\phi}$, indeed, describes the ϕ-dependence of $Y_{\ell m}(\theta,\phi)$; every application of $\mathcal{L}_-$ reduces the power of $e^{i\phi}$ by one. (5.121) states then for the functions $P_{\ell m}(\cos\theta)$

$$\left(\frac{\partial}{\partial\theta} + (m+1)\cot\theta \right) P_{\ell m+1}(\cos\theta) = -(\ell+m+1)(\ell-m)\, P_{\ell m}(\cos\theta) . \quad (5.122)$$

The latter identity can be written, employing again the variable $x = \cos\theta$,

$$\begin{aligned} P_{\ell m}(x) = & \frac{-1}{(\ell+m+1)(\ell-m)} \times \quad (5.123) \\ & \times \left[-(1-x^2)^{\frac{1}{2}} \frac{\partial}{\partial x} + (m+1) \frac{x}{(1-x^2)^{\frac{1}{2}}} \right] P_{\ell m+1}(x) . \end{aligned}$$

We want to demonstrate now that the recursion equation (5.123) leads to the expression

$$P_{\ell m}(x) = \frac{1}{2^\ell \ell!} \frac{(\ell+m)!}{(\ell-m)!} (1-x^2)^{-\frac{m}{2}} \frac{\partial^{\ell-m}}{\partial x^{\ell-m}} (x^2-1)^\ell \quad (5.124)$$

called the *associated Legendre polynomials*. The reader should note that the associated Legendre polynomials, as specified in (5.124), are real. To prove (5.124) we proceed by induction. For $m = \ell$ (5.124) reads

$$\begin{aligned} P_{\ell\ell}(x) &= \frac{(2\ell)!}{2^\ell \ell!} (1-x^2)^{-\frac{\ell}{2}} (x^2-1)^\ell \\ &= (-1)^\ell\, 1\cdot 3\cdot 5 \cdots (2\ell-1)\, \sin^\ell\theta \end{aligned} \quad (5.125)$$

which agrees with (5.114, 5.119). Let us then assume that (5.124) holds for $m+1$, i.e.,

$$P_{\ell m+1}(x) = \frac{1}{2^\ell \ell!} \frac{(\ell+m+1)!}{(\ell-m-1)!} (1-x^2)^{-\frac{m+1}{2}} \frac{\partial^{\ell-m-1}}{\partial x^{\ell-m-1}} (x^2-1)^\ell . \quad (5.126)$$

Then holds, according to (5.123),

$$\begin{aligned} P_{\ell m}(x) = & \frac{-1}{2^\ell \ell!} \frac{(\ell+m)!}{(\ell-m)!} \left[-(1-x^2)^{\frac{1}{2}} \frac{\partial}{\partial x} + (m+1) \frac{x}{(1-x^2)^{\frac{1}{2}}} \right] \times \\ & \times (1-x^2)^{-\frac{m+1}{2}} \frac{\partial^{\ell-m-1}}{\partial x^{\ell-m-1}} (x^2-1)^\ell . \end{aligned} \quad (5.127)$$

By means of

$$\begin{aligned} & -(1-x^2)^{\frac{1}{2}} \frac{\partial}{\partial x} (1-x^2)^{-\frac{m+1}{2}} \frac{\partial^{\ell-m-1}}{\partial x^{\ell-m-1}} (x^2-1)^\ell \\ = & \quad -(1-x^2)^{-\frac{m}{2}} \frac{\partial^{\ell-m}}{\partial x^{\ell-m}} (x^2-1)^\ell \\ & \quad - (m+1) \frac{x}{(1-x^2)^{\frac{1}{2}}} (1-x^2)^{-\frac{m+1}{2}} \frac{\partial^{\ell-m-1}}{\partial x^{\ell-m-1}} \end{aligned} \tag{5.128}$$

one can show that (5.127) reproduces (5.124) and, therefore, that expression (5.124) holds for m if it holds for $m+1$. Since (5.124) holds for $m = \ell$, it holds then for all m.
We want to test if the recursion (5.123) terminates for $m = -\ell$, i.e., if

$$\mathcal{L}_- \, Y_{\ell\ell}(\theta, \phi) \; = \; 0 \tag{5.129}$$

holds. In fact, expression (5.124), which is equivalent to recursive application of $\mathcal{L}_-$, yields a vanishing expression for $m = -\ell - 1$ as long as ℓ is a non-negative integer. In that case $(1-x^2)^\ell$ is a polynomial of degree 2ℓ and, hence, the derivative $\partial^{2\ell+1}/\partial x^{2\ell+1}$ of this expression vanishes.

Constructing $Y_{\ell-\ell} \rightarrow Y_{\ell-\ell+1} \rightarrow \cdots Y_{\ell\ell}$

An alternative route to construct the eigenfunctions $Y_{\ell m}(\theta, \phi)$ determines first a normalized solution of

$$\mathcal{L}_- \, f(\theta, \phi) \quad = \quad 0 \tag{5.130}$$

$$\mathcal{L}_3 \, f(\theta, \phi) \quad = \quad i \, \ell \, f(\theta, \phi) \; , \tag{5.131}$$

identifies $f(\theta, \phi) = Y_{\ell-\ell}(\theta, \phi)$ choosing the proper sign, and constructs then the eigenfunctions $Y_{\ell-\ell+1}$, $Y_{\ell-\ell+2}$, etc. by repeated application of the operator $\mathcal{L}_+$. Such construction reproduces the eigenfunctions $Y_{\ell m}(\theta, \phi)$ as given in (5.106, 5.124) and, therefore, appears not very interesting. However, from such construction emerges an important symmetry property of $Y_{\ell m}(\theta, \phi)$, namely,

$$Y^*_{\ell m}(\theta, \phi) \; = \; (-1)^m \, Y_{\ell-m}(\theta, \phi) \tag{5.132}$$

which reduces the number of spherical harmonics which need to be evaluated independently roughly by half ; therefore, we embark on this construction in order to prove (5.132).
We first determine $Y_{\ell-\ell}(\theta, \phi)$ using (5.106, 5.124). It holds, using $x = \cos\theta$,

$$P_{\ell-\ell}(x) \; = \; \frac{1}{2^\ell \ell!} \frac{1}{(2\ell)!} (1-x^2)^{\frac{\ell}{2}} \frac{\partial^{2\ell}}{\partial x^{2\ell}} (x^2-1)^\ell \; . \tag{5.133}$$

Since the term with the highest power of $(x^2-1)^\ell$ is $x^{2\ell}$, it holds

$$\frac{\partial^{2\ell}}{\partial x^{2\ell}} (x^2-1)^\ell \; = \; (2\ell)! \tag{5.134}$$

and, therefore,

$$P_{\ell-\ell}(x) \; = \; \frac{1}{2^\ell \ell!} (1-x^2)^{\frac{\ell}{2}} \; . \tag{5.135}$$

Due to (5.106, 5.124) one arrives at

$$Y_{\ell-\ell}(\theta,\phi) \;=\; \sqrt{\frac{2\ell+1}{4\pi}\,\frac{1}{(2\ell)!}}\,\frac{1}{2^\ell \ell!}\,\sin^\ell\theta\, e^{-i\ell\phi}\;. \tag{5.136}$$

We note in passing that this expression and the expression (5.120) for $Y_{\ell\ell}$ obey the postulated relationship (5.132).
Obviously, the expression (5.136) is normalized and has the proper sign, i.e., a sign consistent with the family of functions $Y_{\ell m}$ constructed above. One can readily verify that this expression provides a solution of (5.130). This follows from the identity

$$\left(\frac{\partial}{\partial\theta} \;-\; i\cot\theta\,\frac{\partial}{\partial\phi}\right)\sin^\ell\theta\, e^{-i\ell\phi} \;=\; 0\;. \tag{5.137}$$

One can use (5.136) to construct all other $Y_{\ell m}(\theta,\phi)$. According to (5.80) and (5.110) applies the recursion

$$e^{i\phi}\left(\frac{\partial}{\partial\theta} \;+\; i\cot\theta\,\frac{\partial}{\partial\phi}\right) Y_{\ell m}(\theta,\phi) \;=\; \sqrt{(\ell+m+1)(\ell-m)}\,Y_{\ell m+1}(\theta,\phi)\;. \tag{5.138}$$

Employing (5.106), one can conclude for the associated Legendre polynomials

$$\sqrt{\frac{(\ell-m)!}{(\ell+m)!}}\left(\frac{\partial}{\partial\theta} \;-\; m\cot\theta\right)P_{\ell m}(\cos\theta)$$
$$=\; \sqrt{(\ell+m+1)(\ell-m)}\,\sqrt{\frac{(\ell-m-1)!}{(\ell+m+1)!}}\,P_{\ell m+1}(\cos\theta) \tag{5.139}$$

or

$$P_{\ell m+1}(\cos\theta) \;=\; \left(\frac{\partial}{\partial\theta} \;-\; m\cot\theta\right)P_{\ell m}(\cos\theta)\;. \tag{5.140}$$

Introducing again the variable $x = \cos\theta$ leads to the recursion equation [c.f. (5.122, 5.123)]

$$P_{\ell m+1}(x) \;=\; \left(-(1-x^2)^{\frac{1}{2}}\frac{\partial}{\partial x} \;-\; m\,\frac{x}{(1-x^2)^{\frac{1}{2}}}\right)P_{\ell m}(x)\;. \tag{5.141}$$

We want to demonstrate now that this recursion equation leads to the expression

$$P_{\ell m}(x) \;=\; \frac{(-1)^m}{2^\ell \ell!}\,(1-x^2)^{\frac{m}{2}}\,\frac{\partial^{\ell+m}}{\partial x^{\ell+m}}\,(x^2-1)^\ell \tag{5.142}$$

For this purpose we proceed by induction, following closely the proof of eq. (5.124). We first note that for $m = -\ell$ (5.142) yields

$$P_{\ell-\ell}(x) \;=\; \frac{(-1)^\ell}{2^\ell \ell!}\,(1-x^2)^{-\frac{\ell}{2}}\,(x^2-1)^\ell \;=\; \frac{1}{2^\ell \ell!}\,(1-x^2)^{\frac{\ell}{2}} \tag{5.143}$$

wich agrees with (5.135). We then assume that (5.142) holds for m. (5.141) reads then

$$P_{\ell m+1}(x) = \left(-(1-x^2)^{\frac{1}{2}} \frac{\partial}{\partial x} - m \frac{x}{(1-x^2)^{\frac{1}{2}}} \right) \frac{(-1)^m}{2^\ell \ell!} (1-x^2)^{\frac{m}{2}} \frac{\partial^{\ell+m}}{\partial x^{\ell+m}} (x^2-1)^\ell . \tag{5.144}$$

Replacing in (5.128) $m+1 \to -m$ or, equivalently, $m \to -m-1$ yields

$$\begin{aligned} & -(1-x^2)^{\frac{1}{2}} \frac{\partial}{\partial x} (1-x^2)^{\frac{m}{2}} \frac{\partial^{\ell+m}}{\partial x^{\ell+m}} (x^2-1)^\ell \\ = & \quad -(1-x^2)^{\frac{m+1}{2}} \frac{\partial^{\ell+m+1}}{\partial x^{\ell+m+1}} (x^2-1)^\ell \\ & \quad + m \frac{x}{(1-x^2)^{\frac{1}{2}}} (1-x^2)^{\frac{m}{2}} \frac{\partial^{\ell+m}}{\partial x^{\ell+m}} . \end{aligned} \tag{5.145}$$

Hence, (5.144) reads

$$P_{\ell m+1}(x) = \frac{(-1)^{m+1}}{2^\ell \ell!} (1-x^2)^{\frac{m+1}{2}} \frac{\partial^{\ell+m+1}}{\partial x^{\ell+m+1}} (x^2-1)^\ell , \tag{5.146}$$

i.e., (5.142) holds for $m+1$ if it holds for m. Since (5.142) holds for $m = -\ell$ we verified that it holds for all m.

