Irreducible Cartesian Tensors

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Preface

On averaging a physical quantity that depends on several vectors over one of its independent vectors, the resulting average physical quantity can no longer depend on that vector, but rather depends only on the remaining independent vectors. In my research, my first real need to deal with vector quantities was essentially a requirement to classify the nature of averages of certain specific functions in terms of their dependence on the directions of the remaining independent vectors. With a desire to retain as much of the directional character of these dependences as possible, it was recognized that only certain combinations could arise and this simplified the calculations. Several years later, my research involved describing gas transport properties as functions of an external magnetic field but with a need to also keep track of the directions of both the driving force and the flux as well as of the magnetic field. All these directions are naturally expressed in terms of Cartesian vectors. But at the same time, collision processes in the gas are essentially rotational invariants. To obtain a description that retains the best of both these worlds, I enlisted the aid of Professor J. A. R. Coope, and together we formulated the theory in terms of Irreducible Cartesian Tensors. Clearly some of the properties of these quantities were known previously, but we consider that we developed a more general understanding of Irreducible Cartesian Tensors. Professor Coope went on by himself to develop the 3-j tensors and their properties. The papers by Professor Coope and myself form the basis of what is presented in this book. In writing the book, some obvious generalizations arose and some developments that we had thought of doing have been accomplished and presented here for the first time. I had hoped that Professor Coope would have joined me in this endeavour, but unfortunately I could not persuade him to do so.

Chapter 1

Introduction

The method of Irreducible Cartesian Tensors is a means of simultaneously accomplishing two objectives. First, since we live in a 3-dimensional world, we have an inherent sense of a Cartesian vector as having a direction (and also a magnitude). For example, we inherently point in a direction when describing where something is. A Cartesian tensor is just a generalization of that, to when something depends on two or more directions, such as the pressure tensor which describes the direction of the force applied by a fluid to a wall, when the wall's direction is described by the vector normal to its surface. Most objects that we deal with are described in terms of Cartesian directions and this is the natural way we visualize objects in the real world. The second objective deals with the inherent isotropy of space. All directions are equivalent, or if one direction is preferred, then that preference is associated with some phenomena, e.g. gravity. But if we rotate in an arbitrary manner, both the object of interest and the device (or object, e.g. the earth in the case of gravity) responsible for the preference in direction, the physical properties remain unchanged. Such an invariance implies something about the phenomena and how it's description can be quantified. Thus a classification of an object according to its rotational properties is useful. Such a classification can always be made in terms of the irreducible representations of the 3-dimensional rotation group. An irreducible Cartesian tensor belongs to an irreducible representation of the rotation group, but is written in terms of Cartesian directions, thus providing a means of satisfying both objectives.

This book was written with the needs and interests of chemists, physicists and other physical scientists in mind. The subject is an area of mathematics, or more correctly a combination of areas of mathematics, as described in the above paragraph, but the method of presentation draws on physical concepts rather than the definition, theorem, proof presentation commonly used in mathematical presentations. There has been an attempt to make the presentation self-contained, and appendix A gives an introduction to some of the mathematical concepts used in the book, with an attempt to cover both the mathematical as well as the physical (physicist's, chemist's, etc.) way of defining these terms. The book also presents a number of relations between well-known quantities that the author believes are new. A mathematician may find some of these of interest, in particular the chapter on spinors, which presents, to the author's knowledge, a novel way of formulating some of their properties.

In the teaching of physics and chemistry, the presentation of the rotation group is usually associated with the quantum mechanics of angular momentum. It is stressed that these two notions are fundamentally two different things. The description of the orientation of an object and how this changes under a rotation has inherently nothing quantum or even mechanical about it, but merely describes how its orientation is, or could be, changed by a rotation. For example, the direction vector pointing to a tree, can be rotated to point to a bush. Nothing has moved, but a comparison of the sightings can be made and the angle between them measured, possibly for the purpose of taking a picture. In contrast, angular momentum is a mechanical property associated with the physical motion of a physical object. Most of this book involves the properties of the rotation group without any reference to mechanics. But Chapter 11 does discuss a number of aspects of the quantum mechanics of angular momentum and describes these in terms of Irreducible Cartesian Tensors. A combination of these two notions is the classification of tensors of the angular momentum operator according to the irreducible representations of the rotation group. Thus the rotation group enters both as a mechanical property (the angular momentum vector operator) and as a means of mathematically classifying the functions of this operator, see Chap. 11.

It is most common to express the irreducible representations of the 3-dimensional rotation group in terms of spherical harmonics and "spherical tensors", see for example Refs. [1–7]. These are sets of quantities which form irreducible representations of the rotation group, but are also classified by how they rotate about a particular axis, usually chosen as the $\hat{z}$-axis. As such, they have an inherent bias to this axis, and if it is desired to classify an object about some other set of directions, it is necessary to transform or take appropriate linear combinations in order to do this. Both the set of final directions and the initial axis of classification enters into such a computation. Irreducible Cartesian Tensors have an advantage here! Since there is no preferential direction under which these are given, only the desired final set of directions needs to be considered.

A further difficulty with spherical tensors is that they involve complex numbers and phase factors. When working with, and combining, such quantities, it is necessary to be very careful that all phase factors are entered correctly. Irreducible Cartesian Tensors are real, so there is at most a plus or minus sign that must be worried about when applying them. The formula for a particular spherical harmonic usually has to be looked up, with its combinations of sines and cosines of angles. In contrast, the structure of an Irreducible Cartesian Tensor in natural form is immediate, having a definite symmetry, namely being symmetric and traceless between every pair of indices. This can be visualized geometrically. There are normalization factors for both systems so there is no advantage to either system in that regard. But in contrast to the many phase factors in the spherical tensor formalism, even the sign that enters when combining Irreducible Cartesian Tensors is associated with some symmetry property of those tensors involved in the combination.

Manipulations involving, in particular combining, irreducible representations of the rotation group can be given diagrammatic interpretations. Some of these are very well known and have simple structures, in particular the scalar n-j symbols $[n \geq 6]$. These diagrams, being rotational invariants, are the same for both the spherical and Cartesian ways of expressing the irreducible representations. But for more directionally dependent combinations of irreducible representations, the diagrammatic interpretation based on spherical tensors requires an elaboration on phases, see in particular the work by Yutsis and coworkers [7]. In contrast, the diagrammatic interpretation for combining Irreducible Cartesian Tensors needs to worry only about which sets of symmetric traceless indices are to be contracted together.

In many calculations the object of interest is a function of several vectors, some of which may be averaged (integrated) over. The object then remains only a function of those vectors which have not been integrated over. Often that dependence is linear in each of the remaining directions, or at most a small power of each. In such a case, the calculation of the object is equivalent to the calculation of the set of coefficients of the various combinations of the vectors on which the object explicitly depends. Such coefficients are tensors, involving the integration over certain directions, but inherently are rotational invariants since they do not depend on any directions. The method of Irreducible Cartesian Tensors is appropriate for carrying out such calculations since the coefficients are recognized as invariant Cartesian tensors. A classification using symmetry can then reduce the number of independent integrals which need to be calculated. Chapter 4 elaborates on the possible invariants resulting from an integral over a single spatial variable, the direction of the vector $\mathbf{r}$. An introduction to the analogous classification of invariants arising from the trace over a product of angular momentum operators is given in Chap.11. It is the method of Irreducible Cartesian Tensors that suggests using rotational invariants for carrying out such calculations.

It would take an historian to do justice to the multitude of contributions to vector and tensor calculus, and to the number of different terminologies and ways of presenting these quantities. The present work involves Cartesian vectors and tensors, and ignores all aspects of curvilinear coordinates and their associated transformations. Even within this limited perspective, the final result has arisen as a combination of the work of researchers with many different points of view. Such developments occurred in parallel so there is no simple order to the story. I comment here on my connections with the subject and how I remember those influences that brought me to my present understanding of Irreducible Cartesian Tensors.

The author started using a diagrammatic method for the depiction of Cartesian tensors when he was involved in integrating several complicated functions in gas kinetic theory [8]. It was already well known in fluid dynamics and kinetic theory that a second order tensor is conveniently separated into its trace, antisymmetric and symmetric traceless parts, and that these have different physical meanings. Also well known and used in kinetic theory is the fact that integrals over the velocity of scalar, vector and symmetric traceless tensor functions of the velocity are orthogonal, see for example Chapman and Cowling [9]. The later authors used the symbol $\overline{\overline{\mathsf{w}}}$ for the symmetric part of the second order tensor w, $\overset{\circ}{\mathsf{w}}$ for the traceless part and the combination $\overset{\circ}{\overline{\overline{\mathsf{w}}}}$ for the traceless symmetric part of w. In the more recent literature of kinetic theory, the notation $\overset{\circ}{\mathsf{w}}$ is used for the traceless part in Hess' book [10] on vector and tensor calculus, as well as in the book on kinetic theory by McCourt et al [11]. But for the symmetric traceless part, these authors use the simpler symbol $\ulcorner\mathsf{w}\urcorner$ for the symmetric traceless part of w. Kagan and Maximov [12], motivated by the work of Fano and Racah [6], used the notation $[\mathsf{w}]^{(2)}$ for the symmetric traceless part of the second order tensor w, with an obvious generalization to arbitrary tensorial order. It is this notation that the author finds easier to write and generalizable to all situations. This is the notation that was adopted in Ref. [13] and it is the notation that is used in this book.

Writing two vectors side by side to give a quantity with two directions was first done by J. Willard Gibbs, and he called the product a dyad. Linear combinations of such products are called dyadics and the generalizations to several vectors are polyads and polyadics. A book founded on Gibbs' lectures has been written by Wilson [14] and a modern presentation of these ideas is given in the book by Drew [15]. Generally this approach gives what I consider the physical scientist's view of a tensor and is the underlying concept used here in discussing tensors. Mathematicians prefer an abstract definition which I find obscure. These different points of view are discussed in appendix A. The dot product of two vectors is commonly introduced at the same time that one is introduced to vectors. For the double dot contraction between two dyadics w_1 and w_2, Gibbs introduced the obvious boldface colon, $\mathsf{w}_1\boldsymbol{:}\mathsf{w}_2$. But for polyadics, the number of dots that may be required becomes unmanageable. Drew introduced the notation $\mathsf{w}_1^{(p)} \textcircled{p}\ \mathsf{w}_2^{(p)}$ for the p-fold dot product between two polyadics of order p. My colleague and I [16] considered this notation constraining to use, so the

p-fold dot product was changed to $\mathbf{w}_1^{(p)} \odot^p \mathbf{w}_2^{(p)}$. It is this notation which is used here, especially for $p > 2$. The order of contraction is important when the tensors (polyadics) are not symmetric. Here it is chosen to always dot together the nearest vector directions, continuing with that order until all the indicated contractions have been carried out. This is a convention adopted in gas kinetic theory [9] but was not Gibbs' original choice, see the comments in appendix A.2.

The author has always liked a coordinate free approach to writing vectors and tensors, considering them to be quantities in their own right. Other authors prefer to express them as sets of elements labelled according to some coordinate system, whether by Cartesian $x,\ y,\ z$ labels or by the spherical tensor $\ell\ m$ labels. As already stated, the spherical tensor system requires choosing a reference $(\hat{z})$ axis, while the Cartesian labelling again requires choosing which are the $\hat{x},\ \hat{y}$ and $\hat{z}$ directions. Different choices for these reference directions imply that the same vector or tensor be associated with different components. Transformations from one coordinate system to another then always plays a dominant role when discussing a vector or tensor and, from the author's point of view, detracts from studying the inherent properties of the vector or tensor. Obviously then, this book emphasises almost exclusively, the coordinate free representation of vectors and tensors.

This book starts in Chapter 2 with an introduction to vectors and tensors. This is followed by a discussion of the rotational properties of vectors. In keeping with the coordinate free emphasis of the book, this action can be expressed as a tensor acting on the vector to be rotated. Moreover, the rotation tensor is expressed entirely in terms of the unit vector along the axis of rotation and the angle of rotation. A convenient way of writing such a tensor is in terms of a diagrammatic representation. This method of representation is presented in this chapter and is used throughout the book. To complete the description of how a rotation affects a vector, the connections to the standardly used Euler angle description of a rotation are given.

The standard vector operations naturally lead to the introduction of the second order identity tensor $\mathbf{U}$ and the Levi Civita tensor $\boldsymbol{\varepsilon}$. Chapter 3 starts with a proof that these are rotational invariants. The notion of an invariant (to any rotation) mapping between tensor spaces of different order is then introduced. That provides the background for the reduction (under the action of the rotation group) of a given tensor into its irreducible parts and the expression of these irreducible parts in their "natural" form, namely as symmetric traceless tensors in a tensor space of minimal order. This leads to the projection tensors $\mathbf{E}^{(p)}$ and a discussion of various properties of the rotation group. A parentage scheme for the construction of tensors of higher order and the classification of their irreducible parts is described. After reduction of a given tensor to its irreducible parts, it is recognized that the original tensor can then be rebuilt out of these "natural tensors", showing how the irreducible parts contribute to the whole.

Chapter 4 describes Irreducible Cartesian Tensors constructed from one or more vectors. The scalar product between two irreducible tensors of order p is defined and it is shown that, for tensors built from vectors, this scalar product is proportional to the Legendre polynomial of order p. Integrals of products of two irreducible tensors formed from the common vector $\mathbf{r}$ are discussed, and normalizations appropriate for these tensors introduced. This leads to a discussion of expanding an arbitrary tensor product of $\mathbf{r}$ with itself, or more appropriately, of the unit vector $\hat{r}$, in terms of the irreducible Cartesian tensors based on $\hat{r}$. A related problem is the evaluation of the integral of a general tensor product of $\hat{r}$'s. A number of papers have appeared in the literature that list the integrals of products of vector components. Here it is stressed how all these integrals can be expressed in terms of a set of tensor integrals, each of which is evaluated in terms of invariant tensors. The evaluation of an integral involving a certain set of components of $\hat{r}$ then simply involves indentifying which part of the invariant tensor has the same set of directions as does the original integral.

Chapter 5 starts with a review of the eigenvectors of a rotation generator and goes on to find Cartesian vector and tensor basis elements that satisfy these requirements with suitable normalization. These spherical tensors are used to discuss the spherical components of an arbitrary Irreducible Cartesian Tensor. For a tensor built up from a vector $\hat{r}$, these are the spherical harmonics. Some of the basic properties of these functions are derived using Cartesian tensor methods and demonstrate the general connections between Cartesian and spherical tensors. Two phase conventions for spherical tensors arise in the literature, one commonly used in most of the physical and chemical literature, and the other intimately connected to the spinor representation of tensorial quantities, which are discussed in Chapter 10. Both conventions are presented here, but the emphasis is on the former.

Chapter 6 introduces the 3-j coupling tensors together with their normalization factors and certain recursion relations satisfied by them. This material draws heavily on Ref. [17]. The basic properties are summarized in the first section with much of the remaining chapter presenting the detailed computations needed to derive the normalization factors and certain recursion relations. These latter sections are more for those interested in these detailed calculations, but some of the recursion relations get used in later chapters. The immediately useful properties of the 3-j tensors are covered in the following chapter, Chap. 7. In particular, the integral of a product of three Irreducible Cartesian Tensors built on $\hat{r}$ is presented, and the 3-j symbols are obtained.

Chapters 8 and 9 present other properties of the rotation group in terms of Irreducible Cartesian Tensors. Specifically the 6-j and 9-j symbols and the rotation matrices are written in terms of Irreducible Cartesian Tensors. The presentation of the connections between Cartesian tensors and the rotation matrices is believed to be original.

The notion of Irreducible Cartesian Tensors is generalized in Chapter 10 to the case of spinors, namely to the space of tensors based on 2-dimensional complex vectors with irreducibility under the action of the group SU(2). This is the natural extension of the rotation group to include the $\frac{1}{2}$-integer representations of the rotation group. In this complex 2-dimensional space it is necessary to distinguish between contravariant and covariant basis sets and their differing rotational properties. The well known invariant metric $\boldsymbol{\epsilon}$ is shown, with a particular choice of a multiplicative constant, to be idempotent. Interesting properties relating contravariant and covariant basis elements follow from this assertion, as does the anticommutativity of the contraction of contravariant and covariant basis elements. The reduction of spinor tensors is discussed together with their parentage scheme. Finally 3-j spinor tensors are defined and related to 3-j symbols. A start of this program was given in Ref. [16], but most of this chapter is believed to be original. The reason for the novelty of this presentation is interpreted as the difference in outlook, namely here a coordinate free description is taken as far as it can be, whereas the standard treatments emphasize the spinor components.

Finally, various properties of the quantum mechanics of angular momentum are described in Chapter 11 in terms of Irreducible Cartesian Tensors. Orientation kets for the position and momentum unit vectors are introduced and used as bases for the representation of angular momentum states. An extension of these to describe the states of a symmetric top molecule is given. The chapter ends with a discussion of some of the properties of tensors of the angular momentum.

This book is devoted to the study of tensors of 3-dimensional vectors and their behaviour under the 3-dimensional rotation group. This is appropriate for describing the properties of physical systems that are isotropic. But often a physical system in 3-dimensions is not in an isotropic environment. Then classifying the systems properties according to the 3-dimensional rotation group is not really appropriate, rather a classification under a subgroup of the rotation group plus possibly some reflection symmetries (namely under the action of some point group) might be more immediately useful. In such a situation there may be one or more vectors that are invariant to the group action, other than only the rotational invariants. A treatment analogous to that given in this book could be carried out, involving all the invariants to the group appropriate to the symmetry of the system. As a consequence, the reduction of tensors and the embedding of irreducible representations in higher order tensor spaces is completely different in detail from that given in this book. It is expected that it is possible to generalize the methods presented here to cover such symmetry considerations. A very cursory mention of the C_∞, $C_{\infty v}$ and C_n groups are mentioned in Ref. [16]. For groups of higher symmetry, there are fewer invariants, see again the short discusion in Ref. [16]. It is also interesting to speculate how useful the same methods might be in the study of higher dimensional spaces, for example to the Lorentz group in 4-dimensional space-time.

Chapter 2

Vectorial Approach

2.1 An Introduction to Vectors and Tensors

A vector, in the world in which we live, is a quantity with a magnitude and a direction. In this work such a vector is written in boldface, for example $\mathbf{r}$. This is common in much of the physics and chemistry literature, but often an alternative is the use of an arrow, namely $\vec{r}$. In this book, this latter notation is reserved for the designation of a column vector, which implies that there is some coordinate system that has been specified, see Secs. 2.3 and 2.5.2 for examples of the use of this notation. Thus $\mathbf{r}$ is to be thought of as a vector without reference to any coordinate system. Mathematically, $\mathbf{r}$ designates an element of a 3-dimensional vector space over the field of real numbers. It is often useful to separate the magnitude, designated by r, from the directional properties of $\mathbf{r}$ by introducing the unit vector $\hat{r}$, thus $\mathbf{r} = r\hat{r}$. This is the Cartesian description of a vector.

In 3-dimensions one has a subjective notion of three (orthogonal) directions, which are usually referred to as the x, y and z directions, with unit vectors (Cartesian basis vectors) $\hat{x}$, $\hat{y}$ and $\hat{z}$. The vector $\mathbf{r}$ can be described in this coordinate system by its components x, y and z along these directions, namely

$$\mathbf{r} = x\hat{x} + y\hat{y} + z\hat{z}, \tag{2.1}$$

these being equivalent meanings of what is a vector. Standardly the basis set is chosen as a right-handed coordinate system [direct the fingers of the right hand along the $\hat{x}$, curl the tips of the fingers to $\hat{y}$ and then the thumb points along $\hat{z}$]. Any reference in this book to a 3-dimensional coordinate system will always imply that a right-handed coordinate system is to be meant. It should also be emphasized that a coordinate system can be set up in any number of ways, that is, there is nothing unique about the $\hat{x}$, $\hat{y}$ or $\hat{z}$ directions, but a coordinate system is often used by an observer so as to reference where a vector points (relative to the observer's orientation). Stated otherwise, the choice of a coordinate system is always at the whim of the observer and is thus subjective. Note that, as stated in the Introduction, this book emphasizes the coordinate independent properties of vectors and tensors while coordinate systems are used to explicitly explain and illustrate the various quantities and their relations. For ease of writing complicated expressions, the x, y and z components of a vector will sometimes be written as r_j with j referring to x, y and/or z. Thus Eq.

(2.1) can be abbreviated as

$$\mathbf{r} = \sum_j r_j \hat{j}. \tag{2.2}$$

An alternate description of a vector in 3-dimensional space is in terms of its spherical components, r, θ and ϕ. This depends on having a coordinate system, with one direction, usually labelled as the $\hat{z}$-direction, having a very preferred role. In terms of the Cartesian coordinates, the spherical components are

$$r = \sqrt{x^2 + y^2 + z^2} \qquad \cos\theta = z/r, \qquad \tan\phi = y/x, \tag{2.3}$$

and the inverse relation is

$$z = r\cos\theta, \qquad x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi. \tag{2.4}$$

Since the angles are not unique by the addition of multiples of π or 2π, the usual constraints are that $r > 0$, $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$, but sometimes a recognition of the multiplicity of the spherical coordinates is both useful and necessary for an understanding of a particular problem. However it is noticed that both coordinate descriptions of a vector depend on a (subjective) coordinate system. It is an advantage of Cartesian tensor analysis, that such subjective quantities may be eliminated. At least until an observer wishes to compare a direction to the observer's chosen reference frame.

Vectors can be added and multiplied together in a number of different ways. These are:

1. The addition $\mathbf{R} = \mathbf{r}_1 + \mathbf{r}_2$ of two vectors is merely equivalent to adding their Cartesian components, $X = x_1 + x_2$, etc., provided the same coordinate system is used for the description of both vectors. But, of course, there are no simple relations between the spherical components.

2. The most important type of multiplication is the "dot" product, giving the (coordinate independent) scalar product

$$\mathbf{r}_1 \cdot \mathbf{r}_2 = x_1 x_2 + y_1 y_2 + z_1 z_2. \tag{2.5}$$

   This is used to identify the length (magnitude) r of a vector, $r = \sqrt{\mathbf{r}\cdot\mathbf{r}}$, the angle Θ_{12} between two vectors, $\cos(\Theta_{12}) = \hat{r}_1 \cdot \hat{r}_2$, and the special case of orthogonality (perpendicularity), $\mathbf{r}_1 \cdot \mathbf{r}_2 = 0$. The Cartesian basis elements are inherently taken to be orthonormal (both orthogonal and normalized, that is, of unit length), so a Cartesian component of a vector $\mathbf{r}$ can be obtained by the dot product

$$r_j = \hat{j} \cdot \mathbf{r}. \tag{2.6}$$

3. Multiplication by a scalar a affects only the magnitude of the vector

$$\mathbf{r} \to a\mathbf{r}. \tag{2.7}$$

   This implies that the magnitude of the vector is changed, $r \to ar$, while $\hat{r}$ is unchanged.

