

Chapter 6

Quantum Mechanical Addition of Angular Momenta and Spin

In this section we consider composite systems made up of several particles, each carrying orbital angular momentum described by spherical harmonics $Y_{\ell m}(\theta, \phi)$ as eigenfunctions and/or spin. Often the so-called *total angular momentum*, classically speaking the sum of all angular momenta and spins of the composite system, is the quantity of interest, since related operators, sums of orbital angular momentum and of spin operators of the particles, commute with the Hamiltonian of the composite system and, hence, give rise to good quantum numbers. We like to illustrate this for an example involving particle motion. Further below we will consider composite systems involving spin states.

Example: Three Particle Scattering

Consider the scattering of three particles A, B, C governed by a Hamiltonian \mathbf{H} which depends only on the internal coordinates of the system, e.g., on the distances between the three particles, but neither on the position of the center of mass of the particles nor on the overall orientation of the three particle system with respect to a laboratory-fixed coordinate frame.

To specify the dependency of the Hamiltonian on the particle coordinates we start from the nine numbers which specify the Cartesian components of the three position vectors $\vec{r}_A, \vec{r}_B, \vec{r}_C$ of the particles. Since the Hamiltonian does not depend on the position of the center of mass $\vec{R} = (m_A\vec{r}_A + m_B\vec{r}_B + m_C\vec{r}_C)/(m_A + m_B + m_C)$, six parameters must suffice to describe the interaction of the system. The overall orientation of any three particle configuration can be specified by three parameters¹, e.g., by a rotational vector \vec{v} . This eliminates three further parameters from the dependency of the Hamiltonian on the three particle configuration and one is left with three parameters. How should they be chosen?

Actually there is no unique choice. We like to consider a choice which is physically most reasonable in a situation that the scattering proceeds such that particles A and B are bound, and particle C impinges on the compound AB coming from a large distance. In this case a proper choice for a description of interactions would be to consider the vectors $\vec{r}_{AB} = \vec{r}_A - \vec{r}_B$ and $\vec{\rho}_C = (m_A\vec{r}_A + m_B\vec{r}_B)/(m_A + m_B) - \vec{r}_C$, and to express the Hamiltonian in terms of $|\vec{r}_{AB}|, |\vec{\rho}_C|$, and $\angle(\vec{r}_{AB}, \vec{\rho}_C)$. The rotational part of the scattering motion is described then in terms of the unit vectors \hat{r}_{AB} and

¹We remind the reader that, for example, three Eulerian angles α, β, γ are needed to specify a general rotational transformation

$\hat{\rho}_C$, each of which stands for two angles. One may consider then to describe the motion in terms of products of spherical harmonics $Y_{\ell_1 m_1}(\hat{r}_{AB}) Y_{\ell_2 m_2}(\hat{\rho}_C)$ describing rotation of the compound AB and the orbital angular momentum of C around AB.

One can describe the rotational degrees of freedom of the three-particle scattering process through the basis

$$\mathcal{B} = \{ Y_{\ell_1 m_1}(\hat{r}_{AB}) Y_{\ell_2 m_2}(\hat{\rho}_C), \ell_1 = 0, 1, \dots, \ell_{1,max}, -\ell_1 \leq m_1 \leq \ell_1; \ell_2 = 0, 1, \dots, \ell_{2,max}, -\ell_2 \leq m_2 \leq \ell_2 \} \quad (6.1)$$

where $\ell_{1,max}$ and $\ell_{2,max}$ denote the largest orbital and rotational angular momentum values, the values of which are determined by the size of the interaction domain Δ_V , by the total energy E , by the masses m_A, m_B, m_C , and by the moment of inertia I_{A-B} of the diatomic molecule A-B approximately as follows

$$\ell_{1,max} = \frac{\Delta}{\hbar} \sqrt{\frac{2 m_A m_B m_C E}{m_A m_B + m_B m_C + m_A m_C}}, \quad \ell_{2,max} = \frac{1}{\hbar} \sqrt{2 I_{A-B} E}. \quad (6.2)$$

The dimension $d(\mathcal{B})$ of \mathcal{B} is

$$d(\mathcal{B}) = \sum_{\ell_1=0}^{\ell_{1,max}} (2\ell_1 + 1) \sum_{\ell_2=0}^{\ell_{2,max}} (2\ell_2 + 1) = (\ell_{1,max} + 1)^2 (\ell_{2,max} + 1)^2 \quad (6.3)$$

For rather moderate values $\ell_{1,max} = \ell_{2,max} = 10$ one obtains $d(\mathcal{B}) = 14\,641$, a very large number. Such large number of dynamically coupled states would constitute a serious problem in any detailed description of the scattering process, in particular, since further important degrees of freedom, i.e., vibrations and rearrangement of the particles in reactions like $AB + C \rightarrow A + BC$, have not even be considered. The rotational symmetry of the interaction between the particles allows one, however, to separate the 14 641 dimensional space of rotational states $Y_{\ell_1 m_1}(\hat{r}_{AB}) Y_{\ell_2 m_2}(\hat{\rho}_C)$ into subspaces $\mathcal{B}_k, \mathcal{B}_1 \oplus \mathcal{B}_2 \oplus \dots = \mathcal{B}$ such that only states within the subspaces \mathcal{B}_k are coupled in the scattering process. In fact, as we will demonstrate below, the dimensions $d(\mathcal{B}_k)$ of these subspaces does not exceed 100. Such extremely useful transformation of the problem can be achieved through the choice of a new basis set

$$\mathcal{B}' = \left\{ \sum_{\substack{\ell_1, m_1 \\ \ell_2, m_2}} g_{\ell_1, m_1; \ell_2, m_2}^{(n)} Y_{\ell_1 m_1}(\hat{r}_{AB}) Y_{\ell_2 m_2}(\hat{\rho}_C), n = 1, 2, \dots, 14\,641 \right\}. \quad (6.4)$$

The basis set which provides a maximum degree of decoupling between rotational states is of great principle interest since the new states behave in many respects like states with the attributes of a single angular momentum state: to an observer the three particle system prepared in such states may look like a two particle system governed by a single angular momentum state. Obviously, composite systems behaving like elementary objects are common, albeit puzzling, and the following mathematical description will shed light on their ubiquitous appearance in physics, in fact, will make their appearance a natural consequence of the symmetry of the building blocks of matter.

There is yet another important reason why the following section is of fundamental importance for the theory of the microscopic world governed by Quantum Mechanics, rather than by Classical Mechanics. The latter often arrives at the physical properties of composite systems by adding the

corresponding physical properties of the elementary components; examples are the total momentum or the total angular momentum of a composite object which are the sum of the (angular) momenta of the elementary components. Describing quantum mechanically a property of a composite object as a whole and relating this property to the properties of the elementary building blocks is then the quantum mechanical equivalent of the important operation of addition. In this sense, the reader will learn in the following section how to add and subtract in the microscopic world of Quantum Physics, presumably a facility the reader would like to acquire with great eagerness.

Rotational Symmetry of the Hamiltonian

As pointed out already, the existence of a basis (6.4) which decouples rotational states is connected with the rotational symmetry of the Hamiltonian of the three particle system considered, i.e., connected with the fact that the Hamiltonian \mathbf{H} does not depend on the overall orientation of the three interacting particles. Hence, rotations $\mathfrak{R}(\vec{\vartheta})$ of the wave functions $\psi(\vec{r}_{AB}, \vec{\rho}_C)$ defined through

$$\mathfrak{R}(\vec{\vartheta}) \psi(\vec{r}_{AB}, \vec{\rho}_C) = \psi(R^{-1}(\vec{\vartheta}) \vec{r}_{AB}, R^{-1}(\vec{\vartheta}) \vec{\rho}_C) \quad (6.5)$$

do not affect the Hamiltonian. To specify this property mathematically let us denote by \mathbf{H}' the Hamiltonian in the rotated frame, assuming presently that \mathbf{H}' might, in fact, be different from \mathbf{H} . It holds then $\mathbf{H}' \mathfrak{R}(\vec{\vartheta}) \psi = \mathfrak{R}(\vec{\vartheta}) \mathbf{H} \psi$. Since this is true for any $\psi(\vec{r}_{AB}, \vec{\rho}_C)$ it follows $\mathbf{H}' \mathfrak{R}(\vec{\vartheta}) = \mathfrak{R}(\vec{\vartheta}) \mathbf{H}$, from which follows in turn the well-known result that \mathbf{H}' is related to \mathbf{H} through the similarity transformation $\mathbf{H}' = \mathfrak{R}(\vec{\vartheta}) \mathbf{H} \mathfrak{R}^{-1}(\vec{\vartheta})$. The invariance of the Hamiltonian under overall rotations of the three particle system implies then

$$\mathbf{H} = \mathfrak{R}(\vec{\vartheta}) \mathbf{H} \mathfrak{R}^{-1}(\vec{\vartheta}) \quad (6.6)$$

For the following it is essential to note that \mathbf{H} is not invariant under rotations of only \vec{r}_{AB} or $\vec{\rho}_C$, but solely under **simultaneous and identical** rotations of \vec{r}_{AB} or $\vec{\rho}_C$.

Following our description of rotations of single particle wave functions we express (6.5) according to (5.48)

$$\mathfrak{R}(\vec{\vartheta}) = \exp\left(-\frac{i}{\hbar} \vec{\vartheta} \cdot \vec{\mathcal{J}}^{(1)}\right) \exp\left(-\frac{i}{\hbar} \vec{\vartheta} \cdot \vec{\mathcal{J}}^{(2)}\right) \quad (6.7)$$

where the generators $\vec{\mathcal{J}}^{(k)}$ are differential operators acting on \hat{r}_{AB} ($k = 1$) and on $\hat{\rho}_C$ ($k = 2$). For example, according to (5.53) (5.55) holds

$$-\frac{i}{\hbar} \mathcal{J}_1^{(1)} = z_{AB} \frac{\partial}{\partial y_{AB}} - y_{AB} \frac{\partial}{\partial z_{AB}}; \quad -\frac{i}{\hbar} \mathcal{J}_3^{(2)} = \rho_y \frac{\partial}{\partial \rho_x} - \rho_x \frac{\partial}{\partial \rho_y} \quad (6.8)$$

Obviously, the commutation relationships

$$\left[\mathcal{J}_p^{(1)}, \mathcal{J}_q^{(2)}\right] = 0 \quad \text{for } p, q = 1, 2, 3 \quad (6.9)$$

hold since the components of $\vec{\mathcal{J}}^{(k)}$ are differential operators with respect to different variables. One can equivalently express therefore (6.7)

$$\mathfrak{R}(\vec{\vartheta}) = \exp\left(-\frac{i}{\hbar} \vec{\vartheta} \cdot \vec{\mathcal{J}}\right) \quad (6.10)$$

where

$$\vec{\mathbb{J}} = \vec{\mathcal{J}}^{(1)} + \vec{\mathcal{J}}^{(2)} \quad . \quad (6.11)$$

By means of (6.11) we can write the condition (6.6) for rotational invariance of the Hamiltonian in the form

$$\mathbf{H} = \exp\left(-\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathbb{J}}\right) \mathbf{H} \exp\left(+\frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathbb{J}}\right) \quad . \quad (6.12)$$

We consider this equation for infinitesimal rotations, i.e. for $|\vec{\vartheta}| \ll 1$. To order $O(|\vec{\vartheta}|)$ one obtains

$$\mathbf{H} \approx \left(\mathbb{1} - \frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathbb{J}}\right) \mathbf{H} \left(\mathbb{1} + \frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathbb{J}}\right) \approx \mathbf{H} + \frac{i}{\hbar}\mathbf{H}\vec{\vartheta}\cdot\vec{\mathbb{J}} - \frac{i}{\hbar}\vec{\vartheta}\cdot\vec{\mathbb{J}}\mathbf{H} \quad . \quad (6.13)$$

Since this holds for any $\vec{\vartheta}$ it follows $\mathbf{H}\vec{\mathbb{J}} - \vec{\mathbb{J}}\mathbf{H} = 0$ or, componentwise,

$$[\mathbf{H}, \mathbb{J}_k] = 0 \quad , \quad k = 1, 2, 3 \quad . \quad (6.14)$$

We will refer in the following to \mathbb{J}_k , $k = 1, 2, 3$ as the three components of the *total angular momentum operator*.

The property (6.14) implies that the **total** angular momentum is conserved during the scattering process, i.e., that energy, and the eigenvalues of $\vec{\mathbb{J}}^2$ and \mathbb{J}_3 are good quantum numbers. To describe the scattering process of $AB + C$ most concisely one seeks eigenstates \mathfrak{Y}_{JM} of $\vec{\mathbb{J}}^2$ and \mathbb{J}_3 which can be expressed in terms of $Y_{\ell_1 m_1}(\hat{r}_{AB}) Y_{\ell_2 m_2}(\hat{\rho}_C)$.

Definition of Total Angular Momentum States

The commutation property (6.14) implies that the components of the total angular momentum operator (6.12) each individually can have simultaneous eigenstates with the Hamiltonian. We suspect, of course, that the components \mathbb{J}_k , $k = 1, 2, 3$ cannot have simultaneous eigenstates among each other, a supposition which can be tested through the commutation properties of these operators. One can show readily that the commutation relationships

$$[\mathbb{J}_k, \mathbb{J}_\ell] = i\hbar \epsilon_{k\ell m} \mathbb{J}_m \quad (6.15)$$

are satisfied, i.e., the operators \mathbb{J}_k , $k = 1, 2, 3$ do not commute. For a proof one uses (6.9), the properties $[\mathcal{J}_k^{(n)}, \mathcal{J}_\ell^{(n)}] = i\hbar \epsilon_{k\ell m} \mathcal{J}_m^{(n)}$ for $n = 1, 2$ together with the property $[A, B + C] = [A, B] + [A, C]$.

We recognize, however, the important fact that the \mathbb{J}_k obey the Lie algebra of $SO(3)$. According to the theorem above this property implies that one can construct eigenstates \mathfrak{Y}_{JM} of \mathbb{J}_3 and of

$$\mathbb{J}^2 = \mathbb{J}_1^2 + \mathbb{J}_2^2 + \mathbb{J}_3^2 \quad (6.16)$$

following the procedure stated in the theorem above [c.f. Eqs. (5.71–5.81)]. In fact, we will find that the states yield the basis \mathcal{B}' with the desired property of a maximal uncoupling of rotational states.

Before we apply the procedure (5.71–5.81) we want to consider the relationship between \mathfrak{Y}_{JM} and $Y_{\ell_1 m_1}(\hat{r}_{AB}) Y_{\ell_2 m_2}(\hat{\rho}_C)$. In the following we will use the notation

$$\Omega_1 = \hat{r}_{AB} \quad , \quad \Omega_2 = \hat{\rho}_C \quad . \quad (6.17)$$

6.1 Clebsch-Gordan Coefficients

In order to determine \mathfrak{Y}_{JM} we notice that the states $Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 m_2}(\Omega_2)$ are characterized by **four** quantum numbers corresponding to eigenvalues of $[\mathcal{J}^{(1)}]^2$, $\mathcal{J}_3^{(1)}$, $[\mathcal{J}^{(2)}]^2$, and $\mathcal{J}_3^{(2)}$. Since \mathfrak{Y}_{JM} so far specifies solely **two** quantum numbers, two further quantum numbers need to be specified for a complete characterization of the total angular momentum states. The two missing quantum numbers are ℓ_1 and ℓ_2 corresponding to the eigenvalues of $[\mathcal{J}^{(1)}]^2$ and $[\mathcal{J}^{(2)}]^2$. We, therefore, assume the expansion

$$\mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = \sum_{m_1, m_2} (JM | \ell_1 m_1 \ell_2 m_2) Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 m_2}(\Omega_2) \quad (6.18)$$

where the states $\mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \hat{\rho}_C)$ are normalized. The expansion coefficients $(JM | \ell_1 m_1 \ell_2 m_2)$ are called the *Clebsch-Gordan coefficients* which we seek to determine now. These coefficients, or the closely related *Wigner 3j-coefficients* introduced further below, play a cardinal role in the mathematical description of microscopic physical systems. Equivalent coefficients exist for other symmetry properties of multi-component systems, an important example being the symmetry groups $SU(N)$ governing elementary particles made up of two quarks, i.e., mesons, and three quarks, i.e., baryons.

Exercise 6.1.1: Show that $\mathbb{J}^2, \mathbb{J}_3, (\mathcal{J}^{(1)})^2, (\mathcal{J}^{(2)})^2$, and $\vec{\mathcal{J}}^{(1)} \cdot \vec{\mathcal{J}}^{(2)}$ commute. Why can states \mathfrak{Y}_{JM} then not be specified by 5 quantum numbers?

Properties of Clebsch-Gordan Coefficients

A few important properties of *Clebsch-Gordan coefficients* can be derived rather easily. We first notice that \mathfrak{Y}_{JM} in (6.18) is an eigenfunction of \mathbb{J}_3 , the eigenvalue being specified by the quantum number M , i.e.

$$\mathbb{J}_3 \mathfrak{Y}_{JM} = \hbar M \mathfrak{Y}_{JM} . \quad (6.19)$$

Noting $\mathbb{J}_3 = \mathcal{J}_3^{(1)} + \mathcal{J}_3^{(2)}$ and applying this to the l.h.s. of (6.18) yields using the property $\mathcal{J}_3^{(k)} Y_{\ell_k m_k}(\Omega_k) = \hbar m_k Y_{\ell_k m_k}(\Omega_k)$, $k = 1, 2$

$$M \mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = \sum_{m_1, m_2} (m_1 + m_2) (JM | \ell_1 m_1 \ell_2 m_2) Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 m_2}(\Omega_2) . \quad (6.20)$$

This equation can be satisfied only if the *Clebsch-Gordan coefficients* satisfy

$$(JM | \ell_1 m_1 \ell_2 m_2) = 0 \quad \text{for } m_1 + m_2 \neq M \quad . \quad (6.21)$$

One can, hence, restrict the sum in (6.18) to avoid summation of vanishing terms

$$\mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = \sum_{m_1} (JM | \ell_1 m_1 \ell_2 M - m_1) Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 M - m_1}(\Omega_2) \quad . \quad (6.22)$$

We will not adopt such explicit summation since it leads to cumbersome notation. However, the reader should always keep in mind that conditions equivalent to (6.21) hold.