The construction beginning with $Y_{\ell -\ell}$ and continuing with $Y_{\ell -\ell+1}$, $Y_{\ell -\ell+2}$, etc. yields the same eigenfunctions as the previous construction beginning with $Y_{\ell\ell}$ and stepping down the series of functions $Y_{\ell\ell-1}$, $Y_{\ell\ell-2}$, etc. Accordingly, also the associated Legendre polynomials determined this way, i.e., given by (5.142) and by (5.124), are identical. However, one notes that application of (5.124) yields

$$(-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_{\ell -m}(x) = \frac{(-1)^m}{2^\ell \ell!} (1-x^2)^{\frac{m}{2}} \frac{\partial^{\ell+m}}{\partial x^{\ell+m}} (x^2-1)^\ell , \tag{5.147}$$

the r.h.s. of which agrees with the r.h.s. of (5.142). Hence, one can conclude

$$P_{\ell m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_{\ell -m}(x) . \tag{5.148}$$

According to (5.106) this implies for $Y_{\ell m}(\theta, \phi)$ the identity (5.132).

The Legendre Polynomials

The functions

$$P_\ell(x) = P_{\ell 0}(x) \tag{5.149}$$

are called *Legendre polynomials*. According to both (5.124) and (5.142) one can state

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{\partial^\ell}{\partial x^\ell} (x^2-1)^\ell . \tag{5.150}$$

The first few polynomials are

$$P_0(x) \;=\; 1\;, \qquad P_1(x) \;=\; x\;, \qquad P_2(x) \;=\; \tfrac{1}{2}(3x^2 \,-\, 1)$$
$$P_3(x) \;=\; \tfrac{1}{2}\,(5x^3 \,-\, 3x) \qquad . \tag{5.151}$$

Comparision of (5.150) and (5.142) allows one to express the associated Legendre polynomials in terms of Legendre polynomials

$$P_{\ell m}(x) \;=\; (-1)^m\,(1-x^2)^{\frac{m}{2}}\,\frac{\partial^m}{\partial x^m}\,P_\ell(x)\;,\; m \,\geq\, 0 \tag{5.152}$$

and, accordingly, the spherical harmonics for $m \,\geq\, 0$

$$Y_{\ell m}(\theta,\phi) \;=\; \sqrt{\frac{2\ell+1}{4\pi}\,\frac{(\ell-m)!}{(\ell+m)!}}\,(-1)^m\,\sin^m\theta\;\times \tag{5.153}$$
$$\times\;\left(\frac{\partial}{\partial\cos\theta}\right)^m\;P_\ell(\cos\theta)\,e^{im\phi}\;.$$

The spherical harmonics for $m \,<\, 0$ can be obtained using (5.132).

The Legendre polynomials arise in classical electrodynamics as the expansion coefficients of the electrostatic potential around a point charge $q/|\vec{r}_1 - \vec{r}_2|$ where q is the charge, $\vec{r}_1$ is the point where the potential is measured, and $\vec{r}_2$ denotes the location of the charge. In case $q = 1$ and $|\vec{r}_2| \,<\, |\vec{r}_1|$ holds the identity[2]

$$\frac{1}{|\vec{r}_1 \,-\, \vec{r}_2|} \;=\; \sum_{\ell=0}^{\infty}\frac{r_2^\ell}{r_1^{\ell+1}}\,P_\ell(\cos\gamma) \tag{5.154}$$

where γ is the angle between $\vec{r}_1$ and $\vec{r}_2$. Using $x \,=\, \cos\gamma$, $t \,=\, r_2/r_1$, and

$$|\vec{r}_1 \,-\, \vec{r}_2| \;=\; r_1\,\sqrt{1\,-2\,x\,t\,+\,t^2}\;, \tag{5.155}$$

(5.154) can be written

$$w(x,t) \;=\; \frac{1}{\sqrt{1\,-\,2xt\,+\,t^2}} \;=\; \sum_{\ell=0}^{\infty} P_\ell(x)\,t^\ell\;. \tag{5.156}$$

$w(x,t)$ is called a *generating function* of the Legendre polynomials[3].

The generating function allows one to derive useful properties of the Legendre polynomials. For example, in case of $x \,=\, 1$ holds

$$w(1,t) \;=\; \frac{1}{\sqrt{1\,-\,2t\,+\,t^2}} \;=\; \frac{1}{1\,-\,t} \;=\; \sum_{\ell=0}^{\infty} t^\ell\;. \tag{5.157}$$

Comparision with (5.156) yields

$$P_\ell(1) \;=\; 1\;, \qquad \ell \,=\, 0,\,1,\,2,\,\ldots \tag{5.158}$$

[2] see, e.g., "Classical Electrodynamics, 2nd Ed." by J.D. Jackson (John Wiley, New York, 1975), pp. 92

[3] To prove this property see, for example, pp. 45 of "Special Functions and their Applications" by N.N. Lebedev (Prentice-Hall, Englewood Cliffs, N.J., 1965) which is an excellent compendium on special functions employed in physics.

For $w(x,t)$ holds

$$\frac{\partial \ln w(x,t)}{\partial t} \;=\; \frac{x \,-\, t}{1 \,-\, 2xt \,+\, t^2}\;. \tag{5.159}$$

Using $\partial \ln w/\partial t \;=\; (1/w)\,\partial w/\partial t$ and multiplying (5.159) by $w(1 \,-\, 2xt \,+\, t^2)$ leads to the differential equation obeyed by $w(x,t)$

$$(1 \,-\, 2xt \,+\, t^2)\,\frac{\partial w}{\partial t} \;+\; (t \,-\, x)\,w \;=\; 0\;. \tag{5.160}$$

Employing (5.156) and $(\partial/\partial t)\sum_\ell P_\ell(x)t^\ell \;=\; \sum_\ell \ell P_\ell(x)t^{\ell-1}$ this differential equation is equivalent to

$$(1 \,-\, 2xt \,+\, t^2)\sum_{\ell=0}^{\infty}\ell P_\ell(x)\,t^{\ell-1} \;+\; (t \,-\, x)\sum_{\ell=0}^{\infty}P_\ell(x)\,t^\ell \;=\; 0 \tag{5.161}$$

Collecting coefficients with equal powers t^ℓ yields

$$\begin{aligned} 0 \;=\; & P_1(x) \;-\; x\,P_0(x) \\ & +\sum_{\ell=1}^{\infty}\left[(\ell+1)\,P_{\ell+1}(x) \;-\; (2\ell+1)x\,P_\ell(x) \;+\; \ell\,P_{\ell-1}(x)\right]t^\ell \end{aligned} \tag{5.162}$$

The coefficients for all powers t^ℓ must vanish individually. Accordingly, holds

$$P_1(x) \;=\; x\,P_0(x) \tag{5.163}$$

$$(\ell \,+\, 1)\,P_{\ell+1}(x) \;=\; (2\ell \,+\, 1)\,x\,P_\ell(x) \;-\; \ell\,P_{\ell-1}(x) \tag{5.164}$$

which, using $P_0(x) \;=\; 1$ [c.f. (5.151)] allows one to determine $P_\ell(x)$ for $\ell \;=\; 1,\,2,\,\ldots$.

Inversion Symmetry of $Y_{\ell m}(\theta,\phi)$ Under inversion at the origin vectors $\vec{r}$ are replaced by $-\vec{r}$. If the spherical coordinates of $\vec{r}$ are (r,θ,ϕ), then the coordinates of $-\vec{r}$ are $(r,\pi \,-\, \theta,\pi \,+\, \phi)$. Accordingly, under inversion $Y_{\ell m}(\theta,\phi)$ goes over to $Y_{\ell m}(\pi-\theta,\pi+\phi)$. Due to $\cos(\pi-\theta) \;=\; -\cos\theta$ the replacement $\vec{r} \,\rightarrow\, -\vec{r}$ alters $P_{\ell m}(x)$ into $P_{\ell m}(-x)$. Inspection of (5.142) allows one to conclude

$$P_{\ell m}(-x) \;=\; (-1)^{\ell+m}\,P_{\ell m}(x) \tag{5.165}$$

since $\partial^n/\partial(-x)^n \;=\; (-1)^n\partial^n/\partial x^n$. Noting $\exp[im(\pi+\phi)] \;=\; (-1)^m\exp(im\phi)$ we determine

$$Y_{\ell m}(\pi-\theta,\pi+\phi) \;=\; (-1)^\ell\,Y_{\ell m}(\theta,\phi)\;. \tag{5.166}$$

Properties of $Y_{\ell m}(\theta,\phi)$

We want to summarize the properties of the spherical harmonics $Y_{\ell m}(\theta,\phi)$ derived above.

1. The spherical harmonics are eigenfunctions of the angular momentum operators

$$\mathcal{J}^2\,Y_{\ell m}(\theta,\phi) \;=\; \hbar^2\,\ell(\ell+1)\,Y_{\ell m}(\theta,\phi) \tag{5.167}$$

$$\mathcal{J}_3\,Y_{\ell m}(\theta,\phi) \;=\; \hbar\,m\,Y_{\ell m}(\theta,\phi)\;. \tag{5.168}$$

2. The spherical harmonics form an orthonormal basis of the space $\mathbb{C}_\infty(S_2)$ of normalizable, uniquely defined functions over the unit sphere S_2 which are infinitely often differentiable

$$\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi Y^*_{\ell' m'}(\theta,\phi)\, Y_{\ell m}(\theta,\phi) \;=\; \delta_{\ell'\ell}\delta_{m'm} \;. \tag{5.169}$$

3. The spherical harmonics form, in fact, a *complete* basis of $\mathbb{C}_\infty(S_2)$, i.e., for any $f(\theta,\phi) \in \mathbb{C}_\infty(S_2)$ holds

$$f(\theta,\phi) \;=\; \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} C_{\ell m}\, Y_{\ell m}(\theta,\phi) \tag{5.170}$$

$$C_{\ell m} \;=\; \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi\, Y^*_{\ell m}(\theta,\phi) f(\theta,\phi) \;. \tag{5.171}$$

4. The spherical harmonics obey the recursion relationships

$$\mathcal{J}_+\, Y_{\ell m}(\theta,\phi) \;=\; \hbar\sqrt{(\ell+m+1)(\ell-m)}\; Y_{\ell m+1}(\theta,\phi) \tag{5.172}$$

$$\mathcal{J}_-\, Y_{\ell m+1}(\theta,\phi) \;=\; \hbar\sqrt{(\ell+m+1)(\ell-m)}\; Y_{\ell m}(\theta,\phi) \tag{5.173}$$

where $\mathcal{J}_\pm \;=\; \mathcal{J}_1 \,\pm\, i\mathcal{J}_2$.

5. The spherical harmonics are given by the formula

$$Y_{\ell m}(\theta,\phi) \;=\; \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{(-1)^m}{2^\ell \ell!}\,\sin^m\theta \;\times \tag{5.174}$$

$$\times\left(\frac{\partial}{\partial\cos\theta}\right)^m P_\ell(\cos\theta)\, e^{im\phi} \;, \quad m \,\geq\, 0$$

where $(\ell = 1, 2, \ldots)$

$$P_0(x) \;=\; 1 \;, \qquad P_1(x) \;=\; x \;, \tag{5.175}$$

$$P_{\ell+1}(x) \;=\; \tfrac{1}{\ell+1}\,[\,(2\ell\,+\,1)\,x\,P_\ell(x) \;-\; \ell\,P_{\ell-1}(x)\,] \tag{5.176}$$

are the *Legendre polynomials*. The spherical harmonics for $m \,<\, 0$ are given by

$$Y_{\ell -m}(\theta,\phi) \;=\; (-1)^m\, Y^*_{\ell m}(\theta,\phi) \;. \tag{5.177}$$

Note that the spherical harmonics are real, except for the factor $\exp(im\phi)$.