4. The "cross" product $\mathbf{r}_1 \times \mathbf{r}_2$ determines a vector of magnitude $r_1 r_2 \sin(\Theta_{12})$ in the direction perpendicular to both $\mathbf{r}_1$ and $\mathbf{r}_2$ and directed as in the $\hat{z}$-direction of a right-handed coordinate system determined by $\hat{r}_1$ and $\hat{r}_2$ with $\hat{r}_1$ and the part of $\hat{r}_2$ perpendicular to $\hat{r}_1$ being the $\hat{x}$ and $\hat{y}$-directions. In terms of an $\hat{x}$, $\hat{y}$, $\hat{z}$ coordinate system, the cross product has Cartesian components

$$\mathbf{r}_1 \times \mathbf{r}_2 = (y_1 z_2 - z_1 y_2)\hat{x} + (z_1 x_2 - x_1 z_2)\hat{y} + (x_1 y_2 - y_1 x_2)\hat{z}. \tag{2.8}$$

5. The tensor product, sometimes referred to as an outer product or as a direct product, of $\mathbf{r}_1$ and $\mathbf{r}_2$, is written here as $\mathbf{r}_1\mathbf{r}_2$, whereas it is formally indicated in the literature as $\mathbf{r}_1 \otimes \mathbf{r}_2$. This is a quantity with two directions and thus $3 \times 3 = 9$ Cartesian components

$$\mathbf{r}_1\mathbf{r}_2 = \sum_{j\ell} r_{1j} r_{2\ell} \hat{j}\hat{\ell}. \tag{2.9}$$

Another name for such a quantity is that it is a "dyad" [14, 15], a name that appears to be little used at present. This can be immediately generalized by addition of similar products of vectors to give a general "second order" tensor T or "dyadic" [14,15]. Such quantities are also commonly referred to as second "rank" tensors. Since "rank" has an association as the number of linearly independent quantities, this book (attempts to) avoid this usage for classifying the order of a tensor, see also Appendix A. A second order tensor has 9 components, in general all independent of each other, but possibly zero. As such, the best that be done to express T in component form is to expand it as

$$\mathsf{T} = \sum_{j\ell} T_{j\ell} \hat{j}\hat{\ell}, \tag{2.10}$$

with the 9 independent scalars $T_{j\ell}$, which are determined from T according to

$$T_{j\ell} = \hat{j}\cdot\mathsf{T}\cdot\hat{\ell} = \hat{\ell}\hat{j}:\mathsf{T}. \tag{2.11}$$

The colon designates a double dot contraction. The convention that is followed in this work is that nearest indices are contracted together, the same type of convention as usually used in calculating multiple integrals. Thus the doubledot product of four vectors is the product of the scalar products according to

$$\mathbf{r}_1\mathbf{r}_2:\mathbf{r}_3\mathbf{r}_4 = \mathbf{r}_1\cdot(\mathbf{r}_2\cdot\mathbf{r}_3)\mathbf{r}_4 = (\mathbf{r}_1\cdot\mathbf{r}_4)(\mathbf{r}_2\cdot\mathbf{r}_3), \tag{2.12}$$

with the last form valid if the vectors commute (the usual case, but in quantum mechanics, for example, for angular momentum vectors, this may not be the case). It should also be mentioned that this order is NOT that used by Gibbs or Drew [14, 15], see also appendix A.2. The order of carrying out a tensor product is crucially important, e.g., so as to be sure whether it is the first or second direction in the tensor $\mathbf{r}_1\mathbf{r}_2$ that refers to $\mathbf{r}_1$. An immediate consequence of this ordering is that there is a "transpose" operator, which nicely interchanges the two directions. Specifically, for the second order tensor T of Eq. (2.10), the transpose tensor T^t is given by

$$\mathsf{T}^t = \sum_{j\ell} T_{j\ell} \hat{\ell}\hat{j}, \tag{2.13}$$

with the order of the unit vectors interchanged. Clearly this is also equivalent to the interchange of the indices on the amplitude

$$T^t_{j\ell} = T_{\ell j}, \tag{2.14}$$

since each sum over j and ℓ involves the sum over all coordinate directions. Another generalization is to take the tensor product of several vectors, such as the n-fold tensor product

$$\mathsf{T} = \mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n. \tag{2.15}$$

Such a quantity is referred to as an $n\underline{\text{th}}$ order tensor, corresponding to it having n directions. Linear combinations of $n\underline{\text{th}}$ order tensors give the most general $n\underline{\text{th}}$ order tensor which can be written in the form

$$\mathbf{T} = \sum_{jk\ldots\ell} T_{jk\ldots\ell}\hat{j}\hat{k}\cdots\hat{\ell} \tag{2.16}$$

with 3^n Cartesian components

$$T_{jk\ldots\ell} = \mathbf{T} \odot^n \hat{\ell}\cdots\hat{k}\hat{j}, \tag{2.17}$$

which are in general independent. $\odot^n$ denotes the n-fold dot contraction, again with the contraction order starting from the nearest directions and working outwards. This notation has been adopted as a variant of that introduced by Drew [15]. He put the number of contractions (n) inside the circle, but this is considered of limited use since this number will sometimes be the sum of several terms. As mentioned earlier, here nearest directions are contracted together whereas Drew uses the opposite order when carrying out successive contractions. Further comments are made on this point in appendix A.2.

There are many operations and combinations of operations that can be performed with Cartesian tensors, but all are really just combinations of the above. No attempt will be made to exhaust all such possibilities, if that is even possible, but a number of such operations are mentioned since they play certain central roles in the remainder of the book.

Given the $n\underline{\text{th}}$ order tensors $\mathbf{T}$ and $\mathbf{S}$, there is the scalar product $\mathbf{T}\odot^n\mathbf{S}$, which gives a number. In particular, $\mathbf{T}^t \odot^n \mathbf{T}$ is interpreted as the square of the magnitude of the tensor $\mathbf{T}$. [The transpose of an n$\underline{\text{th}}$ order tensor is the *complete* transpose, that is, the reverse order of all directions.] Inherently it has been assumed that the tensors are real (that is, the tensorial components are real), whereas if the tensors are complex, then the scalar product $\mathbf{T}^* \odot^n \mathbf{S}$, * denoting complex conjugation, is more useful. The square of the magnitude of $\mathbf{T}$ is then $\mathbf{T}^{*t}\odot^n\mathbf{T}$, including both the complex conjugation and the transpose. If the tensors are also quantum mechanical operators, then a useful scalar product would be $\mathbf{T}^\dagger \odot^n \mathbf{S}$, with † denoting the operator adjoint. This automatically accounts for the complex conjugation, but a tensor transpose might also be appropriate. In this book, any extra features of this kind are explicitly indicated, with the $\odot^n$ indicating a pure tensor contraction.

The property of being a tensor is only one possible attribute that a quantity can have. While the major emphasis in this book is on the tensorial properties of a quantity, the interplay between tensorial and certain quantum operator properties are discussed in Sec. 11.4.

A further generalization of dot product, is to carry out only a partial contraction of two tensors, namely

$$\mathbf{R} = \mathbf{T} \odot^m \mathbf{S} \qquad\qquad m < n \tag{2.18}$$

is a $2(n-m)$ order tensor, if $\mathbf{T}$ and $\mathbf{S}$ are $n\underline{\text{th}}$ order tensors. On the other hand, if $\mathbf{T}$ is $n\underline{\text{th}}$ order while $\mathbf{S}$ is of order p, then $\mathbf{R}$ is of order $n+p-2m$, provided of course that n and p are both larger that m. A cross product between tensors, $\mathbf{T}\times\mathbf{S}$, or between a vector and a tensor, $\mathbf{r}\times\mathbf{T}$, is another type of operation. Several successive cross products could also be carried out, as long as there are sufficient directions (indices) on the respective tensors to make the operation meaningful. The tensor product also should be mentioned, for example $\mathbf{R} = \mathbf{TS}$ is a tensor of order $m+n$ if $\mathbf{T}$ and $\mathbf{S}$ are respectively of order m and n. Clearly many other operations and combinations of operations can be envisaged.

2.2 The Four Elementary Tensor Operations

All operations on tensors are combinations of the elementary operations that are performed on vectors. Inherently, I consider there to be four of these, though of course others may wish to classify the operations in a different manner. Their order given here is for presentation purposes, while their natural logical appearance was given in the previous section.

First, and simplest, is the tensor product. For two vectors, this gives a second order tensor, such as $\mathbf{r}_1\mathbf{r}_2$. Note that the order is important. It is useful to consider this also as an operation on a vector, namely the left multiplication on $\mathbf{r}_2$ by $\mathbf{r}_1$, or equivalently the right multiplication on $\mathbf{r}_1$ by $\mathbf{r}_2$.

Second is the dot product of two vectors $\mathbf{r}_1\cdot\mathbf{r}_2$. It is useful to visualize this in a different context, namely as the contraction of the tensor product of the two vectors, thus

$$\mathbf{r}_1\cdot\mathbf{r}_2 = \mathbf{U}\mathbf{:}[\mathbf{r}_1\mathbf{r}_2] \tag{2.19}$$

with the unit second order tensor expressed in terms of a basis set as

$$\mathbf{U} \equiv \hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}. \tag{2.20}$$

This special tensor plays a unique role in most everything that follows.

Third is the multiplication by a scalar a, $\mathbf{r} \to a\mathbf{r}$, and its very special case, the identity operation, $\mathbf{r} \to \mathbf{r}$. It is useful to recognize that this can be written in the form of an operation on $\mathbf{r}$, namely

$$a\mathbf{r} = a\mathbf{U}\cdot\mathbf{r}, \tag{2.21}$$

as a contraction by the second order tensor $a\mathbf{U}$ acting on the vector $\mathbf{r}$. The identity operation is recognized as $\mathbf{r} = \mathbf{U}\cdot\mathbf{r}$.

Fourth is the cross product $\mathbf{r}_1\times\mathbf{r}_2$. This can also be written as an action on $\mathbf{r}_1\mathbf{r}_2$ by introducing the Levi Cevita tensor $\boldsymbol{\mathcal{E}}$. This is the third order, completely antisymmetric tensor (a permutation of any two directions of $\boldsymbol{\mathcal{E}}$ gives $-\boldsymbol{\mathcal{E}}$). Written in terms of a basis set, this is

$$\boldsymbol{\mathcal{E}} = \sum_{jk\ell} \varepsilon_{jk\ell}\hat{j}\hat{k}\hat{\ell}, \tag{2.22}$$

with $\varepsilon_{jk\ell} = 1,\ -1,\ 0$ according to whether $jk\ell$ is an even, odd, or not a, permutation of xyz. Equivalently, whether $\hat{j}$, $\hat{k}$ and $\hat{\ell}$ form a right-handed (orthogonal) coordinate system, a left-handed coordinate system, or whether there is a duplication of the same unit vector among the three. Explicitly written out, this gives

$$\boldsymbol{\mathcal{E}} = \hat{x}\hat{y}\hat{z} + \hat{y}\hat{z}\hat{x} + \hat{z}\hat{x}\hat{y} - \hat{y}\hat{x}\hat{z} - \hat{z}\hat{y}\hat{x} - \hat{x}\hat{z}\hat{y}. \tag{2.23}$$

With the aid of $\boldsymbol{\mathcal{E}}$, the cross product can be written,

$$\mathbf{r}_1\times\mathbf{r}_2 = -\mathbf{r}_1\cdot\boldsymbol{\mathcal{E}}\cdot\mathbf{r}_2 = -\boldsymbol{\mathcal{E}}\mathbf{:}\mathbf{r}_1\mathbf{r}_2, \tag{2.24}$$

with the second form illustrating how the cross product is a tensor operation on the vector $\mathbf{r}_2$, and the last form illustrating how this can be considered as a tensor operation on the tensor product of the two vectors. The minus sign is a result of the convention of dotting nearest directions together.

This section has reviewed the four basic tensor operations and introduced the two tensors $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$, which allows one to interpret all vector operations in an operator type of form, namely as some operator acting on a tensor. Clearly these aspects can be applied to arbitrary tensors and generalized in many ways. The two basic tensors $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$ also play a central role in classifying and manipulating representations of the 3-dimensional rotation group.

2.3 Rotations in Two Dimensions

The simplest example of a rotation is the description of a rotation in a plane. Fig. 2.1 illustrates the rotation $R(\theta)$ of a vector $\mathbf{r}$ through an angle θ into its rotated image $R(\theta)\mathbf{r}$.

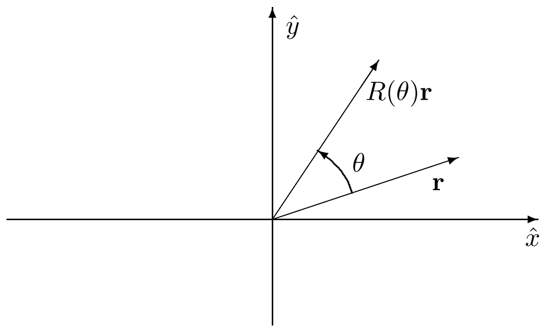


Figure 2.1: Rotation in 2-dimensions

Both the original and rotated vector can be expressed in terms of Cartesian coordinates with a typical coordinate frame indicated in the figure. Specifically, writing

$$\mathbf{r} = x\hat{x} + y\hat{y}, \tag{2.25}$$

it follows from trigonometry that the rotated vector is

$$R(\theta)\mathbf{r} = [x\cos\theta - y\sin\theta]\hat{x} + [y\cos\theta + x\sin\theta]\hat{y}. \tag{2.26}$$

This is often expressed in matrix form as

$$\begin{aligned}
\mathbf{r} \quad &\Longleftrightarrow \quad \begin{pmatrix} x \\ y \end{pmatrix} \\
R(\theta)\mathbf{r} \quad &\Longleftrightarrow \quad \begin{pmatrix} x\cos\theta - y\sin\theta \\ y\cos\theta + x\cos\theta \end{pmatrix} \\
&\Longleftrightarrow \quad \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.
\end{aligned} \tag{2.27}$$

But there is another way of expressing this action. If the initial direction of the vector ($\mathbf{r}$ in this case) is used as one member of a coordinate system, then on rotation, the component of the rotated vector along this direction is reduced by $\cos\theta$ and a component, of length $r\sin\theta$ is produced, in a direction orthogonal to the original direction, formally

$$R(\theta)\mathbf{r} = \cos\theta\mathbf{r} + r\sin\theta\widehat{\mathbf{r}_\perp}. \tag{2.28}$$

It is important to be able to clarify as to what direction the unit vector $\widehat{\mathbf{r}_\perp}$ actually corresponds. Essentially this corresponds to the unit vector $\hat{r}$ being rotated by $\pi/2$ (90°) about an axis that is directed out of the paper and pointing to the reader, so $\widehat{\mathbf{r}_\perp} = R(\pi/2)\hat{r}$. An elaboration of what this is, together with several ways of expressing its effect, is presented in the following subsection.

2.3.1 Rotation by $\pi/2$

One way to describe a (right-handed) rotation of a vector by $\pi/2$ is to recognize that its component along the $\hat{x}$ direction is to be placed along the $\hat{y}$ direction and its component along the $\hat{y}$ direction is to be placed along the $-\hat{x}$ direction. To quantify this, $\hat{x}\cdot\mathbf{r}$ selects out the component of $\mathbf{r}$ along the $\hat{x}$ direction, and placing this quantity along the $\hat{y}$ direction involves multiplying the component by the unit vector $\hat{y}$. Equivalently, the rotation by $\pi/2$ changes $\hat{x}$ to $\hat{y}$ and $\hat{y}$ to $-\hat{x}$, formally

$$R(\pi/2)\hat{x} = \hat{y} \qquad\qquad R(\pi/2)\hat{y} = -\hat{x}. \tag{2.29}$$

This is equivalent to the action (by dot contraction) of the second order tensor $\hat{y}\hat{x} - \hat{x}\hat{y}$ on either basis vector. In this way a rotation by $\pi/2$ is identical to the action of this tensor. Applied to an arbitrary vector $\mathbf{r}$, this rotation can be written

$$R(\pi/2)\mathbf{r} = (\hat{y}\hat{x} - \hat{x}\hat{y})\cdot\mathbf{r} \equiv \mathsf{R}(\pi/2)\cdot\mathbf{r}, \tag{2.30}$$

this defining the second order (rotation) tensor $\mathsf{R}(\pi/2)$. It follows that the unit vector perpendicular to $\hat{r}$ is

$$\widehat{\mathbf{r}_\perp} = \mathsf{R}(\pi/2)\cdot\hat{r}. \tag{2.31}$$

Another way is to think of the plane embedded in 3-dimensional space, with the direction normal to the plane denoted by $\hat{z}$ with a right hand rule relating $\hat{x}$, $\hat{y}$ and $\hat{z}$. Equivalently, $\hat{z} = \hat{x}\times\hat{y}$. Then the appropriate direction perpendicular to $\hat{r}$ is given by

$$\widehat{\mathbf{r}_\perp} = \hat{z}\times\hat{r} = (\hat{y}\hat{x} - \hat{x}\hat{y})\cdot\hat{r}, \tag{2.32}$$

working out the effect of successive cross products [an easier way to do this is discussed in Sec. 2.4]. On making use of writing the cross product in terms of the Levi Cevita tensor, it is seen that the rotation tensor $\mathsf{R}(\pi/2)$ can be written in the two forms

$$\mathsf{R}(\pi/2) = \hat{y}\hat{x} - \hat{x}\hat{y} = -\hat{z}\cdot\boldsymbol{\mathcal{E}}\ . \tag{2.33}$$

Clearly these are the same, but the 3-dimensional sense of the latter plays an important role in the next section.

2.3.2 Tensorial Description of a Rotation

For a general rotation of $\mathbf{r}$ by θ, the action is given by

$$\begin{aligned} R(\theta)\mathbf{r} &= \cos\theta\mathbf{r} + \sin\theta\mathsf{R}(\pi/2)\cdot\mathbf{r} \\ &= [\cos\theta\mathsf{U}^{(2d)} + r\sin\theta\mathsf{R}(\pi/2)]\cdot\mathbf{r} \\ &= \mathsf{R}(\theta)\cdot\mathbf{r}, \end{aligned} \tag{2.34}$$

where

$$\mathsf{U}^{(2d)} \equiv \hat{x}\hat{x} + \hat{y}\hat{y} \tag{2.35}$$

is the tensor identity in 2-dimensions, which is a restriction of the 3-dimensional tensor identity U of Eq. (2.20). The total effect has been expressed in terms of a rotation tensor

$$\begin{aligned} \mathsf{R}(\theta) &= \cos\theta\mathsf{U}^{(2d)} + \sin\theta\mathsf{R}(\pi/2) \\ &= \cos\theta\mathsf{U}^{(2d)} - \sin\theta\hat{z}\cdot\boldsymbol{\mathcal{E}} \\ &= \cos\theta(\hat{x}\hat{x} + \hat{y}\hat{y}) + \sin\theta(\hat{y}\hat{x} - \hat{x}\hat{y}). \end{aligned} \tag{2.36}$$

This has been expressed in a variety of ways. A matrix equivalent of the last form is to represent the unit vectors by the column vectors

$$\hat{x} \Longleftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \hat{y} \Longleftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{2.37}$$

in which case the rotation tensor is equivalent to the matrix

$$\begin{aligned} R(\theta) \quad &\Longleftrightarrow \quad \mathbf{R}(\theta) \Longleftrightarrow \cos\theta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \sin\theta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \\ &\Longleftrightarrow \quad \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \end{aligned} \tag{2.38}$$

which is exactly what appears in Eq. (2.27), but now related to tensorial properties. The above equation has also attempted to emphasize the relation between the "abstract" notion of a rotation, $R(\theta)$, the "tensorial representation" of this rotation when acting on a vector, $\mathbf{R}(\theta)$, and the "matrix representation" of the rotation when acting on the components of a vector. Fundamentally they all relate to the same rotation, the abstract form being the "concept" of the rotation, while the last two describe how the result of the rotation is to be calculated. The matrix form is extremely useful, but it must always be kept in mind that it is expressed in terms of a basis set, so its interpretation is always in terms of that basis set.

The distinction between the abstract notion of a rotation and the calculation of its result is illustrated by considering the rotation of a second order tensor $\mathbf{T}$. Having two directions, each direction must be rotated, thus

$$R(\theta)\mathbf{T} = \mathbf{R}(\theta)\cdot\mathbf{T}\cdot\mathbf{R}(\theta)^t, \tag{2.39}$$

where ^{t} designates the transpose of the rotation tensor $\mathbf{R}(\theta)$, necessary since, of the two directions of the second order tensor $\mathbf{R}(\theta)$, it is the "right-hand" direction of $\mathbf{R}(\theta)$ that is to be dotted into the original direction, while the "left-hand" direction of $\mathbf{R}(\theta)$ is to give the rotated direction.

2.3.3 Group theory aspects

The successive rotations, first by θ_1 and then by θ_2 is equivalent to the rotation by $\theta_1+\theta_2$. While this is intuitive, the formal calculation of this result can be accomplished with the tensorial representation of the rotations, namely

$$\begin{aligned} \mathbf{R}(\theta_2)\cdot\mathbf{R}(\theta_1) &= \Big[\cos(\theta_2)\mathbf{U}^{(2d)} + \sin(\theta_2)\mathbf{R}(\pi/2)\Big]\cdot\Big[\cos(\theta_1)\mathbf{U}^{(2d)} + \sin(\theta_1)\mathbf{R}(\pi/2)\Big] \\ &= [\cos(\theta_2)\cos(\theta_1) - \sin(\theta_2)\sin(\theta_1)]\,\mathbf{U}^{(2d)} \\ &\quad + [\cos(\theta_2)\sin(\theta_1) + \sin(\theta_2)\cos(\theta_1)]\,\mathbf{R}(\pi/2) \\ &= \cos(\theta_1+\theta_2)\mathbf{U}^{(2d)} + \sin(\theta_1+\theta_2)\mathbf{R}(\pi/2). \end{aligned} \tag{2.40}$$

This depends on trigonometric addition formulas and the tensorial product relations

$$\begin{aligned} \mathbf{U}^{(2d)}\cdot\mathbf{U}^{(2d)} &= \mathbf{U}^{(2d)} \\ \mathbf{U}^{(2d)}\cdot\mathbf{R}(\pi/2) &= \mathbf{R}(\pi/2)\cdot\mathbf{U}^{(2d)} = \mathbf{R}(\pi/2) \\ \mathbf{R}(\pi/2)\cdot\mathbf{R}(\pi/2) &= -\mathbf{U}^{(2d)}. \end{aligned} \tag{2.41}$$

The last of these can also be recognized as the rotation by π, or by the detailed calculation

$$(\hat{y}\hat{x} - \hat{x}\hat{y})\cdot(\hat{y}\hat{x} - \hat{x}\hat{y}) = -\hat{y}\hat{y} - \hat{x}\hat{x}. \tag{2.42}$$

It is clear that the result is independent of the order in which the rotations are applied. That is, the rotations in the plane commute.

The special rotation $R(0) = 1$ is the identity, tensorially $\mathbf{R}(0) = \mathbf{U}^{(2d)}$. It also follows from the composition of rotations, that for every rotation $R(\theta)$ there is an inverse rotation

$$R(\theta)^{-1} = R(-\theta) \tag{2.43}$$

on the basis that

$$R(\theta)^{-1}R(\theta) = R(\theta)R(\theta)^{-1} = R(0) = 1. \tag{2.44}$$

The corresponding tensors satisfy the analogous relations. These properties imply that the set of rotations form a group, see Appendix A.1.

The 2-dimensional rotation group, designated formally as SO(2), since it is equivalent (isomorphic) to the set of 2 by 2 matrices which are orthogonal with a positive determinant, has an infinite number of elements, one for each θ (actually continuously infinite). Moreover the elements commute. Thus SO(2) is a commutative (also known as abelian) continuous one parameter group under multiplication, with each element parameterized by an angle θ between 0 and 2π.