The expansion (6.18) constitutes a change of an orthonormal basis

$$\begin{aligned} \mathfrak{B}(\ell_1, \ell_2) &= \{Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 m_2}(\Omega_2), m_1 = -\ell_1, -\ell_1 + 1, \dots, \ell_1, \\ &\quad m_2 = -\ell_2, -\ell_2 + 1, \dots, \ell_2\}, \end{aligned} \quad (6.23)$$

corresponding to the r.h.s., to a new basis $\mathfrak{B}'(\ell_1, \ell_2)$ corresponding to the l.h.s. The orthonormality property implies

$$\int d\Omega_1 \int d\Omega_2 Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 m_2}(\Omega_2) Y_{\ell_1' m_1'}(\Omega_1) Y_{\ell_2' m_2'}(\Omega_2) = \delta_{\ell_1 \ell_1'} \delta_{m_1 m_1'} \delta_{\ell_2 \ell_2'} \delta_{m_2 m_2'}. \quad (6.24)$$

The basis $\mathfrak{B}(\ell_1, \ell_2)$ has $(2\ell_1 + 1)(2\ell_2 + 1)$ elements. The basis $\mathfrak{B}'(\ell_1, \ell_2)$ is also orthonormal² and must have the same number of elements. For each quantum number J there should be $2J + 1$ elements \mathfrak{Y}_{JM} with $M = -J, -J + 1, \dots, J$. However, it is not immediately obvious what the J -values are. Since \mathfrak{Y}_{JM} represents the total angular momentum state and $Y_{\ell_1 m_1}(\Omega_1)$ and $Y_{\ell_2 m_2}(\Omega_2)$ the individual angular momenta one may start from one's classical notion that these states represent angular momentum vectors \vec{J} , $\vec{J}^{(1)}$ and $\vec{J}^{(2)}$, respectively. In this case the range of $|\vec{J}|$ -values would be the interval $[||\vec{J}^{(1)}| - |\vec{J}^{(2)}||, |\vec{J}^{(1)}| + |\vec{J}^{(2)}|]$. This obviously corresponds quantum mechanically to a range of J -values $J = |\ell_1 - \ell_2|, |\ell_1 - \ell_2| + 1, \dots, \ell_1 + \ell_2$. In fact, it holds

$$\sum_{J=|\ell_1-\ell_2}^{\ell_1+\ell_2} (2J + 1) = (2\ell_1 + 1)(2\ell_2 + 1), \quad (6.25)$$

i.e., the basis $\mathfrak{B}'(\ell_1, \ell_2)$ should be

$$\begin{aligned} \mathfrak{B}_2 &= \{\mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2); J = |\ell_1 - \ell_2|, |\ell_1 - \ell_2| + 1, \ell_1 + \ell_2, \\ &\quad M = -J, -J + 1, \dots, J\}. \end{aligned} \quad (6.26)$$

We will show below in an explicit construction of the *Clebsch-Gordan coefficients* that, in fact, the range of values assumed for J is correct. Our derivation below will also yield real values for the *Clebsch-Gordan coefficients*.

Exercise 6.1.2: Prove Eq. (6.25)

We want to state now two summation conditions which follow from the orthonormality of the two basis sets $\mathfrak{B}(\ell_1, \ell_2)$ and $\mathfrak{B}'(\ell_1, \ell_2)$. The property

$$\int d\Omega_1 \int d\Omega_2 \mathfrak{Y}_{JM}^*(\ell_1, \ell_2 | \Omega_1, \Omega_2) \mathfrak{Y}_{J'M'}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = \delta_{JJ'} \delta_{MM'} \quad (6.27)$$

together with (6.18) applied to \mathfrak{Y}_{JM}^* and to $\mathfrak{Y}_{J'M'}$ and with (6.24) yields

$$\sum_{m_1, m_2} (JM | \ell_1 m_1 \ell_2 m_2)^* (J'M' | \ell_1 m_1 \ell_2 m_2) = \delta_{JJ'} \delta_{MM'}. \quad (6.28)$$

²This property follows from the fact that the basis elements are eigenstates of hermitian operators with different eigenvalues, and that the states can be normalized.

The second summation condition starts from the fact that the basis sets $\mathfrak{B}(\ell_1, \ell_2)$ and $\mathfrak{B}'(\ell_1, \ell_2)$ span the **same** function space. Hence, it is possible to expand $Y_{\ell_1 m_1}(\Omega_1)Y_{\ell_2 m_2}(\Omega_2)$ in terms of $\mathfrak{Y}_{JM}(\ell_1, \ell_2|\Omega_1, \Omega_2)$, i.e.,

$$Y_{\ell_1 m_1}(\Omega_1)Y_{\ell_2 m_2}(\Omega_2) = \sum_{J'=|\ell_1-\ell_2|^{\ell_1+\ell_2}} \sum_{M'=-J}^J c_{J'M'} \mathfrak{Y}_{J'M'}(\ell_1, \ell_2|\Omega_1, \Omega_2), \quad (6.29)$$

where the expansion coefficients are given by the respective scalar products in function space

$$c_{J'M'} = \int d\Omega_1 \int d\Omega_2 \mathfrak{Y}_{J'M'}^*(\ell_1, \ell_2|\Omega_1, \Omega_2) Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 m_2}(\Omega_2) \quad . \quad (6.30)$$

The latter property follows from multiplying (6.18) by $\mathfrak{Y}_{J'M'}^*(\ell_1, \ell_2|\Omega_1, \Omega_2)$ and integrating. The orthogonality property (6.27) yields

$$\delta_{JJ'} \delta_{MM'} = \sum_{m_1, m_2} (JM|\ell_1 m_1 \ell_2 m_2) c_{J'M'} \quad . \quad (6.31)$$

Comparison with (6.28) allows one to conclude that the coefficients $c_{J'M'}$ are identical to $(J'M'|\ell_1 m_1 \ell_2 m_2)^*$, i.e.,

$$\begin{aligned} & Y_{\ell_1 m_1}(\Omega_1) Y_{\ell_2 m_2}(\Omega_2) \\ &= \sum_{J'=|\ell_1-\ell_2|^{\ell_1+\ell_2}} \sum_{M'=-J}^J (J'M'|\ell_1 m_1 \ell_2 m_2)^* \mathfrak{Y}_{J'M'}(\ell_1, \ell_2|\Omega_1, \Omega_2), \end{aligned} \quad (6.32)$$

which complements (6.18). One can show readily using the same reasoning as applied in the derivation of (6.28) from (6.18) that the *Clebsch-Gordan coefficients* obey the second summation condition

$$\sum_{JM} (JM|\ell_1 m_1 \ell_2 m_2)^* (JM|\ell_1 m'_1 \ell_2 m'_2) = \delta_{m_1 m'_1} \delta_{m_2 m'_2} \quad . \quad (6.33)$$

The latter summation has not been restricted explicitly to allowed J -values, rather the convention

$$(JM|\ell_1 \ell_2 m_2) = 0 \quad \text{if } J < |\ell_1 - \ell_2|, \text{ or } J > \ell_1 + \ell_2 \quad (6.34)$$

has been assumed.

6.2 Construction of Clebsch-Gordan Coefficients

We will now construct the *Clebsch-Gordan coefficients*. The result of this construction will include all the properties previewed above. At this point we like to stress that the construction will be based on the theorems (5.71–5.81) stated above, i.e., will be based solely on the commutation properties of the operators \vec{J} and $\vec{J}^{(k)}$. We can, therefore, also apply the results, and actually also the properties of *Clebsch-Gordan coefficients* stated above, to composite systems involving spin- $\frac{1}{2}$ states. A similar construction will also be applied to composite systems governed by other symmetry groups, e.g., the group SU(3) in case of meson multiplets involving two quarks, or baryons multiplets involving three quarks.

For the construction of \mathfrak{Y}_{JM} we will need the operators

$$\mathbb{J}_{\pm} = \mathbb{J}_1 + i\mathbb{J}_2 . \quad (6.35)$$

The construction assumes a particular choice of $J \in \{|\ell_1 - \ell_2|, |\ell_1 - \ell_2| + 1, \dots, \ell_1 + \ell_2\}$ and for such J -value seeks an expansion (6.18) which satisfies

$$\mathbb{J}_+ \mathfrak{Y}_{JJ}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = 0 \quad (6.36)$$

$$\mathbb{J}_3 \mathfrak{Y}_{JJ}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = \hbar J \mathfrak{Y}_{JJ}(\ell_1, \ell_2 | \Omega_1, \Omega_2) . \quad (6.37)$$

The solution needs to be normalized. Having determined such \mathfrak{Y}_{JJ} we then construct the whole family of functions $\mathbb{X}_J = \{\mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2), M = -J, -J + 1, \dots, J\}$ by applying repeatedly

$$\mathbb{J}_- \mathfrak{Y}_{JM+1}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = \hbar \sqrt{(J + M + 1)(J - M)} \mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2) . \quad (6.38)$$

for $M = J - 1, J - 2, \dots, -J$.

We embark on the suggested construction for the choice $J = \ell_1 + \ell_2$. We first seek an unnormalized solution \mathcal{G}_{JJ} and later normalize. To find \mathcal{G}_{JJ} we start from the observation that \mathcal{G}_{JJ} represents the state with the largest possible quantum number $J = \ell_1 + \ell_2$ with the largest possible component $M = \ell_1 + \ell_2$ along the z -axis. The corresponding classical total angular momentum vector $\vec{\mathbb{J}}_{\text{class}}$ would be obtained by aligning both $\vec{\mathcal{J}}_{\text{class}}^{(1)}$ and $\vec{\mathcal{J}}_{\text{class}}^{(2)}$ also along the z -axis and adding these two vectors. Quantum mechanically this corresponds to a state

$$\mathcal{G}_{\ell_1+\ell_2, \ell_1+\ell_2}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) \quad (6.39)$$

which we will try for a solution of (6.37). For this purpose we insert (6.39) into (6.37) and replace according to (6.11) \mathbb{J}_+ by $\mathcal{J}_+^{(1)} + \mathcal{J}_+^{(2)}$. We obtain using (5.66, 5.68)

$$\begin{aligned} & (\mathcal{J}_+^{(1)} + \mathcal{J}_+^{(2)}) Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) \\ &= (\mathcal{J}_+^{(1)} Y_{\ell_1 \ell_1}(\Omega_1)) Y_{\ell_2 \ell_2}(\Omega_2) + Y_{\ell_1 \ell_1}(\Omega_1) (\mathcal{J}_+^{(2)} Y_{\ell_2 \ell_2}(\Omega_2)) = 0 . \end{aligned} \quad (6.40)$$

Similarly, we can demonstrate condition (6.25) using (6.11) and (5.64)

$$\begin{aligned} & (\mathcal{J}_3^{(1)} + \mathcal{J}_3^{(2)}) Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) \\ &= (\mathcal{J}_3^{(1)} Y_{\ell_1 \ell_1}(\Omega_1)) Y_{\ell_2 \ell_2}(\Omega_2) + Y_{\ell_1 \ell_1}(\Omega_1) (\mathcal{J}_3^{(2)} Y_{\ell_2 \ell_2}(\Omega_2)) \\ &= \hbar(\ell_1 + \ell_2) Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) . \end{aligned} \quad (6.41)$$

In fact, we can also demonstrate using (??) that $\mathcal{G}_{\ell_1+\ell_2, \ell_1+\ell_2}(\ell_1, \ell_2 | \Omega_1, \Omega_2)$ is normalized

$$\begin{aligned} & \int d\Omega_1 \int d\Omega_2 \mathcal{G}_{\ell_1+\ell_2, \ell_1+\ell_2}(\ell_1, \ell_2 | \Omega_1, \Omega_2) \\ &= \left(\int d\Omega_1 Y_{\ell_1 \ell_1}(\Omega_1) \right) \left(\int d\Omega_2 Y_{\ell_2 \ell_2}(\Omega_2) \right) = 1 . \end{aligned} \quad (6.42)$$

We, therefore, have shown

$$\mathfrak{Y}_{\ell_1+\ell_2, \ell_1+\ell_2}(\ell_1, \ell_2 | \Omega_1, \Omega_2) = Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) . \quad (6.43)$$

We now employ property (6.38) to construct the family of functions $\mathbb{B}_{\ell_{\mu} + \ell_{\nu}} = \{\mathfrak{Y}_{\ell_{\mu} + \ell_{\nu} M}(\ell_{\mu}, \ell_{\nu} | \cancel{\ell_{\mu}}, \cancel{\ell_{\nu}}), M = -(\ell_{\mu} + \ell_{\nu}), \dots, (\ell_{\mu} + \ell_{\nu})\}$. We demonstrate the procedure explicitly only for $M = \ell_1 + \ell_2 - 1$. The r.h.s. of (6.38) yields with $\mathbb{J}_- = \mathcal{J}_-^{(1)} + \mathcal{J}_-^{(2)}$ the expression $\hbar\sqrt{2\ell_1} Y_{\ell_1 \ell_1 - 1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) + \hbar\sqrt{2\ell_2} Y_{\ell_1 \ell_1 - 1}(\Omega_1) Y_{\ell_2 \ell_2 - 1}(\Omega_2)$. The l.h.s. of (6.38) yields $\hbar\sqrt{2(\ell_1 + \ell_2)} \mathfrak{Y}_{\ell_1 + \ell_2 \ell_1 + \ell_2 - 1}(\ell_1, \ell_2 | \Omega_1, \Omega_2)$. One obtains then

$$\begin{aligned} \mathfrak{Y}_{\ell_1 + \ell_2 \ell_1 + \ell_2 - 1}(\ell_1, \ell_2 | \Omega_1, \Omega_2) &= \\ \sqrt{\frac{\ell_1}{\ell_1 + \ell_2}} Y_{\ell_1 \ell_1 - 1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) &+ \sqrt{\frac{\ell_2}{\ell_1 + \ell_2}} Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2 - 1}(\Omega_2). \end{aligned} \quad (6.44)$$

This construction can be continued to obtain all $2(\ell_1 + \ell_2) + 1$ elements of $\mathbb{B}_{\ell_{\mu} + \ell_{\nu}}$ and, thereby, all the *Clebsch-Gordan coefficients* $(\ell_1 + \ell_2 M | \ell_1 m_1 \ell_2 m_2)$. We have provided in Table 1 the explicit form of $\mathfrak{Y}_{JM}(\ell_1 \ell_2 | \Omega_1 \Omega_2)$ for $\ell_1 = 2$ and $\ell_2 = 1$ to illustrate the construction. The reader should familiarize himself with the entries of the Table, in particular, with the symmetry pattern and with the terms $Y_{\ell_1 m_1} Y_{\ell_2 m_2}$ contributing to each \mathfrak{Y}_{JM} .

We like to construct now the family of total angular momentum functions $\mathbb{B}_{\ell_{\mu} + \ell_{\nu} - \cancel{\mu}} = \{\mathfrak{Y}_{\ell_{\mu} + \ell_{\nu} - \cancel{\mu} M}(\ell_{\mu}, \ell_{\nu} | \cancel{\ell_{\mu}}, \cancel{\ell_{\nu}}), M = -(\ell_{\mu} + \ell_{\nu} - \cancel{\mu}), \dots, (\ell_{\mu} + \ell_{\nu} - \cancel{\mu})\}$. We seek for this purpose first an unnormalized solution $\mathcal{G}_{\ell_1 + \ell_2 - 1 \ell_1 + \ell_2 - 1}$ of (6.36, 6.37). According to the condition (6.21) we set

$$\mathcal{G}_{\ell_1 + \ell_2 - 1 \ell_1 + \ell_2 - 1}(\ell_1 \ell_2 | \Omega_1 \Omega_2) = Y_{\ell_1 \ell_1 - 1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) + c Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2 - 1}(\Omega_2) \quad (6.45)$$

for some unknown constant c . One can readily show that (6.37) is satisfied. To demonstrate (6.36) we proceed as above and obtain

$$\begin{aligned} & \left(\mathcal{J}_+^{(1)} Y_{\ell_1 \ell_1 - 1}(\Omega_1) \right) Y_{\ell_2 \ell_2}(\Omega_2) + c Y_{\ell_1 \ell_1}(\Omega_1) \left(\mathcal{J}_+^{(2)} Y_{\ell_2 \ell_2 - 1}(\Omega_2) \right) \\ &= \left(\sqrt{2\ell_1} + c \sqrt{2\ell_2} \right) Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) = 0. \end{aligned} \quad (6.46)$$

To satisfy this equation one needs to choose $c = -\sqrt{\ell_1/\ell_2}$. We have thereby determined $\mathcal{G}_{\ell_1 + \ell_2 - 1 \ell_1 + \ell_2 - 1}$ in (6.45). Normalization yields furthermore

$$\begin{aligned} \mathfrak{Y}_{\ell_1 + \ell_2 - 1 \ell_1 + \ell_2 - 1}(\ell_1 \ell_2 | \Omega_1 \Omega_2) &= \\ \sqrt{\frac{\ell_2}{\ell_1 + \ell_2}} Y_{\ell_1 \ell_1 - 1}(\Omega_1) Y_{\ell_2 \ell_2}(\Omega_2) &- \sqrt{\frac{\ell_1}{\ell_1 + \ell_2}} Y_{\ell_1 \ell_1}(\Omega_1) Y_{\ell_2 \ell_2 - 1}(\Omega_2). \end{aligned} \quad (6.47)$$

This expression is orthogonal to (6.39) as required by (6.27).

Expression (6.47) can serve now to obtain recursively the elements of the family $\mathbb{B}_{\ell_{\mu} + \ell_{\nu} - \cancel{\mu}}$ for $M = \ell_1 + \ell_2 - 2, \ell_1 + \ell_2 - 3, \dots, -(\ell_1 + \ell_2 - 1)$. Having constructed this family we have determined the *Clebsch-Gordan coefficients* $(\ell_1 + \ell_2 - 1 M | \ell_1 m_1 \ell_2 m_2)$. The result is illustrated for the case $\ell_1 = 2, \ell_2 = 1$ in Table 1.

One can obviously continue the construction outlined to determine $\mathfrak{Y}_{\ell_1 + \ell_2 - 2 \ell_1 + \ell_2 - 2}$, etc. and all total angular momentum functions for a given choice of ℓ_1 and ℓ_2 .

Exercise 6.2.1: Construct following the procedure above the three functions $\mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2)$ for $M = \ell_1 + \ell_2 - 2$ and $J = \ell_1 + \ell_2, \ell_1 + \ell_2 - 1, \ell_1 + \ell_2 - 2$. Show that the resulting functions are orthonormal.