6. The spherical harmonics $Y_{\ell 0}$ are

$$Y_{\ell 0}(\theta,\phi) \;=\; \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta) \;. \tag{5.178}$$

7. For the Legendre polynomials holds the orthogonality property

$$\int_{-1}^{+1} dx\; P_\ell(x)\, P(\ell'(x) \;=\; \frac{2}{2\ell\,+\,1}\,\delta_{\ell\ell'} \;. \tag{5.179}$$

8. The spherical harmonics for $\theta = 0$ are

$$Y_{\ell m}(\theta = 0, \phi) \; = \; \delta_{m0} \sqrt{\frac{2\ell + 1}{4\pi}} \; . \tag{5.180}$$

9. The spherical harmonics obey the inversion symmetry

$$Y_{\ell m}(\theta, \phi) \; = \; (-1)^{\ell} \, Y_{\ell m}(\pi - \theta, \pi + \phi) \; . \tag{5.181}$$

10. The spherical harmonics for $\ell = 0, 1, 2$ are given by

$$Y_{00} \; = \; \frac{1}{\sqrt{4\pi}} \tag{5.182}$$

$$Y_{11} \; = \; -\sqrt{\frac{3}{8\pi}} \, \sin\theta \, e^{i\phi} \tag{5.183}$$

$$Y_{10} \; = \; \sqrt{\frac{3}{4\pi}} \, \cos\theta \tag{5.184}$$

$$Y_{22} \; = \; \frac{1}{4}\sqrt{\frac{15}{2\pi}} \, \sin^2\theta \, e^{2i\phi} \tag{5.185}$$

$$Y_{21} \; = \; -\sqrt{\frac{15}{8\pi}} \, \sin\theta \cos\theta \, e^{i\phi} \tag{5.186}$$

$$Y_{20} \; = \; \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} \cos^2\theta \; - \; \frac{1}{2} \right) \tag{5.187}$$

together with (5.177).

11. For the Laplacian holds

$$\nabla^2 \, h(r) \, Y_{\ell m}(\theta, \phi) \; = \; \left[\frac{1}{r} \frac{\partial^2}{\partial r^2} \, r \; - \; \frac{\ell(\ell + 1)}{r^2} \right] \, h(r) \, Y_{\ell m}(\theta, \phi) \; . \tag{5.188}$$

Exercise 5.4.1: Derive expressions (5.86), (5.87).
Exercise 5.4.2: Derive the orthogonality property for the Legendre polynomials (5.179) using the generating function $w(x,t)$ stated in (5.156). For this purpose start from the identity

$$\int_{-1}^{+1} dx \; w(x,t)^2 \; = \; \sum_{\ell,\ell'=0}^{\infty} t^{\ell+\ell'} \int_{-1}^{+1} dx P_{\ell}(x) \, P_{\ell'}(x) \; , \tag{5.189}$$

evaluate the integral on the l.h.s., expand the result in powers of t and equate the resulting powers to those arising on the r.h.s. of (5.189).
Exercise 5.4.3: Construct all spherical harmonics $Y_{3m}(\theta, \phi)$.

5.5 Irreducible Representations

We will consider now the effect of the rotational transformations introduced in (5.42), $\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$, on functions $f(\theta,\phi) \in \mathbb{C}_\infty(\mathbb{S}_{\nvDash})$. We denote the image of a function $f(\theta,\phi)$ under such rotational transformation by $\tilde{f}(\theta,\phi)$, i.e.,

$$\tilde{f}(\theta,\phi) \;=\; \exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right) f(\theta,\phi)\;. \tag{5.190}$$

Since the spherical harmonics $Y_{\ell m}(\theta,\phi)$ provide a complete, orthonormal basis for the function space $\mathbb{C}_\infty(\mathbb{S}_{\nvDash})$ one can expand

$$\tilde{f}(\theta,\phi) \;=\; \sum_{\ell,m} c_{\ell m}\, Y_{\ell m}(\theta,\phi) \tag{5.191}$$

$$c_{\ell m} \;=\; \int_{S_2} d\Omega'\, Y^*_{\ell m}(\theta',\phi') \exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right) f(\theta',\phi') \tag{5.192}$$

One can also represent $\mathbb{C}_\infty(\mathbb{S}_{\nvDash})$

$$\mathbb{C}_\infty(\mathbb{S}_{\nvDash}) \;=\; [\,\{\mathbb{Y}_{\ell\gtrdot},\, \ell \,=\, \nvdash, \nVdash, \ldots\, \infty,\, \gtrdot \,=\, -\ell, -\ell+\nVdash,\, \ldots, \ell\}\,] \tag{5.193}$$

where $[\,\{\quad\}\,]$ denotes closure of a set by taking all possible linear combinations of the elements of the set. The transformations $\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$, therefore, are characterized completely if one specifies the transformation of any $Y_{\ell m}(\theta,\phi)$

$$\tilde{Y}_{\ell m}(\theta,\phi) \;=\; \sum_{\ell',m'} \left[\mathcal{D}(\vec{\vartheta})\right]_{\ell' m';\,\ell m} Y_{\ell m}(\theta,\phi) \tag{5.194}$$

$$\left[\mathcal{D}(\vec{\vartheta})\right]_{\ell' m';\,\ell m} \;=\; \int_{S_2} d\Omega\, Y^*_{\ell' m'}(\theta,\phi) \exp\!\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right) Y_{\ell m}(\theta,\phi)\;, \tag{5.195}$$

i.e., if one specifies the functional form of the coefficients $[\mathcal{D}(\vartheta)]_{\ell' m';\,\ell m}$. These coefficients can be considered the elements of an infinite-dimensional matrix which provides the representation of $\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$ in the basis $\{Y_{\ell m},\, \ell \,=\, 0, 1, \ldots\, \infty,\, m \,=\, -\ell, -\ell+1,\, \ldots, \ell\}$.

We like to argue that the matrix representing the rotational transformations of the function space $\mathbb{C}_\infty(\mathbb{S}_{\nvDash})$, with elements given by (5.195), assumes a particularly simple form, called the irreducible representation. For this purpose we consider the subspaces of $\mathbb{C}_\infty(\mathbb{S}_{\nvDash})$

$$\mathbb{X}_\ell \;=\; [\,\{\mathbb{Y}_{\ell\gtrdot},\, \gtrdot \,=\, -\ell, -\ell+\nVdash,\, \ldots, \ell\}\,] \quad,\; \ell = \nvdash, \nVdash, \nvDash, \ldots \tag{5.196}$$

Comparision with (5.193) shows

$$\mathbb{C}_\infty(\mathbb{S}_{\nvDash}) \;=\; \bigcup_{\ell=\nvdash}^{\infty} \mathbb{X}_\ell\;. \tag{5.197}$$

The subspaces $\mathbb{X}_\ell$ have the important property that (i) they are invariant under rotations $\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$, i.e., $\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)(\mathbb{X}_\ell) \;=\; \mathbb{X}_\ell$, and (ii) they form the lowest dimensional sets $\mathbb{X}_\ell$ obeying $\mathbb{C}_\infty(\mathbb{S}_{\nvDash}) \;=\; \bigcup_\ell \mathbb{X}_\ell$ which have this invariance property.

The invariance of the subspaces $\mathbb{X}_\ell$ under rotations follows from a Taylor expansion of the exponential operator $\exp\left(-\frac{i}{\hbar}\,\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$. One proceeds by expanding first $\vec{\vartheta}\cdot\vec{\mathcal{J}}$ in terms of $\mathcal{J}_+$, $\mathcal{J}_-$, and $\mathcal{J}_3$

$$\vartheta\cdot\vec{\mathcal{J}} \;=\; \frac{1}{2}\vartheta_-\mathcal{J}_+ \;+\; \frac{1}{2}\vartheta_+\mathcal{J}_- \;+\; \vartheta_3\mathcal{J}_3 \tag{5.198}$$

where $\vartheta_\pm \;=\; \vartheta_1 \mp \vartheta_2$. The exponential operator $\exp\left(-\frac{i}{\hbar}\,\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$ can be expanded in powers $(\frac{1}{2}\vartheta_-\mathcal{J}_+ \;+\; \frac{1}{2}\vartheta_+\mathcal{J}_- \;+\; \vartheta_3\mathcal{J}_3)^n$. One employs then the commutation properties

$$[\mathcal{J}_+,\,\mathcal{J}_-] \;=\; 2\hbar\mathcal{J}_3\;, \quad [\mathcal{J}_3,\,\mathcal{J}_\pm] \;=\; \pm\hbar\mathcal{J}_\pm \tag{5.199}$$

which follow readily from (5.56, 5.65). Application of (5.199) allows one to express

$$\exp\left(-\frac{i}{\hbar}\,\vec{\vartheta}\cdot\vec{\mathcal{J}}\right) \;=\; \sum_{n_1,n_2,n_3} c_{n_1,n_2,n_3}\,\mathcal{J}_+^{n_1}\mathcal{J}_-^{n_2}\mathcal{J}_3^{n_3}\;. \tag{5.200}$$

Accordingly, one needs to consider the action of $\mathcal{J}_+^{n_1}\mathcal{J}_-^{n_2}\mathcal{J}_3^{n_3}$ on the subspaces $\mathbb{X}_\ell$. Since the $Y_{\ell m}$ are eigenfunctions of $\mathcal{J}_3$ the action of $\mathcal{J}_3^{n_3}$ reproduces the basis functions of $\mathbb{X}_\ell$, i.e., leaves $\mathbb{X}_\ell$ invariant. The action of $\mathcal{J}_-$ on $Y_{\ell m}$ produces $Y_{\ell m-1}$ or, in case $m \;=\; -\ell$, produces 0, i.e., $\mathcal{J}_-^{n_2}$ also leaves $\mathbb{X}_\ell$ invariant. Similarly, one can conclude that $\mathcal{J}_+^{n_1}$ leaves $\mathbb{X}_\ell$ invariant. Since any additive term in (5.200) leaves $\mathbb{X}_\ell$ invariant, the transformation $\exp\left(-\frac{i}{\hbar}\,\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$ leaves $\mathbb{X}_\ell$ invariant as well. One can conclude then that in the expansion (5.194) only spherical harmonics with $\ell' \;=\; \ell$ contribute or, equivalently, one concludes for the matrix elements (5.195)

$$[\mathcal{D}(\vartheta)]_{\ell' m';\,\ell m} \;=\; \delta_{\ell'\ell}\int_{S_2} d\Omega\, Y^*_{\ell m'}(\theta,\phi)\exp\left(-\frac{i}{\hbar}\,\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)Y_{\ell m}(\theta,\phi)\;. \tag{5.201}$$

From expression (5.200) of the rotational transformations one can also conclude that the $\mathbb{X}_\ell$ are the smallest invariant subspaces of $\mathbb{C}_\infty(\mathbb{S}_{\nvDash})$.
If one orders the basis according to the partitoning (5.197) of $\mathbb{C}_\infty(\mathbb{S}_{\nvDash})$ the matrix representation of $\mathcal{D}(\vartheta)$ assumes a block-diagonal form, with blocks of dimension $1, 3, 5, \ldots$, i.e.,

$$\mathcal{D}(\vartheta) \;=\; \begin{pmatrix} \boxed{1\times 1} & & & & \\ & \boxed{3\times 3} & & & \\ & & \ddots & & \\ & & & \boxed{(2\ell+1)\times(2\ell+1)} & \\ & & & & \ddots \end{pmatrix} \tag{5.202}$$

This representation of $\mathcal{D}(\vartheta)$ is the one wich has blocks of the lowest dimensions possible. The representation is referred to as the *irreducible representation*, other representations are termed *reducible representations*.