As θ is a continuous parameter, it is also possible to consider the derivative of the rotation operator (and tensor). In particular, at an angle of 0, the derivative

$$G \equiv i\frac{dR(\theta)}{d\theta}\Big|_{\theta=0}, \tag{2.45}$$

with $i = \sqrt{-1}$ introduced for later convenience, is the "generator" of the group. The equivalent tensor relation is

$$\mathbf{G} \equiv i\frac{d\mathbf{R}(\theta)}{d\theta}\Big|_{\theta=0} = i(\hat{y}\hat{x} - \hat{x}\hat{y}) = i\mathbf{R}(\pi/2). \tag{2.46}$$

Clearly, because the length of a vector does not change under rotation, its change must be of direction only, and for a differential change, this must be perpendicular to the original direction. A further consequence of the additive nature of the group parameter (the angle θ) is that this also determines the derivative of a general rotation operator according to

$$\frac{dR(\theta)}{d\theta} = \frac{dR(\theta+\delta)}{d\delta}\Big|_{\delta=0} = \frac{dR(\theta)R(\delta)}{d\delta}\Big|_{\delta=0} = -iR(\theta)G = -iGR(\theta). \tag{2.47}$$

The tensorial analog is

$$\frac{d\mathbf{R}(\theta)}{d\theta} = -i\mathbf{G}\cdot\mathbf{R}(\theta) = -i\mathbf{R}(\theta)\cdot\mathbf{G}. \tag{2.48}$$

Again, the form of this result can be interpreted as the requirement that the differential rotation of a vector must be perpendicular to the original direction of the vector.

The generator G is so known because it can be used to generate the group. Equation (2.47) is a differential equation for the rotation $R(\theta)$, whose integrated form is

$$R(\theta) = e^{-iG\theta}. \tag{2.49}$$

Since G is an abstract operator it is necessary to be cautious about carrying out the integration in the same form as one would do with ordinary functions, but as long as the base e for exponentiation is associated with the group identity (as well as its numerical value), then both left and right sides of the equation are group elements and the equation a valid relation. This equation can also be interpreted by making a Taylor series expansion of the exponential

$$R(\theta) = 1 + \sum_{j=1}^{\infty} \frac{(-iG\theta)^j}{j!}, \tag{2.50}$$

in which each term has a definite meaning and the derivative of the series obviously satisfies Eq. (2.47). The tensorial analog of this exponentiation is

$$\mathbf{R}(\theta) = e^{-i\mathbf{G}\theta} = \mathbf{U}^{(2d)} - i\mathbf{G}\theta + \sum_{j=2}^{\infty} \frac{(-i\mathbf{G}\theta\cdot)^{j-1}}{j!}(-i\mathbf{G}\theta), \tag{2.51}$$

with its Taylor series expansion also listed. Since $\mathbf{G}$ is a tensor and products of $\mathbf{G}$ must be "dotted" together, the detailed expression of the series is complicated by the required presence of the "dots". If it is just assumed that they are to be inserted as required, then the equations can be written simply. This is what has been assumed in the exponential form, but some may object and state that the exponential should be written

$$\mathbf{R}(\theta) = e^{-i\mathbf{G}\theta\cdot}\mathbf{U}^{(2d)} \tag{2.52}$$

so as assure that the right-hand side of the equation is a second order tensor. We find it convenient to write equations with implied contractions if there is no ambiguity in the result, and the formal requirement of adding the contractions (unnecessarily) complicates the writing of the equation. Equation (2.51), either in its exponential or series form, or more formally Eq. (2.52), clearly satisfies Eq. (2.48). From the third relation in Eq. (2.41), it follows that the generator $\mathbf{G}$ satisfies $\mathbf{G}\cdot\mathbf{G} = \mathbf{U}^{(2d)}$, which can be used to simplify the series, or the exponential. For the series, it is convenient to divide the terms according to whether they are even or odd in $\mathbf{G}$. Clearly the product of an even number of $\mathbf{G}$'s is always $\mathbf{U}^{(2d)}$, whereas the product of an odd number reduces to $\mathbf{G}$. Thus, in detail, the series can be simplified according to

$$\begin{aligned}\mathbf{R}(\theta) &= \mathbf{U}^{(2d)}\left[1 + \sum_{k=1}^{\infty}\frac{(-i\theta)^{2k}}{(2k)!}\right] + \mathbf{G}\left[\sum_{k=0}^{\infty}\frac{(-i\theta)^{2k+1}}{(2k+1)!}\right] \\ &= \mathbf{U}^{(2d)}\cos\theta - i\mathbf{G}\sin\theta,\end{aligned} \tag{2.53}$$

which is, of course, equivalent to Eq. (2.36). The exponential form can be reduced in a similar manner, by making use of deMoivre's relations

$$\begin{aligned}\mathbf{R}(\theta) &= e^{-i\mathbf{G}\theta\cdot}\mathbf{U}^{(2d)} = [\cos(\mathbf{G}\theta\cdot) - i\sin(\mathbf{G}\theta\cdot)]\,\mathbf{U}^{(2d)} \\ &= \left[\cos\theta\mathbf{U}^{(2d)}\cdot - i\sin\theta\mathbf{G}\cdot\right]\mathbf{U}^{(2d)} \\ &= \cos\theta\mathbf{U}^{(2d)} - i\sin\theta\mathbf{G}.\end{aligned} \tag{2.54}$$

These manipulations illustrate the important role of the group generator. Before leaving this section, it should be mentioned that the group generator described here is hermitian, which is common for operators in quantum mechanics (and in fact G can be given a physical association when applied to certain physical problems), whereas mathematicians often use $-iG$ as the generator. It is for the physicist and chemist that this book is intended, so it is the former convention that is used here.

2.4 Diagrammatic Representation of Tensors

It has already been stressed that the order in which vectors are written is important. Equivalently, how the indices of a tensor are interpreted. The convention that is followed in this work is that nearest indices are always the first to be dotted together. But whatever convention is used, the evaluation of a tensorial expression can get complicated if there are several different tensors that are contracted (dotted) together. This section describes a manner in which differing orders of contraction can be represented diagrammatically. These have been found to be very useful for visualizing complicated tensorial computations. The first type of problem addressed using this tool is how to represent a change of its indices in any arbitrary manner. Most of the examples given in this section involve polyads, since then the results of the various operations are easily written down. It is assumed that the components of the various vectors and tensors given here commute, that is, they are not, e.g., quantum operators.

Note that this discussion as well as the rest of the book, except for the treatment of spinors, Chap. 10, deals exclusively with vectors and tensors in 3-dimensional space.

The simplest operation of changing the order of indices is that of transposing a second order tensor, which has already been mentioned in Sec. 2.1. Now $\boldsymbol{\mathsf{U}}$ dotted directly into a tensor just preserves the tensor, e.g., for the dyad $\mathbf{ab}$,

$$\boldsymbol{\mathsf{U}}\cdot\mathbf{ab} = \mathbf{ab}. \tag{2.55}$$

Starting with this equation and noticing that $\boldsymbol{\mathsf{U}}$ has two directions, leave the first (left-hand) index where it is but dot the second (right-hand) index into $\mathbf{b}$ produces the transpose. This can be written in a geometrical way as

$$\lfloor\mathbf{a}\rfloor\cdot\mathbf{b} = \mathbf{ba}. \tag{2.56}$$

But it is also useful to express this as a tensor operation on the dyad, which can be written as

$$\boldsymbol{\mathsf{UU}}\odot^2\mathbf{ab} = \boldsymbol{\mathsf{UU}}\,\mathbf{:}\,\mathbf{ab} = \mathbf{ba}, \tag{2.57}$$

where the overlapping $\boldsymbol{\mathsf{U}}$'s indicate the order of their four directions. The combination of $\boldsymbol{\mathsf{U}}$'s can also be written in index form as

$$\left(\boldsymbol{\mathsf{UU}}\right)_{ijk\ell} = \boldsymbol{\mathsf{U}}_{ik}\boldsymbol{\mathsf{U}}_{j\ell}. \tag{2.58}$$

Eq. (2.57) also illustrates both the $\odot^2$ and $\mathbf{:}$ form for carrying out the doubledot contraction. While the above examples use only the dyad $\mathbf{ab}$, the transposition of a general second order tensor $\boldsymbol{\mathsf{T}}$ cannot be expressed in the form of Eq. (2.56), but can be expressed in the form of Eq. (2.57), namely

$$\boldsymbol{\mathsf{UU}}\odot^2\boldsymbol{\mathsf{T}}, \tag{2.59}$$

with index interpretation

$$\left[\boldsymbol{\mathsf{UU}}\odot^2\boldsymbol{\mathsf{T}}\right]_{ij} = \sum_{k\ell}\left(\boldsymbol{\mathsf{UU}}\right)_{ijk\ell}\boldsymbol{\mathsf{T}}_{\ell k} = \boldsymbol{\mathsf{T}}_{ji}. \tag{2.60}$$

or as

$$\llcorner \mathsf{T}\cdot \lrcorner \tag{2.61}$$

For a triad, there are several ways of ordering the three vectors. Starting with the obvious order, one transposition of the triad can be indicated by

$$\llcorner \mathbf{a} \lrcorner \cdot \mathbf{bc} = \sqcup\!\!\!\sqcup \odot^2 \mathbf{abc} = \mathbf{bac}. \tag{2.62}$$

which uses the same tensor operator as above. Another example of a transposition can be written in the form

$$\sqcup\!\!\!\sqcup\!\!\!\sqcup \odot^3 \mathbf{abc} = \llcorner \mathbf{ab} \lrcorner \cdot \mathbf{c} = \mathbf{cab}. \tag{2.63}$$

This transposition, acting on a general third order tensor T, has the index interpretation

$$\left(\sqcup\!\!\!\sqcup\!\!\!\sqcup \odot^3 \mathsf{T}\right)_{ijk} = \sum_{\ell mn} \left(\sqcup\!\!\!\sqcup\!\!\!\sqcup\right)_{ijk\ell mn} \mathsf{T}_{nm\ell} = \sum_{\ell mn} \delta_{i\ell}\delta_{jn}\delta_{km} \mathsf{T}_{nm\ell} = \mathsf{T}_{jki}. \tag{2.64}$$

The various possible transpositions of tensors of arbitrary order can be handled in the same way. They can all be written using a combination of U's overlapping each other so that the order of the directions of the combination map the indices of the tensor on which it acts into the desired order.

The second operation on tensors that is associated with U is the contraction of a pair of indices. The simplest form of this is rewriting the dot product as a contraction with U, see Eq. (2.19). This can be applied on any second order tensor T,

$$\mathsf{U} \odot^2 \mathsf{T} = \sum_i \mathsf{T}_{ii}, \tag{2.65}$$

so is also recognized as the trace of the second order tensor. But the contraction

$$\sqcup\!\!\!\sqcup \odot^3 \mathsf{T}^{(3)} \tag{2.66}$$

of the third order tensor $\mathsf{T}^{(3)}$ gives a vector with direction determined by the middle direction of $\mathsf{T}^{(3)}$, having the indicial interpretation

$$\left(\sqcup\!\!\!\sqcup \odot^3 \mathsf{T}^{(3)}\right)_j = \sum_i \mathsf{T}^{(3)}_{iji}. \tag{2.67}$$

No end of variations of contractions and transpositions can be envisaged as the notation is completely flexible.

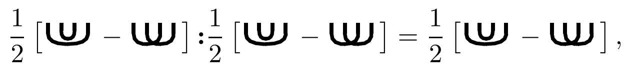
There are only three ways of organizing two U's. These are specifically

$$\text{i)} \quad \mathsf{UU} \qquad \text{ii)} \quad \sqcup\!\!\!\sqcup \qquad \text{iii)} \quad \sqcup\!\!\!\sqcup\,. \tag{2.68}$$

Acting on a second order tensor T, that is taking the double dot product between these fourth order tensors and T, these have the action of: i) replacing T by U times the trace of T, ii) being the identity operation, and iii) transposing the indices on T. But certain linear combinations of these operations are of particular use. It is noticed first that the repeat action of UU gives 3 times a single action. It is useful to take out this factor of 3 so that the result is idempotent, namely

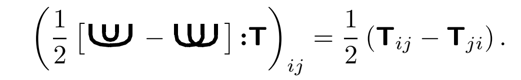
$$\frac{1}{3}\mathsf{UU} : \frac{1}{3}\mathsf{UU} = \frac{1}{3}\mathsf{UU}, \tag{2.69}$$

having the action on a second order tensor of projecting out 1/3 of the part of a second order tensor that corresponds to the trace of the tensor. 1/2 the difference of the second and the third double $\mathbf{U}$ tensors is also idempotent



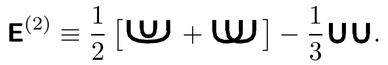
(2.70)

and has the action of projecting out the antisymmetric part of the tensor on which it acts, in indicial form



(2.71)

Clearly the corresponding sum produces the symmetric part of $\mathbf{T}$, but it more useful in the following to also subtract the trace, namely



(2.72)

This tensor is idempotent,

$$\mathbf{E}^{(2)}\mathbf{:}\mathbf{E}^{(2)} = \mathbf{E}^{(2)}, \tag{2.73}$$

and selects out the traceless symmetric part of the second order tensor on which it acts. The indicial equivalent is

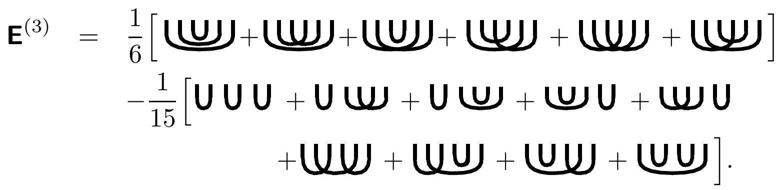
$$\left(\mathbf{E}^{(2)}\mathbf{:}\mathbf{T}\right)_{ij} = \frac{1}{2}\left(\mathbf{T}_{ij} + \mathbf{T}_{ji}\right) - \frac{1}{3}\delta_{ij}\sum_k \mathbf{T}_{kk}. \tag{2.74}$$

It is assumed that the indices label an orthonormal basis. In this way the tensor $\mathbf{T}$ can be divided up into its symmetric traceless, antisymmetric and trace parts, with the identity for second order tensors being the sum

(2.75)

Only the symmetric traceless projector is given a special notation in this book since it has a unique role for the 3-dimensional rotation group, see Sec. 3.3. It is also useful to note that a second order tensor has 9 independent components, and the division according to Eq. (2.75) is into 5 components for the traceless symmetric part, 3 for the antisymmetric part and 1 trace component.

For three $\mathbf{U}$'s, there are 15 ways of permuting the order of the indices. These can be organized in various combinations but only the combination that acts to select out the completely symmetric traceless part of a third order tensor will be considered in detail. By this it is meant that for every pair of indices, the third order tensor is symmetric, and a contraction of any pair of indices with $\mathbf{U}$ gives zero. Such a combination of 3 $\mathbf{U}$'s can be found by starting with the identity and then adding those combinations to make both the first and last sets of three indices symmetric, then subtract a multiple of the combination of all terms in which one pair of the first set of three indices has a $\mathbf{U}$. The multiple must be chosen so that the result is traceless for the first pair of indices, while an overall scale factor can be chosen so that the resultant tensor is idempotent. The result is



(2.76)

The same procedure can be carried out for an arbitrary number of U's. There are in fact $(2n-1)(2n-3)\cdots 3 = (2n-1)!!$ combinations of n U's, but in all cases there is only one unique linear combination of n U's that is symmetric and traceless in the first (and automatically the last) set of n indices. While it may not be desired to explicitly calculate such combinations, the procedure for doing so is nevertheless clear. Choosing the appropriate scale factor, these quantities are idempotent and define the tensors designated in the following as $\mathsf{E}^{(n)}$, one for each integer n. These are elaborated upon, and their properties discussed in greater detail, in Sec. 3.3.

The fourth of the four tensor operations, Sec. 2.2, is the formation of the cross product. This is associated with the Levi Cevita tensor $\boldsymbol{\varepsilon}$, Eq. (2.23) as exemplified by Eq. (2.24). That equation also illustrates how a part of a dyad can be expressed as a vector. The inverse operation

$$\boldsymbol{\varepsilon}\cdot(\mathbf{r}_1\times\mathbf{r}_2) = \mathbf{r}_1\mathbf{r}_2 - \mathbf{r}_2\mathbf{r}_1 \tag{2.77}$$

converts the cross product of two vectors into a dyadic, specifically an antisymmetric dyadic. This can also be applied to find a vector associated with an arbitrary second order tensor T,

$$\mathbf{T} \equiv -\boldsymbol{\varepsilon}:\mathsf{T}. \tag{2.78}$$

Of course this may be zero. For the inverse association, given a vector $\mathbf{T}$, an antisymmetric second order tensor can be obtained,

$$\mathsf{T} = -\mathsf{T}^t = \boldsymbol{\varepsilon}\cdot\mathbf{T}. \tag{2.79}$$

More generally, the antisymmetric part of a second order tensor T, Eq. (2.71), is reproduced from the vector $\mathbf{T}$ by

$$\mathsf{T} - \mathsf{T}^t = \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbf{T}. \tag{2.80}$$

Thus the antisymmetric part of a second order tensor is equivalent to a vector. Combining the two operations together give the two identities

$$\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} = \sqcup\!\sqcup - \sqcup\!\sqcup, \qquad \frac{1}{2}\left[\sqcup\!\sqcup - \sqcup\!\sqcup\right]:\boldsymbol{\varepsilon} = -\boldsymbol{\varepsilon}. \tag{2.81}$$

Note also the idempotency relation (2.70). The minus sign arises because the order of contraction has been taken to work from inside out. Further contractions of the first identity gives

$$\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon} = -2\mathsf{U} \tag{2.82}$$

and

$$\boldsymbol{\varepsilon}\odot^3\boldsymbol{\varepsilon} = -6. \tag{2.83}$$

All these relations can be traced to the evaluation of the direct product of two $\boldsymbol{\varepsilon}$'s,

$$\boldsymbol{\varepsilon}\,\boldsymbol{\varepsilon} = \sqcup\!\sqcup\!\sqcup + \sqcup\!\sqcup\!\sqcup + \sqcup\!\sqcup\!\sqcup - \sqcup\!\sqcup\!\sqcup - \sqcup\!\sqcup\!\sqcup - \sqcup\!\sqcup\!\sqcup \tag{2.84}$$

That is, two $\boldsymbol{\varepsilon}$'s can always be written in terms of combinations of U. This has the important simplifying feature that no tensor need have a product of $\boldsymbol{\varepsilon}$'s in any of its terms.

With the introduction of $\boldsymbol{\varepsilon}$ and the breakdown of the identity for second order tensors, Eq. (2.75), any second order tensor T can be written in the form

$$\mathsf{T} = \mathsf{E}^{(2)}:\mathsf{T} + \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbf{T} + T\mathsf{U}, \tag{2.85}$$

as a sum of its symmetric traceless part, its antisymmetric part expressed in terms of the equivalent vector **T**, and its trace

$$T \equiv \frac{1}{3}\sum_i \mathbf{T}_{ii}. \tag{2.86}$$

Finally it should be recognized that combinations of $\mathbf{U}$ and $\boldsymbol{\varepsilon}$ can occur. To express tensors in which the indices of $\mathbf{U}$ and $\boldsymbol{\varepsilon}$ overlap, it is convenient to think of the three indices on $\boldsymbol{\varepsilon}$, listed according to being a right-handed coordinate system, as being: 1) attached the left-hand side of $\boldsymbol{\varepsilon}$; 2) attached to the free end of the upper branch of the $\boldsymbol{\varepsilon}$; and 3) attached to the free end of the bottom branch of the $\boldsymbol{\varepsilon}$, which is extended so that the three indices have a definite order, see Fig. 2.2.

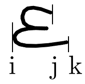
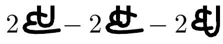


Figure 2.2: Showing the placement of the three indices for the Levi Civita tensor.

Direct products of arbitrary numbers of $\mathbf{U}$'s and $\boldsymbol{\varepsilon}$'s can be of even order, in which case the resultant tensor is expressible, because of Eq. (2.84), entirely in terms of $\mathbf{U}$. Tensors of odd order need one $\boldsymbol{\varepsilon}$, and can be expressed using only one $\boldsymbol{\varepsilon}$. There is thus only one tensor of order 3, namely $\boldsymbol{\varepsilon}$ itself, whereas there are 10 fifth order tensors, each involving one $\mathbf{U}$ and one $\boldsymbol{\varepsilon}$. But according to the parentage scheme of Sec. 3.5, there are only 6 linearly independent combinations of $\mathbf{U}$ and $\boldsymbol{\varepsilon}$ of order 5. There are thus 4 linear relations between the 10 fifth order tensors. One way to produce these relations is to doubledot $\boldsymbol{\varepsilon}$ into Eq. (2.84). Contracting on the left-hand side and collecting terms gives

$$-2\mathbf{U}\boldsymbol{\varepsilon} =$$  (2.87)

This unlikely looking identity can be checked by taking components in a variety of ways. The other three relations can be obtained by taking different cyclic permutations of this equation. Any relation between tensors of odd higher order formed solely from $\boldsymbol{\varepsilon}$ and $\mathbf{U}$'s must be a combination of these relations.

2.5 Rotations in Three Dimensions

A rotation in 3-dimensional space requires both an angle of rotation and an axis about which the rotation is to be made. Thus the rotation $R_{\hat{n}}(\theta)$ is the (right-handed) rotation by an angle θ about the direction of the unit vector $\hat{n}$. The axis $\hat{n}$ describes a plane normal to $\hat{n}$ so, projected onto this plane, the rotation is the same as if the rotation occurred in 2-dimensions.

Given a vector $\mathbf{r}$, it is first necessary to partition this vector into parts in and out of the plane of rotation, equivalently to the parts perpendicular and parallel to $\hat{n}$. The component of $\mathbf{r}$ parallel to $\hat{n}$ is $\hat{n}\cdot\mathbf{r}$, so the part of $\mathbf{r}$ that is parallel to $\hat{n}$ is the vector $\hat{n}\hat{n}\cdot\mathbf{r}$. This part is unaffected by any rotation about the $\hat{n}$ axis. It follows that the part of $\mathbf{r}$ that is perpendicular to $\hat{n}$ is $(\mathbf{U} - \hat{n}\hat{n})\cdot\mathbf{r}$. Now in a rotation, it is this part that is reduced in magnitude by $\cos\theta$ while a component of the rotated vector is formed in the plane of the rotation but perpendicular (with right-hand rule) to the original "in-plane" vector. Clearly this direction is in the dirction of the vector $\hat{n}\times\hat{r}$. Thus the effect of $R_{\hat{n}}(\theta)$ on $\mathbf{r}$ is

$$R_{\hat{n}}(\theta)\mathbf{r} = \hat{n}\hat{n}\cdot\mathbf{r} + \cos\theta(\mathbf{U} - \hat{n}\hat{n})\cdot\mathbf{r} + \sin\theta\hat{n}\times\mathbf{r}, \tag{2.88}$$

with the cross product in the last term responsible for selecting out only that magnitude of $\mathbf{r}$ that is perpendicular to $\hat{n}$. This operation can be expressed in tensorial form

$$R_{\hat{n}}(\theta)\mathbf{r} = \mathsf{R}_{\hat{n}}(\theta)\cdot\mathbf{r} \tag{2.89}$$

with rotation tensor

$$\mathsf{R}_{\hat{n}}(\theta) = \hat{n}\hat{n} + \cos\theta(\mathsf{U} - \hat{n}\hat{n}) - \sin\theta\hat{n}\cdot\boldsymbol{\mathcal{E}}\ . \tag{2.90}$$

In comparison with the 2-dimensional rotation tensor of Eq. (2.36), the rotation by $\pi/2$ is replaced by $-\hat{n}\cdot\boldsymbol{\mathcal{E}}$, which is the same if $\hat{n}$ is the special direction $\hat{z}$ normal to the plane used for the description of 2-dimensional rotations, and there is the introduction of terms for separating the initial vector into parts parallel and perpendicular to the rotation axis $\hat{n}$. Essentially $\mathsf{R}_{\hat{n}}(\theta)$ is the embedding of a two dimensional rotation tensor $\mathsf{R}(\theta)$ in three dimensions, with a selection as to what direction is the rotation axis.