$\mathfrak{Y}_{33}(2, 1 \Omega_1, \Omega_2)$	$Y_{22}(\Omega_1)Y_{11}(\Omega_2)$		
	1		
$\mathfrak{Y}_{32}(2, 1 \Omega_1, \Omega_2)$	$Y_{21}(\Omega_1)Y_{11}(\Omega_2)$	$Y_{22}(\Omega_1)Y_{10}(\Omega_2)$	
$\mathfrak{Y}_{22}(2, 1 \Omega_1, \Omega_2)$	$\sqrt{\frac{2}{3}} \simeq 0.816497$	$\sqrt{\frac{1}{3}} \simeq 0.57735$	
	$-\sqrt{\frac{1}{3}} \simeq -0.57735$	$\sqrt{\frac{2}{3}} \simeq 0.816497$	
$\mathfrak{Y}_{31}(2, 1 \Omega_1, \Omega_2)$	$Y_{20}(\Omega_1)Y_{11}(\Omega_2)$	$Y_{21}(\Omega_1)Y_{10}(\Omega_2)$	$Y_{22}(\Omega_1)Y_{1-1}(\Omega_2)$
$\mathfrak{Y}_{21}(2, 1 \Omega_1, \Omega_2)$	$\sqrt{\frac{2}{5}} \simeq 0.632456$	$\sqrt{\frac{8}{15}} \simeq 0.730297$	$\sqrt{\frac{1}{15}} \simeq 0.258199$
$\mathfrak{Y}_{11}(2, 1 \Omega_1, \Omega_2)$	$-\sqrt{\frac{1}{2}} \simeq -0.707107$	$\sqrt{\frac{1}{6}} \simeq 0.408248$	$\sqrt{\frac{1}{3}} \simeq 0.57735$
	$\sqrt{\frac{1}{10}} \simeq 0.316228$	$-\sqrt{\frac{3}{10}} \simeq -0.547723$	$\sqrt{\frac{3}{5}} \simeq 0.774597$
$\mathfrak{Y}_{30}(2, 1 \Omega_1, \Omega_2)$	$Y_{2-1}(\Omega_1)Y_{11}(\Omega_2)$	$Y_{20}(\Omega_1)Y_{10}(\Omega_2)$	$Y_{21}(\Omega_1)Y_{1-1}(\Omega_2)$
$\mathfrak{Y}_{20}(2, 1 \Omega_1, \Omega_2)$	$\sqrt{\frac{1}{5}} \simeq 0.447214$	$\sqrt{\frac{3}{5}} \simeq 0.774597$	$\sqrt{\frac{1}{5}} \simeq 0.447214$
$\mathfrak{Y}_{10}(2, 1 \Omega_1, \Omega_2)$	$-\sqrt{\frac{1}{2}} \simeq -0.707107$	0	$\sqrt{\frac{1}{2}} \simeq 0.707107$
	$\sqrt{\frac{3}{10}} \simeq 0.547723$	$\sqrt{\frac{6}{5}} \simeq -0.632456$	$\sqrt{\frac{3}{10}} \simeq 0.547723$
$\mathfrak{Y}_{3-1}(2, 1 \Omega_1, \Omega_2)$	$Y_{2-2}(\Omega_1)Y_{11}(\Omega_2)$	$Y_{2-1}(\Omega_1)Y_{10}(\Omega_2)$	$Y_{20}(\Omega_1)Y_{1-1}(\Omega_2)$
$\mathfrak{Y}_{2-1}(2, 1 \Omega_1, \Omega_2)$	$\sqrt{\frac{1}{15}} \simeq 0.258199$	$\sqrt{\frac{8}{15}} \simeq 0.730297$	$\sqrt{\frac{2}{5}} \simeq 0.632456$
$\mathfrak{Y}_{1-1}(2, 1 \Omega_1, \Omega_2)$	$-\sqrt{\frac{1}{3}} \simeq -0.57735$	$-\sqrt{\frac{1}{6}} \simeq -0.408248$	$\sqrt{\frac{1}{2}} \simeq 0.707107$
	$\sqrt{\frac{3}{5}} \simeq 0.774597$	$-\sqrt{\frac{3}{10}} \simeq -0.547723$	$\sqrt{\frac{1}{10}} \simeq 0.316228$
$\mathfrak{Y}_{3-2}(2, 1 \Omega_1, \Omega_2)$		$Y_{2-2}(\Omega_1)Y_{10}(\Omega_2)$	$Y_{2-1}(\Omega_1)Y_{1-1}(\Omega_2)$
$\mathfrak{Y}_{2-2}(2, 1 \Omega_1, \Omega_2)$		$\sqrt{\frac{1}{3}} \simeq 0.57735$	$\sqrt{\frac{2}{3}} \simeq 0.816497$
		$-\sqrt{\frac{2}{3}} \simeq -0.816497$	$\sqrt{\frac{1}{3}} \simeq 0.57735$
$\mathfrak{Y}_{3-3}(2, 1 \Omega_1, \Omega_2)$			$Y_{2-2}(\Omega_1)Y_{1-1}(\Omega_2)$
			1

Table 6.1: Some explicit analytical and numerical values of *Clebsch-Gordan coefficients* and their relationship to the total angular momentum wave functions and single particle angular momentum wave functions.

Exercise 6.2.2: Use the construction for Clebsch-Gordan coefficients above to prove the following formulas

$$\begin{aligned} \langle J, M | \ell, m - \frac{1}{2}, \frac{1}{2}, +\frac{1}{2} \rangle &= \begin{cases} \sqrt{\frac{J+M}{2J}} & \text{for } \ell = J - \frac{1}{2} \\ -\sqrt{\frac{J-M+1}{2J+2}} & \text{for } \ell = J + \frac{1}{2} \end{cases} \\ \langle J, M | \ell, m + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \rangle &= \begin{cases} \sqrt{\frac{J-M}{2J}} & \text{for } \ell = J - \frac{1}{2} \\ \sqrt{\frac{J+M+1}{2J+2}} & \text{for } \ell = J + \frac{1}{2} \end{cases} . \end{aligned}$$

The construction described provides a very cumbersome route to the analytical and numerical values of the *Clebsch-Gordan coefficients*. It is actually possible to state explicit expressions for any single coefficient ($JM|\ell_1 m_1 \ell_2 m_2$). These expressions will be derived now.

6.3 Explicit Expression for the Clebsch-Gordan Coefficients

We want to establish in this Section an explicit expression for the Clebsch-Gordan coefficients ($JM|\ell_1 m_1 \ell_2 m_2$). For this purpose we will employ the spinor operators introduced in Sections 5.9, 5.10.

Definition of Spinor Operators for Two Particles

In contrast to Sections 5.9, 5.10 where we studied single particle angular momentum and spin, we are dealing now with two particles carrying angular momentum or spin. Accordingly, we extend definition (5.287) to two particles

$${}^{(1)}J_k = \frac{1}{2} \sum_{\zeta, \zeta'} a_{\zeta}^{\dagger} \langle \zeta | \sigma_k | \zeta' \rangle a_{\zeta'} \quad (6.48)$$

$${}^{(2)}J_k = \frac{1}{2} \sum_{\zeta, \zeta'} b_{\zeta}^{\dagger} \langle \zeta | \sigma_k | \zeta' \rangle b_{\zeta'} \quad (6.49)$$

where $\zeta, \zeta' = \pm$ and the matrix elements $\langle \zeta | \sigma_k | \zeta' \rangle$ are as defined in Section 5.10. The creation and annihilation operators are again of the boson type with commutation properties

$$[a_{\zeta}, a_{\zeta'}] = [a_{\zeta}^{\dagger}, a_{\zeta'}^{\dagger}] = 0 \quad , \quad [a_{\zeta}, a_{\zeta'}^{\dagger}] = \delta_{\zeta\zeta'} \quad (6.50)$$

$$[b_{\zeta}, b_{\zeta'}] = [b_{\zeta}^{\dagger}, b_{\zeta'}^{\dagger}] = 0 \quad , \quad [b_{\zeta}, b_{\zeta'}^{\dagger}] = \delta_{\zeta\zeta'} \quad . \quad (6.51)$$

The operators $a_{\zeta}, a_{\zeta}^{\dagger}$ and $b_{\zeta}, b_{\zeta}^{\dagger}$ refer to different particles and, hence, commute with each other

$$[a_{\zeta}, b_{\zeta'}] = [a_{\zeta}^{\dagger}, b_{\zeta'}^{\dagger}] = [a_{\zeta}, b_{\zeta'}^{\dagger}] = 0 \quad . \quad (6.52)$$

According to Section 5.10 [cf. (5.254)] the angular momentum / spin eigenstates $|\ell_1 m_1\rangle_1$ and $|\ell_2 m_2\rangle_2$ of the two particles are

$$|\ell_1 m_1\rangle_1 = \frac{(a_+^{\dagger})^{\ell_1+m_1} (a_-^{\dagger})^{\ell_1-m_1}}{\sqrt{(\ell_1+m_1)!} \sqrt{(\ell_1-m_1)!}} |\Psi_0\rangle \quad (6.53)$$

$$|\ell_2 m_2\rangle_2 = \frac{(b_+^{\dagger})^{\ell_2+m_2} (b_-^{\dagger})^{\ell_2-m_2}}{\sqrt{(\ell_2+m_2)!} \sqrt{(\ell_2-m_2)!}} |\Psi_0\rangle \quad . \quad (6.54)$$

It holds, in analogy to Eqs. (5.302, 5.303),

$${}^{(1)}J^2|\ell_1 m_1\rangle_1 = \ell_1(\ell_1 + 1)|\ell_1 m_1\rangle_1, \quad {}^{(1)}J_3|\ell_1 m_1\rangle_1 = m_1|\ell_1 m_1\rangle_1 \quad (6.55)$$

$${}^{(2)}J^2|\ell_2 m_2\rangle_2 = \ell_2(\ell_2 + 1)|\ell_2 m_2\rangle_2, \quad {}^{(2)}J_3|\ell_2 m_2\rangle_2 = m_2|\ell_2 m_2\rangle_2 \quad (6.56)$$

The states $|\ell_1, m_1\rangle_1 |\ell_2, m_2\rangle_2$, which describe a two particle system according to (6.53, 6.54), are

$$|\ell_1, m_1\rangle_1 |\ell_2, m_2\rangle_2 = \frac{(a_+^\dagger)^{\ell_1+m_1}}{\sqrt{(\ell_1+m_1)!}} \frac{(a_-^\dagger)^{\ell_1-m_1}}{\sqrt{(\ell_1-m_1)!}} \frac{(b_+^\dagger)^{\ell_2+m_2}}{\sqrt{(\ell_2+m_2)!}} \frac{(b_-^\dagger)^{\ell_2-m_2}}{\sqrt{(\ell_2-m_2)!}} |\Psi_o\rangle. \quad (6.57)$$

The operator of the total angular momentum/spin of the two particle system is

$$\mathbb{J} = {}^{(1)}\vec{J} + {}^{(2)}\vec{J} \quad (6.58)$$

with Cartesian components

$$\mathbb{J}_k = {}^{(1)}J_k + {}^{(2)}J_k \quad ; \quad k = 1, 2, 3. \quad (6.59)$$

We seek to determine states $|J, M(\ell_1, \ell_2)\rangle$ which are simultaneous eigenstates of the operators $\mathbb{J}^2, \mathbb{J}_3, {}^{(1)}J^2, {}^{(2)}J^2$ which, as usual are denoted by their respective quantum numbers J, M, ℓ_1, ℓ_2 , i.e., for such states should hold

$$\mathbb{J}^2|J, M(\ell_1, \ell_2)\rangle = J(J+1)|J, M(\ell_1, \ell_2)\rangle \quad (6.60)$$

$$\mathbb{J}_3|J, M(\ell_1, \ell_2)\rangle = M|J, M(\ell_1, \ell_2)\rangle \quad (6.61)$$

$${}^{(1)}J^2|J, M(\ell_1, \ell_2)\rangle = \ell_1(\ell_1 + 1)|J, M(\ell_1, \ell_2)\rangle \quad (6.62)$$

$${}^{(2)}J^2|J, M(\ell_1, \ell_2)\rangle = \ell_2(\ell_2 + 1)|J, M(\ell_1, \ell_2)\rangle. \quad (6.63)$$

At this point, we like to recall for future reference that the operators ${}^{(1)}J^2, {}^{(2)}J^2$, according to (5.300), can be expressed in terms of the number operators

$$\hat{k}_1 = \frac{1}{2} (a_+^\dagger a_+ + a_-^\dagger a_-) \quad , \quad \hat{k}_2 = \frac{1}{2} (b_+^\dagger b_+ + b_-^\dagger b_-) \quad , \quad (6.64)$$

namely,

$${}^{(j)}J^2 = \hat{k}_j (\hat{k}_j + 1) \quad , \quad j = 1, 2. \quad (6.65)$$

For the operators \hat{k}_j holds

$$\hat{k}_j |\ell_j, m_j\rangle_j = \ell_j |\ell_j, m_j\rangle_j \quad (6.66)$$

and, hence,

$$\hat{k}_j |J, M(\ell_1, \ell_2)\rangle = \ell_j |J, M(\ell_1, \ell_2)\rangle \quad (6.67)$$

We will also require below the raising and lowering operators associated with the total angular momentum operator (6.59)

$$\mathbb{J}_\pm = \mathbb{J}_1 \pm i\mathbb{J}_2. \quad (6.68)$$

The states $|J, M(\ell_1, \ell_2)\rangle$ can be expressed in terms of Clebsch-Gordan coefficients (6.18) as follows

$$|J, M(\ell_1, \ell_2)\rangle = \sum_{m_1, m_2} |\ell_1, m_1\rangle_1 |\ell_2, m_2\rangle_2 (\ell_1, m_1, \ell_2, m_2 | J, M(\ell_1, \ell_2)) \quad , \quad (6.69)$$

$$|\ell_1 - \ell_2| \leq J \leq \ell_1 + \ell_2 \quad , \quad -J \leq M \leq J.$$

The aim of the present Section is to determine closed expressions for the Clebsch-Gordan coefficients $(\ell_1, m_1, \ell_2, m_2 | J, M(\ell_1, \ell_2))$.

The Operator K^\dagger

The following operator

$$K^\dagger = a_+^\dagger b_-^\dagger - a_-^\dagger b_+^\dagger. \quad (6.70)$$

will play a crucial role in the evaluation of the Clebsch-Gordan-Coefficients. This operator obeys the following commutation relationships with the other pertinent angular momentum / spin operators

$$[\hat{k}_j, K^\dagger] = \frac{1}{2} K^\dagger, \quad j = 1, 2 \quad (6.71)$$

$$[{}^{(j)}J^2, K^\dagger] = K^\dagger \hat{k}_j + \frac{3}{4} K^\dagger, \quad j = 1, 2 \quad (6.72)$$

$$[\mathbb{J}_3, K^\dagger] = 0 \quad (6.73)$$

$$[\mathbb{J}_\pm, K^\dagger] = 0. \quad (6.74)$$

We note that, due to $\mathbb{J}^2 = \frac{1}{2}\mathbb{J}_+\mathbb{J}_- + \frac{1}{2}\mathbb{J}_-\mathbb{J}_+ + \mathbb{J}_3^2$, the relationships (6.73, 6.74) imply

$$[\mathbb{J}^2, K^\dagger] = 0. \quad (6.75)$$

The relationships (6.71–6.73) can be readily proven. For example, using (6.64, 6.50, 6.51) one obtains

$$\begin{aligned} [\hat{k}_1, K^\dagger] &= \frac{1}{2} [a_+^\dagger a_+ + a_-^\dagger a_-, a_+^\dagger b_-^\dagger - a_-^\dagger b_+^\dagger] \\ &= \frac{1}{2} a_+^\dagger [a_+, a_+^\dagger] b_-^\dagger - \frac{1}{2} a_-^\dagger [a_-, a_-^\dagger] b_+^\dagger \\ &= \frac{1}{2} (a_+^\dagger a_+ - a_-^\dagger a_-) = \frac{1}{2} K^\dagger. \end{aligned}$$

A similar calculation yields $[\hat{k}_2, K^\dagger] = \frac{1}{2} K^\dagger$. Employing (6.65) and (6.71) one can show

$$\begin{aligned} [{}^{(j)}J^2, K^\dagger] &= \frac{1}{2} [\hat{k}_j(\hat{k}_j + 1), K^\dagger] \\ &= \frac{1}{2} \hat{k}_j [\hat{k}_j + 1, K^\dagger] + \frac{1}{2} [\hat{k}_j, K^\dagger] (\hat{k}_j + 1) \\ &= \frac{1}{2} \hat{k}_j K^\dagger + \frac{1}{2} K^\dagger (\hat{k}_j + 1) \\ &= K^\dagger \hat{k}_j + \frac{1}{2} [\hat{k}_j, K^\dagger] + \frac{1}{2} K^\dagger \\ &= K^\dagger \hat{k}_j + \frac{3}{4} K^\dagger. \end{aligned}$$

Using $\mathbb{J}_3 = {}^{(1)}J_3 + {}^{(2)}J_3$, expressing ${}^{(k)}J_3$ through the creation and annihilation operators according to (5.288), and applying the relationships (6.71–6.73) yields

$$\begin{aligned} [\mathbb{J}_3, K^\dagger] &= \frac{1}{2} [a_+^\dagger a_+ - a_-^\dagger a_- + b_+^\dagger b_+ - b_-^\dagger b_-, a_+^\dagger b_-^\dagger - a_-^\dagger b_+^\dagger] \\ &= \frac{1}{2} a_+^\dagger [a_+, a_+^\dagger] b_-^\dagger + \frac{1}{2} a_-^\dagger [a_-, a_-^\dagger] b_+^\dagger \\ &\quad - \frac{1}{2} b_+^\dagger a_-^\dagger [b_+, b_+^\dagger] - \frac{1}{2} b_-^\dagger a_+^\dagger [b_-, b_-^\dagger] = 0. \end{aligned}$$

Starting from (5.292) one can derive similarly

$$\begin{aligned} [\mathbb{J}_+, K^\dagger] &= [a_+^\dagger a_- + b_+^\dagger b_-, a_+^\dagger b_- - a_-^\dagger b_+] \\ &= -a_+^\dagger [a_-, a_-^\dagger] b_+^\dagger + b_+^\dagger a_+^\dagger [b_-, b_-^\dagger] = 0. \end{aligned}$$

The property $[\mathbb{J}_-, K^\dagger] = 0$ is demonstrated in an analogous way.

Action of K^\dagger on the states $|J, M(\ell_1, \ell_2)\rangle$

We want to demonstrate now that the action of K^\dagger on the states $|J, M(\ell_1, \ell_2)\rangle$ produces again total angular momentum eigenstates to the same J and M quantum numbers of \mathbb{J}^2 and \mathbb{J}_3 , but for different ℓ_1 and ℓ_2 quantum numbers of the operators ${}^{(1)}J^2$ and ${}^{(2)}J^2$.

The commutation properties (6.73, 6.75) ascertain that under the action of K^\dagger the states $|J, M(\ell_1, \ell_2)\rangle$ remain eigenstates of \mathbb{J}^2 and \mathbb{J}_3 with the same quantum numbers. To demonstrate that the resulting states are eigenstates of ${}^{(1)}J^2$ and ${}^{(2)}J^2$ we exploit (6.72) and (6.62, 6.63, 6.67)

$$\begin{aligned} {}^{(j)}J^2 K^\dagger |J, M(\ell_1, \ell_2)\rangle &= \left([{}^{(j)}J^2, K^\dagger] + K^\dagger {}^{(j)}J^2 \right) |J, M(\ell_1, \ell_2)\rangle \\ &= \left(K^\dagger \hat{k}_j + \frac{3}{4} K^\dagger + K^\dagger \ell_j (\ell_j + 1) \right) |J, M(\ell_1, \ell_2)\rangle \\ &= K^\dagger \left(\ell_j + \frac{3}{4} + \ell_j (\ell_j + 1) \right) |J, M(\ell_1, \ell_2)\rangle \\ &= \left(\ell_j + \frac{1}{2} \right) \left(\ell_j + \frac{3}{2} \right) K^\dagger |J, M(\ell_1, \ell_2)\rangle. \end{aligned}$$

However, this result implies that $K^\dagger |J, M(\ell_1, \ell_2)\rangle$ is a state with quantum numbers $\ell_1 + \frac{1}{2}$ and $\ell_2 + \frac{1}{2}$, i.e., it holds

$$K^\dagger |J, M(\ell_1, \ell_2)\rangle = N |J, M(\ell_1 + \frac{1}{2}, \ell_2 + \frac{1}{2})\rangle. \quad (6.76)$$

Here N is an unknown normalization constant.