Exercise 5.5.1: Representations of the group SO(2)
SO(2) is the set of all 2×2 matrices R which are orthogonal, i.e. for which holds $R^T R = R R^T = 1\!\!1$, and for which $\det R = 1$.
(a) Show that SO(2) with the group operation $\circ$ defined as matrix multiplication, is a group.
(b) Prove that the elements of SO(2) can be completely characterized through a single parameter.
(c) Show that the map $R(\varphi)$

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = R(\varphi) \begin{pmatrix} x \\ y \end{pmatrix}$$

defines a representation of SO(2).
(d) Show that the similarity transformation $T(\varphi)$ defined in the space of non-singular, real 2×2–matrices O through

$$O' = T(\varphi)O = R(\varphi)OR^{-1}(\varphi)$$

with $R(\varphi)$ as in (c) is also a representation of SO(2).
(e) In the space $\mathbb{C}^\infty(\not{K})$ of infinitely often differentiable, and **periodic** functions $f(\alpha)$, i.e. $f(\alpha + 2\pi) = f(\alpha)$, the map $\rho(\varphi)$ defined through

$$f(\alpha) \stackrel{\rho}{\rightarrow} g(\varphi) = f(\alpha - \varphi) = \rho(\varphi) f(\alpha)$$

also defines a representation of SO(2). Determine the generator of $\rho(\varphi)$ in analogy to (5.22, 5.49).
(f) The transformation $\rho(\varphi)$ as defined in (e) leaves the following subspace of functions considered in (e)

$$X_m = \{ f(\alpha) = A\, e^{-im\alpha}, A \in \mathbb{C}, \gtrdot \in \mathbb{N} \}$$

invariant. Give the corresponding expression of $\rho(\varphi)$.

5.6 Wigner Rotation Matrices

We will now take an important first step to determine the functional form of the matrix elements of $\mathcal{D}(\vartheta)$. This step reconsiders the parametrization of rotations by the vector $\vec{\vartheta}$ assumed sofar. The three components $\vartheta_k, k = 1, 2, 3$ certainly allow one to describe any rotation around the origin. However, this parametrization, though seemingly natural, does not provide the simplest mathematical description of rotations. A more suitable parametrization had been suggested by Euler: every rotation $\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$ can be represented also uniquely by three consecutive rotations:

(i) a first rotation around the original x_3–axis by an angle α,

(ii) a second rotation around the new x_2'–axis by an angle β,

(iii) a third rotation around the new x_3''–axis by an angle γ.

The angles α, β, γ will be referred to as Euler angles. The axis x_2' is defined in the coordinate frame which is related to the original frame by rotation (i), the axis x_3'' is defined in the coordinate frame which is related to the original frame by the consecutive rotations (i) and (ii).
The Euler rotation replaces $\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right)$ by

$$e^{-\frac{i}{\hbar}\gamma J_3''} e^{-\frac{i}{\hbar}\beta J_2'} e^{-\frac{i}{\hbar}\alpha J_3} \quad . \tag{5.203}$$

For any $\vartheta \in \mathbb{R}^{\not\models}$ one can find Euler angles $\alpha,\ \beta,\ \gamma \in \mathbb{R}$ such that

$$\exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathcal{J}}\right) \ = \ e^{-\frac{i}{\hbar}\gamma J_3''} e^{-\frac{i}{\hbar}\beta J_2'} e^{-\frac{i}{\hbar}\alpha J_3} \tag{5.204}$$

is satisfied. Accordingly, one can replace (5.194, 5.195) by

$$\tilde{Y}_{\ell m}(\theta,\phi) \ = \ \sum_{\ell',m'} [\mathcal{D}(\alpha,\beta,\gamma)]_{\ell'm';\ell m} \ Y_{\ell m}(\theta,\phi) \tag{5.205}$$

$$[\mathcal{D}(\alpha,\beta,\gamma)]_{\ell'm';\ell m} \ = \ \int_{S_2} d\Omega\, Y^*_{\ell'm'}(\theta,\phi)\ e^{-\frac{i}{\hbar}\gamma J_3''} e^{-\frac{i}{\hbar}\beta J_2'} e^{-\frac{i}{\hbar}\alpha J_3} Y_{\ell m}(\theta,\phi)\ , \tag{5.206}$$

The expression (5.203) has the disadvantage that it employs rotations defined with respect to three different frames of reference. We will demonstrate that (5.203) can be expressed, however, in terms of rotations defined with respect to the original frame. For this purpose we notice that J_2' can be expressed through the similarity transformation

$$J_2' \ = \ e^{-\frac{i}{\hbar}\alpha J_3} J_2\, e^{\frac{i}{\hbar}\alpha J_3} \tag{5.207}$$

which replaces J_2' by the inverse transformation (i), i.e., the transformation from the rotated frame to the original frame, followed by J_2 in the original frame, followed by transformation (i), i.e., the transformation from the original frame to the rotated frame. Obviously, the l.h.s. and the r.h.s. of (5.214) are equivalent. For any similarity transformation involving operators A and S holds

$$e^{S\,A\,S^{-1}} \ = \ S\, e^A\, S^{-1}\ . \tag{5.208}$$

Accordingly, we can write

$$e^{-\frac{i}{\hbar}\beta J_2'} \ = \ e^{-\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\beta J_2}\ e^{\frac{i}{\hbar}\alpha J_3} \tag{5.209}$$

The first two rotations in (5.203), i.e., (i) and (ii), can then be written

$$e^{-\frac{i}{\hbar}\beta J_2'} e^{-\frac{i}{\hbar}\alpha J_3} \ = \ e^{-\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\beta J_2} \tag{5.210}$$

The third rotation in (5.203), in analogy to (5.209), is

$$e^{-\frac{i}{\hbar}\gamma J_3''} \ = \ e^{-\frac{i}{\hbar}\beta J_2'}\ e^{-\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\gamma J_3}\ e^{\frac{i}{\hbar}\alpha J_3}\ e^{\frac{i}{\hbar}\beta J_2'} \tag{5.211}$$

Using (5.209) in this expression one obtains

$$\begin{aligned} e^{-\frac{i}{\hbar}\gamma J_3''} \ &= \ e^{-\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\beta J_2}\ e^{\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\gamma J_3}\ e^{\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\alpha J_3}\ e^{\frac{i}{\hbar}\beta J_2}\ e^{\frac{i}{\hbar}\alpha J_3} \\ &= \ e^{-\frac{i}{\hbar}\gamma J_3''} \ = \ e^{-\frac{i}{\hbar}\alpha J_3}\ e^{-\frac{i}{\hbar}\beta J_2}\ e^{-\frac{i}{\hbar}\gamma J_3}\ e^{\frac{i}{\hbar}\beta J_2}\ e^{\frac{i}{\hbar}\alpha J_3} \end{aligned} \tag{5.212}$$

Multiplication from the left with (5.210) yields the simple result

$$e^{-\frac{i}{\hbar}\gamma J_3''} e^{-\frac{i}{\hbar}\beta J_2'} e^{-\frac{i}{\hbar}\alpha J_3} \;=\; e^{-\frac{i}{\hbar}\alpha J_3}\, e^{-\frac{i}{\hbar}\beta J_2}\, e^{-\frac{i}{\hbar}\gamma J_3}\,, \tag{5.213}$$

i.e., to redefine the three rotations in (5.203) with respect to the original (unprimed) frame one simply needs to reverse the order of the rotations. This allows one to express the rotational trasnformation (5.205, 5.206) by

$$\tilde{Y}_{\ell m}(\theta,\phi) \;=\; \sum_{\ell',m'} [\mathcal{D}(\alpha,\beta,\gamma)]_{\ell' m';\,\ell m}\; Y_{\ell m}(\theta,\phi) \tag{5.214}$$

$$[\mathcal{D}(\alpha,\beta,\gamma)]_{\ell' m';\,\ell m} \;=\; \int_{S_2} d\Omega\, Y^*_{\ell' m'}(\theta,\phi)\; e^{-\frac{i}{\hbar}\alpha J_3}\; e^{-\frac{i}{\hbar}\beta J_2}\; e^{-\frac{i}{\hbar}\gamma J_3} Y_{\ell m}(\theta,\phi)\,. \tag{5.215}$$

The evaluation of the matrix elements (5.215) benefits from the choice of Euler angles for the parametrization of rotational transformations. The eigenvalue property (5.64) yields

$$\int_{S_2} d\Omega\, f(\theta,\phi)\; e^{-\frac{i}{\hbar}\gamma J_3} Y_{\ell m}(\theta,\phi) \;=\; \int_{S_2} d\Omega\, f(\theta,\phi)\; Y_{\ell m}(\theta,\phi)\; e^{-im\gamma}\,. \tag{5.216}$$

Using, in addition, the self-adjointness of the operator $\mathcal{J}_3$ one can state

$$\int_{S_2} d\Omega\, Y^*_{\ell m}(\theta,\phi)\; e^{-\frac{i}{\hbar}\alpha J_3} f(\theta,\phi) \;=\; e^{-im'\alpha} \int_{S_2} d\Omega\, Y^*_{\ell m'}(\theta,\phi)\; f(\theta,\phi)\,. \tag{5.217}$$

Accordingly, one can write

$$[\mathcal{D}(\alpha,\beta,\gamma)]_{\ell m;\,\ell' m'} \;=\; e^{-i\alpha m'} \left(\int_{S_2} d\Omega\, Y^*_{\ell m'}(\theta,\phi)\, e^{-\frac{i}{\hbar}\beta \mathcal{J}_2}\; Y_{\ell m}(\theta,\phi) \right) e^{-i\gamma m}\, \delta_{\ell \ell'} \tag{5.218}$$

Defining the so-called *Wigner rotation matrix*

$$d^{(\ell)}_{m m'}(\beta) \;=\; \int_{S_2} d\Omega\, Y^*_{\ell m'}(\theta,\phi)\, e^{-\frac{i}{\hbar}\beta \mathcal{J}_2}\; Y_{\ell m}(\theta,\phi) \tag{5.219}$$

one can express the rotation matrices

$$[\mathcal{D}(\alpha,\beta,\gamma)]_{\ell m;\,\ell' m'} \;=\; e^{-i\alpha m'}\; d^{(\ell)}_{m' m}(\beta)\; e^{-i\gamma m}\;\; \delta_{\ell \ell'}\,. \tag{5.220}$$

We will derive below [see Eqs. (5.309, 5.310)] an explicit expression for the Wigner rotation matrix (5.219).

5.7 Spin $\frac{1}{2}$ and the group SU(2)

The spin describes a basic and fascinating property of matter. Best known is the spin of the electron, but many other elementary components of matter are endowed with spin-like properties. Examples are the other five members of the lepton family to which the electron belongs, the electron e and the electron neutrino ν_e of the first generation, the muon μ and its neutrino ν_μ of the second

generation, the tau τ and its neutrino ν_τ of the third generation and their antiparticles carry a spin-$\frac{1}{2}$. So do the three generations of six quarks, two of which (in certain linear combinations) make up the vector mesons which carry spin 1, and three of which make up the baryons which carry spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$. There are also the mediators, the gluon, the photon, the two $W^{\pm}$ and the Z^o, particles which mediate the strong and the electro-weak interactions, and which carry spin 1.
The particles mentioned, e.g. the quarks, carry other spin-like properties which together, however, have properties beyond those of single spins. In any case, there is nothing more elementary to matter than the spin property. The presence of this property permeates matter also at larger scales than those of the elementary particles mentioned, leaving its imprint on the properties of nuclei, atoms and molecules; in fact, the spin of the electron is likely the most important property in Chemistry. We may finally mention that the spin is at the heart of many properties of condensed matter systems, like superconductivity and magnetism. It appears to be rather impossible for a Physicist not to be enamored with the spin property. We will find that the spin in its transformation behaviour is closely related to angular momentum states, a relationship, which might be the reason why consideration of rotational symmetry is so often fruitful in the study of matter.
We will consider first only the so-called spin–$\frac{1}{2}$, generalizing then further below. Spin-$\frac{1}{2}$ systems can be related to two states which we denote by χ_+ and χ_-. Such systems can also assume any linear combination $c_+\chi_+ + c_-\chi_-$, $c_\pm \in \mathbb{C}$, as long as $|c_+|^2 + |c_-|^2 = 1$. If we identify the states χ_+ and χ_- with the basis of a Hilbert space, in which we define the scalar product between any state $|1\rangle = a_+\chi_+ + a_-\chi_-$ and $|2\rangle = b_+\chi_+ + b_-\chi_-$ as $\langle 1|2\rangle = a_+^* b_+ + a_-^* b_-$, then allowed symmetry transformations of spin states are described by 2×2-matrices U with complex-valued matrix elements U_{jk}. Conservation of the scalar product under symmetry transformations requires the property $U\,U^\dagger = U^\dagger U = 1\!\!1$ where $U^\dagger$ denotes the adjoint matrix with elements $\left[U^\dagger\right]_{jk} = U^*_{kj}$. We will specify for the transformations considered $\det U = 1$. This specification implies that we consider transformations save for overall factors $e^{i\phi}$ since such factors are known not to affect any observable properties.
The transformation matrices are then elements of the set

$$SU(2) \;=\; \{\,\text{complex}\,2\times 2\ \text{matrices}\,U;\ U\,U^\dagger \;=\; U^\dagger U \;=\; 1\!\!1,\ \det U \;=\; 1\,\} \tag{5.221}$$