If only the set of rotations about the same ($\hat{n}$) axis is considered, then these have the same properties as those discussed for the rotations in a plane. Namely they form a commutative 1-parameter group of rotations. Necessarily they have a generator $G_{\hat{n}}$, so that abstractly

$$R_{\hat{n}}(\theta) = e^{-iG_{\hat{n}}\theta}. \tag{2.91}$$

The tensorial analog $\mathsf{G}_{\hat{n}}$ of the abstract generator $G_{\hat{n}}$ is

$$\mathsf{G}_{\hat{n}} = -i\hat{n}\cdot\boldsymbol{\mathcal{E}}\ . \tag{2.92}$$

This can be verified by differentiating Eq. (2.90). An exponentiation of this generator can be calculated, but it is first necessary to know how the powers of $\mathsf{G}_{\hat{n}}$ behave.

Specifically the square of $\mathsf{G}_{\hat{n}}$ is

$$\begin{aligned}\mathsf{G}_{\hat{n}}\cdot\mathsf{G}_{\hat{n}} &= -(\hat{n}\cdot\boldsymbol{\mathcal{E}}\ )\cdot(\hat{n}\cdot\boldsymbol{\mathcal{E}}\ ) = -\hat{n}\cdot(\boldsymbol{\mathcal{E}}\cdot\boldsymbol{\mathcal{E}}\ )\cdot\hat{n} \\ &= -\hat{n}\cdot\left(\mathsf{UU} - \mathsf{UU}\right)\cdot\hat{n} = \mathsf{U} - \hat{n}\hat{n}.\end{aligned} \tag{2.93}$$

An alternate but direct proof of this can be made by introducing the right-handed coordinate system $\hat{n},\ \hat{p},\ \hat{q}$. It follows that $\hat{n}\cdot\boldsymbol{\mathcal{E}}\ = \hat{p}\hat{q} - \hat{q}\hat{p}$, so that the contraction of the square of the generator leads to

$$\mathsf{G}_{\hat{n}}\cdot\mathsf{G}_{\hat{n}} = \hat{p}\hat{p} + \hat{q}\hat{q}, \tag{2.94}$$

which is exactly equal to $\mathsf{U} - \hat{n}\hat{n}$. It is also useful to consider the following general rationale for this identification, since it is indicative of the kind of reasoning that can be applied to a number of tenorial reductions. This goes as follows:

1) One direction of each $\boldsymbol{\mathcal{E}}$ is dotted into a direction of the other $\boldsymbol{\mathcal{E}}$. This requires those two directions to be equal. 2) One direction of each $\boldsymbol{\mathcal{E}}$ is dotted into $\hat{n}$. 3) Since $\boldsymbol{\mathcal{E}}$ is completely antisymmetic, all three directions must be different, and since the two $\boldsymbol{\mathcal{E}}$'s have two directions in common, it follows that the third direction of each $\boldsymbol{\mathcal{E}}$ must also be the same. 4) Since only the direction $\hat{n}$ is preferentially selected out, the above "third" direction can be either of those two directions perpendicular to $\hat{n}$, so a sum of both possibilities is what will appear. 5) Lastly, since the order of dotting of one $\boldsymbol{\mathcal{E}}$ is in opposite order to the other $\boldsymbol{\mathcal{E}}$, the resulting contraction should be negative, this compensating the i^2 that appears in $\mathsf{G}_{\hat{n}}\cdot\mathsf{G}_{\hat{n}}$. This set of reasonings imply Eq. (2.94).

It follows that the cube of $\mathsf{G}_{\hat{n}}$ is $\mathsf{G}_{\hat{n}}$, and all even powers are the same $\mathsf{U} - \hat{n}\hat{n}$, formally

$$\begin{aligned}(\mathsf{G}_{\hat{n}})^{2j+1} &= \mathsf{G}_{\hat{n}} && \text{for all integer } j \text{ including } j = 0 \\ (\mathsf{G}_{\hat{n}})^{2j} &= \mathsf{U} - \hat{n}\hat{n} && \text{for all integer } j > 0.\end{aligned} \tag{2.95}$$

These results are now used to express the tensorial form of the exponentiation of the 3-dimensional rotation generator.

The tensorial form for the exponential of the rotation generator can be calculated via deMoivre's relations according to

$$\begin{aligned}\mathbf{R}_{\hat{n}}(\theta) &= e^{-i\mathbf{G}_{\hat{n}}\theta}\cdot\mathbf{U}\\ &= [\cos(\mathbf{G}_{\hat{n}}\theta) - i\sin(\mathbf{G}_{\hat{n}}\theta)]\cdot\mathbf{U}\\ &= \mathbf{U} + [\cos(\mathbf{G}_{\hat{n}}\theta) - \mathbf{U} - i\sin(\mathbf{G}_{\hat{n}}\theta)]\cdot\mathbf{U}\\ &= \mathbf{U} + [\cos\theta - 1]\,[\mathbf{U} - \hat{n}\hat{n}] - i\sin\theta\mathbf{G}_{\hat{n}}.\end{aligned} \tag{2.96}$$

This is equivalent to Eq. (2.90). Note that the separation of a $\mathbf{U}$ is introduced so that the combination $\cos(\mathbf{G}_{\hat{n}}\theta) - \mathbf{U}$, which is a power series in $\mathbf{G}_{\hat{n}}^2$, can be obtained and simplified according to Eq. (2.95).

2.5.1 The 3-dimensional rotation group

If a vector is rotated by an angle θ_1 about axis $\hat{n}_1$, and subsequently rotated by an angle θ_2 about axis $\hat{n}_2$, the composite of the two actions is intuitively a rotation that should be describable as the rotation by some angle θ about some axis $\hat{n}$. The objective is to verify this by finding the resultant angle θ and axis $\hat{n}$ in terms of the originally applied angles θ_1 and θ_2 and axes $\hat{n}_1$ and $\hat{n}_2$. This is done here using the tensorial form for their rotations, namely

$$\begin{aligned}\mathbf{R}_{\hat{n}_2}(\theta_2)\cdot\mathbf{R}_{\hat{n}_1}(\theta_1) &= [\hat{n}_2\hat{n}_2 + \cos(\theta_2)(\mathbf{U} - \hat{n}_2\hat{n}_2) - \sin(\theta_2)\hat{n}_2\cdot\boldsymbol{\mathcal{E}}\,]\\ &\quad\cdot[\hat{n}_1\hat{n}_1 + \cos(\theta_1)(\mathbf{U} - \hat{n}_1\hat{n}_1) - \sin(\theta_1)\hat{n}_1\cdot\boldsymbol{\mathcal{E}}\,]\\ &\stackrel{?}{=} \mathbf{R}_{\hat{n}}(\theta) = \hat{n}\hat{n} + \cos\theta(\mathbf{U} - \hat{n}\hat{n}) - \sin\theta\hat{n}\cdot\boldsymbol{\mathcal{E}}\,.\end{aligned} \tag{2.97}$$

The validity of this equation can be demonstrated by checking that both sides have the same trace, antisymmetric and symmetric parts. First is the trace, which is calculated by taking the contraction of Eq. (2.97) with $\mathbf{U}$, which after simplification is

$$\begin{aligned}\mathbf{U}:\mathbf{R}_{\hat{n}}(\theta) &= 4\,[\cos(\theta_1/2)\cos(\theta_2/2) - \sin(\theta_1/2)\sin(\theta_2/2)\hat{n}_1\cdot\hat{n}_2]^2 - 1\\ &= 2\cos\theta + 1 = 4\cos(\theta/2)^2 - 1.\end{aligned} \tag{2.98}$$

It follows that the angle θ of the combined rotation is given by

$$\cos(\theta/2) = \cos(\theta_1/2)\cos(\theta_2/2) - \sin(\theta_1/2)\sin(\theta_2/2)\hat{n}_1\cdot\hat{n}_2. \tag{2.99}$$

On the basis that $0 \le \theta \le \pi$, the latter equation determines the angle θ uniquely. It should be emphasized that there is a choice of phase in taking the square root and that the choice presented is so that the relation becomes an identity as θ_1 and/or θ_2 approach 0. If one or more of the angles is larger than π, then it may be necessary to be careful to find the root that is consistent with the notion of how the pair of rotations has been carried out, see the discussion in the following two paragraphs. The axis direction can be obtained by looking at the antisymmetric part of Eq. (2.97), equivalently by taking (1/2) the doubledot contraction with $\boldsymbol{\mathcal{E}}$, compare Eq. (2.82). After simplification and recognizing that the result can be factored into the product of scalar and vector factors,

$$\begin{aligned} \frac{1}{2}\boldsymbol{\mathcal{E}}:\mathbf{R}_{\hat{n}}(\theta) &= 2\left[\cos(\theta_1/2)\cos(\theta_2/2) - \sin(\theta_1/2)\sin(\theta_2/2)\hat{n}_1\cdot\hat{n}_2\right] \\ &\quad\times\left[\sin(\theta_1/2)\cos(\theta_2/2)\hat{n}_1 + \sin(\theta_2/2)\cos(\theta_1/2)\hat{n}_2\right. \\ &\qquad\qquad \left.- \sin(\theta_1/2)\sin(\theta_2/2)\hat{n}_1\times\hat{n}_2\right] \\ &= \sin\theta\hat{n}. \end{aligned} \tag{2.100}$$

It is easily shown that the magnitude of the product is exactly $\sin\theta$, consistent with Eq. (2.99), so that

$$\hat{n} = \frac{\sin(\theta_1/2)\cos(\theta_2/2)\hat{n}_1 + \sin(\theta_2/2)\cos(\theta_1/2)\hat{n}_2 - \sin(\theta_1/2)\sin(\theta_2/2)\hat{n}_1\times\hat{n}_2}{\sin(\theta/2)} \tag{2.101}$$

is indeed a unit vector. Finally, it is checked whether the doubledot contraction with $\hat{n}\hat{n}$ gives $\hat{n}\hat{n}:\mathbf{R}(\theta) = 1$. This can be shown to be true, but is a lengthy calculation which is not reproduced here. A simpler approach to deducing these properties of a product of rotations is via the method of spinors, see Sec. 10.2.1.

Clearly, with this product, the identity rotation is $\mathbf{R}_{\hat{n}}(0)$ in any direction $\hat{n}$ and the inverse of the rotation $\mathbf{R}_{\hat{n}}(\theta)$ is the rotation $\mathbf{R}_{-\hat{n}}(\theta)$, namely by an angle θ about the opposite direction. This retains the condition that a rotation angle is between 0 and π. Thus the rotations form a group. It is useful to picture the group elements as being equivalent to the projected 3-sphere P_3 of radius π, with a rotation of angle θ about axis $\hat{n}$ being the point in the sphere in the direction $\hat{n}$ at a radius θ. It is a projected sphere since a rotation of angle π about either the positive or negative directions $\pm\hat{n}$ is the same rotation, thus points on opposite ends of a diagonal must be identified. This is illustrated in Fig. 2.3.

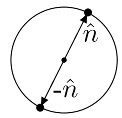


Figure 2.3: Opposite points on the diameter of the sphere of radius π designate equivalent rotations

It is useful to consider the effect of a sequence of rotations, starting from an initial orientation, which is usually thought of having no rotation ($\theta = 0$), but it is possible to start from any orientation. As a body is rotated, the sequence of rotations is conveniently described by mapping out a path in P_3. If, in particular, the body returns to its original orientation, then this is given by a closed path. There are two different classes of paths (homotopy classes), namely those that lie entirely within the sphere, and those that jump from one end of a diagonal to the other [5]. In the first class it is always possible to continuously deform the path to a point - which means looking at a set of paths (each a sequence of rotations), each slightly different one from the other, and each covering a smaller range of orientations - until the path no longer moves from its original point. In contrast, if a sequence of rotations involves the rotation by larger and larger angles, say from 0 to 2π about the same axis, then at π, there is a jump from one end of a diagonal to the other. This path is equivalent to starting from the origin, going out to the surface of P_3, jumping to the other end of the diagonal and coming back to the origin from that side of the sphere. In such a case the path on P_3 can not be continuously deformed to a point. Such paths form the second homotopy class. Of course, if there are two jumps across diagonals in the path describing the sequence of rotations, it is always possible to continuously deform one jump to exactly compensate for the other, with the net result that this path is equivalent to making no jump and the path can thus be deformed to a point. That there are two classes of paths is central to the existence of both single-valued and double-valued representations of the rotation group. For the explicit rotation of vectors and representations on the tensor product of the 3-dimensional vector space, see Chap. 3, all representations are single-valued so there is no special consequence of the existnce of the second homotopy class. Double-valued representations and the importance of the existence of a second homotopy class arise when dealing with represention on vector spaces of even dimension, which is the spinor case, see Chap. 10.

Since $\hat{n}$ and θ arising from a product of rotations involve the cross product $\hat{n}_1 \times \hat{n}_2$, which depends on the order of application of the rotations, it follows that rotations about different axes do not commute. The same must also be true of their generators. This can be seen explicitly by the commutation of their tensorial forms

$$\begin{aligned} &\mathbf{G}_{\hat{n}_2} \cdot \mathbf{G}_{\hat{n}_1} - \mathbf{G}_{\hat{n}_1} \cdot \mathbf{G}_{\hat{n}_2} \\ &= -\hat{n}_2 \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon} \cdot \hat{n}_1 + \hat{n}_1 \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon} \cdot \hat{n}_2 = -\hat{n}_1 \hat{n}_2 + \hat{n}_2 \hat{n}_1 \\ &= \boldsymbol{\varepsilon} \cdot (\hat{n}_2 \times \hat{n}_1) = i \mathbf{G}_{\hat{n}_2 \times \hat{n}_1}. \end{aligned} \tag{2.102}$$

As long as $\hat{n}_1$ and $\hat{n}_2$ are different, then the three directions $\hat{n}_1$, $\hat{n}_2$ and $\hat{n}_2 \times \hat{n}_1$ provide three different directions about which rotations can occur, and thus span all possible rotation generators. For the special case that $\hat{n}_2 = \hat{x}$ and $\hat{n}_1 = \hat{y}$, this commutation relation is

$$\mathbf{G}_{\hat{x}} \cdot \mathbf{G}_{\hat{y}} - \mathbf{G}_{\hat{y}} \cdot \mathbf{G}_{\hat{x}} = i \mathbf{G}_{\hat{z}}. \tag{2.103}$$

Such a commutation relation is the same as that for angular momentum, reasonably so since angular momentum deals with the rotation of a physical system. What must be clearly distinguished though, is that the $\mathbf{G}_{\hat{n}}$ could be generating the effect of a rotation on a set of mathematical objects, having nothing to do with rotating a physical system. Thus the rotation generators that one is dealing with here are of a very general nature, so should not be equated with the physical notion of angular momentum. They just happen to have the same commutation properties since the set of angular momentum operators is just the special case that generate rotations of a physical system. In fact, the rotation of angular momentum tensors will be discussed in Chap. 11, so the distinction between an angular momentum and a general rotation generator needs to be recognized. But the algebraic similarity between the properties of the angular momentum operators and the rotation generators means that one can appeal to well known angular momentum properties to deduce similar relations for the rotation generators.

It follows by analogy with the angular momentum commutation rules, that if raising and lowering generators are defined as

$$\mathbf{G}_+ \equiv \mathbf{G}_{\hat{x}} + i \mathbf{G}_{\hat{y}} \qquad \mathbf{G}_- \equiv \mathbf{G}_{\hat{x}} - i \mathbf{G}_{\hat{y}}, \tag{2.104}$$

then these satisfy the raising and lowering relations

$$\mathbf{G}_{\hat{z}} \cdot \mathbf{G}_+ = \mathbf{G}_+ \cdot (\mathbf{G}_{\hat{z}} + \mathbf{U}) \qquad \mathbf{G}_{\hat{z}} \cdot \mathbf{G}_- = \mathbf{G}_- \cdot (\mathbf{G}_{\hat{z}} - \mathbf{U}) \tag{2.105}$$

while the Casimir operator

$$\mathbf{G}^2 \equiv \mathbf{G}_{\hat{x}} \cdot \mathbf{G}_{\hat{x}} + \mathbf{G}_{\hat{y}} \cdot \mathbf{G}_{\hat{y}} + \mathbf{G}_{\hat{z}} \cdot \mathbf{G}_{\hat{z}} \tag{2.106}$$

commutes with all generators

$$\mathbf{G}^2 \cdot \mathbf{G}_{\hat{n}} = \mathbf{G}_{\hat{n}} \cdot \mathbf{G}^2. \tag{2.107}$$

These relations have been expressed using the $\hat{x}$, $\hat{y}$, $\hat{z}$ coordinate axes, but any set of orthogonal axes labelled according to a right-handed coordinate system would do just as well.

2.5.2 Eulerian Angles

This book emphasizes a coordinate free description of vectors and tensors (in 3-dimensions). In contrast, most books describe vectors and tensors only in terms of their coordinates. A connection beteen the two descriptions requires choosing some fixed coordinate system, whose axes are usually labelled $\hat{x}$, $\hat{y}$ and $\hat{z}$. It is emphasized that in this book, this coordinate system is taken as being right-handed and fixed in space, sometimes referred to as a lab-fixed frame. In reference to this basis, the spherical coordinates r, θ and ϕ of a vector $\mathbf{r}$ are given by Eqs. (2.1-2.4). A standard form for representing a rotation in 3-dimensional space is by means of the Eulerian angles α, β and γ. These are defined by considering the rotation being made up of three rotations: first is a rotation about the $\hat{z}$-axis by angle α; second by a rotation about a new $\hat{y}$-axis, usually labelled $\hat{y}'$, by angle β; and lastly about a new $\hat{z}$-axis, labelled $\hat{z}''$ by angle γ, specifically, any rotation can be written in the form

$$R_{\hat{n}}(\theta) = R_{\hat{z}''}(\gamma) R_{\hat{y}'}(\beta) R_{\hat{z}}(\alpha). \tag{2.108}$$

The details of the connection between the axis-angle and Euler angle representations of a rotation are given later in this subsection. But first it is necessary to describe in detail the rotated axes.

The $\hat{y}'$ and $\hat{z}''$ axes are obtained by considering unit vectors initially aligned along the lab-fixed $\hat{y}$ and $\hat{z}$ axes and allowing these unit vectors to rotate with the prescribed rotations. It is necessary to be very clear in this regard, since the lab-fixed axes remain fixed! Only a pair of unit vectors initially aligned along them change! Thus the coordinate system itself does not rotate, but remains fixed.

The new axes arise because of the previous rotations, thus $\hat{y}'$ is explicitly given by

$$\hat{y}' = \mathsf{R}_{\hat{z}}(\alpha)\cdot\hat{y} = \hat{y}\cos\alpha - \hat{x}\sin\alpha, \tag{2.109}$$

where $\hat{y}$ designates a unit vector initially aligned along the $\hat{y}$-direction. Analogously, $\hat{z}''$ is

$$\hat{z}'' = \mathsf{R}_{\hat{y}'}(\beta)\cdot\hat{z} = \hat{z}\cos\beta + \hat{x}'\sin\beta, \tag{2.110}$$

where $\hat{x}'$ is the unit vector obtained from rotating a unit vector initially aligned along the $\hat{x}$-axis by the α rotation, namely

$$\hat{x}' = \mathsf{R}_{\hat{z}}(\alpha)\cdot\hat{x} = \hat{x}\cos\alpha + \hat{y}\sin\alpha. \tag{2.111}$$

Substituting the definition of $\hat{x}'$ into Eq. (2.110), the axis for the final rotation is

$$\hat{z}'' = \hat{z}\cos\beta + \sin\beta[\hat{x}\cos\alpha + \hat{y}\sin\alpha]. \tag{2.112}$$

The form of the last equation shows that β and α are the angles associated with the spherical coordinates that specifies the orientation of the final rotation axis, or equivalently, the set of rotations that take a unit vector along the lab-fixed $\hat{z}$-axis into the unit vector $\hat{z}''$.

Such a rotation is labelled as active, as are all rotations in this book, unless specifically described otherwise. That is, a rotation rotates the vector (or other object) on which it acts, but leaves the coordinate system fixed. In contrast, a passive rotation leaves the vector fixed but rotates the coordinate system, thus changing the description of the unchanged vector. The literature has both, not always stating which interpretation of a rotation is being considered, which is confusing. I prefer the active interpretation and that is what is presented both here, inherently in the presentation of Secs. 2.3 and 2.5, and in the rest of the book.

While on the question of how any vector aligned along a fixed axis would be rotated, consider also the $\hat{x}'''$ and $\hat{y}'''$ directions. [It has not been stated, but understood, that the α rotation produces primed directions, carrying out the β rotation as well gives double primed directions and carrying out the γ rotation as well gives triple primed directions. Since the γ rotation is about the $\hat{z}''$ axis, it follows that $\hat{z}''' = \hat{z}''$.] As an intermediary for this calculation, the direction

$$\begin{aligned} \hat{x}'' &= \mathbf{R}_{\hat{y}'}(\beta)\cdot\hat{x}' = \hat{x}'\cos\beta - \hat{z}'\sin\beta \\ &= \cos\beta[\hat{x}\cos\alpha + \hat{y}\sin\alpha] - \hat{z}\sin\beta \end{aligned} \tag{2.113}$$

is needed. It follows that

$$\begin{aligned} \hat{x}''' &= \mathbf{R}_{\hat{z}''}(\gamma)\cdot\hat{x}'' = \hat{x}''\cos\gamma + \hat{y}''\sin\gamma \\ &= \hat{x}[\cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma] + \hat{y}[\sin\alpha\cos\beta\cos\gamma \\ &\quad + \cos\alpha\sin\gamma] - \hat{z}\sin\beta\cos\gamma \end{aligned} \tag{2.114}$$

and

$$\begin{aligned} \hat{y}''' &= \mathbf{R}_{\hat{z}''}(\gamma)\cdot\hat{y}'' = \hat{y}''\cos\gamma - \hat{x}''\sin\gamma \\ &= \hat{x}[-\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma] + \hat{y}[\cos\alpha\cos\gamma \\ &\quad - \sin\alpha\cos\beta\sin\gamma] + \hat{z}\sin\beta\sin\gamma. \end{aligned} \tag{2.115}$$

If the components of an arbitrary vector $\mathbf{v}$ are written as a column vector

$$\mathbf{v} = v_x\hat{x} + v_y\hat{y} + v_z\hat{z} \iff \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} \equiv \vec{v}, \tag{2.116}$$

denoted here by $\vec{v}$, then the action of an active rotation of the vector, namely

$$\begin{aligned} \mathbf{R}_{\hat{z}''}(\gamma)\cdot\mathbf{R}_{\hat{y}'}(\beta)\cdot\mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{v} &= v_x\hat{x}''' + v_y\hat{y}''' + v_z\hat{z}''' \\ &\equiv v'_x\hat{x} + v'_y\hat{y} + v'_z\hat{z}, \end{aligned} \tag{2.117}$$

is given by the action on the column vector by the rotation matrix

$$R(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma & \cos\alpha\cos\gamma-\sin\alpha\cos\beta\sin\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}, \tag{2.118}$$

namely

$$\vec{v}' = R(\alpha,\beta,\gamma)\vec{v}. \tag{2.119}$$

It is emphasized that the basis for $\vec{v}$, the rotated vector $\vec{v}'$, and this matrix is the lab-fixed frame $\hat{x}$, $\hat{y}$, $\hat{z}$. That is, all components are with respect to the same fixed reference frame.