One can generalize property (6.76) and state

$$(K^\dagger)^n |J, M(\ell_1, \ell_2)\rangle = N' |J, M(\ell_1 + \frac{n}{2}, \ell_2 + \frac{n}{2})\rangle \quad (6.77)$$

where N' is another normalization constant. We consider now the case that $(K^\dagger)^n$ acts on the simplest total angular momentum / spin state, namely, on the state

$$|j_1 + j_2, j_1 + j_2(j_1, j_2)\rangle = |j_1, j_1\rangle_1 |j_2, j_2\rangle_2, \quad (6.78)$$

a state which has been used already in the construction of Clebsch-Gordan coefficients in Section 6.2. Application of $(K^\dagger)^n$ to this state yields, according to (6.77),

$$\begin{aligned} |j_1 + j_2, j_1 + j_2(j_1 + \frac{n}{2}, j_2 + \frac{n}{2})\rangle \\ = N(n, j_1 + \frac{n}{2}, j_1 + \frac{n}{2}) (K^\dagger)^n |j_1 + j_2, j_1 + j_2(j_1, j_2)\rangle \end{aligned} \quad (6.79)$$

where we denoted the associated normalization constant by $N(n, j_1 + \frac{n}{2}, j_2 + \frac{n}{2})$.

It is now important to notice that any state of the type $|J, J(\ell_1, \ell_2)\rangle$ can be expressed through the r.h.s. of (6.79). For this purpose one needs to choose in (6.79) n, j_1, j_2 as follows

$$J = j_1 + j_2 \quad , \quad \ell_1 = j_1 + \frac{n}{2} \quad , \quad \ell_2 = j_2 + \frac{n}{2} \quad (6.80)$$

which is equivalent to

$$\begin{aligned} n &= \ell_1 + \ell_2 - J \\ j_1 &= \ell_1 - \frac{n}{2} = \frac{1}{2}(J + \ell_1 - \ell_2) \\ j_2 &= \ell_2 - \frac{n}{2} = \frac{1}{2}(J + \ell_2 - \ell_1) . \end{aligned} \quad (6.81)$$

Accordingly, holds

$$\begin{aligned} |J, J(\ell_1, \ell_2)\rangle &= N(\ell_1 + \ell_2 - J, \ell_1, \ell_2) (K^\dagger)^{\ell_1 + \ell_2 - J} \times \\ &\times \left| \frac{1}{2}(J + \ell_1 - \ell_2) \right\rangle_1 \times \\ &\times \left| \frac{1}{2}(J + \ell_2 - \ell_1) \right\rangle_2 . \end{aligned} \quad (6.82)$$

The normalization constant appearing here is actually

$$N(\ell_1 + \ell_2 - J, \ell_1, \ell_2) = \left[\frac{(2J + 1)!}{(\ell_1 + \ell_2 - J)!(\ell_1 + \ell_2 + J + 1)!} \right]^{\frac{1}{2}} . \quad (6.83)$$

The derivation of this expression will be provided further below (see page 158 ff).

Strategy for Generating the States $|J, M(\ell_1, \ell_2)\rangle$

Our construction of the states $|J, M(\ell_1, \ell_2)\rangle$ exploits the expression (6.82) for $|J, J(\ell_1, \ell_2)\rangle$. The latter states, in analogy to the construction (5.104, 5.105) of the spherical harmonics, allow one to obtain the states $|J, M(\ell_1, \ell_2)\rangle$ for $-J \leq M \leq J$ as follows

$$|J, M(\ell_1, \ell_2)\rangle = \Delta(J, M) (\mathbb{J}_-)^{J-M} |J, J(\ell_1, \ell_2)\rangle \quad (6.84)$$

$$\Delta(J, M) = \left[\frac{(J + M)!}{(2J)!(J - M)!} \right]^{\frac{1}{2}} . \quad (6.85)$$

Combining (6.84) with (6.82, 6.57) and exploiting the fact that \mathbb{J}_- and K^\dagger commute [c.f. (6.74)] yields

$$\begin{aligned} |J, M(\ell_1, \ell_2)\rangle &= \frac{N(\ell_1 + \ell_2 - J, \ell_1, \ell_2) \Delta(J, M)}{\sqrt{(J + \ell_1 - \ell_2)!(J + \ell_2 - \ell_1)!}} \times \\ &\times (K^\dagger)^{\ell_1 + \ell_2 - J} (\mathbb{J}_-)^{J-M} (a_+^\dagger)^{J + \ell_1 - \ell_2} (b_+^\dagger)^{J + \ell_2 - \ell_1} |\Psi_o\rangle \end{aligned} \quad (6.86)$$

Our strategy for the evaluation of the Clebsch-Gordan-coefficients is to expand (6.86) in terms of monomials

$$\left(a_+^\dagger\right)^{\ell_1+m_1} \left(a_-^\dagger\right)^{\ell_1-m_1} \left(b_+^\dagger\right)^{\ell_2+m_2} \left(b_-^\dagger\right)^{\ell_2-m_2} |\Psi_o\rangle, \quad (6.87)$$

i.e., in terms of $|\ell_1, m_1\rangle_1 |\ell_2, m_2\rangle_2$ [cf. (6.57)]. Comparison with (6.69) yields then the Clebsch-Gordan-coefficients.

Expansion of an Intermediate State

We first consider the expansion of the following factor appearing in (6.86)

$$|G_{st}^r\rangle = \mathbb{J}_- \left(a_+^\dagger\right)^s \left(b_+^\dagger\right)^t |\Psi_o\rangle \quad (6.88)$$

in terms of monomials (6.87). For this purpose we introduce the generating function

$$I(\lambda, x, y) = \exp(\lambda \mathbb{J}_-) \exp\left(x a_+^\dagger\right) \exp\left(y b_+^\dagger\right) |\Psi_o\rangle. \quad (6.89)$$

Taylor expansion of the two exponential operators yields immediately

$$I(\lambda, x, y) = \sum_{r,s,t} \frac{\lambda^r x^s y^t}{r! s! t!} |G_{st}^r\rangle, \quad (6.90)$$

i.e., $I(\lambda, x, y)$ is a generating function for the states $|G_{st}^r\rangle$ defined in (6.88).

The desired expansion of $|G_{st}^r\rangle$ can be obtained from an alternate evaluation of $I(\lambda, x, y)$ which is based on the properties

$$a_\zeta f(a_\zeta^\dagger) |\Psi_o\rangle = \frac{\partial}{\partial a_\zeta^\dagger} f(a_\zeta^\dagger) |\Psi_o\rangle \quad b_\zeta f(b_\zeta^\dagger) |\Psi_o\rangle = \frac{\partial}{\partial b_\zeta^\dagger} f(b_\zeta^\dagger) |\Psi_o\rangle \quad (6.91)$$

which, in analogy to (5.264), follows from the commutation properties (6.50–6.52). One obtains then using

$$\mathbb{J}_- = a_-^\dagger a_+ + b_-^\dagger b_+ \quad (6.92)$$

and noting $[a_+, a_-^\dagger] = [b_+, b_-^\dagger] = 0$ [cf. (6.50)]

$$\begin{aligned} \exp(\lambda \mathbb{J}_-) f(a_+^\dagger) g(b_+^\dagger) |\Psi_o\rangle &= \exp\left(a_-^\dagger a_+\right) f(a_+^\dagger) \exp\left(b_-^\dagger b_+\right) g(b_+^\dagger) |\Psi_o\rangle \\ &= \sum_u \frac{\lambda^u}{u!} \left(a_-^\dagger a_+\right)^u f(a_+^\dagger) \times \\ &\quad \times \sum_v \frac{\lambda^v}{v!} \left(b_-^\dagger b_+\right)^v g(b_+^\dagger) |\Psi_o\rangle \\ &= \sum_u \frac{\left(\lambda a_-^\dagger\right)^u}{u!} \left(\frac{\partial}{\partial a_+^\dagger}\right)^u f(a_+^\dagger) \times \\ &\quad \times \sum_v \frac{\left(\lambda b_-^\dagger\right)^v}{v!} \left(\frac{\partial}{\partial b_+^\dagger}\right)^v g(b_+^\dagger) |\Psi_o\rangle \\ &= f\left(a_+^\dagger + \lambda a_-^\dagger\right) g\left(b_+^\dagger + \lambda b_-^\dagger\right) |\Psi_o\rangle. \end{aligned} \quad (6.93)$$

We conclude

$$I(\lambda, x, y) = \exp\left(a_+^\dagger + \lambda a_-^\dagger\right) \exp\left(b_+^\dagger + \lambda b_-^\dagger\right) |\Psi_o\rangle. \quad (6.94)$$

One can infer from this result the desired expressions for $|G_{st}^r\rangle$. Expanding the exponentials in (6.94) yields

$$\begin{aligned} I(\lambda, x, y) &= \sum_{s,t} \frac{x^s}{s!} \frac{y^t}{t!} \left(a_+^\dagger + \lambda a_-^\dagger\right)^s \left(b_+^\dagger + \lambda b_-^\dagger\right)^t |\Psi_o\rangle \\ &= \sum_{s,t} \frac{x^s}{s!} \frac{y^t}{t!} \sum_t \sum_v \binom{s}{u} \binom{t}{v} \times \\ &\quad \times \left(a_+^\dagger\right)^{s-u} \lambda^u \left(a_-^\dagger\right)^u \left(b_+^\dagger\right)^{t-v} \lambda^v \left(b_-^\dagger\right)^v |\Psi_o\rangle \\ &= \sum_{r,s,t} \frac{\lambda^r}{r!} \frac{x^s}{s!} \frac{y^t}{t!} \sum_q r! \binom{s}{q} \binom{t}{r-q} \times \\ &\quad \times \left(a_+^\dagger\right)^{s-q} \left(a_-^\dagger\right)^q \left(b_+^\dagger\right)^{t-r+q} \left(b_-^\dagger\right)^{r-q} |\Psi_o\rangle \end{aligned} \quad (6.95)$$

Comparison with (6.90) allows one to infer

$$\begin{aligned} |G_{s,t}^r\rangle &= \sum_q r! \binom{s}{q} \binom{t}{r-q} \times \\ &\quad \times \left(a_+^\dagger\right)^{s-q} \left(a_-^\dagger\right)^q \left(b_+^\dagger\right)^{t-r+q} \left(b_-^\dagger\right)^{r-q} |\Psi_o\rangle \end{aligned} \quad (6.96)$$

and, using the definition (6.88), one can write the right factor in (6.86)

$$\begin{aligned} &(\mathbb{J}_-)^{J-M} \left(a_+^\dagger\right)^{J+\ell_1-\ell_2} \left(b_+^\dagger\right)^{J+\ell_2-\ell_1} |\Psi_o\rangle \\ &= \sum_q \frac{(J-M)!(J+\ell_1-\ell_2)!(J+\ell_2-\ell_1)!}{q!(J+\ell_1-\ell_2-q)!(J-M-q)!(M+\ell_2-\ell_1+q)!} \times \\ &\quad \times \left(a_+^\dagger\right)^{J+\ell_1-\ell_2-q} \left(a_-^\dagger\right)^q \left(b_+^\dagger\right)^{M+\ell_2-\ell_1+q} \left(b_-^\dagger\right)^{J-M-q} |\Psi_o\rangle \end{aligned} \quad (6.97)$$

Final Result

Our last step is to apply the operator $(K^\dagger)^{\ell_1+\ell_2-J}$ to expression (6.97), to obtain the desired expansion of $|J, M(\ell_1, \ell_2)\rangle$ in terms of states $|\ell_1, m_1\rangle_1 |\ell_2, m_2\rangle_2$. With K^\dagger given by (6.70) holds

$$\begin{aligned} (K^\dagger)^{\ell_1+\ell_2-J} &= \sum_s \binom{\ell_1+\ell_2-J}{s} (-1)^s \\ &\quad \left(a_+^\dagger\right)^{\ell_1+\ell_2-J-s} \left(b_+^\dagger\right)^{\ell_1+\ell_2-J-s} \left(a_-^\dagger\right)^s \left(b_-^\dagger\right)^s. \end{aligned} \quad (6.98)$$

Operation of this operator on (6.97) yields, using the commutation property (6.50),

$$|J, M(\ell_1, \ell_2)\rangle = \sum_{s,q} (-1)^s \quad (6.99)$$

$$\frac{(\ell_1 + \ell_2 - J)!(J - M)!(J + \ell_1 - \ell_2)!(J + \ell_2 - \ell_1)!}{s!(\ell_1 + \ell_2 - J - s)!q!(J + \ell_1 - \ell_2 - q)!(J - M - q)!(M + \ell_2 - \ell_1 + q)!} \\ \left(a_+^\dagger\right)^{2\ell_1 - q - s} \left(a_-^\dagger\right)^{q + s} \left(b_+^\dagger\right)^{M + \ell_2 - \ell_1 + q + s} \left(b_-^\dagger\right)^{\ell_1 + \ell_2 - M - q - s} |\Psi_0\rangle$$

The relationships (6.53,6.54) between creation operator monomials and angular momentum states allow one to write this

$$|J, M(\ell_1, \ell_2)\rangle = \frac{N(\ell_1 + \ell_2 - J, \ell_1, \ell_2) \Delta(J, M)}{\sqrt{(J + \ell_1 - \ell_2)!(J + \ell_2 - \ell_1)!}} \sum_{s,q} (-1)^s \times \quad (6.100) \\ \times \frac{(\ell_1 + \ell_2 - J)!(J - M)!(J + \ell_1 - \ell_2)!(J + \ell_2 - \ell_1)!}{s!(\ell_1 + \ell_2 - J - s)!q!(J + \ell_1 - \ell_2 - q)!(J - M - q)!(M + \ell_2 - \ell_1 + q)!} \\ \times \sqrt{(2\ell_1 - q - s)!(q + s)!} \\ \times \sqrt{(M + \ell_2 - \ell_1 + q + s)!(\ell_1 + \ell_2 - M - q - s)!} \\ \times |\ell_1, \ell_1 - q - s\rangle_1 |\ell_2, M - \ell_1 + q + s\rangle_2$$

One can conclude that this expression reproduces (6.69) if one identifies

$$m_1 = \ell_1 - q - s, \quad m_2 = M - \ell_1 + q + s. \quad (6.101)$$

Note that $m_1 + m_2 = M$ holds. The summation over q corresponds then to the summation over m_1, m_2 in (6.69) since, according to (6.101), $q = \ell_1 - m_1 - s$ and $m_2 = M - m_1$. The Clebsch-Gordan coefficients are then finally

$$(\ell_1, m_1, \ell_2, m_2 | J, M) = \sqrt{2J + 1} \left[\frac{\ell_1 + \ell_2 - J}{(\ell_1 + \ell_2 + J + 1)!} \frac{(\ell_1 - \ell_2 + J)!(-\ell_1 + \ell_2 + J)!}{(\ell_1 + \ell_2 + J + 1)!} \right]^{\frac{1}{2}} \\ \times [(\ell_1 + m_1)!(\ell_1 - m_1)!(\ell_2 + m_2)!(\ell_2 - m_2)!(J + M)!(J - M)!]^{\frac{1}{2}} \\ \times \sum_s \frac{(-1)^s}{s!(\ell_1 - m_1 - s)!(\ell_2 + m_2 - s)!} \\ \times \frac{1}{(\ell_1 + \ell_2 - J - s)!(J - \ell_1 - m_2 + s)!(J - \ell_2 + m_1 + s)!} \quad (6.102)$$

The Normalization

We want to determine now the expression (6.83) of the normalization constant $N(\ell_1 + \ell_2 - J, \ell_1, \ell_2)$ defined through (6.82). For this purpose we introduce

$$j_1 = \frac{1}{2}(J + \ell_1 - \ell_2), \quad j_2 = \frac{1}{2}(J + \ell_2 - \ell_1), \quad n = \ell_1 + \ell_2 - J. \quad (6.103)$$

To determine $N = N(\ell_1 + \ell_2 - J, \ell_1, \ell_2)$ we consider the scalar product $\langle J, J(\ell_1, \ell_2) | J, J(\ell_1, \ell_2) \rangle = 1$. Using (6.82) and (6.103) this can be written

$$1 = N^2 \langle \psi(j_1, j_2, n) | \psi(j_1, j_2, n) \rangle \quad (6.104)$$

where

$$|\psi(j_1, j_2, n)\rangle = (K^\dagger)^n |j_1, j_1\rangle_1 |j_2, j_2\rangle_2. \quad (6.105)$$

The first step of our calculation is the expansion of $\psi(j_1, j_2, n)$ in terms of states $|j'_1, m_1\rangle_1 |j'_2, m_2\rangle_2$. We employ the expression (6.57) for these states and the expression (6.70) for the operator K^\dagger . Accordingly, we obtain

$$\begin{aligned} |\psi(j_1, j_2, n)\rangle &= \frac{1}{\sqrt{(2j_1)!(2j_2)!}} \sum_s \binom{n}{s} (a_+^\dagger b_-^\dagger)^{n-s} (-1)^s (a_-^\dagger b_+^\dagger)^s \\ &\quad (a_+^\dagger)^{2j_1} (b_+^\dagger)^{2j_2} |\Psi_o\rangle = \\ &= \frac{n!}{\sqrt{(2j_1)!(2j_2)!}} \sum_s \frac{(-1)^s \sqrt{(2j_1+n-s)!s!(2j_2+s)!(n-s)!}}{s!(n-s)!} \\ &\quad \frac{(a_+^\dagger)^{2j_1-n-s} (a_-^\dagger)^s (b_+^\dagger)^{2j_2+s} (b_-^\dagger)^{n-s}}{\sqrt{(2j_1+n-s)!s!(2j_2+s)!(n-s)!}} |\Psi_o\rangle. \end{aligned} \quad (6.106)$$

The orthonormality of the states occurring in the last expression allows one to write (6.104)

$$\begin{aligned} 1 &= N^2 \frac{(n!)^2}{(2j_1)!(2j_2)!} \sum_s \frac{(2j_1+n-s)!(2j_2+s)!}{s!(n-s)!} \\ &= (n!)^2 \sum_s \binom{2j_1+n-s}{2j_1} \binom{2j_2+s}{2j_2} \end{aligned} \quad (6.107)$$

The latter sum can be evaluated using

$$\left(\frac{1}{1-\lambda}\right)^{n_1+m_1} = \sum_{m_1} \binom{n_1+m_1}{n_1} \lambda^{m_1} \quad (6.108)$$

a property which follows from

$$\frac{\partial}{\partial \lambda} \left(\frac{1}{1-\lambda}\right)^{n_1+1} \Big|_{\lambda=0} = \frac{(n_1+1)!}{n_1!} \quad (6.109)$$

and Taylor expansion of the left hand side of (6.108). One obtains then, applying (6.108) twice,

$$\left(\frac{1}{1-\lambda}\right)^{n_1+1} \left(\frac{1}{1-\lambda}\right)^{n_2+1} = \sum_{m_1, m_2} \binom{n_1+m_1}{n_1} \binom{n_2+m_2}{n_2} \lambda^{m_1+m_2} \quad (6.110)$$

which can be written

$$\left(\frac{1}{1-\lambda}\right)^{n_1+n_2+2} = \sum_r \left[\sum_s \binom{n_1+r-s}{n_1} \binom{n_2+s}{n_2} \right] \lambda^r \quad (6.111)$$

Comparison with (6.108) yields the identity

$$\sum_s \binom{n_1+r-s}{n_1} \binom{n_2+s}{n_2} = \binom{n_1+n_2+r+1}{n_1+n_2+1}. \quad (6.112)$$

Applying this to (6.107) yields

$$\begin{aligned} 1 &= N^2 (n!)^2 \binom{2j_1 + 2j_2 + n + 1}{2j_1 + 2j_2 + 1} \\ &= N^2 \frac{n!(2j_1 + 2j_2 + n + 1)!}{(2j_1 + 2j_2 + 1)!}. \end{aligned} \quad (6.113)$$

Using the identities (6.103) one obtains the desired result (6.83).