One can show readily that this set forms a group with the groups binary operation being matrix multiplication.
How can the elements of SU(2) be parametrized. As complex 2×2 matrices one needs, in principle, eight real numbers to specify the matrix elements, four real and four imaginary parts of $U_{jk}, j,k = 1,2$. Because of the unitarity condition $U^\dagger U = 1\!\!1$ which are really four equations in terms of real quantities, one for each matrix element of $U^\dagger U$, and because of $\det U = 1$, there are together five conditions in terms of real quantities to be met by the matrix elements and, hence, the degrees of freedom of the matrices U are three real quantities. The important feature is that all $U \in$ SU(2) can be parametrized by an exponential operator

$$U \;=\; \exp\Big(-i\,\vec{\vartheta}\cdot\vec{S}\Big) \tag{5.222}$$

where the vector $\vec{S}$ has three components, each component $S_k, k = 1,2,3$ representing a 2×2 matrix. One can show that the unitarity condition requires these matrices to be hermitian, i.e. $[S_k]_{mn} = ([S_k]_{nm})^*$, and the condition $\det U = 1$ requires the S_k to have vanishing trace. There exist three such linear independent matrices, the simplest choice being

$$S_1 = \frac{1}{2}\sigma_1, \quad S_2 = \frac{1}{2}\sigma_2, \quad S_3 = \frac{1}{2}\sigma_3 \tag{5.223}$$

where σ_k, $k = 1, 2, 3$ are the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.224}$$

Algebraic Properties of the Pauli Matrices

The Pauli matrices (5.224) provide a basis in terms of which all traceless, hermitian 2×2–matrices A can be expandend. Any such A can be expressed in terms of three real parameters x, y, z

$$A = \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix}, \quad x,\, y,\, z, \in \mathbb{R}\,. \tag{5.225}$$

In fact, it holds,

$$A = x\,\sigma_1 + y\,\sigma_2 + z\,\sigma_3\,. \tag{5.226}$$

The Pauli matrices satisfy very special commutation and anti-commutation relationships. One can readily verify the *commutation property*

$$\sigma_j\,\sigma_k - \sigma_k\,\sigma_j = [\sigma_j,\, \sigma_k]_- = 2i\epsilon_{jk\ell}\,\sigma_\ell \tag{5.227}$$

which is essentially identical to the Lie algebra (5.31) of the group SO(3). We will show below that a 2-1–homomorphic mapping exists between SU(2) and SO(3) which establishes the close relationship between the two groups.
The Pauli matrices obey the following *anti-commutation properties*

$$\sigma_j\,\sigma_k + \sigma_k\,\sigma_j = [\sigma_j,\, \sigma_k]_+ = 2\delta_{jk}1\!\!1\,, \tag{5.228}$$

i.e.

$$\left(\sigma^j\right)^2 = 1\!\!1\,; \quad \sigma^j\sigma^k = -\,\sigma^k\sigma^j \quad \text{for } j \neq k \tag{5.229}$$

which can also be readily verified. According to this property the Pauli matrices generate a 3-dimensional *Clifford algebra* C_3. Clifford algebras play an important role in the mathematical structure of physics, e.g. they are associated with the important fermion property of matter. At this point we will state a useful property, namely,

$$(\vec{\sigma}\cdot\vec{a})\,(\vec{\sigma}\cdot\vec{b}) = \vec{a}\cdot\vec{b}\,1\!\!1 + i\vec{\sigma}\cdot(\vec{a}\times\vec{b}) \tag{5.230}$$

where $\vec{a}$, $\vec{b}$ are vectors commuting with $\vec{\sigma}$, but their comonents must not necessarily commute with each other, i.e., it might hold $a_jb_k - b_ka_j \neq 0$. The proof of this relation rests on the commutation relationship and the anti-commutation relationship (5.227, 5.229) and avoids commuting the components a_j and b_k. In fact, one obtains

$$(\vec{\sigma}\cdot\vec{a})\,(\vec{\sigma}\cdot\vec{b}) = \textstyle\sum_{j,k=1}^{3}\sigma^j\sigma^k\,a_jb_k = \\ \textstyle\sum_{j=1}^{3}(\sigma^j)^2\,a_jb_j + \sum_{\substack{j,k=1\\ j>k}}^{3}\sigma^j\sigma^k\,a_jb_k + \sum_{\substack{j,k=1\\ j<k}}^{3}\sigma^j\sigma^k\,a_jb_k\,. \tag{5.231}$$

Using $(\sigma^j)^2 = 1$ the first term on the r.h.s. yields $\vec{a} \cdot \vec{b}$. The two remaining terms yield using $\sigma^j \sigma^k = -\sigma^k \sigma^j$ for $j \neq k$ and altering 'dummy' summation indices

$$\begin{gathered}\sum_{\substack{j,k=1\\ j>k}}^{3} \sigma^j \sigma^k \, (a_j b_k - a_k b_j) = \\ \tfrac{1}{2} \sum_{\substack{j,k=1\\ j>k}}^{3} \sigma^j \sigma^k \, (a_j b_k - a_k b_j) - \tfrac{1}{2} \sum_{\substack{j,k=1\\ j>k}}^{3} \sigma^k \sigma^j \, (a_j b_k - a_k b_j) = \\ \tfrac{1}{2} \sum_{\substack{j,k=1\\ j>k}}^{3} (\sigma^j \sigma^k - \sigma^k \sigma^j) \, (a_j b_k - a_k b_j) \, . \end{gathered} \tag{5.232}$$

The commutation property (5.227) leads to

$$i \sum_{\substack{j,k=1\\ j>k}}^{3} \epsilon_{jk\ell} \sigma_l \, (a_j b_k - a_k b_j) = i \sum_{\ell=1}^{3} \sigma_\ell \left(\vec{a} \times \vec{b} \right)_\ell \, . \tag{5.233}$$

This result together with (5.231) proves (5.230).
In the special case $\vec{a} = \vec{b} \in \mathbb{R}^{\not\Vdash}$ holds

$$(\vec{\sigma} \cdot \vec{a})^2 = \vec{a}^{\,2} 1\!\!1 \, . \tag{5.234}$$

5.8 Generators and Rotation Matrices of SU(2)

Sofar there is nothing which relates the transformations U, i.e. (5.222), to rotations in space. This relationship emerges, however, through the algebra obeyed by the operators S_k

$$[S_k, \, S_\ell] = i \, \epsilon_{k\ell m} \, S_m \tag{5.235}$$

which is identical to that of the generators of SO(3). The algebra of the generators of a transformation is such a basic property that the 'accident' that the generators of spin transformations behave in this respect like the generators of 3-dimensional rotations makes spins appear in their physical behaviour like rotations. Well almost like it, since there is a slight difference: when you interprete the 3-component $\vec{\vartheta}$ in (5.222) as a rotation vector and you rotate once, let say around the x_2–axis by 360^o, spin changes sign; only a 720^o rotation leaves the spin invariant. We like to derive this result now by evaluating the transformations of SU(2) explicitly. For this purpose we choose to replace (5.222) by the Euler form

$$\exp(-i\gamma S_3) \exp(-i\beta S_2) \exp(-i\alpha S_3) \quad . \tag{5.236}$$

The matrix elements of this 2×2 operator can be labelled by the basis states χ_+ and χ_-, however, we like to draw in this respect also on a close analogy to angular momentum states which developes if one considers the operators $S^2 = S_1^2 + S_2^2 + S_3^2$ and S_3. Noticing the idempotence of the S_k's

$$S_k^2 = \frac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.237}$$

one obtains $S^2 = \frac{3}{4} 1\!\!1 = \frac{1}{2}(\frac{1}{2} + 1) 1\!\!1$ and, hence,

$$S^2 \, \chi_\pm = \frac{1}{2}(\frac{1}{2} + 1) \, \chi_\pm \quad ; \quad S_3 \, \chi_\pm = \pm \frac{1}{2} \, \chi_\pm \quad . \tag{5.238}$$

This result implies that the states $\chi_\pm$ behave in relation to the generators of SU(2) like an angular momentum state $|\frac{1}{2} \pm \frac{1}{2}\rangle$ in relation to the generators of SO(3). We may, therefore, use the label $|\frac{1}{2} \pm \frac{1}{2}\rangle$ for the states $\chi_\pm$.
We obtain with this notation for the transformations (5.236)

$$\begin{aligned} &\langle \tfrac{1}{2}m \mid \exp(-i\gamma S_3)\exp(-i\beta S_2)\exp(-i\alpha S_3) \mid \tfrac{1}{2}m'\rangle \\ &= e^{-i\gamma m}\,\langle \tfrac{1}{2}m \mid \exp(-i\beta S_2) \mid \tfrac{1}{2}m'\rangle\, e^{-i\alpha m'} \\ &= e^{-i\gamma m}\, d^{(\frac{1}{2})}_{mm'}(\beta) e^{-i\alpha m'} \end{aligned} \tag{5.239}$$

where we made use of the notation (5.219).
In order to determine the Wigner matrix in (5.219,5.239) one expands the exponential operator $\exp(-i\beta S_2)$. For this purpose one needs to determine the powers of $-i\beta S_2$. The idempotence property of S_k yields particularly simple expressions for these powers, namely,

$$(-\beta S_2)^{2n} = (-1)^n \left(\frac{\beta}{2}\right)^{2n} 1\!\!1 \tag{5.240}$$

$$(-\beta S_2)^{2n+1} = (-1)^n \left(\frac{\beta}{2}\right)^{2n+1} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad . \tag{5.241}$$

Taylor expansion of the exponential operator yields then

$$\exp(-i\beta S_2) = \left[\sum_{n=0}^{\infty} (-1)^n \left(\frac{\beta}{2}\right)^{2n}\right] 1\!\!1 + \left[\sum_{n=0}^{\infty} (-1)^n \left(\frac{\beta}{2}\right)^{2n+1}\right] \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{5.242}$$

The expressions in brackets [...] can be identified with the Taylor expansion of the cos- and sin-functions and one obtains for the rotation matrices

$$\left(d^{(\frac{1}{2})}_{mm'}(\beta) \right) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} . \tag{5.243}$$

We note the property of this rotation matrix

$$\left(d^{(\frac{1}{2})}_{mm'}(2\pi) \right) = -\,1\!\!1 \quad ; \tag{5.244}$$

i.e. rotation by 360^o changes the sign of the spin state.
The complete matrix elements (5.239) in the notation (5.220) are

$$[\mathcal{D}(\alpha,\beta,\gamma)]_{\ell m;\ell' m'} = \begin{pmatrix} \cos\frac{\beta}{2}\, e^{-i(\frac{\alpha}{2}+\frac{\gamma}{2}} & -\sin\frac{\beta}{2}\, e^{i(\frac{\alpha}{2}-\frac{\gamma}{2}} \\ \sin\frac{\beta}{2}\, e^{i(-\frac{\alpha}{2}+\frac{\gamma}{2}} & \cos\frac{\beta}{2}\, e^{i(\frac{\alpha}{2}+\frac{\gamma}{2}} \end{pmatrix} . \tag{5.245}$$

5.9 Constructing Spin States with Larger Quantum Numbers Through Spinor Operators

In this section we like to demonstrate, following Jourdan and Schwinger, that states $|\ell m\rangle$ for higher quantum numbers $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$, $m = -\ell, -\ell+1, \ldots \ell$ can be constructed formally from spin states $\chi_\pm$ if one considers the two properties $\chi_\pm$ to be carried by two kinds of **bosons**, i.e. identical particles any number of which can exist in the same state χ_+ and χ_-. One cannot consider the entities carrying the spin–$\frac{1}{2}$ to be particles in the ordinary sense for it can be shown that spin–$\frac{1}{2}$ particles have fermion character, i.e. no two such particles can exist in the same state.