The rotation specified by the Euler angles α, β and γ can be calculated in two different ways, each as the product of three rotations, namely

$$\mathbf{R}_{\hat{z}''}(\gamma)\cdot\mathbf{R}_{\hat{y}'}(\beta)\cdot\mathbf{R}_{\hat{z}}(\alpha) = \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{R}_{\hat{z}}(\gamma). \tag{2.120}$$

The first order is what has been previously described and is standardly given as the definition of the action of the Euler angles while the second form has the order of rotations reversed, and is simpler, in that each rotation is about a lab-fixed axis. That these produce the same result depends on a fascinating relation, exemplified by

$$\mathbf{R}_{\hat{y}'}(\beta)\cdot\mathbf{R}_{\hat{z}}(\alpha) = \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{R}_{\hat{y}}(\beta), \tag{2.121}$$

where $\hat{y}'$ is given by Eq. (2.109). The physical meaning of this relation can be visualized by contrasting how a vector initially aligned along the $\hat{z}$ direction is rotated. In the second version, such a vector is first rotated around the y-axis by β, so it lies in the xz-plane, then about the z-axis which rotates the result in an xy-plane. The first version of Eq. (2.121) gets the same net result by first rotating about the z-axis, for which nothing happens, so that the whole effect is by the rotation by β, but this must be about an axis perpendicular to both the $\hat{z}$ and desired final orientation of the vector. This is exactly the $\hat{y}'$ direction. Two mathematical proofs of this relation and its consequence, Eq. (2.120), are given below, neither of which appears to be discussed in the literature.

Proof by composition

A relation equivalent to Eq. (2.121) is obtained as a combination of two applications of the composition rule of Eq. (2.97). Let

$$\mathbf{R}_{\hat{m}}(\psi) \equiv \mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{R}_{\hat{z}}(-\alpha) \tag{2.122}$$

be the rotation resulting as a product of these two rotations. Then according to Eqs. (2.99) and (2.101), the angle ψ and axis direction $\hat{m}$ are given by

$$\cos(\psi/2) = \cos(\alpha/2)\cos(\beta/2) \tag{2.123}$$

and

$$\hat{m} = \frac{-\sin(\alpha/2)\cos(\beta/2)\hat{z} + \sin(\beta/2)\cos(\alpha/2)\hat{y} - \sin(\alpha/2)\sin(\beta/2)\hat{x}}{\sin(\psi/2)}. \tag{2.124}$$

Then the final product

$$\mathbf{R}_{\hat{n}}(\theta) = \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{R}_{\hat{m}}(\psi) \tag{2.125}$$

has an angle determined by

$$\cos(\theta/2) = \cos(\psi/2)\cos(\alpha/2) - \sin(\psi/2)\sin(\alpha/2)\hat{z}\cdot\hat{m} = \cos(\beta/2), \tag{2.126}$$

so that $\theta = \beta$. The corresponding axis of rotation is

$$\begin{aligned}\hat{n} &= \frac{\sin(\psi/2)\cos(\alpha/2)\hat{m} + \sin(\alpha/2)\cos(\psi/2)\hat{z} - \sin(\psi/2)\sin(\alpha/2)\hat{m}\times\hat{z}}{\sin(\beta/2)} \\ &= -\sin\alpha\hat{x} + \cos\alpha\hat{y} = \mathbf{R}_{\hat{z}}(\alpha)\cdot\hat{y},\end{aligned} \tag{2.127}$$

which has been identified as $\hat{y}'$. Thus the identity

$$\mathbf{R}_{\hat{y}'}(\beta) = \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{R}_{\hat{z}}(-\alpha) \tag{2.128}$$

has been proven, which on multiplying on the right with $\mathbf{R}_{\hat{z}}(\alpha)$, gives Eq. (2.121). Either by repeating the procedure, or by just relabelling, it also follows that

$$\mathbf{R}_{\hat{z}''}(\gamma) = \mathbf{R}_{\hat{y}'}(\beta)\cdot\mathbf{R}_{\hat{z}}(\gamma)\cdot\mathbf{R}_{\hat{y}'}(-\beta). \tag{2.129}$$

The combination of these two identities then proves Eq. (2.120).

Proof using generators

This approach is again to prove the intermediary result, Eq. (2.128). Thus consider the product of the three rotations on the right-hand side of Eq. (2.128). The object is to identify to what rotation this corresponds. Thus set

$$\begin{aligned}\mathbf{S}(\alpha,\beta) &\equiv \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{R}_{\hat{z}}(-\alpha) \\ &= e^{-i\alpha\mathbf{G}_{\hat{z}}}\cdot e^{-i\beta\mathbf{G}_{\hat{y}}}\cdot e^{i\alpha\mathbf{G}_{\hat{z}}},\end{aligned} \tag{2.130}$$

with the individual rotations expressed as exponentials of their generators. Then the derivative of this equation with respect to β gives

$$\begin{aligned}i\frac{\partial}{\partial\beta}\mathbf{S}(\alpha,\beta) &= \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{G}_{\hat{y}}\cdot\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{R}_{\hat{z}}(-\alpha) \\ &= \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{G}_{\hat{y}}\cdot\mathbf{R}_{\hat{z}}(-\alpha)\cdot\mathbf{S}(\alpha,\beta) \equiv \mathbf{G}_{\alpha}\cdot\mathbf{S}(\alpha,\beta),\end{aligned} \tag{2.131}$$

defining $\mathbf{G}_{\alpha}$. This equation is immediately reintegrated with respect to β, and using the fact that $\mathbf{S}(\alpha,0) = \mathbf{U}$, this gives

$$\mathbf{S}(\alpha,\beta) = e^{-i\beta\mathbf{G}_{\alpha}}\cdot \tag{2.132}$$

as a rotation generated by the modified generator

$$\mathbf{G}_{\alpha} = \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{G}_{\hat{y}}\cdot\mathbf{R}_{\hat{z}}(-\alpha), \tag{2.133}$$

that depends on α through a similarity transformation. This generator can be further identified by using the same method, namely differentiation, but now twice, thus

$$\begin{aligned}i\frac{\partial}{\partial\alpha}\mathbf{G}_{\alpha} &= \mathbf{R}_{\hat{z}}(\alpha)\cdot\left[\mathbf{G}_{\hat{z}}\cdot\mathbf{G}_{\hat{y}} - \mathbf{G}_{\hat{y}}\cdot\mathbf{G}_{\hat{z}}\right]\cdot\mathbf{R}_{\hat{z}}(-\alpha) \\ &= -i\mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{G}_{\hat{x}}\cdot\mathbf{R}_{\hat{z}}(-\alpha).\end{aligned} \tag{2.134}$$

This has made use of the commutation relation of the generators, Eq. (2.103). In the same way, the second derivative gives

$$\begin{aligned}-\frac{\partial^2}{\partial\alpha^2}\mathbf{G}_{\alpha} &= -i\mathbf{R}_{\hat{z}}(\alpha)\cdot\left[\mathbf{G}_{\hat{z}}\cdot\mathbf{G}_{\hat{x}} - \mathbf{G}_{\hat{x}}\cdot\mathbf{G}_{\hat{z}}\right]\cdot\mathbf{R}_{\hat{z}}(-\alpha) \\ &= \mathbf{R}_{\hat{z}}(\alpha)\cdot\mathbf{G}_{\hat{y}}\cdot\mathbf{R}_{\hat{z}}(-\alpha) = \mathbf{G}_{\alpha}.\end{aligned} \tag{2.135}$$

Thus $\mathbf{G}_\alpha$ can be written in the form

$$\mathbf{G}_\alpha = \mathbf{A}\cos\alpha + \mathbf{B}\sin\alpha \tag{2.136}$$

for some tensors $\mathbf{A}$ and $\mathbf{B}$, which can be identified by the values of $\mathbf{G}_\alpha$ and its derivative at $\alpha = 0$ to give

$$\begin{aligned}\mathbf{G}_\alpha &= \mathbf{G}_{\hat{y}}\cos\alpha - \mathbf{G}_{\hat{x}}\sin\alpha \\ &= -i\boldsymbol{\mathcal{E}}\cdot[\hat{y}\cos\alpha - \hat{x}\sin\alpha] = -i\boldsymbol{\mathcal{E}}\cdot\hat{y}' \\ &= \mathbf{G}_{\hat{y}'}.\end{aligned} \tag{2.137}$$

As a consequence, $\mathbf{S}(\alpha,\beta)$ is recognized as the rotation tensor $\mathbf{R}_{\hat{y}'}(\beta)$, which was to be shown. Such an identification can also be made for the other trannsformation, Eq. (2.129), and a combination of the two gives Eq. (2.120).

Euler angle to axis-angle representation

The rotation, Eq (2.120), determined by the Euler angles must be equivalent to the rotation by some angle θ about some axis $\hat{n}$. These quantities can be determined in many ways, but possibly the simplest is from the matrix, Eq. (2.118). First the trace must be equal to $2\cos\theta + 1$, so on simplification and choosing the sign of the square root that is consistent for small angles, θ is determined by

$$\cos(\theta/2) = \cos(\beta/2)\cos[(\alpha+\gamma)/2]. \tag{2.138}$$

The coordinates of the rotation axis can be determined from the antisymmetric part of the matrix, e.g., the z component is $1/[2\sin\theta]$ the difference of the yx and xy components of the matrix. After simplification the axis can be written in the form

$$\hat{n} = \frac{\sin(\beta/2)\,\{\sin[(\gamma-\alpha)/2]\hat{x} + \cos[(\gamma-\alpha)/2]\hat{y}\} + \cos(\beta/2)\sin[(\alpha+\gamma)/2]\hat{z}}{\sqrt{1-\cos^2(\beta/2)\cos^2[(\alpha+\gamma)/2]}}. \tag{2.139}$$

A check on the correctness of θ and $\hat{n}$ is that it reduces properly for small Euler angles.

The inverse calculation, of calculating the Euler angles from $\hat{n}$ and θ, can be accomplished by inverting the above relations. Specifically, the difference between γ and α can be calculated from the ratio

$$\tan[(\gamma-\alpha)/2] = n_x/n_y. \tag{2.140}$$

After some algebra, the sum of γ and α is found to be given by

$$\cos[(\gamma+\alpha)/2] = \cos(\theta/2)/\sqrt{n_z^2 + (1-n_z^2)\cos^2(\theta/2)} \tag{2.141}$$

and with this, β can be calculated from Eq. 2.138.

2.5.3 Passive Rotations

It is well known that one can describe rotations either actively or passively, essentially by the active rotation of the object being considered, or passively by rotating the coordinate system. To get the same relation between object and coordinate system after the rotation, it is necessary that the passive rotation of the coordinate system be opposite to the active rotation of the object. Thus, if the active rotation is by a rotation by θ about the $\hat{n}$ axis, the equivalent passive rotation is by $-\theta$ about $\hat{n}$, or what is an equal description, by θ about the $-\hat{n}$ axis. Such rotations are inverse to one another. Since the standard description of a rotation is in terms of Euler coordinates, if $R(\alpha,\beta,\gamma)$ is the active rotation, then $R(-\gamma,-\beta,-\alpha)$ is the equivalent passive rotation, that is, the passive rotation that produces the same relation between object and coordinate system as does the active rotation. But often a (passive) rotation of the coordinate system is described by Euler angles in the standard sequence namely to first rotate by α about the $\hat{x}$ axis, then rotate by β about the new $\hat{y}$ axis, and finally rotate by γ about the final $\hat{z}$ axis. Clearly, such a passive rotation is not equivalent to an active rotation using the same Euler angles. Not only must the signs of the Euler angles be changed, but also the order of these rotations must be inverted. It is useful to understand how the coordinates of an object change when the coordinate system is rotated in an arbitrary way. This subsection is devoted to commenting on these questions.

The rotation of the basis vectors $\hat{x}$, $\hat{y}$ and $\hat{z}$ by Euler angles α, β and γ give $\hat{x}'''$, $\hat{y}'''$ and $\hat{z}''' = \hat{z}''$, as given by Eqs. (2.114), (2.115) and (2.112). This can be expressed in matrix form as

$$\begin{pmatrix} \hat{x}''' \\ \hat{y}''' \\ \hat{z}''' \end{pmatrix} = \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma & \sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma & -\sin\beta\cos\gamma \\ -\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma & \cos\alpha\cos\gamma-\sin\alpha\cos\beta\sin\gamma & \sin\beta\sin\gamma \\ \sin\beta\cos\alpha & \sin\beta\sin\alpha & \cos\beta \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix}. \tag{2.142}$$

The matrix in this equation is denoted here by $R_B(\alpha,\beta,\gamma)$ (B for basis rotation) and is seen to be the transpose of the matrix $R(\alpha,\beta,\gamma)$ of Eq. (2.118). Since the matrix $R(\alpha,\beta,\gamma)$ is a real orthogonal matrix, the transpose is also the inverse, so

$$R_B(\alpha,\beta,\gamma) = R^t(\alpha,\beta,\gamma) = R^{-1}(\alpha,\beta,\gamma) = R(-\gamma,-\beta,-\alpha). \tag{2.143}$$

Thus the passive rotation matrix for rotation $\alpha,\ \beta,\ \gamma$ is equal to the active rotation matrix for rotation $-\gamma,\ -\beta,\ -\alpha$. It may also be of use to contrast the nature of the column vectors in Eq. (2.142) with those of Eq. (2.116). In Eq. (2.116), the components of the column vector are in one-to-one correspondence with the components of the vector $\mathbf{v}$, according to an assignment that

$$\hat{x} \Longleftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \hat{y} \Longleftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \hat{z} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{2.144}$$

whereas each element in the column vector of Eq. (2.142) is a vector, so this is a shorthand for describing how three vectors are related to three other vectors. That is, the column vectors in Eq. (2.142) have a composite structure, being a set of 3-dimensional vectors arranged to form a column vector while the elements in the column vector in Eq. (2.116) have no directional association and are pure numbers, the connection of the latter to a 3-dimensional vector being only through the association of the total column vector with a 3-dimensional vector.

To elaborate further on the properties of a passive rotation, consider a vector $\mathbf{v}$ expressed in terms of its components with respect to a fixed basis set, $\hat{x}$, $\hat{y}$, $\hat{z}$ and with respect to the rotated basis set $\hat{x}'''$, $\hat{y}'''$, $\hat{z}'''$, thus

$$\mathbf{v} = v_x\hat{x} + v_y\hat{y} + v_z\hat{z} = v_x'''\hat{x}''' + v_y'''\hat{y}''' + v_z'''\hat{z}'''. \tag{2.145}$$

The components of $\mathbf{v}$ with respect to the rotated basis can be obtained by taking the appropriate dot products, for example, $v_x''' = \hat{x}'''\cdot\mathbf{v}$, or in column vector form

$$\vec{v}\,''' \equiv \begin{pmatrix} v_x''' \\ v_y''' \\ v_z''' \end{pmatrix} = \begin{pmatrix} \hat{x}''' \\ \hat{y}''' \\ \hat{z}''' \end{pmatrix}\cdot\mathbf{v} = R_B \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix}\cdot\mathbf{v} = R_B \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = R_B\vec{v}. \tag{2.146}$$

In summary, since $R_B = R^{-1}$, the matrices that describe how the components of a vector rotate actively and passively are inverse to one another. Moreover, this shows that a passive rotation of a vector with rotation R^{-1} is equivalent (that is, the components of $\mathbf{v}$ are changed in the same way) to an active rotation of the vector with rotation R.

While active and passive rotations with the same set of Euler angles change the components of a vector in very different ways, a closer similarity is obtained by considering a passive rotation with Euler angles of opposite sign to those of the active rotation with which it is to be compared. [Note that these are NOT equivalent active and passive rotations.] For simplicity, consider the rotation of a vector initially aligned along the $\hat{x}$ axis and simplify the discussion by restricting the (active and passive) rotations so that $\gamma = 0$. The two rotations affect the components of $\mathbf{v}$ as follows:

A. The active rotation of a unit vector aligned along the $\hat{x}$ direction, first by α about the $\hat{z}$ axis and then by β about the $\hat{y}'$ direction gives a vector in coordinate representation with basis set $\hat{x}$, $\hat{y}$ and $\hat{z}$

$$\vec{v} \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} \cos\alpha\cos\beta \\ \sin\alpha\cos\beta \\ -\sin\beta \end{pmatrix} \equiv \vec{v}_A. \tag{2.147}$$

The subscript A is used here to indicate "active". This can be obtained directly by carrying out the rotations or by multiplying the rotation matrix of Eq. (2.118) (with $\gamma = 0$) into the above initial column vector, that is, in matrix form, $\vec{v}_A = R(\alpha, \beta, 0)\vec{v}$. The angle of rotation is determined by $\cos(\theta/2) = \cos(\beta/2)\cos(\alpha/2)$ about the axis

$$\hat{n}_A = \frac{\sin(\beta/2)[\cos(\alpha/2)\hat{y} - \sin(\alpha/2)\hat{x}] + \cos(\beta/2)\sin(\alpha/2)\hat{z}}{\sqrt{1 - \cos^2(\beta/2)\cos^2(\alpha/2)}}. \tag{2.148}$$

P. Consider now the passive rotation first by $-\alpha$ about the $\hat{z}$ axis and then by $-\beta$ about the axis $\hat{y}_P$ resulting from the rotation of the $\hat{y}$ axis. It is stressed again that this is NOT the rotation inverse to that in paragraph A. In this (passive) rotation, the object, a unit vector lying along the initial $\hat{x}$ direction remains fixed. In terms of describing the object in terms of the new coordinate frame, the $-\alpha$ rotation puts the object in the $\hat{x}_P$-$\hat{y}_P$ plane (which is also the $\hat{x}$-$\hat{y}$ plane) while the $-\beta$ rotation rotates the $\hat{x}_P$ and $\hat{z}$ axes in such a way that the object acquires a negative $\hat{z}_P$ component (for positive β). Thus, in the rotated coordinate system, the object, namely the unit vector $\hat{x}$, is described by the coordinates

$$\vec{v} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} \cos\alpha\cos\beta \\ \sin\alpha \\ -\cos\alpha\sin\beta \end{pmatrix} \equiv \vec{v}_P. \tag{2.149}$$

This can also be obtained according to $\vec{v}_P = R(0, \beta, \alpha)\vec{v}$. The angle of this rotation is the same as for the active rotation, but the axis of rotation is (subscript P for "passive")

$$\hat{n}_P = \frac{\sin(\beta/2)[\sin(\alpha/2)\hat{x} + \cos(\alpha/2)\hat{y}] + \sin(\alpha/2)\cos(\beta/2)\hat{z}}{\sqrt{1 - \cos^2(\beta/2)\cos^2(\alpha/2)}}. \tag{2.150}$$

The difference arises entirely from the different orders in which the individual Euler angle rotations are carried out, exemplifying the consequences of the fact that rotations about different axes do not generally commute.

Chapter 3

Tensors and their Rotational Reduction

The object of this chapter is to describe how a tensor behaves under rotation and how it is often possible to reduce it (group theory reduction) into rotationally independent parts, that is, into parts which cannot be transformed one into another by any rotation. Provided no further reduction is possible, these parts are irreducible representations of the rotation group.

A summary of the notation already introduced in Chap. 2 may be useful. As has already been used, a tensor is an object with two or more directions. This is indicated here, and in much of the physics literature, by writing a tensor in sans serif, in contrast to writing a vector (really also a tensor but with only one direction) in boldface. The order (number of directions) will usually be indicated with a superscript in parentheses as, for example, $\mathsf{T}^{(p)}$ for a tensor of pth order. The letter p will be used to designate a tensor of generic order while an exception to the above rule is that a second order tensor will not have its order indicated since such tensors are so common and play a central role in most operations. In particular, the basic rotation tensor $\mathsf{R}_{\hat{n}}(\theta)$ of Eq. (2.90) is of second order, as is U. It is also necessary to distinguish the actual directions that a tensor may have according to the sequence in which the directions appear, the latter is thus referred to as the sequence of directions. Thus for the second order tensor $\hat{x}\hat{y}$, there are two directions, the first pointing in the $\hat{x}$ direction while the second index is in the $\hat{y}$ direction. Again, it is generally of importance to consider particular components of a tensor and these are obtained by contraction. For example, given a third order tensor $\mathsf{T}^{(3)}$, the second order tensor $\mathsf{V}^{(2)} \equiv \hat{n}\cdot\mathsf{T}^{(3)}$ is the component of the third order tensor along the $\hat{n}$ direction, such a component happens in this case to be a second order tensor. Such flexibility in notation is used throughout this book. An explicit indication of the order is given when the author has judged that it is needed for clarity, but otherwise the order may or may not be explicitly indicated.

When rotating a tensor, it is implied that all the directions of the tensor are rotated. Clearly it is also possible to consider rotating only a subset of the directions of a tensor, with the possible objective of studying how the result depends on the non-rotated subset. Another possibility is that a tensor is a function of some other object having directions, such as a vector. In this case, the inherent rotation of the tensor is only of the directions of the tensor, leaving the independent variable (e.g., vector) fixed. Somewhat obviously, it will likely occur that a rotation of the tensor is equivalent to some rotation of the independent variable before inserting it into the functional that defines the tensor. Thus this separation of rotational properties could be useful for clarifying the dependence of a tensor function on its independent variables. Such generalizations are not emphasized in this work except for the odd comment.

The rotation of a pth order tensor $\mathbf{T}^{(p)}$ by an angle θ about axis $\hat{n}$ gives a pth order tensor $R_{\hat{n}}(\theta)\mathbf{T}^{(p)}$ in which all p directions of $\mathbf{T}^{(p)}$ have been rotated. The implementation of this rotation can be accomplished by dotting the corresponding rotation tensor $\mathbf{R}_{\hat{n}}(\theta)$ into each direction of the p indices of $\mathbf{T}^{(p)}$, in detail

$$
\begin{aligned}
R_{\hat{n}}(\theta)\mathbf{T}^{(p)} &= \left[\lfloor\lfloor \cdots \lfloor \mathbf{R}_{\hat{n}}(\theta) \rfloor \cdot \mathbf{R}_{\hat{n}}(\theta) \cdots \rfloor \cdot \mathbf{R}_{\hat{n}}(\theta) \rfloor \cdot \mathbf{R}_{\hat{n}}(\theta) \right] \odot^p \mathbf{T}^{(p)} \\
&\equiv \mathbf{R}_{\hat{n}}^{(p)}(\theta) \odot^p \mathbf{T}^{(p)}. \qquad (3.1)
\end{aligned}
$$

The complexity of this expression is due to the need to take the first direction, rotate it and make it the first direction of the rotated tensor, take the second direction of the tensor, rotate it and make it the second direction of the rotated tensor, etc. As a shorthand notation, the tensor for rotating a tensor of rank p is denoted by $\mathbf{R}_{\hat{n}}^{(p)}(\theta)$. While the coordinate free description of tensors and tensor operations is emphasized and used almost exclusively in this book, utilizing the diagrammatic representation of tensor operations described in Sec. 2.4, it may help the reader to also see some of these tensor relations in index form. Thus Eq. (3.1 can be written out in index form as

$$
\left[R_{\hat{n}}(\theta)\mathbf{T}^{(p)}\right]_{ij\ldots\ell} = \sum_{i'j'\ldots\ell'} \left[\mathbf{R}_{\hat{n}}(\theta)\right]_{ii'} \left[\mathbf{R}_{\hat{n}}(\theta)\right]_{jj'} \cdots \left[\mathbf{R}_{\hat{n}}(\theta)\right]_{\ell\ell'} \mathbf{T}^{(p)}_{i'j'\ldots\ell'}. \qquad (3.2)
$$

This illustrates that each index is transformed in turn, maintaining the order of indices while rotating the tensor.