6.4 Symmetries of the Clebsch-Gordan Coefficients

The Clebsch-Gordan coefficients obey symmetry properties which reflect geometrical aspects of the operator relationship (6.11)

$$\vec{\mathbb{J}} = \vec{\mathcal{J}}^{(1)} + \vec{\mathcal{J}}^{(2)}. \quad (6.114)$$

For example, interchanging the operators $\vec{\mathcal{J}}^{(1)}$ and $\vec{\mathcal{J}}^{(2)}$ results in

$$\vec{\mathbb{J}} = \vec{\mathcal{J}}^{(2)} + \vec{\mathcal{J}}^{(1)}. \quad (6.115)$$

This relationship is a trivial consequence of (6.114) as long as $\vec{\mathbb{J}}$, $\vec{\mathcal{J}}^{(1)}$, and $\vec{\mathcal{J}}^{(2)}$ are vectors in \mathbb{R}^3 . For the quantum mechanical addition of angular momenta the Clebsch Gordan coefficients $(\ell_1, m_1, \ell_2, m_2 | J, M)$ corresponding to (6.114) show a simple relationship to the Clebsch Gordan coefficients $(\ell_2, m_2, \ell_1, m_1 | J, M)$ corresponding to (6.115), namely,

$$(\ell_1, m_1, \ell_2, m_2 | J, M) = (-1)^{\ell_1 + \ell_2 - J} (\ell_2, m_2, \ell_1, m_1 | J, M). \quad (6.116)$$

If one takes the negatives of the operators in (6.114) one obtains

$$\vec{\mathbb{J}} = -\vec{\mathcal{J}}^{(1)} - \vec{\mathcal{J}}^{(2)}. \quad (6.117)$$

The respective Clebsch-Gordan coefficients $(\ell_1, -m_1, \ell_2, -m_2 | J, -M)$ are again related in a simple manner to the coefficients $(\ell_1, m_1, \ell_2, m_2 | J, M)$

$$(\ell_1, m_1, \ell_2, m_2 | J, M) = (-1)^{\ell_1 + \ell_2 - J} (\ell_1, -m_1, \ell_2, -m_2 | J, -M). \quad (6.118)$$

Finally, one can interchange also the operator $\vec{\mathbb{J}}$ on the l.h.s. of (6.114) by, e.g., $\vec{\mathcal{J}}^{(1)}$ on the r.h.s. of this equation

$$\vec{\mathcal{J}}^{(1)} = \vec{\mathcal{J}}^{(2)} - \vec{\mathbb{J}}. \quad (6.119)$$

The corresponding symmetry property of the Clebsch-Gordan coefficients is

$$(\ell_1, m_1, \ell_2, m_2 | J, M) = (-1)^{\ell_2 + m_2} \sqrt{\frac{2J + 1}{2\ell_1 + 1}} (\ell_2, -m_2, J, M | \ell_1, m_1). \quad (6.120)$$

The symmetry properties (6.116), (6.118), and (6.120) can be readily derived from the expression (6.102) of the Clebsch-Gordan coefficients. We will demonstrate this now.

To derive relationship (6.116) one expresses the Clebsch-Gordan coefficient on the r.h.s. of (6.116) through formula (6.102) by replacing (ℓ_1, m_1) by (ℓ_2, m_2) and, vice versa, (ℓ_2, m_2) by (ℓ_1, m_1) , and

seeks then to relate the resulting expression to the original expression (6.102) to prove identity with the l.h.s. Inspecting (6.102) one recognizes that only the sum

$$S(\ell_1, m_1, \ell_2, m_2 | J, M) = \sum_s \frac{(-1)^s}{s!(\ell_1 - m_1 - s)!(\ell_2 + m_2 - s)!} \\ \times \frac{1}{(\ell_1 + \ell_2 - J - s)!(J - \ell_1 - m_2 + s)!(J - \ell_2 + m_1 + s)!} \quad (6.121)$$

is affected by the change of quantum numbers, the factor in front of S being symmetric in (ℓ_1, m_1) and (ℓ_2, m_2) . Correspondingly, (6.116) implies

$$S(\ell_1, m_1, \ell_2, m_2 | J, M) = (-1)^{\ell_1 + \ell_2 - J} S(\ell_2, m_2, \ell_1, m_1 | J, M). \quad (6.122)$$

To prove this we note that S on the r.h.s. reads, according to (6.121),

$$S(\ell_2, m_2, \ell_1, m_1 | J, M) = \sum_s \frac{(-1)^s}{s!(\ell_2 - m_2 - s)!(\ell_1 + m_1 - s)!} \\ \times \frac{1}{(\ell_1 + \ell_2 - J - s)!(J - \ell_2 - m_1 + s)!(J - \ell_1 + m_2 + s)!}. \quad (6.123)$$

Introducing the new summation index

$$s' = \ell_1 + \ell_2 - J - s \quad (6.124)$$

and using the equivalent relationships

$$s = \ell_1 + \ell_2 - J - s', \quad -s = J - \ell_1 - \ell_2 + s' \quad (6.125)$$

to express s in terms of s' in (6.123) one obtains

$$S(\ell_2, m_2, \ell_1, m_1 | J, M) = \sum_{s'} \frac{(-1)^{-s'}}{(\ell_1 + \ell_2 - J - s')!(J - \ell_1 - m_2 + s')!(J - \ell_2 + m_1 + s')!} \\ \times \frac{1}{s'!(\ell_1 - m_1 - s')!(\ell_2 + m_2 - s')!}. \quad (6.126)$$

Now it holds that $\ell_1 + \ell_2 - J$ in (6.124) is an integer, irrespective of the individual quantum numbers ℓ_1, ℓ_2, J being integer or half-integer. This fact can best be verified by showing that the construction of the eigenstates of $(\vec{J}^{(1)} + \vec{J}^{(2)})^2$ and $(\vec{J}^{(1)} + \vec{J}^{(2)})_3$ in Sect. 6.2 does, in fact, imply this property. Since also s in (6.102) and, hence, in (6.122) is an integer, one can state that s' , as defined in (6.124), is an integer and, accordingly, that

$$(-1)^{-s'} = (-1)^{s'} \quad (6.127)$$

holds in (6.126). Reordering the factorials in (6.126) to agree with the ordering in (6.121) leads one to conclude the property (6.122) and, hence, one has proven (6.116).

To prove (6.118) we note that in the expression (6.102) for the Clebsch-Gordan coefficients the prefactor of S , the latter defined in (6.121), is unaltered by the change $m_1, m_2, M \rightarrow -m_1, -m_2, -M$. Hence, (6.118) implies

$$S(\ell_1, m_1, \ell_2, m_2 | J, M) = (-1)^{\ell_1 + \ell_2 - J} S(\ell_1, -m_1, \ell_2, -m_2 | J, -M). \quad (6.128)$$

We note that according to (6.121) holds

$$\begin{aligned} S(\ell_1, -m_1, \ell_2, -m_2 | J, -M) &= \sum_s \frac{(-1)^s}{s!(\ell_1 + m_1 - s)!(\ell_2 - m_2 - s)!} \\ &\times \frac{1}{(\ell_1 + \ell_2 - J - s)!(J - \ell_1 + m_2 + s)!(J - \ell_2 - m_1 + s)!}. \end{aligned} \quad (6.129)$$

Introducing the new summation index s' as defined in (6.124) and using the relationships (6.125) to replace, in (6.129), s by s' one obtains

$$\begin{aligned} S(\ell_1, -m_1, \ell_2, -m_2 | J, -M) &= \\ &(-1)^{\ell_1 + \ell_2 - J} \sum_s \frac{(-1)^{-s'}}{(\ell_1 + \ell_2 - J - s')!(J - \ell_1 - m_1 + s')!(J - \ell_2 - m_2 + s')!} \\ &\times \frac{1}{s'!(\ell_2 + m_2 - s')!(\ell_1 - m_1 - s')!}. \end{aligned} \quad (6.130)$$

For reasons stated already above, (6.127) holds and after reordering of the factorials in (6.130) to agree with those in (6.121) one can conclude (6.128) and, hence, (6.118).

We want to prove finally the symmetry property (6.120). Following the strategy adopted in the proof of relationships (6.116) and (6.118) we note that in the expression (6.102) for the Clebsch-Gordan coefficients the prefactor of S , the latter defined in (6.121), is symmetric in the pairs of quantum numbers (ℓ_1, m_1) , (ℓ_2, m_2) and (J, M) , except for the factor $\sqrt{2J+1}$ which singles out J . However, in the relationship (6.120) this latter factor is already properly 'repaired' such that (6.120) implies

$$S(\ell_1, m_1, \ell_2, m_2 | J, M) = (-1)^{\ell_2 + m_2} S(\ell_2, -m_2, J, M | \ell_1, m_1). \quad (6.131)$$

According to (6.121) holds

$$\begin{aligned} S(\ell_2, -m_2, J, M | \ell_1, m_1) &= \sum_s \frac{(-1)^s}{s!(\ell_2 + m_2 - s)!(J + M - s)!} \\ &\times \frac{1}{(\ell_2 + J - \ell_1 - s)!(\ell_1 - \ell_2 - M + s)!(\ell_1 - J - m_2 + s)!}. \end{aligned} \quad (6.132)$$

Introducing the new summation index

$$s' = \ell_2 + m_2 - s \quad (6.133)$$

and, using the equivalent relationships

$$s = \ell_2 + m_2 - s', \quad -s = -\ell_2 - m_2 + s' \quad (6.134)$$

to replace s by s' in (6.132), one obtains

$$S(\ell_1, -m_1, \ell_2, -m_2 | J, -M) = (-1)^{\ell_2+m_2} \sum_s \frac{(-1)^{-s'}}{(\ell_2 + m_2 - s')! s'! (J - \ell_2 + m_1 + s')!} \times \frac{1}{(J - \ell_1 - m_2 + s')! (\ell_1 - m_1 - s')! (\ell_1 + \ell_2 - J - s')!}. \quad (6.135)$$

Again for the reasons stated above, (6.127) holds and after reordering of the factorials in (6.135) to agree with those in (6.121) one can conclude (6.131) and, hence, (6.120).

6.5 Example: Spin–Orbital Angular Momentum States

Relativistic quantum mechanics states that an electron moving in the Coulomb field of a nucleus experiences a coupling $\sim \vec{\mathcal{J}} \cdot \vec{S}$ between its angular momentum, described by the operator $\vec{\mathcal{J}}$ and wave functions $Y_{\ell m}(\hat{r})$, and its spin- $\frac{1}{2}$, described by the operator \vec{S} and wave function $\chi_{\frac{1}{2}\pm\frac{1}{2}}$. As a result, the eigenstates of the electron are given by the eigenstates of the total angular momentum-spin states

$$\mathcal{Y}_{jm}(\ell, \frac{1}{2} | \hat{r}) = \sum_{m', \sigma} (\ell, m', \frac{1}{2}, \sigma | j, m) Y_{\ell m'}(\hat{r}) \chi_{\frac{1}{2}\sigma} \quad (6.136)$$

which have been defined in (6.18). The states are simultaneous eigenstates of $(\mathcal{J}^{(tot)})^2$, $\mathcal{J}_3^{(tot)}$, \mathcal{J}^2 , and S^2 and, as we show below, also of the spin-orbit coupling term $\sim \vec{\mathcal{J}} \cdot \vec{S}$. Here $\mathcal{J}^{(tot)}$ is defined as

$$\vec{\mathcal{J}}^{(tot)} = \vec{\mathcal{J}} + \vec{S}. \quad (6.137)$$

Here we assume for \vec{S} the same units as for $\vec{\mathcal{J}}$, namely, \hbar , i.e., we define

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma} \quad (6.138)$$

rather than (5.223).

Two-Dimensional Vector Representation

One can consider the functions $\chi_{\frac{1}{2}\pm\frac{1}{2}}$ to be represented alternatively by the basis vectors of the space \mathbb{C}^k

$$\chi_{\frac{1}{2}\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{\frac{1}{2}-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (6.139)$$

The states $\mathcal{Y}_{jm}(\ell, \frac{1}{2} | \hat{r})$, accordingly, can then also be expressed as two-dimensional vectors. Using

$$m' = m - \sigma; \quad \sigma = \pm\frac{1}{2} \quad (6.140)$$

one obtains

$$\begin{aligned} \mathcal{Y}_{jm}(\ell, \frac{1}{2} | \hat{r}) &= (\ell, m - \frac{1}{2}, \frac{1}{2}, \frac{1}{2} | j, m) Y_{\ell m - \frac{1}{2}}(\hat{r}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &+ (\ell, m + \frac{1}{2}, -\frac{1}{2}, \frac{1}{2} | j, m) Y_{\ell m + \frac{1}{2}}(\hat{r}) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \quad (6.141)$$

or

$$\mathcal{Y}_{jm}(\ell, \frac{1}{2}|\hat{r}) = \begin{pmatrix} (\ell, m - \frac{1}{2}, \frac{1}{2}, \frac{1}{2}|j, m) Y_{\ell m - \frac{1}{2}}(\hat{r}) \\ (\ell, m + \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}|j, m) Y_{\ell m + \frac{1}{2}}(\hat{r}) \end{pmatrix}. \quad (6.142)$$

In this expression the quantum numbers (ℓ, m') of the angular momentum state are integers. According to (6.140), m is then half-integer and so must be j . The triangle inequalities (6.220) state in the present case $|\ell - \frac{1}{2}| \leq j \leq \ell + \frac{1}{2}$ and, therefore, we conclude $j = \ell \pm \frac{1}{2}$ or, equivalently, $\ell = j \pm \frac{1}{2}$. The different Clebsch-Gordon coefficients in (6.141) have the values

$$(j - \frac{1}{2}, m - \frac{1}{2}, \frac{1}{2}, \frac{1}{2}|j, m) = \sqrt{\frac{j+m}{2j}} \quad (6.143)$$

$$(j - \frac{1}{2}, m + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}|j, m) = \sqrt{\frac{j-m}{2j}} \quad (6.144)$$

$$(j + \frac{1}{2}, m - \frac{1}{2}, \frac{1}{2}, \frac{1}{2}|j, m) = -\sqrt{\frac{j-m+1}{2j+2}} \quad (6.145)$$

$$(j + \frac{1}{2}, m + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}|j, m) = \sqrt{\frac{j+m+1}{2j+2}} \quad (6.146)$$

which will be derived below (see pp. 170). Accordingly, the spin-orbital angular momentum states (6.141, 6.142) are

$$\mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}) = \begin{pmatrix} \sqrt{\frac{j+m}{2j}} Y_{j - \frac{1}{2} m - \frac{1}{2}}(\hat{r}) \\ \sqrt{\frac{j-m}{2j}} Y_{j - \frac{1}{2} m + \frac{1}{2}}(\hat{r}) \end{pmatrix} \quad (6.147)$$

$$\mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}) = \begin{pmatrix} -\sqrt{\frac{j-m+1}{2j+2}} Y_{j + \frac{1}{2} m - \frac{1}{2}}(\hat{r}) \\ \sqrt{\frac{j+m+1}{2j+2}} Y_{j + \frac{1}{2} m + \frac{1}{2}}(\hat{r}) \end{pmatrix}. \quad (6.148)$$

Eigenvalues

For the states (6.147, 6.148) holds

$$(\vec{\mathcal{J}} + \vec{S})^2 \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) = \hbar^2 j(j+1) \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) \quad (6.149)$$

$$(\vec{\mathcal{J}} + \vec{S})_3 \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) = \hbar m \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) \quad (6.150)$$

$$\mathcal{J}^2 \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) = \hbar^2 (j \mp \frac{1}{2})(j \mp \frac{1}{2} + 1) \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) \quad (6.151)$$

$$S^2 \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) = \frac{3}{4} \hbar^2 \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2}|\hat{r}) \quad (6.152)$$

Furthermore, using

$$(\mathcal{J}^{(tot)})^2 = (\vec{\mathcal{J}} + \vec{S})^2 = \mathcal{J}^2 + S^2 + 2\vec{\mathcal{J}} \cdot \vec{S} \quad (6.153)$$

or, equivalently,

$$2\vec{\mathcal{J}} \cdot \vec{S} = (\mathcal{J}^{(tot)})^2 - \mathcal{J}^2 - S^2 \quad (6.154)$$

one can readily show that the states $\mathcal{Y}_{jm}(\ell, \frac{1}{2}|\hat{r})$ are also eigenstates of $\vec{\mathcal{J}} \cdot \vec{S}$. Employing (6.149, 6.151, 6.152) one derives

$$\begin{aligned} 2\vec{\mathcal{J}} \cdot \vec{S} \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}) &= \hbar^2 [j(j+1) - (j - \frac{1}{2})(j + \frac{1}{2}) - \frac{3}{4}] \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}) \\ &= \hbar^2 (j - \frac{1}{2}) \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}) \end{aligned} \quad (6.155)$$

and

$$\begin{aligned} 2\vec{\mathcal{J}} \cdot \vec{S} \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}) &= \hbar^2 [j(j+1) - (j + \frac{1}{2})(j + \frac{3}{2}) - \frac{3}{4}] \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}) \\ &= \hbar^2 (-j - \frac{3}{2}) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}). \end{aligned} \quad (6.156)$$

Orthonormality Properties

The construction (6.141) in terms of Clebsch-Gordon coefficients produces normalized states. Since eigenstates of hermitean operators, i.e., of $(\vec{\mathcal{J}} + \vec{S})^2$, $(\vec{\mathcal{J}} + \vec{S})_3$, \mathcal{J}^2 with different eigenvalues are orthogonal, one can conclude the orthonormality property

$$\int_{-\pi}^{+\pi} \sin \theta d\theta \int_0^{2\pi} d\phi [\mathcal{Y}_{j'm'}^*(\ell', \frac{1}{2}|\theta, \phi)]^T \mathcal{Y}_{jm}^*(\ell, \frac{1}{2}|\theta, \phi) = \delta_{jj'} \delta_{mm'} \delta_{\ell\ell'} \quad (6.157)$$

where we have introduced the angular variables θ, ϕ to represent \hat{r} and used the notation $[\dots]^T$ to denote the transpose of the two-dimensional vectors $\mathcal{Y}_{j'm'}^*(\ell', \frac{1}{2}|\theta, \phi)$ which defines the scalar product

$$\begin{pmatrix} a^* \\ b^* \end{pmatrix}^T \begin{pmatrix} c \\ d \end{pmatrix} = (a^* \ b^*) \begin{pmatrix} c \\ d \end{pmatrix} = a^* c + b^* d. \quad (6.158)$$

The Operator $\vec{\sigma} \cdot \hat{r}$

Another important property of the spin-orbital angular momentum states (6.147, 6.148) concerns the effect of the operator $\vec{\sigma} \cdot \hat{r}$ on these states. In a representation defined by the states (6.139), this operator can be represented by a 2×2 matrix.