Definition of Spinor Creation and Annihilation Operators

We present the states $\chi_\pm$ through creation operators $b_\pm^\dagger$ which when applied to a formal vacuum state $|\Psi_0\rangle$ generate $\chi_\pm$, i.e.

$$b_+^\dagger|\Psi_0\rangle \;=\; \chi_+ \quad ; \quad b_-^\dagger|\Psi_0\rangle \;=\; \chi_- \quad . \tag{5.246}$$

The corresponding adjoint operators are denoted by b_+ and b_-. The boson character of the operators $b^\dagger = (b_+^\dagger, b_-^\dagger)^T$ and $b = (b_+, b_-)^T$ is expressed through the commutation relationships ($\zeta, \zeta' = +, -$)

$$\left[b_\zeta, b_{\zeta'}\right] = \left[b_\zeta^\dagger, b_{\zeta'}^\dagger\right] = 0 \tag{5.247}$$

$$\left[b_\zeta, b_{\zeta'}^\dagger\right] = \delta_{\zeta\zeta'} \; . \tag{5.248}$$

For the vacuum state $|\Psi_0\rangle$ holds

$$b_\pm\,|\Psi_0\rangle \;=\; 0 \tag{5.249}$$

In the following will refer to $b^\dagger = (b_+^\dagger, b_-^\dagger)^T$ and $b = (b_+, b_-)^T$ as spinor creation and annihilation operators. These operators are associated with a given spatial reference system. We consider, therefore, also operators of the type

$$x\,b^\dagger \;=\; x_+ b_+^\dagger \;+\; x_- b_-^\dagger \quad ; \; x^* b \;=\; x_+^* b_+ \;+\; x_-^* b_- \tag{5.250}$$

which for $x^* x \;=\; x_+^* x_+ \;+\; x_-^* x_- \;=\; 1$ represent spinor operators in an arbitrary reference system. For example, using (5.243) the creation operators in a coordinate system rotated by an angle β around the y–axis are

$$\left(b'_+\right)^\dagger \;=\; \cos\frac{\beta}{2}\,b_+^\dagger \;+\; \sin\frac{\beta}{2}\,b_-^\dagger \quad ; \quad \left(b'_-\right)^\dagger \;=\; -\sin\frac{\beta}{2}\,b_+^\dagger \;+\; \cos\frac{\beta}{2}\,b_-^\dagger \; . \tag{5.251}$$

One can show using this property and (5.247,5.248) that $\left(b'_\zeta\right)^\dagger$ and b'_ζ obey the commutation relationships

$$\left[b'_\zeta, b'_{\zeta'}\right] = \left[b'^\dagger_\zeta, b'^\dagger_{\zeta'}\right] = 0 \tag{5.252}$$

$$\left[b'_\zeta, b'^\dagger_{\zeta'}\right] = \delta_{\zeta\zeta'} \; . \tag{5.253}$$

The States $|\Psi(j,m)\rangle$

The operators $b_\pm^\dagger$ allow one to construct a set of states which represent $j+m$–fold and $j-m$–fold χ_+ and χ_- states as follows

$$|\Psi\,(j,m)\rangle = \frac{\left(b_+^\dagger\right)^{j+m}}{\sqrt{(j+m)!}}\frac{\left(b_-^\dagger\right)^{j-m}}{\sqrt{(j-m)!}}|\Psi_0\rangle \; . \tag{5.254}$$

We will show below that these states are orthonormal and form spin states with higher quantum numbers, i.e. $j \;=\; 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots \; ; \; m \;=\; -j, -j+1, \ldots j$.

5.10 Algebraic Properties of Spinor Operators

We want to establish first a few important and useful algebraic properties which result from the commutation relationships (5.247, 5.248) and from (5.249).

The Spinor Derivative Operator

A most important operation is the action of the annihilation operators b_+ and b_- on operators which can be expressed as polynomials, possibly infinite power series, in $b_+^\dagger$ and $b_-^\dagger$. An example is the monomial $\left(b_+^\dagger\right)^{j+m} \left(b_-^\dagger\right)^{j-m}$ which generates the states (5.254). We will derive the result, well-known for the quantum mechanical harmonic oscillator, that the annihilation operators play a role similar to the differential operator in calculus.
For this purpose we consider the following polynomial of creation operators

$$f(b_+^\dagger) \;=\; \sum_{n=0}^{N} c_n \left(b_+^\dagger\right)^n \;. \tag{5.255}$$

In order to determine how this operator is modified by multiplication from the left by b_+ we note

$$b_+ f(b_+^\dagger)\,|\text{state}\rangle \;=\; \left[\, b_+,\; f(b_+^\dagger)\,\right]\;|\text{state}\rangle \;+\; f(b_+^\dagger)\, b_+\,|\text{state}\rangle\;. \tag{5.256}$$

In the special case $|\text{state}\rangle \;=\; |\Psi_0\rangle$ this reads using (5.249)

$$b_+ f(b_+^\dagger)\,|\Psi_0\rangle \;=\; \left[\, b_+,\; f(b_+^\dagger)\,\right]\;|\Psi_0\rangle\;. \tag{5.257}$$

Equations (5.256) and (5.257) motivate us to determine the commutator $\left[\, b_+,\; f(b_+^\dagger)\,\right]$ which for (5.255) is

$$\left[b_+, f\left(b^\dagger\right)\right] = \sum_n c_n \left[b_+, \left(b_+^\dagger\right)^n\right]. \tag{5.258}$$

Obviously, we need to evaluate $\left[b_+, \left(b_+^\dagger\right)^n\right]$. We will show that for this commutator holds

$$\left[b_+, \left(b_+^\dagger\right)^n\right] \;=\; n\left(b_+^\dagger\right)^{n-1}\;. \tag{5.259}$$

The property is obviously true for $n = 0$. If it is true for n then using (5.248) we obtain

$$\begin{aligned}
\left[b_+, \left(b_+^\dagger\right)^{n+1}\right] &= \left[b_+, \left(b_+^\dagger\right)^n b_+^\dagger\right] \\
&= \left[b_+, \left(b_+^\dagger\right)^n\right] b_+^\dagger + \left(b_+^\dagger\right)^n \left[b_+, b_+^\dagger\right] \\
&= n\left(b_+^\dagger\right)^{n-1} b_+^\dagger + \left(b_+^\dagger\right)^n \\
&= (n+1)\left(b_+^\dagger\right)^n\;,
\end{aligned} \tag{5.260}$$

i.e. the property holds also for $n+1$. By induction we can conclude that (5.259) holds for all $n \in \mathbb{N}$. One can finally conclude for polynomials (5.255)

$$\left[b_+, f(b_+^\dagger)\right] = f'(b_+^\dagger) \tag{5.261}$$

where $f'(x) = \frac{df}{dx}$. Similarly, one can prove

$$\left[b_-, f(b_-^\dagger)\right] = f'(b_-^\dagger) \tag{5.262}$$

Because of the commutation relationships (5.247) the more general property for polynomials $f(b_+^\dagger, b_-^\dagger)$ in $b_+^\dagger$ and $b_-^\dagger$ holds ($\zeta = +, -$)

$$\left[b_\zeta, f(b_+^\dagger, b_-^\dagger)\right] = \frac{\partial}{\partial b_\zeta^\dagger} f(b_+^\dagger, b_-^\dagger) \,. \tag{5.263}$$

According to (5.257) we can conclude in particular

$$b_\zeta \, f(b_+^\dagger, b_-^\dagger) \, |\Psi_0\rangle = \frac{\partial}{\partial b_\zeta^\dagger} f(b_+^\dagger, b_-^\dagger) \, |\Psi_0\rangle \,. \tag{5.264}$$

This demonstrates the equivalence of the spinor operators b_ζ and the derivative operation. Equation (5.263) corresponds to the product rule of calculus $\partial_k f(\vec{x}) g(\vec{x}) = (\partial_k f(\vec{x})) g(\vec{x}) + f(\vec{x})(\partial_k g(\vec{x}))$ which can be written $(\partial_k f(\vec{x}) - f(\vec{x})\partial_k)\, g(\vec{x}) = [\partial_k, f(\vec{x})]\, g(\vec{x}) = (\partial_k f(\vec{x})) g(\vec{x})$ or

$$[\partial_k, f(\vec{x})] = \partial_k f(\vec{x}) \,. \tag{5.265}$$

Generating Function of the States $|\Psi(j,m)\rangle$

We want to prove now the property

$$\exp\left(x b^\dagger\right) |\Psi_0\rangle = \sum_{j=0,\frac{1}{2},1,\dots}^{\infty} \; \sum_{m=-j}^{j} \phi_{jm}(x) \, \Psi(j,m) \tag{5.266}$$

where $x b^\dagger$ has been defined in (5.250) and where $\phi_{jm}(x)$ represents the function of the two variables x_+ and x_- closely related to $|\Psi(j,m)\rangle$

$$\phi_{jm}(x) = \frac{x_+^{j+m} x_-^{j-m}}{\sqrt{(j+m)!\,(j-m)!}} \,. \tag{5.267}$$

$\exp\left(x b^\dagger\right) |\Psi_0\rangle$ is called a *generating function* of $|\Psi(j,m)\rangle$.
In order to derive (5.266) we compare the terms

$$\phi_{jm}(x) \, \Psi(j,m) = \frac{\left(x_+ b_+^\dagger\right)^{j+m}}{(j+m)!} \frac{\left(x_- b_-^\dagger\right)^{j-m}}{(j-m)!} |\Psi_0\rangle. \tag{5.268}$$

with the s–th term in the binomial expansion of $(a+b)^n$

$$\frac{n!}{s!\,(n-s)!}a^{n-s}b^s\ . \tag{5.269}$$

Defining

$$\begin{aligned} j+m &= N-s \\ j-m &= s\ . \end{aligned} \tag{5.270}$$

one obtains

$$\begin{aligned} \phi_{jm}(x)\,\Psi(j,m) &= \frac{\left(x_+b_+^\dagger\right)^{N-s}}{(N-s)!}\frac{\left(x_-b_-^\dagger\right)^{s}}{s!}|\Psi_0\rangle \\ &= \frac{1}{N!}\left[\frac{N!}{(N-s)!s!}\right]\left(x_+b_+^\dagger\right)^{N-s}\left(x_-b_-^\dagger\right)^{s}|\Psi_0\rangle. \end{aligned} \tag{5.271}$$

Summation over s from $s=0$ to $s=N$ yields

$$\begin{aligned} & \frac{1}{N!}\sum_{s=0}^{N}\left[\frac{N!}{(N-s)!s!}\right]\left(x_+b_+^\dagger\right)^{N-s}\left(x_-b_-^\dagger\right)^{s}|\Psi_0\rangle \\ =\ & \frac{1}{N!}\left(x_+b_+^\dagger+x_-b_-^\dagger\right)^{N}|\Psi_0\rangle \\ =\ & \frac{1}{(2j)!}\left(x_+b_+^\dagger+x_-b_-^\dagger\right)^{2j}|\Psi_0\rangle \end{aligned} \tag{5.272}$$

The summation over s can be written in terms of j and m using (5.270)

$$\sum_{s=0}^{N}\rightarrow\sum_{j-m=0}^{2j}\rightarrow\sum_{m=-j}^{j}\ . \tag{5.273}$$

Change of the summation indices allows one to conclude

$$\begin{aligned} & \sum_{m=-j}^{j}\phi_{jm}(x)\,\Psi(j,m) \\ =\ & \frac{1}{(2j)!}\left(x_+b_+^\dagger+x_-b_-^\dagger\right)^{2j}|\Psi_0\rangle \\ =\ & \frac{1}{(2j)!}\left(xb^\dagger\right)^{2j}|\Psi_0\rangle. \end{aligned} \tag{5.274}$$

Summing this expression over $2j=0,1,2,\ldots$, i.e. chosing the summation index $j=0,\frac{1}{2},1,\frac{3}{2},2,\ldots$, leads to

$$\begin{aligned} \sum_{j=0,\frac{1}{2},1,\ldots}^{\infty}\ \sum_{m=-j}^{j}\phi_{jm}(x)\,|\Psi(j,m)\rangle &= \sum_{j=0,\frac{1}{2},1,\ldots}^{\infty}\frac{1}{2j!}\left(xb^\dagger\right)^{2j}|\Psi_0\rangle \\ &= \sum_{u=0,1,\ldots}^{\infty}\frac{1}{u!}\left(xb^\dagger\right)^{u}|\Psi_0\rangle \\ &= exp\left(xb^\dagger\right)|\Psi_0\rangle \end{aligned} \tag{5.275}$$

which concludes our derivation. The generating function allows one to derive various properties of the states $|\Psi(j,m)\rangle$ and will be used for this purpose below.