It is also of use to note that the generator for rotating a pth order tensor is the linear combination of the generators for the individual directions of the tensor, carefully organized so that the order of the directions of the tensor is preserved. Formally this can be obtained by differentiating Eq. (3.1) to give

$$
\begin{aligned}
G_{\hat{n}}\mathbf{T}^{(p)} &= \Big[\lfloor\lfloor \cdots \lfloor \mathbf{G}_{\hat{n}} \rfloor \cdots \rfloor\rfloor + \lfloor\lfloor \cdots \lfloor \mathbf{U} \rfloor \cdot \mathbf{G}_{\hat{n}} \cdots \rfloor\rfloor + \cdots \\
&\quad + \lfloor\lfloor \cdots \lfloor \mathbf{U} \rfloor \cdots \rfloor \cdot \mathbf{G}_{\hat{n}} \rfloor + \lfloor\lfloor \cdots \lfloor \mathbf{U} \rfloor \cdots \rfloor\rfloor \cdot \mathbf{G}_{\hat{n}} \Big] \odot^p \mathbf{T}^{(p)} \\
&\equiv \mathbf{G}_{\hat{n}}^{(p)} \odot^p \mathbf{T}^{(p)} \qquad (3.3)
\end{aligned}
$$

as the sum of the generators rotating each of the individual p directions of the tensor. In index form this is

$$
\begin{aligned}
\left[G_{\hat{n}}\mathbf{T}^{(p)}\right]_{ij\ldots\ell} &= \sum_{i'j'\ldots\ell'} \Big\{ \left[\mathbf{G}_{\hat{n}}\right]_{ii'} \delta_{jj'} \cdots \delta_{\ell\ell'} + \delta_{ii'} \left[\mathbf{G}_{\hat{n}}\right]_{jj'} \cdots \delta_{\ell\ell'} \\
&\quad + \delta_{ii'}\delta_{jj'} \cdots \left[\mathbf{G}_{\hat{n}}\right]_{\ell\ell'} \Big\} \mathbf{T}^{(p)}_{i'j'\ldots\ell'}. \qquad (3.4)
\end{aligned}
$$

The exponentiation of the abstract generator to give the abstract finite rotation operator

$$R_{\hat{n}}(\theta) = e^{-iG_{\hat{n}}\theta} \tag{3.5}$$

and of the tensor generator to give the finite rotation tensor

$$\mathbf{R}^{(p)}_{\hat{n}}(\theta) = e^{-i\mathbf{G}^{(p)}_{\hat{n}}\theta} \tag{3.6}$$

both follow from the one-parameter nature of rotations about a given axis $\hat{n}$, just as in Eq. (2.91) for the rotation of a vector.

Since a tensor generator for a pth order tensor is the sum of the corresponding generator tensors for the p vector directions making up the pth order tensor and since individual generators for the vector directions act on separate directions, the algebraic properties of the pth order tensor generators are the same as for the vector generators. Specifically, the commutation properties are the same

$$\mathbf{G}^{(p)}_{\hat{\ell}} \odot^p \mathbf{G}^{(p)}_{\hat{m}} - \mathbf{G}^{(p)}_{\hat{m}} \odot^p \mathbf{G}^{(p)}_{\hat{\ell}} = i\mathbf{G}^{(p)}_{\hat{n}}, \tag{3.7}$$

where $\hat{\ell},\ \hat{m},\ \hat{n}$ are a set of unit vectors forming a right-handed coordinate system. It is an immediate consequence of these commutation relations that the pth order tensorial form for the Casimir invariant

$$\mathbf{G}^{(p)2} \equiv \mathbf{G}^{(p)2}_{\hat{\ell}} + \mathbf{G}^{(p)2}_{\hat{m}} + \mathbf{G}^{(p)2}_{\hat{n}} \tag{3.8}$$

commutes with all pth order tensor generators, for example

$$\mathbf{G}^{(p)2} \odot^p \mathbf{G}^{(p)}_{\hat{n}} = \mathbf{G}^{(p)}_{\hat{n}} \odot^p \mathbf{G}^{(p)2}. \tag{3.9}$$

This tensor is particularly useful in classifying irreducible Cartesian tensors so its detailed nature is important and is now described.

To get a sense of the general structure of $\mathbf{G}^{(p)2}$, the cases of $p = 1$ and $p = 2$ are worked out in detail. First for $p = 1$, the generator for rotations about, for example, the $\hat{n}$ axis is $\mathbf{G}_{\hat{n}} = -i\hat{n}\cdot\boldsymbol{\mathcal{E}}$, so $\mathbf{G}^{(1)2}$ is

$$\mathbf{G}^{(1)2} = -\lfloor \cdot\boldsymbol{\mathcal{E}} \rfloor \cdot \boldsymbol{\mathcal{E}} = -\boldsymbol{\mathcal{E}} : \boldsymbol{\mathcal{E}} = 2\mathbf{U}. \tag{3.10}$$

Since $\mathbf{U}$ is the identity operator for vectors, it follows that all vectors are eigentensors of $\mathbf{G}^{(1)2}$ with eigenvalue 2. For $p = 2$, the rotation generator about, for example, the $\hat{n}$ axis is

$$\mathbf{G}^{(2)}_{\hat{n}} = -i\left[\hat{n}\cdot\boldsymbol{\mathcal{E}}\cdot\lfloor\mathbf{U}\mathbf{U}\rfloor + \lfloor\hat{n}\cdot\boldsymbol{\mathcal{E}}\rfloor\right]. \tag{3.11}$$

The square of this is

$$\mathbf{G}^{(2)}_{\hat{n}} : \mathbf{G}^{(2)}_{\hat{n}} = 2\lfloor\mathbf{U}\mathbf{U}\rfloor - \hat{n}\mathbf{U}\hat{n} - \lfloor\hat{n}\hat{n}\rfloor - 2\hat{n}\cdot\boldsymbol{\mathcal{E}}\cdot\lfloor\hat{n}\cdot\boldsymbol{\mathcal{E}}\rfloor. \tag{3.12}$$

Summing over the three axes, the Casimir invariant becomes

$$\mathbf{G}^{(2)2} = 4\lfloor\mathbf{U}\mathbf{U}\rfloor + 2\lfloor\mathbf{U}\mathbf{U}\rfloor - 2\mathbf{U}\mathbf{U}. \tag{3.13}$$

Now for the general pth order Casimir invariant there are p terms in which the generators are dotted together and $p(p-1)$ terms in which the generators are for different indices. Since the doubledot contraction of two $\boldsymbol{\mathcal{E}}$'s gives $-2\mathbf{U}$, every term of the first type contributes 2 times the

pth order identity to $\mathsf{G}^{(p)2}$, thus a total contribution of $2p$ times the identity. For $p=2$ this is the first term in Eq. (3.13). Each of the other terms involves a pair of indices which has the structure of the last two terms in Eq. (3.13), namely $2\mathsf{W} - 2\mathsf{U}\mathsf{U}$, but embedded in the $2p$ order tensor in such a way that all the other $p-2$ indices are connected as in the identity. For example, for $p=3$, the three possibilities combine together to give

$$2\underbrace{\left(\mathsf{W} - \mathsf{U}\mathsf{U}\right)} + 2\mathsf{W}\mathsf{J} - 2\mathsf{W}\mathsf{U} + 2\,\mathsf{U}\mathsf{W} - 2\mathsf{U}\mathsf{U}\mathsf{U} \tag{3.14}$$

The combined structure is thus

$$\mathsf{G}^{(p)2} = 2p\underbrace{\cdots\mathsf{U}\cdots} + 2\sum_{\text{perm}}\underbrace{\cdots\left(\mathsf{W} - \mathsf{U}\mathsf{U}\right)\cdots} \tag{3.15}$$

with the sum over all the $p(p-1)/2$ permutations of which pair of directions are transformed by $\mathsf{W} - \mathsf{W}$. It is necessary that the remaining $p-2$ terms of right and left hand indices are connected as in the identity. Expressed in index form, this quantity is

$$\left[\mathsf{G}^{(p)2}\right]_{ijk\ldots\ell,i'j'k'\ldots\ell'} = 2p\delta_{ii'}\delta_{jj'}\delta_{kk'}\cdots\delta_{\ell\ell'} + 2\sum_{\text{perm}}\left[\delta_{ij'}\delta_{ji'} - \delta_{ij}\delta_{i'j'}\right]\delta_{kk'}\cdots\delta_{\ell\ell'}. \tag{3.16}$$

This is then the form for the Casimir invariant for pth order tensors.

Two other useful combinations of the generators are the raising and lowering operators, namely

$$\mathsf{G}^{(p)}_{\pm} \equiv \mathsf{G}^{(p)}_{\hat{x}} \pm i\mathsf{G}^{(p)}_{\hat{y}}. \tag{3.17}$$

While these are written here using the $\hat{x}$, $\hat{y}$, $\hat{z}$ coordinate system, they could be written in terms of any right-handed coordinate system. But in later work, see for example Chap. 5, it is this coordinate system which will be used for explicitly writing down spherical tensors. The raising and lowering operators satisfy relations analogous to those for the vector raising and lowering operators of Eq. (2.105), namely

$$\mathsf{G}^{(p)}_{\hat{z}}\odot^{p}\mathsf{G}^{(p)}_{\pm} = \mathsf{G}^{(p)}_{\pm}\odot^{p}\left(\mathsf{G}^{(p)}_{\hat{z}} \pm \mathsf{U}^{(p)}\right). \tag{3.18}$$

This is what defines them as raising and lowering operators, and makes them useful when studying spherical tensors. In this equation the identity for pth-order tensors has been abbreviated as

$$\mathsf{U}^{(p)} \equiv \underbrace{\cdots\mathsf{U}\cdots}. \tag{3.19}$$

As stated earlier, the object of this chapter is to examine the rotational properties of a general tensor. But before doing this it is useful to examine the two tensors U and $\boldsymbol{\varepsilon}$, which have the special property of being invariant (unchanged) by any rotation. The discussion of the rotation of these tensors also exemplifies how the rotation of a general tensor can be carried out.

3.1 The Rotational Invariance of U and ε

The rotation of the identity tensor U can be calculated according to

$$\begin{aligned} R_{\hat{n}}(\theta)\mathsf{U} &= \left[\underbrace{\mathsf{R}_{\hat{n}}(\theta)}\cdot\mathsf{R}_{\hat{n}}(\theta)\right]:\mathsf{U} = \mathsf{R}_{\hat{n}}(\theta)\cdot\mathsf{U}\cdot\mathsf{R}^{t}_{\hat{n}}(\theta) \\ &= \mathsf{R}_{\hat{n}}(\theta)\cdot\mathsf{R}^{t}_{\hat{n}}(\theta) = \mathsf{R}_{\hat{n}}(\theta)\cdot\mathsf{R}^{-1}_{\hat{n}}(\theta) = \mathsf{R}_{\hat{n}}(\theta)\cdot\mathsf{R}_{\hat{n}}(-\theta) = \mathsf{U}. \end{aligned} \tag{3.20}$$

Since $\mathbf{U}$ has only two directions, the rotation of the second direction can be accomplished by dotting the transpose of the rotation tensor into the right-hand side of $\mathbf{U}$. Furthermore, the transpose of the rotation operator is the same as the inverse of the original rotation, or equivalently, the rotation with the opposite angle (about the same axis). It is also useful to carry out this calculation in detail, specifically

$$\begin{aligned} R_{\hat{n}}(\theta)\mathbf{U} &= \mathbf{R}_{\hat{n}}(\theta)\cdot\mathbf{R}^t_{\hat{n}}(\theta) \\ &= [\hat{n}\hat{n} + \cos\theta(\mathbf{U} - \hat{n}\hat{n}) - \sin\theta\hat{n}\cdot\boldsymbol{\varepsilon}\,]\cdot[\hat{n}\hat{n} + \cos\theta(\mathbf{U} - \hat{n}\hat{n}) + \sin\theta\hat{n}\cdot\boldsymbol{\varepsilon}\,] \\ &= \hat{n}\hat{n} + \cos^2\theta(\mathbf{U} - \hat{n}\hat{n}) - \sin^2\theta\hat{n}\cdot\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}\cdot\hat{n}. \end{aligned} \tag{3.21}$$

It is noted that all cross terms in the product vanish. Then making use of the relation, Eq. (2.81), the last two terms combine to eliminate any dependence on θ. Finally, the sum gives only $\mathbf{U}$.

An alternate, and formally simpler approach for proving the rotational invariance of $\mathbf{U}$, is to show that the generator of a rotation acting on $\mathbf{U}$ gives zero. From Eq. (3.3), a rotation generator acting on the second rank tensor $\mathbf{U}$ is

$$\begin{aligned} G_{\hat{n}}\mathbf{U} &= \left[\lfloor\mathbf{G}_{\hat{n}}\rfloor + \lfloor\mathbf{U}\rfloor\cdot\mathbf{G}_{\hat{n}}\right]:\mathbf{U} \\ &= \mathbf{U}\cdot\mathbf{G}^t_{\hat{n}} + \mathbf{G}_{\hat{n}}\cdot\mathbf{U} = -\mathbf{G}_{\hat{n}} + \mathbf{G}_{\hat{n}} = \mathbf{0}. \end{aligned} \tag{3.22}$$

Thus a rotation generator acting on $\mathbf{U}$ produces nothing new, so that $\mathbf{U}$ is unchanged by a rotation.

The proof that $\boldsymbol{\varepsilon}$ is a rotational invariant is a bit more elaborate. The generator method is examined first, after which the full effect of a rotation is considered.

According to Eq. (3.3), a rotation of $\boldsymbol{\varepsilon}$ is generated by

$$\begin{aligned} G_{\hat{n}}\boldsymbol{\varepsilon} &= \left[\lfloor\lfloor\mathbf{G}_{\hat{n}}\rfloor\rfloor + \lfloor\lfloor\mathbf{U}\rfloor\cdot\mathbf{G}_{\hat{n}}\rfloor + \lfloor\lfloor\mathbf{U}\rfloor\rfloor\cdot\mathbf{G}_{\hat{n}}\right]\odot^3\boldsymbol{\varepsilon} \\ &= i\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}\cdot\hat{n} - i\lfloor\hat{n}\cdot\boldsymbol{\varepsilon}\rfloor:\boldsymbol{\varepsilon} - i\hat{n}\cdot\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} \\ &= -i\left[-\lfloor\hat{n}\rfloor + \hat{n}\mathbf{U} - \hat{n}\mathbf{U} + \mathbf{U}\hat{n} + \lfloor\hat{n}\rfloor - \mathbf{U}\hat{n}\right] \\ &= \mathbf{0}. \end{aligned} \tag{3.23}$$

Since this gives a null result, the rotation generator produces nothing new with the consequence that $\boldsymbol{\varepsilon}$ is a rotational invariant.

Finally, the rotation of $\boldsymbol{\varepsilon}$ by a finite angle θ is obtained according to Eq. (3.1) as

$$R_{\hat{n}}(\theta)\boldsymbol{\varepsilon} = \left[\lfloor\lfloor\mathbf{R}_{\hat{n}}(\theta)\rfloor\cdot\mathbf{R}_{\hat{n}}(\theta)\rfloor\cdot\mathbf{R}_{\hat{n}}(\theta)\right]\odot^3\boldsymbol{\varepsilon} \tag{3.24}$$

The computation of the contractions indicated in this tensor is straightforward, but lengthy and requires care. After straightforward simplification the result is

$$R_{\hat{n}}(\theta)\boldsymbol{\varepsilon} = \cos^3\theta\boldsymbol{\varepsilon} + (\cos^3\theta - 1)\left(\hat{n}\cdot\boldsymbol{\varepsilon}\cdot\lfloor\hat{n}\rfloor - \hat{n}\hat{n}\cdot\boldsymbol{\varepsilon} - \hat{n}\cdot\boldsymbol{\varepsilon}\,\hat{n}\right). \tag{3.25}$$

It is shown in the following paragraph, that the tensor in parentheses is equal to $-\boldsymbol{\varepsilon}$, with the consequence that

$$R_{\hat{n}}(\theta)\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}, \tag{3.26}$$

proving again that $\boldsymbol{\varepsilon}$ is a rotational invariant.

Lemma The tensor in parentheses in Eq. (3.25) is $-\boldsymbol{\mathcal{E}}$.

This can be done by introducing the right-handed coordinate system $\hat{n},\ \hat{\ell},\ \hat{m}$ associated with the unit vector $\hat{n}$, noting in particular that

$$\hat{n}\cdot\boldsymbol{\mathcal{E}} = \hat{\ell}\hat{m} - \hat{m}\hat{\ell}. \tag{3.27}$$

It follows that

$$\begin{aligned} &\hat{n}\hat{n}\cdot\boldsymbol{\mathcal{E}} + \hat{n}\cdot\boldsymbol{\mathcal{E}}\,\hat{n} - \hat{n}\cdot\boldsymbol{\mathcal{E}}\cdot\hat{n}\,\mathbf{U} \\ &\quad = \hat{n}(\hat{\ell}\hat{m} - \hat{m}\hat{\ell}) + (\hat{\ell}\hat{m} - \hat{m}\hat{\ell})\hat{n} - \hat{\ell}\hat{n}\hat{m} + \hat{m}\hat{n}\hat{\ell} \\ &\quad = \hat{n}\hat{\ell}\hat{m} + \hat{\ell}\hat{m}\hat{n} + \hat{m}\hat{n}\hat{\ell} - \hat{n}\hat{m}\hat{\ell} - \hat{m}\hat{\ell}\hat{n} - \hat{\ell}\hat{n}\hat{m} = \boldsymbol{\mathcal{E}}. \end{aligned} \tag{3.28}$$

The formula in the last line treats all unit vectors in the right-handed coordinate system the same, being symmetric to a cyclic permutation and antisymmetric to an anticyclic permutation of the coordinate axes. Thus it is independent of the coordinate system and equal to $\boldsymbol{\mathcal{E}}$. If one is unhappy with the $\hat{n},\ \hat{\ell},\ \hat{m}$ coordinate system, one could express $\hat{n}$ in terms of a fixed basis set, say $\hat{n} = x\hat{x} + y\hat{y} + z\hat{z}$, with $x,\ y,\ z$ equal respectively to $\sin\theta\cos\phi,\ \ \sin\theta\sin\phi,\ \ \cos\theta$. On substitution into the tensor combination of Eq. (3.28), it can easily be shown that the cross terms, e.g. those proportional to xy, vanish, while the diagonal terms are all proportional to $\boldsymbol{\mathcal{E}}$ according to Eq. (2.23). The sum then gives $\boldsymbol{\mathcal{E}}$.

It should of course also be stated that the rotational invariance of $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$ is connected to the fact that taking a dot product or cross product is the same in any coordinate system. That is, since $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$ are the underlying tensors that carry out these operations, their rotational invariance is to be expected.

3.2 Invariant Embedding and Tensorial Reduction

By invariant, it is meant, unchanged by any rotation, but some elaboration of that will be made shortly. The notion of embedding is discussed first, then tensorial reduction. It should be clearly stated at the outset that the "tensorial" reduction discussed in this section emphasizes the reduction in tensorial order. That this is related to the group theoretical reduction with respect to the rotation group is shown in Sec. 3.4. Behind this association is the understanding that any rotational invariant (tensor) is a combination of $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$, which essentially arises from the fact that the only operations on tensors are the four described in Sec. 2.2, which are, besides the straightforward tensor product, all implemented by $\mathbf{U}$ or $\boldsymbol{\mathcal{E}}$.

3.2.1 Invariant Embedding

The four elementary tensor operations of Sec. 2.2 can be applied to tensors in any number of different ways. Thus, for example, given tensors $\mathbf{T}^{(p)}$ and $\mathbf{T}^{(q)}$, the tensor product $\mathbf{T}^{(p)}\mathbf{T}^{(q)}$ of order $p+q$ can be formed. In particular, the tensor product of $\mathbf{T}^{(p)}$ and $\mathbf{U}$ is the $p+2$th order tensor

$$\mathbf{T}^{(p+2)} \equiv \mathbf{T}^{(p)}\mathbf{U}. \tag{3.29}$$

Now the rotation of this tensor has the same properties as rotating the original tensor $\mathbf{T}^{(p)}$ because $\mathbf{U}$ in a rotational invariant. In this way $\mathbf{T}^{(p)}$ has been invariantly embedded in a tensor of higher order, specifically here of order $p+2$. Embedded, because the tensorial order has been increased, and invariantly, because the rotational properties are unchanged. To make sure that this notion of invariance is clear, it is elaborated upon further. First of all, it is to be understood that $\mathbf{T}^{(p+2)}$ is not necessarily a rotational invariant, nor is $\mathbf{T}^{(p)}$, only that these two tensors have the same rotational properties. That is, the embedding is invariant, not the tensors. "Same rotational properties" may also be subject to misinterpretation, and is not necessarily easy to describe, since the two tensors are of different order, so equality can not be used. But under a rotation by an arbitrary angle θ about an arbitrary axis $\hat{n}$, each tensor will develop terms which can be classified by their number of factors of $\hat{n}$, $\cos\theta$ and $\sin\theta$. The same rotational properties is to mean that there is a 1-1 correspondence between the terms with the same numbers of these factors. It should also be possible to consider that the relative amplitudes of these factors in the rotated tensor are the same.

The same discussion can be made if an embedding is made by using the tensor product with $\boldsymbol{\mathcal{E}}$, namely

$$\mathbf{T}^{(p+3)} \equiv \mathbf{T}^{(p)} \boldsymbol{\mathcal{E}}\,, \tag{3.30}$$

except that now the tensorial order is increased by 3. Other possibilities are to dot $\mathbf{U}$ and/or $\boldsymbol{\mathcal{E}}$ into the initial tensor,

$$\mathbf{T}^{(p)} \equiv \mathbf{T}^{(p)} \cdot \mathbf{U}, \qquad \mathbf{T}^{(p+1)} \equiv \mathbf{T}^{(p)} \cdot \boldsymbol{\mathcal{E}}\,, \tag{3.31}$$

but now the contraction with $\mathbf{U}$ has no effect (that is, it is just an identity transformation) while the contraction with $\boldsymbol{\mathcal{E}}$ inceases the tensorial order by 1. The latter is again an invariant embedding. Continuing along this same line of thinking, there is the possibility of a doubledot contraction with $\mathbf{U}$ and/or $\boldsymbol{\mathcal{E}}$, but in both cases, the order of the resultant tensor is less than the initial order. Such a transformation is here called a reduction (in tensorial order) whose more detailed discussion is made in the following paragraph. Note that the tensor product and the dot product could be carried out with any set of directions of the tensor, and the directions of the resulting tensor ordered in any way.

Returning to the discussion of embeddings, it is noticed that a variety of embeddings could be successively carried out, adding any number of $\mathbf{U}$'s and $\boldsymbol{\mathcal{E}}$'s to increase the order of the tensor to any value. Whether this is a useful exercize or not is a separate question, but that such a structure can occur needs to be recognized. It also needs to be recognized that the resulting tensor has the same rotational and related attributes (such as any physical interpretation) as the original tensor, but dressed up (or disguised) to look very different.