We want to show that the operator $\vec{\sigma} \cdot \hat{r}$ in the basis

$$\begin{aligned} \{(\mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}), \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}))\}, \\ j = \frac{1}{2}, \frac{3}{2} \dots ; m = -j, -j + 1, \dots + j \} \end{aligned} \quad (6.159)$$

assumes the block-diagonal form

$$\vec{\sigma} \cdot \hat{r} = \begin{pmatrix} 0 & -1 & & & \\ -1 & 0 & & & \\ & & 0 & -1 & \\ & & -1 & 0 & \\ & & & & \ddots \end{pmatrix} \quad (6.160)$$

where the blocks operate on two-dimensional subspaces spanned by $\{\mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}), \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r})\}$. We first demonstrate that $\vec{\sigma} \cdot \hat{r}$ is block-diagonal. This property follows from the commutation relationships

$$[\mathcal{J}_k^{(tot)}, \vec{\sigma} \cdot \hat{r}] = 0, \quad k = 1, 2, 3 \quad (6.161)$$

where \mathcal{J}_k^{tot} is defined in (6.137). To prove this we consider the case $k = 1$. For the l.h.s. of (6.161) holds, using (6.137),

$$\begin{aligned} & [\mathcal{J}_1 + S_1, \sigma_1 x_1 + \sigma_2 x_2 + \sigma_3 x_3] \\ &= \sigma_2 [\mathcal{J}_1, x_2] + [S_1, \sigma_2] x_2 + \sigma_3 [\mathcal{J}_1, x_3] + [S_1, \sigma_3] x_3. \end{aligned} \quad (6.162)$$

The commutation properties [cf. (5.53) for \mathcal{J}_1 and (5.228), (6.138) for $\vec{\sigma}$ and S_1]

$$[\mathcal{J}_1, x_2] = -i\hbar [x_2 \partial_3 - x_3 \partial_2, x_2] = i\hbar x_3 \quad (6.163)$$

$$[\mathcal{J}_1, x_3] = -i\hbar [x_2 \partial_3 - x_3 \partial_2, x_3] = -i\hbar x_2 \quad (6.164)$$

$$[S_1, \sigma_2] = \frac{\hbar}{2} [\sigma_1, \sigma_2] = i\hbar \sigma_3 \quad (6.165)$$

$$[S_1, \sigma_3] = \frac{\hbar}{2} [\sigma_1, \sigma_3] = -i\hbar \sigma_2 \quad (6.166)$$

allow one then to evaluate the commutator (6.161) for $k = 1$

$$[\mathcal{J}_1^{(tot)}, \vec{\sigma} \cdot \hat{r}] = i\hbar (\sigma_2 x_3 + \sigma_3 x_2 - \sigma_3 x_2 - \sigma_2 x_3) = 0. \quad (6.167)$$

One can carry out this algebra in a similar way for the $k = 2, 3$ and, hence, prove (6.161).

Since the differential operators in $\mathcal{J}_k^{(tot)}$ do not contain derivatives with respect to r , the property (6.161) applies also to $\vec{\sigma} \cdot \hat{r}$, i.e., it holds

$$[\mathcal{J}_k^{(tot)}, \vec{\sigma} \cdot \hat{r}] = 0, \quad k = 1, 2, 3. \quad (6.168)$$

From this follows

$$\begin{aligned} & (\mathcal{J}^{(tot)})^2 \vec{\sigma} \cdot \hat{r} \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r}) \\ &= \vec{\sigma} \cdot \hat{r} (\mathcal{J}^{(tot)})^2 \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r}) \\ &= \hbar^2 j(j+1) \vec{\sigma} \cdot \hat{r} \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r}), \end{aligned} \quad (6.169)$$

i.e., $\vec{\sigma} \cdot \hat{r} \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r})$ is an eigenstate of $(\mathcal{J}^{(tot)})^2$ with eigenvalue $\hbar^2 j(j+1)$. One can prove similarly that this state is also an eigenstate of $\mathcal{J}_3^{(tot)}$ with eigenvalue $\hbar m$. Since in the space spanned by the basis (6.159) only two states exist with such eigenvalues, namely, $\mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r})$, one can conclude

$$\vec{\sigma} \cdot \hat{r} \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}) = \alpha_{++}(jm) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}) + \alpha_{+-}(jm) \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}) \quad (6.170)$$

and, similarly,

$$\vec{\sigma} \cdot \hat{r} \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}) = \alpha_{-+}(jm) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r}) + \alpha_{--}(jm) \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r}). \quad (6.171)$$

We have denoted here that the expansion coefficients $\alpha_{\pm\pm}$, in principle, depend on j and m . We want to demonstrate now that the coefficients $\alpha_{\pm\pm}$, actually, do not depend on m . This property follows from

$$[\mathcal{J}_{\pm}^{(tot)}, \vec{\sigma} \cdot \hat{r}] = 0 \quad (6.172)$$

which is a consequence of (6.168) and the definition of $\mathcal{J}_{\pm}^{(tot)}$ [c.f. (6.35)]. We will, hence, use the notation $\alpha_{\pm\pm}(j)$

Exercise 6.5.1: Show that (6.172) implies that the coefficients $\alpha_{\pm\pm}$ in (6.170, 6.171) are independent of m .

We want to show now that the coefficients $\alpha_{++}(j)$ and $\alpha_{--}(j)$ in (6.170, 6.171) vanish. For this purpose we consider the parity of the operator $\vec{\sigma} \cdot \hat{r}$ and the parity of the states $\mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r})$, i.e., their property to change only by a factor ± 1 under spatial inversion. For $\vec{\sigma} \cdot \hat{r}$ holds

$$\vec{\sigma} \cdot \hat{r} \rightarrow \vec{\sigma} \cdot (-\hat{r}) = -\vec{\sigma} \cdot \hat{r}, \quad (6.173)$$

i.e., $\vec{\sigma} \cdot \hat{r}$ has odd parity. Replacing the \hat{r} -dependence by the corresponding (θ, ϕ) -dependence and noting the inversion symmetry of spherical harmonics [c.f. (5.166)]

$$Y_{j+\frac{1}{2}m\pm\frac{1}{2}}(\pi - \theta, \pi + \phi) = (-1)^{j+\frac{1}{2}} Y_{j+\frac{1}{2}m\pm\frac{1}{2}}(\theta, \phi) \quad (6.174)$$

one can conclude for $\mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r})$ as given by (6.142)

$$\mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\theta, \phi) \rightarrow \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\pi - \theta, \pi + \phi) = (-1)^{j+\frac{1}{2}} \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\theta, \phi). \quad (6.175)$$

Similarly follows for $\mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r})$

$$\mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\theta, \phi) \rightarrow (-1)^{j-\frac{1}{2}} \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\theta, \phi). \quad (6.176)$$

We note that $\mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2}|\hat{r})$ and $\mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2}|\hat{r})$ have opposite parity. Since $\vec{\sigma} \cdot \hat{r}$ has odd parity, i.e., when applied to the states $\mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r})$ changes their parity, we can conclude $\alpha_{++}(j) = \alpha_{--}(j) = 0$. The operator $\vec{\sigma} \cdot \hat{r}$ in the two-dimensional subspace spanned by $\mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2}|\hat{r})$ assumes then the form

$$\vec{\sigma} \cdot \hat{r} = \begin{pmatrix} 0 & \alpha_{+-}(j) \\ \alpha_{-+}(j) & 0 \end{pmatrix}. \quad (6.177)$$

Since $\vec{\sigma} \cdot \hat{r}$ must be a hermitean operator it must hold $\alpha_{-+}(j) = \alpha_{+-}^*(j)$.

According to (5.230) one obtains

$$(\vec{\sigma} \cdot \hat{r})^2 = \mathbb{1}. \quad (6.178)$$

This implies $|\alpha_{+-}(j)| = 1$ and, therefore, one can write

$$\vec{\sigma} \cdot \hat{r} = \begin{pmatrix} 0 & e^{i\beta(j)} \\ e^{-i\beta(j)} & 0 \end{pmatrix}, \quad \beta(j) \in \mathbb{R}. \quad (6.179)$$

One can demonstrate that $\vec{\sigma} \cdot \hat{r}$ is, in fact, a real operator. For this purpose one considers the operation of $\vec{\sigma} \cdot \hat{r}$ for the special case $\phi = 0$. According to the expressions (6.147, 6.148) for

$\mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \theta, \phi)$ and (5.174–5.177) one notes that for $\phi = 0$ the spin-angular momentum states are entirely real such that $\vec{\sigma} \cdot \hat{r}$ must be real as well. One can conclude then

$$\vec{\sigma} \cdot \hat{r} = \pm \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6.180)$$

where the sign could depend on j .

We want to demonstrate finally that the “–”-sign holds in (6.180). For this purpose we consider the application of $\vec{\sigma} \cdot \hat{r}$ in the case of $\theta = 0$. According to (5.180) and (6.147, 6.148) the particular states $\mathcal{Y}_{j\frac{1}{2}}(j - \frac{1}{2}, \frac{1}{2} | \hat{r})$ and $\mathcal{Y}_{j\frac{1}{2}}(j + \frac{1}{2}, \frac{1}{2} | \hat{r})$ at $\theta = 0$ are

$$\mathcal{Y}_{j\frac{1}{2}}(j - \frac{1}{2}, \frac{1}{2} | \theta = 0, \phi) = \begin{pmatrix} \sqrt{\frac{j+\frac{1}{2}}{4\pi}} \\ 0 \end{pmatrix} \quad (6.181)$$

$$\mathcal{Y}_{j\frac{1}{2}}(j + \frac{1}{2}, \frac{1}{2} | \theta = 0, \phi) = \begin{pmatrix} -\sqrt{\frac{j+\frac{1}{2}}{4\pi}} \\ 0 \end{pmatrix}. \quad (6.182)$$

Since $\vec{\sigma} \cdot \hat{r}$, given by

$$\vec{\sigma} \cdot \hat{r} = \sigma_1 \sin \theta \cos \phi + \sigma_2 \sin \theta \sin \phi + \sigma_3 \cos \theta, \quad (6.183)$$

in case $\theta = 0$ becomes in the standard representation with respect to the spin- $\frac{1}{2}$ states $\chi_{\frac{1}{2}\pm\frac{1}{2}}$ [c.f. (5.224)]

$$\vec{\sigma} \cdot \hat{r} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{\text{space } \chi_{\frac{1}{2}\pm\frac{1}{2}}}, \quad \text{for } \theta = 0 \quad (6.184)$$

one can conclude from (6.181, 6.182)

$$\vec{\sigma} \cdot \hat{r} \mathcal{Y}_{j\frac{1}{2}}(j - \frac{1}{2}, \frac{1}{2} | \theta = 0, \phi) = -\mathcal{Y}_{j\frac{1}{2}}(j + \frac{1}{2}, \frac{1}{2} | \theta = 0, \phi), \quad \text{for } \theta = 0. \quad (6.185)$$

We have, hence, identified the sign of (6.180) and, therefore, have proven (6.160). The result can also be stated in the compact form

$$\vec{\sigma} \cdot \hat{r} \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r}) = -\mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2} | \hat{r}) \quad (6.186)$$

The Operator $\vec{\sigma} \cdot \hat{p}$

The operator $\vec{\sigma} \cdot \hat{p}$ plays an important role in relativistic quantum mechanics. We want to determine its action on the wave functions $f(r) \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r})$. Noting that $\hat{p} = -i\hbar\nabla$ is a first order differential operator it holds

$$\vec{\sigma} \cdot \hat{p} f(r) \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r}) = ((\vec{\sigma} \cdot \hat{p} f(r))) \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r}) + f(r) \vec{\sigma} \cdot \hat{p} \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r}) \quad (6.187)$$

Here $((\dots))$ denotes again confinement of the diffusion operator ∂_r to within the double bracket. Since $f(r)$ is independent of θ and ϕ follows

$$((\vec{\sigma} \cdot \hat{p} f(r))) = -i\hbar((\partial_r f(r))) \vec{\sigma} \cdot \hat{r}. \quad (6.188)$$

Using (6.186) for both terms in (6.187) one obtains

$$\vec{\sigma} \cdot \hat{\vec{p}} f(r) \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r}) = \left[i\hbar \partial_r f(r) - f(r) \vec{\sigma} \cdot \hat{\vec{p}} \vec{\sigma} \cdot \hat{r} \right] \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2} | \hat{r}). \quad (6.189)$$

The celebrated property of the Pauli matrices (5.230) allows one to express

$$\vec{\sigma} \cdot \hat{\vec{p}} \vec{\sigma} \cdot \hat{r} = \hat{\vec{p}} \cdot \hat{r} + i \vec{\sigma} \cdot (\hat{\vec{p}} \times \hat{r}). \quad (6.190)$$

For the test function $h(\vec{r})$ holds

$$\begin{aligned} \hat{\vec{p}} \cdot \hat{r} h &= -i\hbar \nabla \cdot \left(\frac{\vec{r}}{r} h \right) = -i\hbar \frac{\hbar}{r} \nabla \cdot \vec{r} - i\hbar \vec{r} \cdot \nabla \frac{h}{r} \\ &= -i\hbar \frac{3}{r} h - i\hbar h \vec{r} \cdot \nabla \frac{1}{r} - i\hbar \hat{r} \cdot \nabla h. \end{aligned} \quad (6.191)$$

Using $\nabla(1/r) = -\vec{r}/r^3$ and $\hat{r} \cdot \nabla h = \partial_r h$ one can conclude

$$\hat{\vec{p}} \cdot \hat{r} h = -i\hbar \left(\frac{2}{r} + \partial_r \right) h \quad (6.192)$$

The operator $\hat{\vec{p}} \times \hat{r}$ in (6.190) can be related to the angular momentum operator. To demonstrate this we consider one of its cartesian components, e.g.,

$$\begin{aligned} (\hat{\vec{p}} \times \hat{r})_1 h &= -i\hbar (\partial_2 \frac{x_3}{r} - \partial_3 \frac{x_2}{r}) h \\ &= -i\hbar \frac{1}{r} (\partial_2 x_3 - \partial_3 x_2) h - i\hbar h (x_3 \partial_2 \frac{1}{r} - x_2 \partial_3 \frac{1}{r}). \end{aligned} \quad (6.193)$$

Using $\partial_2(1/r) = -x_2/r^3$, $\partial_3(1/r) = -x_3/r^3$ and $\partial_2 x_3 = x_3 \partial_2$, $\partial_3 x_2 = x_2 \partial_3$ we obtain

$$(\hat{\vec{p}} \times \hat{r})_1 h = -i\hbar \frac{1}{r} (x_3 \partial_2 - x_2 \partial_3) h = -\frac{1}{r} \mathcal{J}_1 h \quad (6.194)$$

where \mathcal{J}_1 is defined in (5.53). Corresponding results are obtained for the other components of $\hat{\vec{p}} \times \hat{r}$ and, hence, we conclude the intuitively expected identity

$$\hat{\vec{p}} \times \hat{r} = -\frac{1}{r} \vec{\mathcal{J}}. \quad (6.195)$$

Altogether we obtain, using $\partial_r \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r}) = 0$ and $\vec{\sigma} = 2\vec{S}/\hbar$,

$$\vec{\sigma} \cdot \hat{\vec{p}} f(r) \mathcal{Y}_{jm}(j \pm \frac{1}{2}, \frac{1}{2} | \hat{r}) = i \left[\hbar \partial_r + \frac{2\hbar}{r} + \frac{1}{r} \frac{\vec{\mathcal{J}} \cdot \vec{S}}{\hbar} \right] f(r) \mathcal{Y}_{jm}(j \mp \frac{1}{2}, \frac{1}{2} | \hat{r}) \quad (6.196)$$

Using (6.155, 6.156) this yields finally

$$\vec{\sigma} \cdot \hat{\vec{p}} f(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) = i\hbar \left[\partial_r + \frac{j + \frac{3}{2}}{r} \right] f(r) \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) \quad (6.197)$$

$$\vec{\sigma} \cdot \hat{\vec{p}} g(r) \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) = i\hbar \left[\partial_r + \frac{\frac{1}{2} - j}{r} \right] g(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) \quad (6.198)$$

To demonstrate the validity of this key result we note that according to (5.230, 5.99) holds

$$(\vec{\sigma} \cdot \hat{p})^2 = -\hbar^2 \nabla^2 = \frac{\hbar^2}{r} \frac{\partial^2}{\partial r^2} r + \frac{\mathcal{J}^2}{r^2}. \quad (6.199)$$

We want to show that eqs. (6.197, 6.198), in fact, are consistent with this identity. We note

$$\begin{aligned} & (\vec{\sigma} \cdot \hat{p})^2 f(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) \\ &= \hbar \vec{\sigma} \cdot \hat{p} [i\partial_r + \frac{i}{r}(j + \frac{3}{2})] f(r) \mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) \\ &= \hbar^2 [i\partial_r + \frac{i}{r}(\frac{1}{2} - j)] [i\partial_r + \frac{i}{r}(j + \frac{3}{2})] f(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) \\ &= \hbar^2 [-\partial_r^2 - \frac{2}{r}\partial_r + \frac{j + \frac{3}{2}}{r^2} - \frac{(\frac{1}{2} - j)(j + \frac{3}{2})}{r^2}] f(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) \\ &= \hbar^2 [-\partial_r^2 - \frac{2}{r}\partial_r + \frac{j^2 + 2j + \frac{3}{4}}{r^2}] f(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) \end{aligned} \quad (6.200)$$

and, using (5.101), $j^2 + 2j + \frac{3}{4} = (j + \frac{1}{2})(j + \frac{3}{2})$, as well as (6.151), i.e.,

$$\hbar^2 (j + \frac{1}{2})(j + \frac{3}{2}) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) = \mathcal{J}^2 \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) \quad (6.201)$$

yields

$$(\vec{\sigma} \cdot \hat{p})^2 f(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r}) = \left(\frac{\hbar^2}{r} \partial_r^2 r + \frac{\mathcal{J}^2}{r^2} \right) f(r) \mathcal{Y}_{jm}(j + \frac{1}{2}, \frac{1}{2} | \hat{r})$$

which agrees with (6.199).

Evaluation of Relevant Clebsch-Gordan Coefficients

We want to determine now the Clebsch-Gordan coefficients (6.143–6.146). For this purpose we use the construction method introduced in Sec. 6.2. We begin with the coefficients (6.143, 6.144) and, adopting the method in Sec. 6.2, consider first the case of the largest m -value $m = j$. In this case holds, according to (6.43),

$$\mathcal{Y}_{jj}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) = Y_{j-\frac{1}{2}j-\frac{1}{2}}(\hat{r}) \chi_{\frac{1}{2}\frac{1}{2}}. \quad (6.202)$$

The Clebsch-Gordan coefficients are then

$$(j - \frac{1}{2}, j - \frac{1}{2}, \frac{1}{2}, \frac{1}{2} | j, j) = 1 \quad (6.203)$$

$$(j - \frac{1}{2}, j + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} | j, j) = 0 \quad (6.204)$$

$$(6.205)$$

which agrees with the expressions (6.143, 6.144) for $m = j$.