Orthonormality of the States $|\Psi(j,m)\rangle$

We want to show now that the states (5.254) are orthonormal, i.e. that

$$\langle \Psi(j,m)|\Psi(j',m')\rangle \;=\; \delta_{jj'}\delta_{mm'} \tag{5.276}$$

holds. For this purpose we consider the inner product

$$\begin{aligned} &\langle e^{\left(xb^\dagger\right)}\Psi_0|e^{\left(yb^\dagger\right)}\Psi_0\rangle \\ =& \sum_{j,m,j',m'} \phi_{jm}(x^*)\,\phi_{j'm'}(y)\,\langle \Psi(j,m)|\Psi(j',m')\rangle\;. \end{aligned} \tag{5.277}$$

To evaluate this expression we first notice

$$\left[e^{\left(xb^\dagger\right)}\right]^\dagger \;=\; e^{(x^*b)}\;. \tag{5.278}$$

which allows us to replace the l.h.s. of (5.277) by $\langle \Psi_0|e^{(x^*b)}e^{\left(yb^\dagger\right)}\Psi_0\rangle$. In order to evaluate the operator $e^{(x^*b)}e^{\left(yb^\dagger\right)}$ we notice that the derivative property (5.264) implies

$$b_\zeta e^{\left(yb^\dagger\right)}|\Psi_0\rangle = y_\zeta e^{\left(yb^\dagger\right)}|\Psi_0\rangle\;. \tag{5.279}$$

One can generalize this to

$$(b_\zeta)^s\, e^{\left(yb^\dagger\right)}|\Psi_0\rangle = y_\zeta^s e^{\left(yb^\dagger\right)}|\Psi_0\rangle\;. \tag{5.280}$$

The commutation properties $[b_+,b_-]=0$, $[b_+^\dagger,b_-^\dagger]=0$ and $[b_-,b_+^\dagger]=0$ allow one to state that for any polynomial $f(b_+,b_-)$ holds

$$f(b_+,b_-)e^{\left(yb^\dagger\right)}|\Psi_0\rangle = f(y_+,y_-)e^{\left(yb^\dagger\right)}|\Psi_0\rangle \tag{5.281}$$

and, hence, one can write

$$\begin{aligned} &\langle e^{\left(xb^\dagger\right)}\Psi_0|e^{\left(yb^\dagger\right)}\Psi_0\rangle \\ =& \;\langle \Psi_0|e^{(x^*y)}e^{\left(yb^\dagger\right)}\Psi_0\rangle \\ =& \;e^{(x^*y)}\,\langle \Psi_0|e^{\left(yb^\dagger\right)}\Psi_0\rangle \end{aligned} \tag{5.282}$$

where we defined $x^*y \;=\; x_+^*y_+ \,+\, x_-^*y_-$. According to (5.249) for any non-vanishing integer s holds

$$\langle \Psi_0|b^s\Psi_0\rangle \;=\; 0 \tag{5.283}$$

and, therefore, we can conclude

$$\langle e^{\left(xb^\dagger\right)}\Psi_0|e^{\left(yb^\dagger\right)}\Psi_0\rangle \;=\; e^{(x^*y)} \tag{5.284}$$

and comparing (5.282) and (5.277)

$$\sum_{j,m,j',m'} \phi_{jm}(x^*)\,\phi_{j'm'}(y)\,\langle \Psi(j,m)\,|\Psi(j',m')\rangle \;=\; e^{(x^* y)}\;. \tag{5.285}$$

Following steps similar to those in Eqs. (5.268–5.275) one can show

$$e^{(x^* y)} \;=\; \sum_{j,m} \phi_{jm}(x^*)\,\phi_{jm}(y)\,. \tag{5.286}$$

from which follows immediately the orthonormality property (5.276).

New Representation of Spin $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ States

We want to demonstrate now that the states $|\Psi(j,m)\rangle$ as given in (5.254) are eigenstates of operators J^2 and J_3 with eigenvalues $j(j+1)$ and m where J^2 and J_3 are representations of the spin operators $S^2 = S_1^2 + S_2^2 + S_3^2$ and S_3 defined in 5.223, 5.224). One defines corresponding operators J_k through

$$J_k = \frac{1}{2}\sum_{\zeta,\zeta'} b^\dagger_\zeta < \zeta\,|\sigma_k|\,\zeta' > b_{\zeta'}\;, \tag{5.287}$$

where σ_k, $k = 1,2,3$ denote the Pauli spin matrices (5.224). In our present notation the matrix elements $< \zeta\,|\sigma_k|\,\zeta' >$ for $\zeta = \pm$ correspond to the matrix elements $< \zeta\,|\sigma_k|\,\zeta' >$ for $\sigma = \pm\frac{1}{2}$. The operators are explicitly, using $< +|\sigma_1|+ > = < -|\sigma_1|- > = 0$, $< +|\sigma_1|- > = < -|\sigma_1|+ > = 1$, etc.,

$$\begin{aligned} J_1 &= \frac{1}{2}\left(b^\dagger_+ b_- + b^\dagger_- b_+\right) \\ J_2 &= \frac{1}{2i}\left(b^\dagger_+ b_- - b^\dagger_- b_+\right) \\ J_3 &= \frac{1}{2}\left(b^\dagger_+ b_+ - b^\dagger_- b_-\right)\;. \end{aligned} \tag{5.288}$$

The three operators obey the Lie algebra of SU(2)

$$[J_i, J_j] = i\epsilon_{ijk} J_k\;. \tag{5.289}$$

This property is derived as follows

$$\begin{aligned} [J_i, J_j] &= \frac{1}{4}\sum_{n,n',m,m'} < n\,|\sigma_i|\,m >< n'\,|\sigma_j|\,m' > \left[b^\dagger_n b_m, b^\dagger_{n'} b_{m'}\right] \\ &= \frac{1}{4}\sum_{n,n',m,m'} < n\,|\sigma_i|\,m >< n'\,|\sigma_j|\,m' > \{b^\dagger_n \left[b_m, b^\dagger_{n'}\right] b_{m'} \\ &\quad + b^\dagger_{n'}\left[b^\dagger_n, b_{m'}\right] b_m\} \\ &= \frac{1}{4}\sum_{n,n',m,m'} < n\,|\sigma_i|\,m >< n'\,|\sigma_j|\,m' > \{b^\dagger_n b_{m'}\delta_{mn'} - b^\dagger_{n'} b_m \delta_{m'n}\} \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{4} \sum_{n,m,m'} < n\,|\sigma_i|\,m >< m\,|\sigma_j|\,m' > b_n^\dagger b_{m'} \\
&\quad -\frac{1}{4} \sum_{n',m,m'} < n'\,|\sigma_j|\,m' >< m'\,|\sigma_i|\,m > b_{n'}^\dagger b_m \\
&= \frac{1}{4} \sum_{n,m} < n\,|[\sigma_i, \sigma_j]|\,m > b_n^\dagger b_m \\
&= \frac{1}{4} \sum_{n,m,k} < n\,|2i\epsilon_{ijk}\sigma_k|\,m > b_n^\dagger b_m \\
&= i\epsilon_{ijk} \frac{1}{2} \sum_{n,m} < n\,|\sigma_k|\,m > b_n^\dagger b_m \\
&= i\epsilon_{ijk} J_k \; .
\end{aligned} \tag{5.290}$$

$|\Psi\,(j,m)\rangle$ as Eigenstates of J^2 and J_3

We wish to show now that the states $|\Psi\,(j,m)\rangle$ are eigenstates of J^2 and J_3. To this end we note

$$J^2 \;=\; J_1^2 \;+\; J_2^2 \;+\; J_3^2 \;=\; \frac{1}{2}\,J_+J_- \;+\; \frac{1}{2}\,J_-J_+ \;+\; J_3^2 \quad . \tag{5.291}$$

Here we have defined

$$\begin{aligned}
J_+ &= J_1 \;+\; iJ_2 &= b_+^\dagger b_- \\
J_- &= J_1 \;-\; iJ_2 &= b_-^\dagger b_+ \; .
\end{aligned} \tag{5.292}$$

The commutation relationships (5.289) yield

$$[J_-,\, J_+] \;=\; [J_1 \,-\, iJ_2,\, J_1 \,+\, iJ_2] \;=\; -i\,[J_2,\, J_1] \;+\; i\,[J_1,\, J_2] \;=\; -2\,J_3 \tag{5.293}$$

from which we can conclude the property

$$\frac{1}{2}\,J_-J_+ \;=\; \frac{1}{2}\,J_+J_- \;-\; J_3 \quad . \tag{5.294}$$

Hence,

$$J^2 \;=\; J_+J_- \;+\; J_3^2 \;-\; J_3 \;=\; J_3\,(J_3 \,-\, 1) \;+\; J_+J_- \quad . \tag{5.295}$$

The last result together with (5.292), (5.288) yields first the expression

$$J^2 \;=\; \frac{1}{4}\,(\,b^\dagger{}_+\,b_+ \,-\, b^\dagger{}_-b_-\,)\,(\,b^\dagger{}_+\,b_+ \,-\, b^\dagger{}_-b_- \,-\, 2\,) \;+\; b^\dagger{}_+b_-b^\dagger{}_-b_+ \quad . \tag{5.296}$$

which results in

$$\begin{aligned}
J^2 \;=\; \tfrac{1}{4}\,(\,& b^\dagger{}_+\,b_+\,b^\dagger{}_+\,b_+ \;+\; b^\dagger{}_+\,b_+\,b^\dagger{}_-b_- \;-\; 2\,b^\dagger{}_+\,b_+ \;-\; b^\dagger{}_-b_-\,b^\dagger{}_+\,b_+ \\
&+ b^\dagger{}_-b_-b^\dagger{}_-b_- \;+\; 2\,b^\dagger{}_-b_- \;+\; 4\,b^\dagger{}_+b_-b^\dagger{}_-b_+\,)
\end{aligned} \tag{5.297}$$

The last term on the r.h.s. can be written

$$\begin{aligned} b^\dagger{}_+ b_- b^\dagger{}_- b_+ &= b^\dagger{}_+ b_+ \;+\; b^\dagger{}_+ b_+ b^\dagger{}_- b_- \\ &= b^\dagger{}_+ b_+ \;+\; \frac{1}{2} b^\dagger{}_+ b_+ b^\dagger{}_- b_- \;+\; \frac{1}{2} b^\dagger{}_- b_- b^\dagger{}_+ b_+ \;. \end{aligned} \tag{5.298}$$

One can then state

$$\begin{aligned} J^2 &= \frac{1}{4} \Big[(b^\dagger{}_+ b_+)^2 \;+\; b^\dagger{}_+ b_+ b^\dagger{}_- b_- \;+\; b^\dagger{}_- b_- b^\dagger{}_+ b_+ \\ &\quad + (b^\dagger{}_- b_-)^2 \;+\; 2\, b^\dagger{}_+ b_+ \;+\; 2\, b^\dagger{}_- b_- \Big] \;. \end{aligned} \tag{5.299}$$