3.2.2 Reduction and Natural Tensors

The inverse process to invariant embedding is invariant reduction, namely the reduction in tensorial order. This can also be envisaged as stripping away redundant directions to expose the tensor or tensors that carry the essential rotational features of the original tensor. This can be carried out by double contraction with $\mathbf{U}$ and/or $\boldsymbol{\mathcal{E}}$, thus

$$\mathbf{T}^{(p-2)} = \mathbf{T}^{(p)} : \mathbf{U} \quad \text{and} \quad \mathbf{T}^{(p-1)} = \mathbf{T}^{(p)} : \boldsymbol{\mathcal{E}} \tag{3.32}$$

reduce the tensorial order by 2 and 1, respectively. Another possibility is to triple dot with $\boldsymbol{\mathcal{E}}$,

$$\mathbf{T}^{(p-3)} = \mathbf{T}^{(p)} \odot^3 \boldsymbol{\mathcal{E}}\,, \tag{3.33}$$

decreasing the order by 3. Of course this procedure can be repeated as long as there are directions remaining in the tensor with which a contraction may be made. It is also possible, and actually necessary to consider contractions in any order and with any set of directions in the original tensor. The possible outcomes of any such operation is now considered.

The doubledot contraction of a pair of directions of the tensor $\mathsf{T}^{(p)}$ with U can be classified as having three possible outcomes:

1. the result gives zero (the tensor is annihilated by this action) - then the original tensor is classified as being traceless in that pair of directions.
2. the resultant tensor of order $p-2$ has the same rotational properties as does the original tensor.
3. The resultant tensor of order $p-2$ has different rotational properties than does the original tensor.

The following examples illustrate these cases:
a) If $\mathbf{r}_1$ and $\mathbf{r}_2$ are orthogonal, then the contraction

$$\mathsf{U}\!:(\mathbf{r}_1\mathbf{r}_2) = \mathbf{0} \tag{3.34}$$

exemplifies the first case, but maybe a better example is

$$\mathsf{U}\!:(\mathbf{r}_1\mathbf{r}_2 - \mathbf{r}_2\mathbf{r}_1) = \mathbf{0}, \tag{3.35}$$

which is valid for arbitrary $\mathbf{r}_1$ and $\mathbf{r}_2$. Essentially a doubledot contraction with U annihilates any tensor that is antisymmetric in the directions into which U is doubledotted.
b) The doubledot contraction

$$\mathsf{U}\!:(\mathsf{U}\mathbf{r}_1\mathbf{r}_2) = 3\mathbf{r}_1\mathbf{r}_2 \tag{3.36}$$

merely undoes the embedding of the second order tensor $\mathbf{r}_1\mathbf{r}_2$ into a fourth order tensor and it is clear that $\mathbf{r}_1\mathbf{r}_2$ and its embedded form have the same rotational properties, exemplifying the second case.
c) If the same fourth order tensor is contracted with U in a different way, namely

$$(\mathsf{U}\mathbf{r}_1\mathbf{r}_2)\!:\!\mathsf{U} = \mathsf{U}(\mathbf{r}_1\!\cdot\!\mathbf{r}_2), \tag{3.37}$$

this produces a rotationally invariant tensor, which does not have the same rotational properties as the original tensor, exemplifying the third case. A slightly different aspect is the contraction

$$\underbrace{\lfloor\cdot\mathsf{U}\mathbf{r}_1\mathbf{r}_2\cdot\rfloor} = \mathbf{r}_2\mathbf{r}_1 \tag{3.38}$$

that produces 1/3 of the transpose of Eq. (3.36) while the contraction between the second and third directions produces 1/3 of Eq. (3.36).

The discussion of possible outcomes by doubledot contraction is continued by using $\boldsymbol{\varepsilon}$. Again there are three possible results, essentially of the same nature as above, but in cases 2 and 3, the reduction in order is to $p-1$. The three cases are respectively exemplified by

$$\begin{aligned} \boldsymbol{\varepsilon} : (\mathsf{U}\mathbf{r}_1\mathbf{r}_2) &= \mathbf{0} \\ \boldsymbol{\varepsilon} : (\boldsymbol{\varepsilon}\cdot\mathbf{r}) &= -2\mathbf{r} \end{aligned} \tag{3.39}$$

and

$$\boldsymbol{\varepsilon} : (\mathbf{r}_1\mathbf{r}_2) = -\mathbf{r}_1\times\mathbf{r}_2. \tag{3.40}$$

Finally there is the triple dot contraction with $\boldsymbol{\mathcal{E}}$. Clearly the outcome of this has the same three possibilities as listed above. One example is

$$\boldsymbol{\mathcal{E}} \odot^3 (\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) = -\mathbf{r}_1\cdot\mathbf{r}_2\times\mathbf{r}_3, \tag{3.41}$$

and examples of the other possibilities are easily found.

Given a tensor $\mathbf{T}^{(p)}$, if after one reduction in order there is a nonzero outcome, then another reduction can be carried out, and the process can be repeated. The question arises as to when does this process end. Clearly the answer to this question is when the reduction yields a null tensor. In particular, when contracting with $\mathbf{U}$, the nonzero tensor of minimal order found by a sequence of reductions must be traceless in every pair of directions, otherwise $\mathbf{U}$ doubledotted into some pair of directions would give a nonzero result and lead to a nonzero tensor of smaller order. Likewise, the tensor of minimal order must be symmetric in every pair of directions, otherwise doubledotting with $\boldsymbol{\mathcal{E}}$ would give a nonzero tensor of smaller order. The consequence of this discussion is that any tensor of minimal order must be traceless and symmetric in every pair of directions. Such a tensor, namely one that is traceless and symmetric in all pairs of directions, will henceforth be referred to as a **natural tensor**.

It should be mentioned that different sequences of reduction on the same initial tensor may yield different tensors of minimal order, and the orders of two tensors of minimal order may be different. An example illustrating this is the two sequences of reduction of $\mathbf{T}^{(4)} \equiv \mathbf{U}\mathbf{r}_1\mathbf{r}_2$. First consider contracting twice with $\mathbf{U}$ in the following manner:

$$\begin{aligned} \mathbf{U}{:}\mathbf{T}^{(4)} &= 3\mathbf{r}_1\mathbf{r}_2, \\ \mathbf{U}{:}\left(\mathbf{U}{:}\mathbf{T}^{(4)}\right) &= 3(\mathbf{r}_1\cdot\mathbf{r}_2). \end{aligned} \tag{3.42}$$

This gives a scalar. In contrast, consider the triple dot product with $\boldsymbol{\mathcal{E}}$ on the right hand side, to give the vector

$$\mathbf{T}^{(4)} \odot^3 \boldsymbol{\mathcal{E}} = -\mathbf{r}_1\times\mathbf{r}_2. \tag{3.43}$$

All of these results are nonzero, unless $\mathbf{r}_1$ and $\mathbf{r}_2$ are either orthogonal or parallel. Essentially then, $\mathbf{T}^{(4)}$ may be considered to be composed of three different natural tensors, specifically it can be written as the sum of three embedded natural tensors

$$\begin{aligned} \mathbf{T}^{(4)} &\equiv \mathbf{U}\mathbf{r}_1\mathbf{r}_2 \\ &= \mathbf{U}\left[\frac{1}{2}(\mathbf{r}_1\mathbf{r}_2 + \mathbf{r}_2\mathbf{r}_1) - \frac{1}{3}(\mathbf{r}_1\cdot\mathbf{r}_2)\mathbf{U}\right] + \frac{1}{2}\mathbf{U}\boldsymbol{\mathcal{E}}\cdot(\mathbf{r}_1\times\mathbf{r}_2) + \frac{1}{3}(\mathbf{r}_1\cdot\mathbf{r}_2)\mathbf{U}\mathbf{U}, \end{aligned} \tag{3.44}$$

namely of the second order natural tensor in square brackets, the vector $\mathbf{r}_1\times\mathbf{r}_2$, and the scalar $\mathbf{r}_1\cdot\mathbf{r}_2$. It is also noted that the natural tensor of second order does not arise by direct tensorial reduction of the above $\mathbf{T}^{(4)}$. To obtain all natural tensors embedded in a given tensor $\mathbf{T}^{(p)}$ appears then to require the procedure: i) find one natural tensor by tensorial reduction; ii) embed this to form a tensor of the original order and in a manner consistent with the original reduction procedure, this really just involves adding $(1/3\mathbf{U})$'s and $(-2\boldsymbol{\mathcal{E}}\cdot)$'s in the opposite order in which the original reduction was done, and must reproduce the discovered natural tensor if the same (original) reduction is carried out on the embedded natural tensor; iii) subtract the embedded natural tensor from the original tensor to get $\mathbf{T}^{(p)'}$. This tensor is missing the already discovered tensor of natural form; iv) carry out a different sequence of tensorial reductions to discover another natural tensor; v) repeat this procedure until there is nothing left to reduce.

It is noticed that symmetric traceless tensors have unique properties. In fact these correspond exactly to the irreducible representations of the three dimensional rotation group. But before addressing this connection, it is useful to identify tensors which can be used to project out the symmetric traceless part of a given tensor, these special tensors are denoted as the tensors $\mathbf{E}^{(p)}$.

3.3 The Natural Projection Tensors $\mathbf{E}^{(p)}$

The object is to find a tensor $\mathbf{E}^{(p)}$ which, when contracted p times with a pth order tensor $\mathbf{T}^{(p)}$, produces the symmetric traceless part of $\mathbf{T}^{(p)}$. Necessarily this tensor $\mathbf{E}^{(p)}$ will have $2p$ directions. It is also useful if it is idempotent,

$$\mathbf{E}^{(p)} \odot^p \mathbf{E}^{(p)} = \mathbf{E}^{(p)}, \tag{3.45}$$

so that if $\mathbf{T}^{(p)}$ is already symmetric traceless, it does not change the tensor. Moreover, since $\mathbf{E}^{(p)}$ is to pick out the symmetric traceless part of *any* pth order tensor, this projector can have no preferential directions, so it must be a rotational invariant. Again, since it is an even ordered invariant tensor, it can be expressed entirely in terms of combinations of $\mathbf{U}$.

Clearly $\mathbf{E}^{(p)}$ must be symmetric and traceless in the lefthand set of p indices since it is to project out traceless symmetric tensors, but since it is to be sensitive to all the directions of the tensor on which it acts, it must also be symmetric in the righthand set of p directions as well. [It will also turn out to be traceless in the righthand set of directions.] Essentially $\mathbf{E}^{(p)}$ must be a modification of the identity

$$\mathbf{U}^{(p)} = \underbrace{\lfloor \cdots \mathbf{U} \cdots \rfloor} \tag{3.46}$$

having p $\mathbf{U}$'s connecting the two sets (lefthand set and righthand set) of p directions, which has been symmetrized in both sets of directions, and then made traceless in each set of directions. As a shorthand notation, curly brackets with a superscript factor is used to indicate that whatever is within the brackets is symmetrized, for example

$$\Big\{\mathbf{abc}\Big\}^{(3)} \equiv \frac{1}{3!}\left[\mathbf{abc} + \mathbf{bca} + \mathbf{cab} + \mathbf{bac} + \mathbf{acb} + \mathbf{cba}\right]. \tag{3.47}$$

Thus the symmetrization of the above identity in both sets of indices is written as

$$\Big\{\underbrace{\lfloor \cdots \lfloor \Big\}^{(p)} \Big\{ \rfloor \cdots \rfloor} \Big\}^{(p)} \tag{3.48}$$

Each trace condition gives rise to a $\mathbf{U}$ in the lefthand symmetrized set of directions, and necessarily also in the righthand symmetrized set, since there are p directions in each set, so $\mathbf{E}^{(p)}$ must be expressible as the sum

$$\mathbf{E}^{(p)} = \sum_{t=0}^{[\frac{1}{2}p]} c_t^{(p)} \Big\{(\mathbf{U})^t(\underbrace{\lfloor)^{p-2t}\Big\}^{(p)}\Big\{(\rfloor}\,)^{p-2t}(\mathbf{U})^t\Big\}^{(p)} \tag{3.49}$$

of terms in which each set of p directions has t $\mathbf{U}$'s and $p-2t$ connections to the other set of p directions, with each set being symmetrized. The coefficients $c_t^{(p)}$ are to be determined by the traceless and idempotency conditions while the upper limit of the sum is to the largest integer less than or equal to $\frac{1}{2}p$. A trace (doubledot contraction with U) on the lefthand set of p directions gives a number of different terms because the result of the contraction is different, depending on whether the contraction involves zero, one, or two U's in the expansion term. Specifically, the contraction of the sum gives

$$
\begin{aligned}
&\mathsf{U}{:}\mathsf{E}^{(p)} = 0 \\
&= \sum_{t=0}^{[\frac{1}{2}p]} c_t^{(p)} \Big[2t(2p-2t+1) \Big\{ (\mathsf{U})^{t-1} (\mathsf{U})^{p-2t} \Big\}^{(p-2)} \Big\{ (\mathsf{U})^{p-2t} (\mathsf{U})^{t} \Big\}^{(p)} \\
&+(p-2t)(p-2t-1) \Big\{ (\mathsf{U})^{t} (\mathsf{U})^{p-2t-2} \Big\}^{(p)} \Big\{ (\mathsf{U})^{p-2t-2} (\mathsf{U})^{t+1} \Big\}^{(p)} \Big]. \qquad (3.50)
\end{aligned}
$$

Collecting equal tensorial terms together gives the recursion relation

$$
c_t^{(p)} = -\frac{(p-2t+2)(p-2t+1)}{2t(2p-2t+1)} c_{t-1}^{(p)}. \qquad (3.51)
$$

This recursion relation is identical to that for the Legendre polynomials. The idempotency condition implies the condition $c_0^{(p)} = 1$, so the expansion coefficients are determined to be

$$
c_t^{(p)} = (-1)^t \frac{p!^2}{(2p)!} \binom{p}{t} \binom{2p-2t}{p}. \qquad (3.52)
$$

This completes the computation of the projectors $\mathsf{E}^{(p)}$.

Explicitly, $\mathsf{E}^{(0)} = 1$ and $\mathsf{E}^{(1)} = \mathsf{U}$, while $\mathsf{E}^{(2)}$ and $\mathsf{E}^{(3)}$ are written out in diagrammatical form in Eqs. (2.72) and (2.76). Indicial representations of these latter two tensors are

$$
\left[\mathsf{E}^{(2)}\right]_{ij,i'j'} = \frac{1}{2}\left[\delta_{ii'}\delta_{jj'} + \delta_{ij'}\delta_{ji'}\right] - \frac{1}{3}\delta_{ij}\delta_{i'j'} \qquad (3.53)
$$

and

$$
\begin{aligned}
\left[\mathsf{E}^{(3)}\right]_{ijk,i'j'k'} &= \frac{1}{6}[\delta_{ii'}(\delta_{jj'}\delta_{kk'} + \delta_{jk'}\delta_{kj'}) + \delta_{ij'}(\delta_{ji'}\delta_{kk'} + \delta_{jk'}\delta_{ki'}) + \delta_{ik'}(\delta_{ji'}\delta_{kj'} + \delta_{jj'}\delta_{ki'})] \\
&\quad -\frac{1}{15}[\delta_{ij}(\delta_{kk'}\delta_{i'j'} + \delta_{ki'}\delta_{j'k'} + \delta_{kj'}\delta_{i'k'}) + \delta_{ik}(\delta_{jk'}\delta_{i'j'} + \delta_{ji'}\delta_{j'k'} + \delta_{jj'}\delta_{i'k'}) \\
&\qquad +\delta_{jk}(\delta_{ik'}\delta_{i'j'} + \delta_{ii'}\delta_{j'k'} + \delta_{ij'}\delta_{i'k'})]. \qquad (3.54)
\end{aligned}
$$

In this equation for $\mathsf{E}^{(3)}$, it is noticed that while the expansion coefficients are $c_0^{(3)} = 1$ and $c_1^{(3)} = -3/5$, the factors that appear in this equation take into account the 6 terms in the first combination and the 9 terms in the second, associated with the normalization factors in the symmetrization operation, Eq. (3.47). Analogous expressions for the higher ordered projectors could be written out, but the explicit equations for these tensors are rarely needed, rather what they do is clear, namely to project out the traceless symmetric part of the tensor upon which they act.

3.3.1 Contraction of $\mathsf{E}^{(p)}$

For any projection operator, the trace determines the dimension of the space onto which the projector maps any object. The analog of the trace is the p-fold contraction between the left and right indices of $\mathbf{E}^{(p)}$. Rather than carry this out completely, the intermediate contraction $\underbrace{\lfloor\cdot\mathbf{E}^{(p)}\cdot\rfloor}$ is calculated. This can be accomplished by examining the terms in Eq. (3.49). For given t, the contraction becomes

$$
\begin{aligned}
&\left\{(\mathbf{U})^t(\underbrace{\mathbf{U})^{p-2t}\right\}^{(p)}\cdot\left\{(\mathbf{U}}\,)^{p-2t}(\mathbf{U})^t\right\}^{(p)} \\
&= \frac{(p-2t)(p+2t+2)}{p^2}\left\{(\mathbf{U})^t(\underbrace{\mathbf{U})^{p-2t-1}\right\}^{(p-1)}\left\{(\mathbf{U}}\,)^{p-2t-1}(\mathbf{U})^t\right\}^{(p-1)} \\
&+\frac{4t^2}{p^2}\left\{(\mathbf{U})^{t-1}(\underbrace{\mathbf{U})^{p-2t+1}\right\}^{(p-1)}\left\{(\mathbf{U}}\,)^{p-2t+1}(\mathbf{U})^{t-1}\right\}^{(p-1)},
\end{aligned}
\tag{3.55}
$$

after taking into account all the possible ways in which the contraction can be carried out. In the sum over t, the second term, involving $(\mathbf{U})^{t-1}$, can be written in the form of the first term, by replacing t with $t+1$, while the new limits on the sum for this second term can be replaced by the limits appropriate for the first term. The coefficient for the combination is then

$$
\begin{aligned}
& c_t^{(p)}\frac{(p-2t)(p+2t+2)}{p^2}+c_{t+1}^{(p)}\frac{4(t+1)^2}{p^2} \\
&= c_t^{(p)}\frac{(p-2t)}{p^2}\left[p+2t+2-\frac{2(t+1)(p-2t-1)}{2p-2t-1}\right] \\
&= c_t^{(p)}\frac{(p-2t)(2p+1)}{p(2p-2t-1)}=\frac{2p+1}{2p-1}c_t^{(p-1)},
\end{aligned}
\tag{3.56}
$$

where the detailed properties of the expansion coefficients, Eq. (3.52), have been used. It follows that

$$
\underbrace{\lfloor\cdot\mathbf{E}^{(p)}\cdot\rfloor}\;=\frac{2p+1}{2p-1}\mathbf{E}^{(p-1)}. \tag{3.57}
$$

That the result is symmetric and traceless in both left and right sets of $p-1$ indices implies that it is a multiple of $\mathbf{E}^{(p-1)}$. Repeating this contraction $p-2$ times and recognizing that $\mathbf{E}^{(1)}=\mathbf{U}$, so that $\underbrace{\lfloor\cdot\mathbf{E}^{(1)}\cdot\rfloor}=3$, implies that

$$
\underbrace{\lfloor\cdots\underbrace{\lfloor\odot^p\mathbf{E}^{(p)}\odot^p\rfloor}\cdots\rfloor}=2p+1 \tag{3.58}
$$

is the dimension of the range of $\mathbf{E}^{(p)}$. This result is also found by a direct count of independent variables, see Sec. 3.4.1.

3.3.2 Selection of a direction of $\mathbf{E}^{(p)}$

It is often desirable to treat one direction of a symmetric traceless set as special, for example it may be contracted in a different way than the others. This is particularly the case when examining various properties of the 3-j tensors, see Chap. 6.

The starting point for this selection is to consider the contraction $\mathbf{U}\cdot\mathbf{E}^{(p)}$. This of course does nothing in itself. It is noted that the remaining directions on the lefthand side of $\mathbf{E}^{(p)}$ are symmetric and traceless among themselves, so this can be elaborated as

$$
\mathbf{E}^{(p)}=\underbrace{\lfloor\mathbf{E}^{(p-1)}\rfloor}\;\odot^p\mathbf{E}^{(p)}. \tag{3.59}
$$

Now expand $\mathsf{E}^{(p)}$ according to Eq. (3.49). This expansion and the subsequent calculation of the contraction gives

$$
\begin{aligned}
\mathsf{E}^{(p)} &= \sum_t c_t^{(p)} \mathsf{E}^{(p-1)} \odot^p \left\{ (\mathsf{U})^t (\;)^{p-2t} \right\}^{(p)} \left\{ (\;)^{p-2t} (\mathsf{U})^t \right\}^{(p)} \\
&= \sum_t c_t^{(p)} \left[\frac{p-2t}{p} \mathsf{E}^{(p-1)} \odot^{p-1} \left\{ (\mathsf{U})^t (\;)^{p-2t-1} \right\}^{(p-1)} \left\{ (\;)^{p-2t-1} (\mathsf{U})^t \right\}^{(p)} \right. \\
&\qquad \left. + \frac{2t}{p} \mathsf{E}^{(p-1)} \odot^{p-1} \left\{ (\mathsf{U})^{t-1} (\;)^{p-2t} \right\}^{(p-2)} \left\{ (\;)^{p-2t} (\mathsf{U})^t \right\}^{(p)} \right] \\
&= \mathsf{E}^{(p-1)} \odot^{p-1} \left((\;)^{p-1} \left\{ (\;)^{p-1} \right\}^{(p)} \right. \\
&\qquad \left. - \frac{p-1}{2p-1} \mathsf{E}^{(p-1)} \odot^{p-1} \left((\;)^{p-2} \left\{ (\;)^{p-2} \mathsf{U} \right\}^{(p)} \right. \right. \quad . \qquad (3.60)
\end{aligned}
$$

The contraction of the selected direction into the lefthand symmetric set of directions has two possibilities, listed as $p-2t$ possibilities of being contracted to a U associated with the righthand set of symmetric directions, and $2t$ possibilities of being contracted into a U lying entirely in the lefthand set. Because of the presence of $\mathsf{E}^{(p-1)}$, only the first two terms of the t expansion contribute, which is the advantage of explicitly inserting this projector into Eq. (3.59). The final result is obtained by inserting the value of the expansion coefficients $c_t^{(p)}$. Equation (3.60) gives the result of treating the lefthand index in a special manner. Clearly the transpose of this formula can be used to describe the selection of the righthand direction. And of course this could be iterated to select out 2 or more directions for special treatment. Such generalizations are not explicitly carried out here.

3.4 Natural Tensors as Irreducible Representations

A natural tensor was defined in the last section as a tensor completely symmetric between all directions of the tensor and traceless in all pairs of directions. It is now shown that these tensors are irreducible representations of the rotation group. A first step in this process is to note that any rotation retains symmetry, because all directions undergo the same transformation, and also retains the traceless conditions, since the act of taking a trace is the same as doubledotting U with that pair of directions, the latter operation being invariant to a rotation. Thus a symmetric traceless tensor remains so under any rotation. The only question that remains is whether the symmetric traceless tensor can be separated into two or more parts which are unconnected by any rotation. Intuitively the answer to this question is no, but that does not provide a proof. The following proof has two steps: first the dimension (the maximum number of independent elements) of a symmetric traceless tensor of order p is found; second it is shown that a symmetric traceless tensor is an eigentensor of the Casimir invariant G^2, showing that such tensors belong to an irreducible representation of the rotation group. Then from the known properties of the three dimensional rotation group, since the dimension found is exactly the dimension of the correspondingly found irreducible representation, there is no redundancy and such tensors uniquely correspond to the irreducible representation. These two steps are now carried out.