For $m = j - 1$ one can state, according to (6.45),

$$\mathcal{Y}_{jj-1}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) = \sqrt{\frac{2j-1}{2j}} Y_{j-\frac{1}{2}j-\frac{3}{2}} \chi_{\frac{1}{2}\frac{1}{2}} + \sqrt{\frac{1}{2j}} Y_{j-\frac{1}{2}j-\frac{1}{2}} \chi_{\frac{1}{2}-\frac{1}{2}} \quad (6.206)$$

The corresponding Clebsch-Gordan coefficients are then

$$(j - \frac{1}{2}, j - \frac{3}{2}, \frac{1}{2}, \frac{1}{2} | j, j - 1) = \sqrt{\frac{2j - 1}{2j}} \quad (6.207)$$

$$(j - \frac{1}{2}, j - \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} | j, j - 1) = \sqrt{\frac{1}{2j}} \quad (6.208)$$

$$(6.209)$$

which again agrees with the expressions (6.143, 6.144) for $m = j - 1$.

Expression (6.206), as described in Sec. 6.2, is obtained by applying the operator [c.f. (6.137)]

$$\mathcal{J}_-^{(tot)} = \mathcal{J}_- + S_- \quad (6.210)$$

to (6.202). The further Clebsch-Gordan coefficients $(\dots | jj - 2), (\dots | jj - 3)$, etc., are obtained by iterating the application of (6.210). Let us verify then the expression (6.143, 6.144) for the Clebsch-Gordan coefficients by induction. (6.143, 6.144) implies for $j = m$

$$\mathcal{Y}_{jm}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) = \sqrt{\frac{j + m}{2j}} Y_{j - \frac{1}{2}m - \frac{1}{2}} \chi_{\frac{1}{2}\frac{1}{2}} + \sqrt{\frac{j - m}{2j}} Y_{j - \frac{1}{2}m + \frac{1}{2}} \chi_{\frac{1}{2} - \frac{1}{2}}. \quad (6.211)$$

Applying $\mathcal{J}_-^{(tot)}$ to the l.h.s. and $\mathcal{J}_- + S_-$ to the r.h.s. [c.f. (6.210)] yields

$$\begin{aligned} \sqrt{(j + m)(j - m + 1)} \mathcal{Y}_{jm-1}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) = & \\ & \sqrt{\frac{j + m}{2j}} \sqrt{(j + m - 1)(j - m + 1)} Y_{j - \frac{1}{2}m - \frac{3}{2}} \chi_{\frac{1}{2}\frac{1}{2}} \\ & + \sqrt{\frac{j + m}{2j}} Y_{j - \frac{1}{2}m - \frac{1}{2}} \chi_{\frac{1}{2} - \frac{1}{2}} \\ & + \sqrt{\frac{j - m}{2j}} \sqrt{(j + m)(j - m)} Y_{j - \frac{1}{2}m - \frac{1}{2}} \chi_{\frac{1}{2} - \frac{1}{2}} \end{aligned}$$

or

$$\begin{aligned} \mathcal{Y}_{jm-1}(j - \frac{1}{2}, \frac{1}{2} | \hat{r}) = & \\ & \sqrt{\frac{j + m - 1}{2j}} Y_{j - \frac{1}{2}m - \frac{3}{2}} \chi_{\frac{1}{2}\frac{1}{2}} + \\ & \left((j - m) \sqrt{\frac{1}{2j(j - m + 1)}} + \sqrt{\frac{1}{2j(j - m + 1)}} \right) Y_{j - \frac{1}{2}m - \frac{1}{2}} \chi_{\frac{1}{2} - \frac{1}{2}} \\ = & \sqrt{\frac{j + m - 1}{2j}} Y_{j - \frac{1}{2}m - \frac{3}{2}} \chi_{\frac{1}{2}\frac{1}{2}} + \sqrt{\frac{j - m + 1}{2j}} Y_{j - \frac{1}{2}m - \frac{1}{2}} \chi_{\frac{1}{2} - \frac{1}{2}}. \end{aligned}$$

This implies

$$(j - \frac{1}{2}, m - \frac{3}{2}, \frac{1}{2}, \frac{1}{2} | j, m - 1) = \sqrt{\frac{j + m - 1}{2j}} \quad (6.212)$$

$$(j - \frac{1}{2}, m - \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} | j, m - 1) = \sqrt{\frac{j - m + 1}{2j}} \quad (6.213)$$

which is in agreement with (6.143, 6.144) for $j = m - 1$. We have, hence, proven (6.143, 6.144) by induction.

The Clebsch-Gordan coefficients (6.146) can be obtained from (6.143) by applying the symmetry relationships (6.116, 6.120). The latter relationships applied together read

$$\begin{aligned} (\ell_1, m_1, \ell_2, m_2 | \ell_3, m_3) &= (-1)^{\ell_2 + \ell_3 - \ell_1 + \ell_2 + m_2} \times \\ &\times \sqrt{\frac{2\ell_3 + 1}{2\ell_1 + 1}} (\ell_3, m_3, \ell_2, -m_2 | \ell_1, m_1) \end{aligned} \quad (6.214)$$

For

$$(j, m, \frac{1}{2}, \frac{1}{2} | j + \frac{1}{2}, m + \frac{1}{2}) = \sqrt{\frac{j + m + 1}{2j + 1}}, \quad (6.215)$$

which follows from (6.143), the relationship (6.214) yields

$$(j, m, \frac{1}{2}, \frac{1}{2} | j + \frac{1}{2}, m + \frac{1}{2}) = \sqrt{\frac{2j + 2}{2j + 1}} (j + \frac{1}{2}, m + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} | j, m) \quad (6.216)$$

and, using (6.215), one obtains

$$(j + \frac{1}{2}, m + \frac{1}{2}, \frac{1}{2}, -\frac{1}{2} | j, m) = \sqrt{\frac{j + m + 1}{2j + 2}}. \quad (6.217)$$

Similarly, one can obtain expression (6.144) from (6.144).

6.6 The $3j$ -Coefficients

The *Clebsch-Gordan coefficients* describe the quantum mechanical equivalent of the addition of two classical angular momentum vectors $\vec{J}_{\text{class}}^{(1)}$ and $\vec{J}_{\text{class}}^{(2)}$ to obtain the total angular momentum vector $\vec{J}_{\text{class}}^{(\text{tot})} = \vec{J}_{\text{class}}^{(1)} + \vec{J}_{\text{class}}^{(2)}$. In this context $\vec{J}_{\text{class}}^{(1)}$ and $\vec{J}_{\text{class}}^{(2)}$ play the same role, leading quantum mechanically to a symmetry of the *Clebsch-Gordan coefficients* ($JM | \ell_1 m_1 \ell_2 m_2$) with respect to exchange of $\ell_1 m_1$ and $\ell_2 m_2$. However, a higher degree of symmetry is obtained if one rather considers classically to obtain a vector $\vec{J}_{\text{class}}^{(-\text{tot})}$ with the property $\vec{J}_{\text{class}}^{(1)} + \vec{J}_{\text{class}}^{(2)} + \vec{J}_{\text{class}}^{(-\text{tot})} = 0$. Obviously, all three vectors $\vec{J}_{\text{class}}^{(1)}$, $\vec{J}_{\text{class}}^{(2)}$ and $\vec{J}_{\text{class}}^{(-\text{tot})}$ play equivalent roles.

The coefficients which are the quantum mechanical equivalent to $\vec{J}_{\text{class}}^{(1)} + \vec{J}_{\text{class}}^{(2)} + \vec{J}_{\text{class}}^{(-\text{tot})} = 0$ are the $3j$ -coefficients introduced by Wigner. They are related in a simple manner to the *Clebsch-Gordan coefficients*

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1 - j_2 + m_3} (2j_3 + 1)^{-\frac{1}{2}} (j_3 - m_3 | j_1 m_1, j_2 m_2) \quad (6.218)$$

where we have replaced the quantum numbers $J, M, \ell_1, m_1, \ell_2, m_2$ by the set $j_1, m_1, j_2, m_2, j_3, m_3$ to reflect in the notation the symmetry of these quantities.

We first like to point out that conditions (6.21, 6.34) imply

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0 \text{ if not } m_1 + m_2 + m_3 = 0 \quad (6.219)$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0 \text{ if not } |j_1 - j_2| \leq j_3 \leq j_1 + j_2. \quad (6.220)$$

The latter condition $|j_1 - j_2| \leq j_3 \leq j_1 + j_2$, the so-called triangle condition, states that j_1, j_2, j_3 form the sides of a triangle and the condition is symmetric in the three quantum numbers.

According to the definition of the $3j$ -coefficients one would expect symmetry properties with respect to exchange of j_1, m_1 , j_2, m_2 and j_3, m_3 and with respect to sign reversals of all three values m_1, m_2, m_3 , i.e. with respect to altogether 12 symmetry operations. These symmetries follow the equations

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} \\ &= (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \end{aligned} \quad (6.221)$$

where the results of a cyclic, anti-cyclic exchange and of a sign reversal are stated. In this way the values of 12 $3j$ -coefficients are related.

However, there exist even further symmetry properties, discovered by Regge, for which no known classical analogue exists. To represent the full symmetry one expresses the $3j$ -coefficients through a 3×3 -matrix, the Regge-symbol, as follows

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{bmatrix} -j_1 + j_2 + j_3 & j_1 - j_2 + j_3 & j_1 + j_2 - j_3 \\ j_1 - m_1 & j_2 - m_2 & j_3 - m_3 \\ j_1 + m_1 & j_2 + m_2 & j_3 + m_3 \end{bmatrix}. \quad (6.222)$$

The Regge symbol vanishes, except when all elements are non-negative integers and each row and column has the same integer value $\Sigma = j_1 + j_2 + j_3$. The Regge symbol also vanishes in case that two rows or columns are identical and Σ is an odd integer. The Regge symbol reflects a remarkable degree of symmetry of the related $3j$ -coefficients: One can exchange rows, one can exchange columns and one can reflect at the diagonal (transposition). In case of a non-cyclic exchange of rows and columns the $3j$ -coefficient assumes a prefactor $(-1)^\Sigma$. These symmetry operations relate altogether 72 $3j$ -coefficients.

The reader may note that the entries of the Regge-symbol, e.g., $-j_1 + j_2 + j_3$, are identical to the integer arguments which enter the analytical expression (6.102) of the Clebsch-Gordan coefficients, safe for the prefactor $\sqrt{2j_3 + 1}$ which is cancelled according to the definition (6.218) relating $3j$ -coefficients and Clebsch-Gordan coefficients. The two integer entries $J - \ell_1 - m_2$ and $J - \ell_2 + m_1$ in (6.102) are obtained each through the difference of two entries of the Regge-symbol.

Because of its high degree of symmetry the Regge symbol is very suited for numerical evaluations of the $3j$ -coefficients. For this purpose one can use the symmetry transformations to place the smallest element into the upper left corner of the Regge symbol. Assuming this placement the Regge symbol can be determined as follows (n_{11} is the smallest element!)

$$\begin{bmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{bmatrix} = (-1)^{n_{23}+n_{32}} \sqrt{\frac{n_{12}!n_{13}!n_{21}!n_{31}!}{(\Sigma + 1)!n_{11}!n_{22}!n_{33}!n_{23}!n_{32}!}} \sum_{n=0}^{n_{11}} s_n \quad (6.223)$$

where

$$\Sigma = n_{11} + n_{12} + n_{13} = j_1 + j_2 + j_3 \quad (6.224)$$

$$s_0 = \frac{n_{23}!}{(n_{23}-n_{11})!} \frac{n_{32}!}{(n_{32}-n_{11})!} \quad (6.225)$$

$$s_n = -\frac{(n_{11}+1-n)(n_{22}+1-n)(n_{33}+1-n)}{n(n_{23}-n_{11}+n)(n_{32}-n_{11}+n)} s_{n-1} . \quad (6.226)$$

We like to state finally a few explicit analytical expressions for *Clebsch-Gordan coefficients* which were actually obtained using (6.223-6.226) by means of a symbolic manipulation package (Mathematica)

$$(1m|2m_1 1m_2) = \frac{(-1)^{1+m+m_1} \delta(m, m_1 + m_2) \sqrt{(2-m_1)!} \sqrt{(2+m_1)!}}{\sqrt{10} \sqrt{(1-m)!} \sqrt{(1+m)!} \sqrt{(1-m_2)!} \sqrt{(1+m_2)!}} \\ 1 \geq |m| \wedge 1 \geq |m_2| \wedge 2 \geq |m_1| \quad (6.227)$$

$$(2m|2m_1 1m_2) = \frac{(-1)^{m+m_1} (m+2m_2) \delta(m, m_1 + m_2) \sqrt{(2-m_1)!} (2+m_1)!}{\sqrt{6} \sqrt{(2-m)!} \sqrt{(2+m)!} \sqrt{(1-m_2)!} \sqrt{(1+m_2)!}} \\ 1 \geq |m_2| \wedge 2 \geq |m| \wedge 2 \geq |m_1| \quad (6.228)$$

$$(3m|2m_1 1m_2) = \frac{(-1)^{2m_1-2m_2} \sqrt{7} \delta(m, m_1 + m_2) \sqrt{(3-m)!} \sqrt{(3+m)!}}{\sqrt{105} \sqrt{(2-m)!} \sqrt{(2+m)!} \sqrt{(1-m_2)!} \sqrt{(1+m_2)!}} \\ 1 \geq |m_2| \wedge 2 \geq |m_1| \wedge 3 \geq |m| \quad (6.229)$$

$$(0m|\frac{1}{2}m_1 \frac{1}{2}m_2) = \frac{i(-1)^{1-m_2} \delta(0, m) \delta(-m_1, m_2)}{\sqrt{2}} \\ \frac{1}{2} \geq |m_1| \quad (6.230)$$

$$(1m|\frac{1}{2}m_1 \frac{1}{2}m_2) = \frac{(-1)^{2m_1-2m_2} \sqrt{3} \delta(m, m_1 + m_2) \sqrt{(1-m)!} \sqrt{(1+m)!}}{\sqrt{6} \sqrt{(\frac{1}{2}-m_1)!} \sqrt{(\frac{1}{2}+m_1)!} \sqrt{(\frac{1}{2}-m_2)!} \sqrt{(\frac{1}{2}+m_2)!}} \\ \frac{1}{2} \geq |m_1| \wedge \frac{1}{2} \geq |m_2| \wedge 1 \geq |m| \quad (6.231)$$

Here is an explicit value of a Clebsch-Gordan coefficient:

$$(70\frac{1}{2} - 15\frac{1}{2} | 120 - 10 \ 60\frac{1}{2} - 5\frac{1}{2}) = \\ \frac{4793185293503147294940209340 \sqrt{127} \sqrt{142}}{\sqrt{35834261990081573635135027068718971996984731222241334046198355}} \\ \simeq 0.10752786393409395427444450130056540562826159542886 \quad (6.232)$$

We also illustrate the numerical values of a sequence of 3j-coefficients in Figure 6.1.

For the basis $\{\mathfrak{Y}_{JM}(\ell_1, \ell_2 | \Omega_1, \Omega_2), \ell_1, \ell_2 = 1, 2, \dots, J = |\ell_1 - \ell_2|, \dots, \ell_1 + \ell_2, M = -J, \dots, J\}$ each of the blocks in (6.233) is further block-diagonalized as follows

$$\begin{array}{c}
 \boxed{\begin{array}{c} (2\ell_1 + 1) \quad (2\ell_1 + 1) \\ (2\ell_2 + 1) \times (2\ell_2 + 1) \end{array}} = \\
 \\
 \boxed{\begin{array}{c} (2|\ell_1 - \ell_2| + 1) \\ \times (2|\ell_1 - \ell_2| + 1) \end{array}} \\
 \\
 \boxed{\begin{array}{c} (2|\ell_1 - \ell_2| + 3) \\ \times (2|\ell_1 - \ell_2| + 3) \end{array}} \\
 \dots \\
 \boxed{\begin{array}{c} (2(\ell_1 + \ell_2) + 1) \\ \times (2(\ell_1 + \ell_2) + 1) \end{array}}
 \end{array} \tag{6.234}$$

Partitioning in smaller blocks is not possible.

Exercise 6.6.1: Prove Eqs. (6.233, 6.234)

Exercise 6.6.2: How many overall singlet states can be constructed from four spin- $\frac{1}{2}$ states $|\frac{1}{2}m_1\rangle_{(1)}|\frac{1}{2}m_2\rangle_{(2)}|\frac{1}{2}m_3\rangle_{(3)}|\frac{1}{2}m_4\rangle_{(4)}$? Construct these singlet states in terms of the product wave functions above.

Exercise 6.6.3: Two triplet states $|1m_1\rangle_{(1)}|1m_2\rangle_{(2)}$ are coupled to an overall singlet state $\mathfrak{Y}_{00}(1, 1)$. Show that the probability of detecting a triplet substate $|1m_1\rangle_{(1)}$ for arbitrary polarization (m_2 -value) of the other triplet is $\frac{1}{3}$.

6.7 Tensor Operators and Wigner-Eckart Theorem

In this Section we want to discuss operators which have the property that they impart angular momentum and spin properties onto a quantum state. Such operators T can be characterized through their behaviour under rotational transformations.

Let $T|\psi\rangle$ denote the state obtained after the operator T has been applied and let $\mathcal{R}(\vec{\vartheta})$ denote a rotation in the representation of $\text{SO}(3)$ or $\text{SU}(2)$ which describes rotational transformations of the quantum states under consideration, e.g. the operator (5.42) in case (i) of the position representation of single particle wave functions or the operator (5.222) in case (ii) of single particle spin operators. Note that in the examples mentioned the operator T would be defined within the same representation as $\mathcal{R}(\vec{\vartheta})$. This implies, for example, that in

case (i) T is an operator $\mathbb{C}_\infty(\mathbb{K}) \rightarrow \mathbb{C}_\infty(\mathbb{K})$ acting on single particle wave functions, e.g. a multiplicative operator $T\psi(\vec{r}) = f(\vec{r})\psi(\vec{r})$ or a differential operator $T\psi(\vec{r}) = \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right)\psi(\vec{r})$;

case (ii) the operator T could be a spin operator S_k defined in (5.223), e.g. $S^2 = S_1^2 + S_2^2 + S_3^2$ or any other polynomial of S_k .

The operator T may also act on multi-particle states like $Y_{\ell_1 m_1}(\hat{r}_1)Y_{\ell_2 m_2}(\hat{r}_2)$. In fact, some of the examples considered below involve tensor operators T of this type.