Defining the operator

$$\hat{k} \;=\; \frac{1}{2} \,(\, b^\dagger{}_+ b_+ \;+\; b^\dagger{}_- b_- \,) \tag{5.300}$$

one can write finally

$$J^2 \;=\; \hat{k}\,(\,\hat{k} \;+\; 1\,) \quad . \tag{5.301}$$

Obviously, the states (5.254) are eigenstates of $b^\dagger{}_+ b_+$ and $b^\dagger{}_- b_-$ with eigenvalues $j + m$ and $j - m$, respectively, and eigenstates of $\hat{k}$ with eigenvalues j. One can then conclude

$$J^2\, |\Psi\,(j,m)\rangle \;=\; j\,(\,j \;+\; 1\,)\, |\Psi\,(j,m)\rangle \tag{5.302}$$

$$J_3\, |\Psi\,(j,m)\rangle \;=\; m\, |\Psi\,(j,m)\rangle \;. \tag{5.303}$$

One can furthermore derive readily

$$J_+ |\Psi\,(j,m)\rangle \;=\; \sqrt{(j+m+1)\,(j-m)}\, |\Psi\,(j,m+1)\rangle \tag{5.304}$$

$$J_- \,|\Psi\,(j,m)\rangle \;=\; \sqrt{(j+m)\,(j-m+1)} |\Psi\,(j,m-1)\rangle \;. \tag{5.305}$$

Exercise 5.10.1: The system investigated in this section is formally identical to a 2-dimensional isotropic harmonic oscillator governed by the Hamiltonian

$$H \;=\; \hbar\omega(b_1^+ b_1 \;+\; b_2^+ b_2 \;+\; 1)\,;\; [b_j, b_k^+] \;=\; \delta_{jk}\,,\; j \;=\; 1,2\;.$$

(a) Show that the eigenstates are given by

$$|n_1, n_2\rangle \;=\; \frac{1}{\sqrt{n_1!}} \left(b_1^+\right)^{n_1} |0\rangle_1 \frac{1}{\sqrt{n_2!}} \left(b_2^+\right)^{n_2} |0\rangle_2$$

where the vacuum states are defined through $b_j |0\rangle_j \;=\; 0$. State the corresponding eigenvalues and the degree of degeneracy, i.e., the number of states to the possible energy eigenvalues.
(b) Show that the three operators

$$I_1 \;=\; \frac{1}{2}(b_1^+ b_2 \;+\; b_2^+ b_1)\,,\; I_2 \;=\; \frac{1}{2i}(b_1^+ b_2 \;-\; b_2^+ b_1)\,,\; I_3 \;=\; \frac{1}{2}(b_1^+ b_1 \;+\; b_2^+ b_2)$$

satisfy the Lie algebra of SU(2), i.e. $[I_j, I_k] \;=\; i\epsilon_{jk\ell} I_\ell$. Construct, using operators $I_\pm \;=\; I_1 \pm iI_2$ and the subspace $\{|n_1,n_2\rangle,\, n \;=\; n_1 + n_2$ fixed, $n_1 \;=\; 0,1,2,\ldots,n\}$ eigenstates of $I^2 \;=\; I_1^2 + I_2^2 + I_3^2$ and of I_3

$$I^2 ||\lambda, m\rangle \;=\; \lambda ||\lambda, m\rangle\,;\; I_3 ||\lambda, m\rangle \;=\; m ||\lambda, m\rangle$$

where $\lambda \;=\; 0, 1\; 2, \ldots\,,\, m = -\lambda, -\lambda+1, \ldots, \lambda$. Show $\lambda \;=\; \frac{n_1+n_2}{2}(\frac{n_1+n_2}{2} \;+\; 1)$ and $m \;=\; \frac{1}{2}(n_1 \;-\; n_2)$.

5.11 Evaluation of the Elements $d^{j}_{m\,m'}(\beta)$ of the Wigner Rotation Matrix

The spinor algorithm allows one to derive expressions for the Wigner rotation matrix elements $d^{j}_{m\,m'}(\beta)$. For this purpose we note that the states $|\Psi(jm)\rangle$ in a rotated coordinate system according to (5.254) are

$$|\Psi'\left(j,m'\right)\rangle = \frac{\left(b'^{\dagger}_{+}\right)^{j+m'}}{\sqrt{(j+m')!}}\frac{\left(b'^{\dagger}_{-}\right)^{j-m'}}{\sqrt{(j-m')!}}|\Psi_0\rangle \tag{5.306}$$

where $b'^{\dagger}_{+}$ and $b'^{\dagger}_{-}$ are given by (5.251). On the other side the states $|\Psi'\left(j,m'\right)\rangle$ are related to the states $|\Psi\left(j,m\right)\rangle$ in the original coordinate system by

$$|\Psi'\left(j,m'\right)\rangle \;=\; \sum_{m=-j}^{j} d^{(j)}_{m\,m'}(\beta)\,|\Psi\left(j,m\right)\rangle\;. \tag{5.307}$$

Comparision of (5.306) and (5.307) shows that the elements of the rotation matrix can be obtained by binomial expansion of $b'^{\dagger}_{+}$ and $b'^{\dagger}_{-}$ in terms of $b^{\dagger}_{+}$ and $b^{\dagger}_{-}$. For this purpose we expand

$$\begin{aligned}
&\left(b'^{\dagger}_{+}\right)^{j+m'}\left(b'^{\dagger}_{-}\right)^{j-m'} \;=\\
&\left(\cos\tfrac{\beta}{2}b^{\dagger}_{+}\,+\,\sin\tfrac{\beta}{2}b^{\dagger}_{-}\right)^{j+m'}\left(-\sin\tfrac{\beta}{2}b^{\dagger}_{+}\,+\,\cos\tfrac{\beta}{2}b^{\dagger}_{-}\right)^{j-m'} \;=\\
&\textstyle\sum_{\sigma'=0}^{j+m'}\sum_{\sigma=0}^{j-m'}\begin{pmatrix} j+m' \\ \sigma' \end{pmatrix}\left(\cos\tfrac{\beta}{2}\right)^{\sigma'}\left(\sin\tfrac{\beta}{2}\right)^{j+m'-\sigma'}\\
&\begin{pmatrix} j-m' \\ \sigma \end{pmatrix}\left(-\sin\tfrac{\beta}{2}\right)^{\sigma}\left(\cos\tfrac{\beta}{2}\right)^{j-m'-\sigma}\left(b^{\dagger}_{+}\right)^{\sigma'+\sigma}\left(b^{\dagger}_{-}\right)^{2j-\sigma'-\sigma}
\end{aligned} \tag{5.308}$$

The latter sum involves terms $(b^{\dagger}_{+})^{j+m}(b^{\dagger}_{-})^{j-m}$ for $\sigma'+\sigma \;=\; j+m$ and $2j-\sigma'-\sigma \;=\; j-m$. One may expect that these two conditions restrict both σ' and σ. However, both conditions are satisfied for $\sigma' \;=\; j+m-\sigma$. The combination of σ,σ' values which yields $(b^{\dagger}_{+})^{j+m}(b^{\dagger}_{-})^{j-m}$ is then $\sigma' \;=\; j+m-\sigma$. The prefactor of $(b^{\dagger}_{+})^{j+m}(b^{\dagger}_{-})^{j-m}$ which according to (5.306,5.307) can be identified with the elements $d^{(j)}_{m\,m'}(\beta)$ of the rotation matrix can then be written

$$\begin{aligned}
d^{(j)}_{m\,m'}(\beta) \;&=\; \sqrt{\frac{(j+m)!(j-m)!}{(j+m')!(j-m')!}}\sum_{\sigma=0}^{j-m'}\begin{pmatrix} j+m' \\ j+m-\sigma \end{pmatrix}\begin{pmatrix} j-m' \\ \sigma \end{pmatrix}\times\\
&\times(-1)^{j-m'-\sigma}\left(\sin\frac{\beta}{2}\right)^{2j-m-m'-2\sigma}\left(\cos\frac{\beta}{2}\right)^{m+m'+2\sigma}\;.
\end{aligned} \tag{5.309}$$

In case $j=1$ this expression yields, for example,

$$(d^{(1)}_{m'\,m}) \;=\; \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & \frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1-\cos\beta) \\ -\frac{1}{\sqrt{2}}\sin\beta & \cos\beta & \frac{1}{\sqrt{2}}\sin\beta \\ \frac{1}{2}(1-\cos\beta) & -\frac{1}{\sqrt{2}}\sin\beta & \frac{1}{2}(1+\cos\beta) \end{pmatrix} \tag{5.310}$$

and in case $j \;=\; \frac{1}{2}$ it reduces to (5.243).

5.12 Mapping of SU(2) onto SO(3)

The representation (5.310) establishes a mapping of SU(2) onto SO(3). This can be shown by applying to the matrix $A = (d^{(1)}_{m'\,m})$ in (5.310) the similarity transformation

$$\tilde{A} = U^\dagger A U \tag{5.311}$$

where U is the 3×3 unitary matrix which establishes the transformation

$$\begin{pmatrix} \frac{1}{\sqrt{2}}(-x_1 - ix_2) \\ x_3 \\ \frac{1}{\sqrt{2}}(x_1 - ix_2) \end{pmatrix} = U \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \; ; \quad U = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix} . \tag{5.312}$$

The choice of this transformation derives from a property shown further below, namely that the component of the vector on the l.h.s. of (5.312) transforms like an angular momentum state $|1\,m\rangle$. Hence, the matrix $\tilde{A}$ should represent a rotation around the x_2–axis in the space of vectors $(x_1, x_2, x_3) \in \mathbb{R}^{\not\Vdash}$. Evaluation of $\tilde{A}$ yields

$$\begin{aligned} \tilde{A} = \tfrac{1}{4} & \begin{pmatrix} -1 & 0 & 1 \\ i & 0 & i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 1 + \cos\beta & \sqrt{2}\sin\beta & 1 - \cos\beta \\ -\sqrt{2}\sin\beta & 2\cos\beta & \sqrt{2}\sin\beta \\ 1 - \cos\beta & -\sqrt{2}\sin\beta & 1 + \cos\beta \end{pmatrix} \times \\ \times & \begin{pmatrix} -1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} = \tfrac{1}{4} \begin{pmatrix} -2\cos\beta & -2\sqrt{2}\sin\beta & 2\cos\beta \\ 2i & 0 & 2i \\ -2\sin\beta & 2\sqrt{2}\cos\beta & 2\sin\beta \end{pmatrix} \times \\ \times & \begin{pmatrix} -1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \end{pmatrix} = \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \end{aligned} \tag{5.313}$$

which, in fact, is the expected element of SO(3), i.e., the orthogonal 3×3 matrix which describes a rotation around the x_2–axis.
It is of interest to trace the mapping from SU(2) onto SO(3) as represented by (5.310) to the SU(2) transformation assumed in deriving the general result (5.309) and the particular matrix (5.310). The SU(2) transformation entered in (5.308) and had the form (5.251). Replacing the latter transformation by its negative form, i.e.,

$$(b'_+)^\dagger = -\cos\frac{\beta}{2}\, b^\dagger_+ - \sin\frac{\beta}{2}\, b^\dagger_- \quad ; \quad (b'_-)^\dagger = \sin\frac{\beta}{2}\, b^\dagger_+ - \cos\frac{\beta}{2}\, b^\dagger_- \,. \tag{5.314}$$

leaves (5.308) unaltered except for a factor $(-1)^{2j}$ which multiplies then also the final result (5.309). This factor implies, however, that the the representation (5.309) does not distinguish between SU(2) transformations (5.251) and (5.314) in case of integer j–values, e.g. in case of $j = 1$. One can, therefore, conclude that the mapping from SU(2) onto SO(3) is a 2–1 mapping.