Rotations transform $|\psi\rangle$ as $|\psi'\rangle = \mathcal{R}(\vec{\vartheta})|\psi\rangle$ and $T|\psi\rangle$ as $\mathcal{R}(\vec{\vartheta})T|\psi\rangle$. The latter can be written $T'|\psi'\rangle$ where T' denotes T in the rotated frame given by

$$T' = \mathcal{R}(\vec{\vartheta})T\mathcal{R}^{-1}(\vec{\vartheta}) \quad . \quad (6.235)$$

The property that T imparts onto states $|\psi\rangle$ angular momentum or spin corresponds to T behaving as an angular momentum or spin state multiplying $|\psi\rangle$. The latter implies that T transforms like an angular momentum or spin state $|k m\rangle$, i.e. that T belongs to a family of operators $\{T_{kq}, q = -k, -k+1, \dots, k\}$ such that

$$T'_{kq} = \sum_{q'=-k}^k \mathcal{D}_{q'q}^{(k)}(\vec{\vartheta}) T_{kq'} \quad . \quad (6.236)$$

In this equation $\mathcal{D}_{q'q}^{(k)}(\vec{\vartheta})$ denotes the rotation matrix

$$\mathcal{D}_{q'q}^{(k)}(\vec{\vartheta}) = \langle kq' | \mathcal{R}(\vec{\vartheta}) | kq \rangle \quad . \quad (6.237)$$

The operators $T \in \{T_{kq}, q = -k, -k+1, \dots, k\}$ with the transformation property (6.236, 6.237) are called *tensor operators of rank k*.

Examples of Tensor Operators

The multiplicative operators $\mathbb{C}_\infty(\mathbb{K}) \rightarrow \mathbb{C}_\infty(\mathbb{K})$

$$\mathbb{Y}_{\Gamma_{II}}(\vec{\omega}) \stackrel{\text{def}}{=} \sqrt{\frac{2}{\Gamma_{II}}} \mathbb{Y}_{\Gamma_{II}}(\vec{\omega}) \quad (6.238)$$

are tensor operators of rank k . Examples are

$$\begin{aligned}
 Y_{00} &= \frac{1}{\sqrt{4\pi}} \\
 Y_{1\pm 1} &= \mp \sqrt{\frac{3}{8\pi}} r \sin\theta e^{\pm i\phi} = \mp \sqrt{\frac{3}{8\pi}} (x_1 \pm ix_2) \\
 Y_{10} &= \sqrt{\frac{3}{4\pi}} r \cos\theta = \sqrt{\frac{3}{4\pi}} x_3 \\
 Y_{2\pm 2} &= \frac{1}{4} \sqrt{\frac{15}{2\pi}} r^2 \sin^2\theta e^{\pm 2i\phi} = \frac{1}{4} \sqrt{\frac{15}{2\pi}} (x_1 \pm ix_2)^2 \\
 Y_{2\pm 1} &= \mp \sqrt{\frac{15}{8\pi}} r^2 \sin\theta e^{\pm i\phi} = \mp \sqrt{\frac{15}{8\pi}} (x_1 \pm ix_2) x_3 \\
 Y_{20} &= \sqrt{\frac{5}{4\pi}} r^2 \left(\frac{3}{2} \cos^2\theta - \frac{1}{2} \right) = \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} x_3^2 - \frac{r^2}{2} \right)
 \end{aligned} \tag{6.239}$$

These operators can be expressed in terms of the coordinates x_1, x_2, x_3 . The fact that these operators form tensor operators of rank 1, 2, 3 follows from the transformation properties of the spherical harmonics derived in Section 1.3.

Exercise 6.7.1: Show that the following set of spin operators

$$\begin{aligned}
 T_{00} &= 1 \\
 T_{1\pm 1} &= \mp \frac{1}{\sqrt{2}} S_{\pm} \\
 T_{10} &= S_3 \\
 T_{2\pm 2} &= (S^{\pm})^2 \\
 T_{2\pm 1} &= \mp (S_3 S^{\pm} + S^{\pm} S_3) \\
 T_{20} &= \sqrt{\frac{2}{3}} (3S_3^2 - S^2)
 \end{aligned}$$

are tensor operators of rank 0, 1, 2.

Exercise 6.7.2: Express the transformed versions of the following operators (a) $T = x_1^2 - x_2^2$ and (b) $S_2 S_3$ in terms of Wigner rotation matrices and untransformed operators.

For the following it is important to note that the rotation matrix elements (6.237) do not require that the rotation $\mathcal{R}^{-1}(\vec{\vartheta})$ is expressed in terms of Euler angles according to (5.203), but rather any rotation and any parametrization can be assumed. In fact, we will assume presently that the rotation is chosen as follows

$$\mathcal{R}(\vec{\vartheta}) = \exp(\vartheta_+ L_+ + \vartheta_- L_- + \vartheta_3 L_3) \tag{6.240}$$

where we have defined $\vartheta_{\pm} = \frac{1}{2}(\vartheta_1 \mp i\vartheta_2)$ and $L_{\pm} = L_1 \pm iL_2$. This choice of parametrization allows us to derive conditions which are equivalent to the property (6.235 - 6.237), but are far easier to ascertain for any particular operator.

The conditions can be derived if we consider the property (6.235 - 6.237) for transformations characterized by infinitesimal values of $\vartheta_+, \vartheta_-, \vartheta_3$. We first consider a rotation with $\vec{\vartheta} = (\vartheta_+, 0, 0)^T$ in case of small ϑ_+ . The property (6.235 - 6.237) yields first

$$\mathcal{R}(\vec{\vartheta}) T_{kq} \mathcal{R}^{-1}(\vec{\vartheta}) = \sum_{q'=-k}^k \langle kq' | \mathcal{R}(\vec{\vartheta}) | kq \rangle T_{kq'}. \quad (6.241)$$

Using $\mathcal{R}(\vec{\vartheta}) = \mathbb{1} + \vartheta_+ L_+ + O(\vartheta_+^2)$ this equation can be rewritten neglecting terms of order $O(\vartheta_+^2)$

$$(\mathbb{1} + \vartheta_+ L_+) T_{kq} (\mathbb{1} - \vartheta_+ L_+) = \sum_{q'=-k}^k \langle kq' | \mathbb{1} + \vartheta_+ L_+ | kq \rangle T_{kq'}. \quad (6.242)$$

from which follows by means of $\langle kq' | \mathbb{1} | kq \rangle = \delta_{qq'}$ and by subtracting T_{kq} on both sides of the equation

$$\vartheta_+ [L_+, T_{kq}] = \sum_{q'=-k}^k \vartheta_+ \langle kq' | L_+ | kq \rangle T_{kq'}. \quad (6.243)$$

From (5.80) follows $\langle kq' | L_+ | kq \rangle = -i\sqrt{(k+q+1)(k-q)}\delta_{q'q+1}$ and, hence,

$$[L_+, T_{kq}] = -iT_{kq+1} \sqrt{(k+q+1)(k-q)}. \quad (6.244)$$

Similar equations can be derived for infinitesimal rotations of the form $\vec{\vartheta} = (0, \vartheta_-, 0)^T, (0, 0, \vartheta_3)^T$. Expressing the results in terms of the angular momentum operators J_+, J_-, J_3 yields

$$[J_+, T_{kq}] = \hbar T_{kq+1} \sqrt{(k+q+1)(k-q)} \quad (6.245)$$

$$[J_-, T_{kq}] = \hbar T_{kq-1} \sqrt{(k+q)(k-q+1)} \quad (6.246)$$

$$[J_3, T_{kq}] = \hbar q T_{kq}. \quad (6.247)$$

These properties often can be readily demonstrated for operators and the transformation properties (6.235 - 6.237) be assumed then.

Exercise 6.7.3: Derive Eqs. (6.246, 6.247).

Exercise 6.7.4: Is the 1-particle Hamiltonian

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(|\vec{r}|) \quad (6.248)$$

a tensor operator?

Exercise 6.7.5: Consider a system of two spin- $\frac{1}{2}$ particles for which the first spin is described by the operator $\vec{S}^{(1)}$ and the second spin by the operator $\vec{S}^{(2)}$. Show that $\vec{S}^{(1)} \cdot \vec{S}^{(2)}$ is a tensor operator of rank 0 in the space of the products of the corresponding spin states $|\frac{1}{2}m_1\rangle_{(1)}|\frac{1}{2}m_2\rangle_{(2)}$. For this purpose state first the proper rotation operator $\mathcal{R}(\vec{\vartheta})$ and note then that $\vec{S}^{(1)} \cdot \vec{S}^{(2)}$ commutes with the generators of the rotation of $|\frac{1}{2}m_1\rangle_{(1)}|\frac{1}{2}m_2\rangle_{(2)}$.

Exercise 6.7.6: Form tensor operators of rank 1 in terms of the three components of ∇ acting on the space of 1-particle wave functions.

6.8 Wigner-Eckart Theorem

A second important property of tensor operators T_{kq} beside (6.235 - 6.237) is that their matrix elements $\langle \ell_1 m_1 \gamma_1 | T_{kq} | \ell_2 m_2 \gamma_2 \rangle$ obey simple relationships expressed in terms of Clebsch-Gordan coefficients. $|\ell_1 m_1 \gamma_1\rangle$ denotes an angular momentum (spin) state, possibly the total angular momentum-spin state of a composite system, which is characterized also by a set of other quantum numbers γ_1 which are not affected by the rotational transformation $\mathcal{R}(\vec{\vartheta})$. The relationships among the matrix elements $\langle \ell_1 m_1 \gamma_1 | T_{kq} | \ell_2 m_2 \gamma_2 \rangle$ are stated by the Wigner-Eckart theorem which we will derive now. Starting point of the derivation is the fact that the states $T_{kq} | \ell_2 m_2 \gamma_2 \rangle$ behave like angular momentum states of a composite system of two particles each carrying angular momentum or spin, i.e. behave like $|kq\rangle | \ell_1 m_1 \rangle$. To prove this we consider the transformation of $T_{kq} | \ell_2 m_2 \gamma_2 \rangle$

$$\begin{aligned} \mathcal{R}(\vec{\vartheta}) T_{kq} | \ell_2 m_2 \gamma_2 \rangle &= \mathcal{R}(\vec{\vartheta}) T_{kq} \mathcal{R}^{-1}(\vec{\vartheta}) \mathcal{R}(\vec{\vartheta}) | \ell_2 m_2 \gamma_2 \rangle \\ &= \sum_{q' m'_2} \mathcal{D}_{q'q}^{(k)} T_{kq'} \mathcal{D}_{m'_2 m_2}^{(\ell_2)} | \ell_2 m'_2 \gamma_2 \rangle \end{aligned} \quad (6.249)$$

which demonstrates, in fact, the stated property. One can hence, construct states $\Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2)$ which correspond to total angular momentum states. These states according to (6.18) are defined through

$$\Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2) = \sum_{q, m_2} (\ell_1 m_1 | kq \ell_2 m_2) T_{kq} | \ell_2 m_2 \gamma_2 \rangle. \quad (6.250)$$

We want to show now that these states are eigenstates of $J^2 = J_1^2 + J_2^2 + J_3^2$ and of J_3 where J_1, J_2, J_3 are the generators of the rotation $\mathcal{R}(\vec{\vartheta})$. Before we proceed we like to point out that the states $| \ell_2 m_2 \gamma_2 \rangle$ are also eigenstates of J^2, J_3 , i.e.

$$J^2 | \ell_2 m_2 \gamma_2 \rangle = \hbar^2 \ell_2 (\ell_2 + 1) | \ell_2 m_2 \gamma_2 \rangle \quad ; \quad J_3 | \ell_2 m_2 \gamma_2 \rangle = \hbar m_2 | \ell_2 m_2 \gamma_2 \rangle. \quad (6.251)$$

The corresponding property for $\Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2)$ can be shown readily as follows using (6.247), $J_3 | \ell_2 m_2 \gamma_2 \rangle = \hbar m_2 \gamma_2 | \ell_2 m_2 \gamma_2 \rangle$ and the property (6.21) of Clebsch-Gordan coefficients

$$\begin{aligned} J_3 \Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2) &= \sum_{q, m_2} (\ell_1 m_1 | kq \ell_2 m_2) \underbrace{(J_3 T_{kq} - T_{kq} J_3 + T_{kq} J_3)}_{=\hbar q T_{kq}} | \ell_2 m_2 \gamma_2 \rangle \\ &= \hbar \sum_{q, m_2} \underbrace{(\ell_1 m_1 | kq \ell_2 m_2)}_{\sim \delta_{m_1, q+m_2}} (q + m_2) T_{kq} | \ell_2 m_2 \gamma_2 \rangle \\ &= \hbar m_1 \sum_{q, m_2} (\ell_1 m_1 | kq \ell_2 m_2) T_{kq} | \ell_2 m_2 \gamma_2 \rangle \end{aligned} \quad (6.252)$$

Similarly, one can show that $\Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2)$ is an eigenstate of J^2 with eigenvalue $\hbar^2 \ell_1 (\ell_1 + 1)$. The hermitian property of J_3 and J^2 implies that states $\Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2)$ are orthogonal to $|\ell'_1 m'_1\rangle$ in case of different quantum numbers ℓ_1, m_1 , i.e.

$$\langle \ell'_1 m'_1 | \Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2) = C \delta_{\ell_1 \ell'_1} \delta_{m_1 m'_1} \quad (6.253)$$

Exercise 6.8.1: Show that $\Phi_{\ell_1 m_1}(k, \ell_2 | \gamma_2)$ is an eigenstate of J^2 with eigenvalue $\hbar^2 \ell_1 (\ell_1 + 1)$.

In order to evaluate the matrix elements $\langle \ell_1 m_1 \gamma_1 | T_{kq} | \ell_2 m_2 \gamma_2 \rangle$ we express using the equivalent of (6.32)

$$T_{kq} | \ell_2 m_2 \gamma_2 \rangle = \sum_{\ell_1 m_1} (\ell_1 m_1 | kq \ell_2 m_2) \Phi_{\ell_1 m_1} (k \ell_2 | \gamma_2) \quad (6.254)$$

and orthogonality property (6.253)

$$\langle \ell_1 m_1 \gamma_1 | T_{kq} | \ell_2 m_2 \gamma_2 \rangle = \langle \ell_1 m_1 \gamma_1 | \Phi_{\ell_1 m_1} (k \ell_2 | \gamma_2) \rangle (\ell_1 m_1 | kq \ell_2 m_2). \quad (6.255)$$

At this point the important property can be proven that $\langle \ell_1 m_1 \gamma_1 | \Phi_{\ell_1 m_1} (k \ell_2 | \gamma_2) \rangle$ is independent of m_1 , i.e. the matrix elements $\langle \ell_1 m_1 \gamma_1 | T_{kq} | \ell_2 m_2 \gamma_2 \rangle$ can be reduced to an m_1 -independent factor, its m_1 -dependence being expressed solely through a Clebsch-Gordan coefficient. To prove this property we consider $\langle \ell_1 m_1 \gamma_1 | \Phi_{\ell_1 m_1} (k \ell_2 | \gamma_2) \rangle$ for a different m_1 value, say $m_1 + 1$. Using

$$| \ell_1 m_1 + 1 \gamma_1 \rangle = \frac{1}{\sqrt{(\ell_1 + m_1 + 1)(\ell_1 - m_1)}} J_+ | \ell_1 m_1 \gamma_1 \rangle \quad (6.256)$$

and noting that the operator adjoint to J_+ is J_- , one obtains

$$\begin{aligned} \langle \ell_1 m_1 + 1 \gamma_1 | \Phi_{\ell_1 m_1 + 1} (k \ell_2 | \gamma_2) \rangle &= \\ \frac{1}{\sqrt{(\ell_1 + m_1 + 1)(\ell_1 - m_1)}} \langle \ell_1 m_1 \gamma_1 | J_- \Phi_{\ell_1 m_1 + 1} (k \ell_2 | \gamma_2) \rangle &= \\ \langle \ell_1 m_1 \gamma_1 | \Phi_{\ell_1 m_1} (k \ell_2 | \gamma_2) \rangle & \end{aligned} \quad (6.257)$$

which establishes the m_1 -independence of $\langle \ell_1 m_1 \gamma_1 | \Phi_{\ell_1 m_1} (k \ell_2 | \gamma_2) \rangle$. In order to express the m_1 -independence explicitly we adopt the following notation

$$\langle \ell_1 m_1 \gamma_1 | \Phi_{\ell_1 m_1} (k \ell_2 | \gamma_2) \rangle = (-1)^{k - \ell_2 + \ell_1} \frac{1}{\sqrt{2\ell_1 + 1}} \langle \ell_1, \gamma_1 || T_k || \ell_2, \gamma_2 \rangle. \quad (6.258)$$

We can then finally express the matrix elements of the tensor operators T_{kq} as follows

$$\langle \ell_1 m_1, \gamma_1 | T_{kq} | \ell_2 m_2, \gamma_2 \rangle = (\ell_1 m_1 | kq \ell_2 m_2) (-1)^{k - \ell_2 + \ell_1} \frac{1}{\sqrt{2\ell_1 + 1}} \langle \ell_1, \gamma_1 || T_k || \ell_2, \gamma_2 \rangle \quad (6.259)$$

The so-called reduced matrix element $\langle \ell_1, \gamma_1 || T_k || \ell_2, \gamma_2 \rangle$ is determined by applying (6.259) to a combination of magnetic quantum numbers m'_1, q', m'_2 , e.g. $m'_1 = q' = m'_2 = 0$, for which the l.h.s. can be evaluated as easily as possible. One can then evaluate also the corresponding Clebsch-Gordan coefficient $(\ell_1 m'_1 | kq' \ell_2 m'_2)$ and determine

$$\langle \ell_1, \gamma_1 || T_k || \ell_2, \gamma_2 \rangle = \sqrt{2\ell_1 + 1} \frac{\langle \ell_1 m'_1, \gamma_1 | T_{kq'} | \ell_2 m'_2, \gamma_2 \rangle}{(-1)^{k - \ell_2 + \ell_1} (\ell_1 m'_1 | kq' \ell_2 m'_2)} \quad (6.260)$$

Exercise 6.8.2: Determine the matrix elements of the gradient operator ∇ of the type

$$\int d^3 r F(\vec{r}) \nabla G(\vec{r}) \quad (6.261)$$

when the functions $F(\vec{r})$ and $G(\vec{r})$ are of the type $f(r)Y_{\ell m}(\hat{r})$. For this purpose relate ∇ to a tensor operator T_{1q} , evaluate the matrix for $m_1 = q = m_2 = 0$ using

$$\begin{aligned} \cos\theta Y_{\ell m}(\theta, \phi) &= \\ \sqrt{\frac{(\ell+1-m)(\ell+1+m)}{(2\ell+1)(2\ell+3)}} Y_{\ell+1m}(\theta, \phi) &+ \sqrt{\frac{(\ell-m)(\ell+m)}{(2\ell-1)(2\ell+1)}} Y_{\ell-1m}(\theta, \phi) \\ \sin\theta Y_{\ell m}(\theta, \phi) &= \\ \frac{\ell(\ell+1)}{\sqrt{(2\ell+1)(2\ell+3)}} Y_{\ell+1m}(\theta, \phi) &- \frac{\ell(\ell-1)}{\sqrt{2\ell-1)(2\ell+1)}} Y_{\ell-1m}(\theta, \phi) \end{aligned}$$

and express the remaining matrix elements using the Wigner–Eckart theorem. (The necessary evaluations are cumbersome, but a very useful exercise!)

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