3.4.1 Dimension of symmetric traceless tensors of order p

The number of independent components of a symmetric tensor is obtained first, then the number of traceless conditions is subtracted. There are three possible components (unit vectors) that can be assigned to each direction in a pth order tensor, these will be referred to here as the $\hat{x}$, $\hat{y}$ and $\hat{z}$ components for definiteness. If m of these are assigned to $\hat{x}$, then there are $p-m$ indices to be assigned to $\hat{y}$ and $\hat{x}$. The latter can be assigned in $p-m+1$ ways correponding to whether there are 0, 1, 2 $\cdots$, or $p-m$ $\hat{y}$'s with the remaining components assigned to $\hat{z}$. Since the range of m is from 0 to p, the number of symmetric terms is the sum

$$D_{\mathrm{sym}}(p)=\sum_{m=0}^{p}(p+1-m)=(p+1)(p+1)-\frac{p(p+1)}{2}=\frac{(p+1)(p+2)}{2}. \tag{3.61}$$

Now the tensor must be traceless in all pairs of indices, so that there are $p(p-1)/2$ traceless conditions. It follows that the dimension of traceless symmetric tensors of order p is

$$D_p=D_{\mathrm{sym}}(p)-\frac{p(p-1)}{2}=2p+1. \tag{3.62}$$

This result was also obtained by calculating the trace of the projector $\mathbf{E}^{(p)}$, see Eq. (3.58). It is immediately recognized that this is the dimension of the irreducible representation of the rotation group having maximum weight p. Thus it needs to be shown that the eigenvalue of the Casimir invariant is $p(p+1)$ so that any traceless symmetric tensor of order p corresponds to an irreducible representation of maximum weight p.

3.4.2 The Casimir invariant eigenvalue for a symmetric traceless tensor

Since symmetric traceless tensors are distinguished by having a projector $\mathbf{E}^{(p)}$, it is sufficient for classifying the action of the Casimir invariant on symmetric traceless tensors, to consider only the action of the corresponding Casimir invariant $\mathbf{G}^{(p)2}$ on this projector. In carrying out this contraction it is noted that of the terms in the sum over permutations in Eq. (3.15), the $\Cup$ terms are merely permutations of the identity, and contribute the same as the identity when acting on $\mathbf{E}^{(p)}$, since $\mathbf{E}^{(p)}$ is symmetric in each of the left and right hand sets of indices. Moreover, the $\cup\cup$ terms involve traces over pairs of indices in the left and right sets of indices, which vanish because of the traceless nature of $\mathbf{E}^{(p)}$. It follows that all nonzero terms in the contraction are proportional to $\mathbf{E}^{(p)}$ and add together to a total multiple $2p+2p(p-1)/2=p(p+1)$ of the projector, that is

$$\mathbf{G}^{(p)2}\odot^{p}\mathbf{E}^{(p)}=p(p+1)\mathbf{E}^{(p)}. \tag{3.63}$$

Thus symmetric traceless tensors of order p belong to the irreducible representation of the three dimensional rotation group having highest weight p. Moreover, since the dimension of this tensor space is $2p+1$, as shown above, this representation is a single irreducible representation of the rotation group of weight p.

3.5 Parentage Scheme

The tensor product of p vectors is a particular form of a pth order tensor. A reduction of this tensor product into all its natural tensors, assuming all vectors are inherently different, can provide a means of classifying all the possible natural tensors that constitute the tensor product. One way of carrying out this procedure is to build up the tensor product by adding one vector at a time and reduce the product into its natural tensors after each addition. Correctly, the natural tensors should be embedded to form pth order tensors to provide a common format for the reduction, but as far as providing a classification of all possible natural tensors which are contained in the tensor product, the last step is unnecessary.

Thus the implementation of the above classification procedure is as follows:

1. Start with the scalar 1. This uses 0 vectors, so is associated with a tensor product of $p = 0$, and is a rotational invariant, so is of weight $\ell = 0$.

2. Add one vector. This is a natural tensor having weight 1, formed from only one vector, so is associated with order $p = 1$ and weight $\ell = 1$.

3. At each successive stage, say the pth, add a vector to each natural tensor associated with the $(p-1)$th stage.

4. For each tensor product of a vector and a natural tensor of weight ℓ greater than 0, reduce this by using the three operations, a) dot product the vector into the natural tensor, b) cross product the vector into the natural tensor, and c) form the symmetric traceless combination of the vector and the natural tensor. These give natural tensors of weights $\ell - 1$, ℓ and $\ell + 1$. This exhausts the possible number of independent variables since the tensor product has $3(2\ell + 1)$ variables while the sum of the three natural tensors into which the product has been reduced has $(2\ell - 1) + (2\ell + 1) + (2\ell + 3) = 3(2\ell + 1)$ variables. Thus this is a complete reduction of the tensor product.

5. Repeat the last two steps until the desired order has been reached.

The result of this procedure is best represented in diagrammatic form, see Figure 3.1, whose form first appeared in Ref. [13]. The diagonal and horizontal lines describe the parentage, namely each order p, weight ℓ natual tensor gives rise to the three $p+1$ order natural tensors of weights $\ell - 1$, ℓ and $\ell + 1$. The exception being when the weight is 0, in which case there is only the possibility of increasing the weight to 1. It is then merely adding up the numbers of parentage lines from lower order natural tensors, to get the number of natural tensors of a given weight. In particular, a 3rd order tensor can always be decomposed into one natural tensor of weight 3, two of weight 2, 3 of weight 1 and 1 scalar (weight 0). Moreover, the weight 3 tensor is formed by successively symmetrizing and making traceless the tensor product after adding each vector, actually this procedure only needs to be done once, namely to the tensor product of the three vectors. In contrast, the 3 weight 1 tensors are formed by the three parentage schemes, namely: i) dot the third vector into the symmetric traceless part of the tensor product of the first two vectors; ii) cross product the second vector into the first, and then take the cross product of the result with the third vector; and iii) dot product the first two vectors and multiply the result by the third vector. These are just the interpretations of the three paths leading to the order 3, weight 1 position in the Figure. The count of the number of variables in these natural tensors is $7 + (2 \times 5) + (3 \times 3) + 1 = 27$, which is exactly 3^3, the number of components in a 3rd order tensor, so this decomposition is consistent in its count of the number of independent variables.

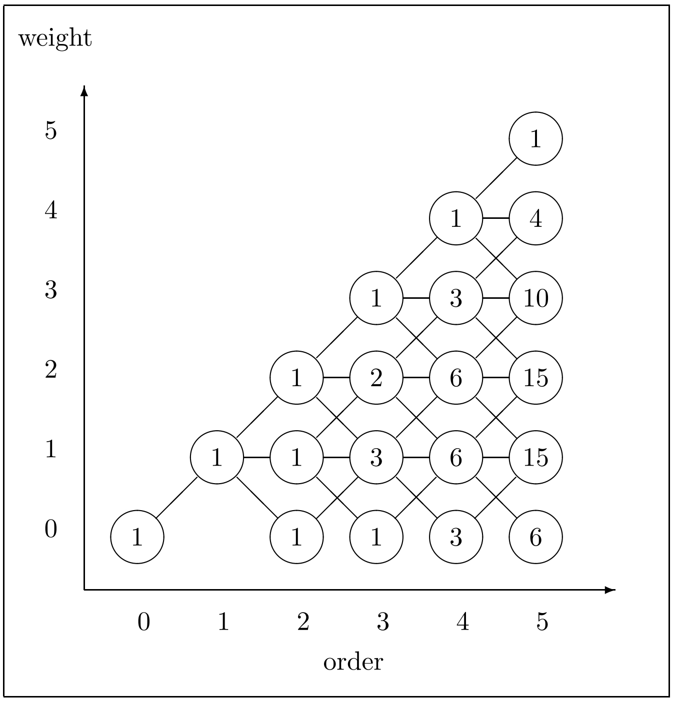


Figure 3.1: Parentage Scheme. The number of linearly independent irreducible representations of weight ℓ in a tensor of order p.

3.6 Method of Characters

Given a representation of a group, a standard group theoretical method for discovering what irreducible representations are present in this representation is the method of group characters. Essentially this depends on the orthogonality of the characters $\chi_j(g)$ for the different irreducible representations. For a group G of finite order h_G, this orthogonality is the sum over the group elements

$$\sum_{g \in G} \chi_j(g)\chi_k(g) = \delta_{jk} h_G. \tag{3.64}$$

Since the rotation group is of infinite order, the sum must be replaced by an integral over the group elements. The group elements are parameterized by the angle of rotation θ and the axis of rotation $\hat{n}$, so it is natural to express the integration over the group elements as an integration over these parameters. But it is necessary to introduce a density of group elements $\varpi(\theta)$ in order to assign a (relative) number of group elements to a given volume in parameter space. The calculation of this density is usually based on fairly general and abstract group theoretical arguments [3, 5]. Here a derivation is given directly based on the above parameterization of the rotation group. This is done in the first subsection. After that, the character of a general pth tensor is discussed, as well as that of a particular symmetric traceless tensor. It is seen that for a Cartesian tensor having a certain symmetry, the symmetry dominates the analysis of its group theoretical properties. This is somewhat obvious since the classification of natural tensors is fundamentally based on symmetry (and trace, which is another kind of symmetry) properties.

3.6.1 Group Density

It is desired to find a function ϖ of the parameters θ and $\hat{n}$ such that the product of the group density ϖ and the parameter volume element $\theta^2 d\theta d\hat{n}$, namely $\varpi\theta^2 d\theta d\hat{n}$, is a measure of the number of group elements in this parameter volume. Here the parameterization of the rotation group is the projective 3 sphere P_3, see Sec. 2.5.1. This calculation can be accomplished by recognizing that a group element can be used to map a parameter volume from a reference parameter set to any other parameter set. Then the ratio of group densities is the inverse of the ratio of parameter volumes. A simplification of this calculation is provided by the recognition that all axis directions are equivalent, so the density depends only on the angle of rotation. Moreover, it is a property of the rotation group, that a group similarity transformation is equivalent to changing the axis of rotation, but maintaining the same angle of rotation [compare Eqs. (2.121-2.137) and related discussion]. Thus, in any representation, the character of a group element, being the trace of the representation matrix, is independent of the direction of the axis. As a consequence, both the group density and the character of any representation depend only on the angle of rotation θ.

Since there is only a θ dependence of the group density, it is sufficient to examine a single axis direction $\hat{n}$ and to calculate how a small parameter volume at the origin ($\theta = 0$) is transformed into a parameter volume at finite θ. As it doesn't matter what shape is chosen for the reference parameter volume, it is convenient to choose a pointed cylindrical wedge at the origin, see Fig. 3.2, with axis along the $\hat{n}$ direction of length ϕ , apex angle α and cylindrical angle β, these three angles are all to be considered infinitesimal. The arc length of the infinitesimal volume at radius ϕ is then $\alpha\phi$, surface area at this radius $(1/2)\beta(\alpha\phi)^2$, and volume $(1/6)\alpha^2\beta\phi^3$. This volume element determines, of course, the set of group elements of the rotation group within the parameter volume element, which is clearly specified by the four limiting parameter sets (rotations) $(0,\ \hat{n})$, $(\phi,\ \hat{n})$, $(\phi,\ \hat{n}_1)$ and $(\phi,\ \hat{n}_2)$. The two other directions besides $\hat{n}$ are the axes along the other two edges of the pointed wedge, being given by

$$\hat{n}_1 \simeq \hat{n} + \alpha\hat{\ell} \qquad \hat{n}_2 \simeq \hat{n}_1 + \alpha\beta\hat{m}, \tag{3.65}$$

where $\hat{\ell} \perp \hat{n}$ is along one side of the wedge, and $\hat{m} = \hat{n}\times\hat{\ell}$, these correspond to the general orthogonal basis set introduced at the beginning of the chapter.

Now rotate this set of rotations described by the wedge by an angle θ about the axis $\hat{n}$. Then the four limiting rotations are transformed into the rotations

$$\begin{array}{ll} R_{\hat{n}}(\theta)R_{\hat{n}}(0) = R_{\hat{n}}(\theta), & R_{\hat{n}}(\theta)R_{\hat{n}}(\phi) = R_{\hat{n}}(\theta+\phi) \\ R_{\hat{n}}(\theta)R_{\hat{n}_1}(\phi) = R_{\hat{n}'_1}(\phi'), & R_{\hat{n}}(\theta)R_{\hat{n}_2}(\phi) = R_{\hat{n}'_2}(\phi''). \end{array} \tag{3.66}$$

The first two rotations correspond to the obvious sets of parameters $(\theta,\ \hat{n})$ and $(\theta+\phi,\ \hat{n})$ while the last two require detailed calculation. Expanding the combining rules, Eqs. (2.99) and (2.101), according to the smallness of ϕ, α and β, it is found that their angles are $\phi' \simeq \phi'' \simeq \theta + \phi$ while their axes are

$$\hat{n}'_1 \simeq \hat{n} + \alpha\frac{\phi}{2}\left(\hat{\ell}\cot\frac{\theta}{2} + \hat{m}\right)$$

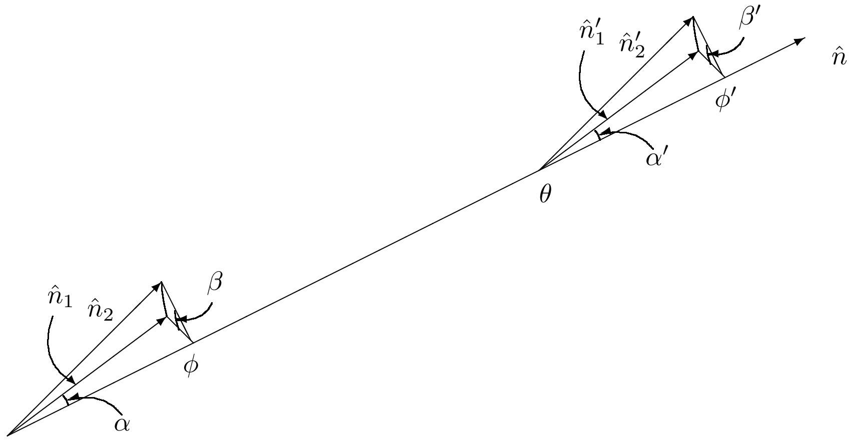


Figure 3.2: The pointed wedge used for calculating the group density

$$\hat{n}'_2 \simeq \hat{n}'_1 + \alpha\beta\frac{\phi}{2}\left(\hat{m}\cot\frac{\theta}{2} - \hat{\ell}\right). \tag{3.67}$$

These four sets of parameters set out a pointed wedge with apex at $(\theta,\ \hat{n})$ and edge lengths ϕ. The circular sector at the base has a radius of $\alpha(\phi/2)\csc(\theta/2)\theta$ and arc length $\beta\alpha(\phi/2)\csc(\theta/2)\theta$, the last θ factor being a first approximation to the radius of the parameter space at the base points. As a consequence the volume of this wedge is $(1/24)\alpha^2\beta\phi^3\csc^2(\theta/2)\theta^2$. It folows that the group density at θ is related to the density at 0 by the inverse ratio of wedge volumes, namely

$$\begin{aligned}\varpi(\theta) &= \frac{(1/6)\alpha^2\beta\phi^3}{(1/24)\csc^2(\theta/2)\alpha^2\beta\phi^3\theta^2}\varpi(0) \\ &= \frac{4\sin^2(\theta/2)}{\theta^2}\varpi(0) = \frac{2(1-\cos\theta)}{\theta^2}\varpi(0).\end{aligned} \tag{3.68}$$

Since an element of volume in the parameter space is $\theta^2 d\theta d\hat{n}$, $\varpi(0)$ is chosen to be $1/8\pi^2$, so that

$$\int_0^\pi \int \varpi(\theta)d\hat{n}\theta^2 d\theta = \frac{1}{4\pi^2}\int_0^\pi \int d\hat{n}(1-\cos\theta)d\theta = 1 \tag{3.69}$$

provides a normalized integral over group parameters associated with an equal weighting of group elements. In terms of Euler angles this integral is

$$\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi}\sin\beta d\beta d\alpha d\gamma = 1. \tag{3.70}$$

This can be proved using the Jacobian of the relations (2.138) and (2.139) between θ and $\hat{n}$ and the Euler angles $\alpha,\ \beta$ and γ.

3.6.2 Classification of Tensors of order p via characters

As stated in the introduction to this chapter, since rotating a tensor does not change its order, it follows that tensors of a particular order, say p, provide a representation of the rotation group. The matrix form for this represention can be obtained by listing the 3^p components of the tensor in order, equating the tensor to a 3^p-dimensional vector. Translating the effect of a rotation into this vector space description of the tensor produces the $3^p \times 3^p$ matrix representation of the rotation group. The object is then to reduce this representation, or at least to classify what irreducible representations are present in this representation of the rotation group. The character of the representation provides a means of doing this. In general it is necessary to have the representation matrix before calculating its trace (character), but for a general tensor of order p, having no prescribed symmetry, the character can be calculated in an indirect manner. This case is considered first, then the character of a second order natural tensor is calculated, which illustrates some of the care that must be taken when carrying out such a calculation. The character of a general natural tensor is more easily calculated after a connection to spherical tensors is made, this being done in Chap. 5.

The General pth Order Tensor

For a general pth order tensor, each of the p directions is to be rotated. Thus the rotation of such a tensor is equivalent to simultaneously rotating p vectors. Since the trace of the matrix for rotating a vector is

$$\Gamma^{(1)}(\theta) = \mathbf{U}{:}\mathbf{R}_{\hat{n}}(\theta) = 2\cos\theta + 1, \tag{3.71}$$

the character for the general pth order tensor is the pth power of this, namely

$$\Gamma^{(p)}(\theta) = (2\cos\theta + 1)^p. \tag{3.72}$$

Given that the irreducible representations of the rotation group are parameterized by their highest weight ℓ and dependence on angle of rotation θ, see Eq. (5.10),

$$\chi_\ell(\theta) = 1 + \sum_{m=1}^{\ell} 2\cos(m\theta) = \frac{\sin\left[(\ell+\frac{1}{2})\theta\right]}{\sin(\theta/2)}, \tag{3.73}$$

the number of irreducible representations of highest weight ℓ that can occur in a tensor of order p is

$$n_\ell^{(p)} = \frac{1}{\pi}\int_0^\pi \chi_\ell(\theta)\Gamma^{(p)}(\theta)(1-\cos\theta)d\theta. \tag{3.74}$$

These are the same numbers as appear in the parentage scheme, see Fig. 3.1.

Second Order Symmetric Traceless Tensors

Since a second order symmetric traceless tensor is a special second order tensor, its rotation is a special case of the rotation of a second order tensor. Thus it is appropriate to restrict the rotation tensor $\mathbf{R}_{\hat{n}}^{(2)}(\theta)$ to act on symmetric traceless tensors. This can be accomplished by projecting the rotation tensor onto this symmetry, namely

$$\mathbf{T} \equiv \mathbf{E}^{(2)}{:}\mathbf{R}_{\hat{n}}^{(2)}(\theta){:}\mathbf{E}^{(2)}. \tag{3.75}$$

A detailed computation of this fourth order tensor can be written down by carrying out the contractions and this is written below, but in a matrix form corresponding to its components in a Cartesian coordinate system. But only the character (trace) of this representation is wanted. Several ways of carrying out this calculation are discussed. Strictly Cartesian methods are discussed in this section, but there are a number of different ways to view this calculation. The general method based on the connection to spherical tensors, as given in Chap. 5, is also applicable.

The first method is very detailed and depends on having an explicit matrix form for the representation. Since a second order tensor has 9 components, an order for these components needs to be selected, so that Eq. (3.75) can be written as a 9×9 matrix. For the subsequent discussion the rotation axis is chosen to be the $\hat{z}$-direction and the choice of order of the tensor components to be

$$T_{xx},\ T_{xy},\ T_{xz},\ T_{yx},\ T_{yy},\ T_{yz},\ T_{zx},\ T_{zy},\ T_{zz}. \tag{3.76}$$

In terms of this order of the components, the matrix form of Eq. (3.75) is

$$\begin{pmatrix} c^2-\frac{1}{3} & -sc & 0 & -sc & s^2-\frac{1}{3} & 0 & 0 & 0 & -\frac{1}{3} \\ sc & \frac{1}{2}(c^2-s^2) & 0 & \frac{1}{2}(c^2-s^2) & -sc & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}c & 0 & 0 & -\frac{1}{2}s & \frac{1}{2}c & -\frac{1}{2}s & 0 \\ sc & \frac{1}{2}(c^2-s^2) & 0 & \frac{1}{2}(c^2-s^2) & -sc & 0 & 0 & 0 & 0 \\ s^2-\frac{1}{3} & sc & 0 & sc & c^2-\frac{1}{3} & 0 & 0 & 0 & -\frac{1}{3} \\ 0 & 0 & \frac{1}{2}s & 0 & 0 & \frac{1}{2}c & \frac{1}{2}s & \frac{1}{2}c & 0 \\ 0 & 0 & \frac{1}{2}c & 0 & 0 & -\frac{1}{2}s & \frac{1}{2}c & -\frac{1}{2}s & 0 \\ 0 & 0 & \frac{1}{2}s & 0 & 0 & \frac{1}{2}c & \frac{1}{2}s & \frac{1}{2}c & 0 \\ -\frac{1}{3} & 0 & 0 & 0 & -\frac{1}{3} & 0 & 0 & 0 & \frac{2}{3} \end{pmatrix}. \tag{3.77}$$

In this matrix, c is used as an abbreviation for $\cos\theta$ and s for $\sin\theta$. It is now easy to calculate the trace of this matrix, which is found to be

$$\begin{aligned} \Gamma(\theta) &= 2\left(c^2 - \frac{1}{3}\right) + c^2 - s^2 + 2c + \frac{2}{3} \\ &= 3c^2 - s^2 + 2c = 2\cos(2\theta) + 2\cos\theta + 1. \end{aligned} \tag{3.78}$$

This is recognized as the character for the irreducible representation of the rotation group of maximum weight 2.

What might appear as an easier approach is to recognize that there are only 5 independent parameters that determines a second order symmetric traceless tensor, essentially that such a tensor can be written in the form

$$\begin{aligned} \mathsf{T} &= \frac{1}{2}\left(T_{xx} - T_{yy}\right)\left(\hat{x}\hat{x} - \hat{y}\hat{y}\right) + T_{zz}\left(\hat{z}\hat{z} - \frac{1}{2}\hat{x}\hat{x} - \frac{1}{2}\hat{y}\hat{y}\right) \\ &\quad + T_{xy}\left(\hat{x}\hat{y} + \hat{y}\hat{x}\right) + T_{xz}\left(\hat{x}\hat{z} + \hat{z}\hat{x}\right) + T_{yz}\left(\hat{y}\hat{z} + \hat{z}\hat{y}\right). \end{aligned} \tag{3.79}$$

This has used the traceless condition $T_{xx} + T_{yy} + T_{zz} = 0$ to eliminate the sum $T_{xx} + T_{yy}$, and the symmetry conditions $T_{yx} = T_{xy}$, $T_{zx} = T_{xz}$ and $T_{zy} = T_{yz}$. But now the rotational properties of the independent set of parameters is needed. For a rotation about the $\hat{z}$-direction, any z component is unchanged while the x and y components of any vector $\mathbf{v} = v_x\hat{x} + v_y\hat{y}$ are changed according to

$$\begin{aligned} R_{\hat{z}}(\theta)v_x\hat{x} &= v_x\left[\cos\theta\hat{x} + \sin\theta\hat{y}\right] \\ R_{\hat{z}}(\theta)v_y\hat{y} &= v_y\left[\cos\theta\hat{y} - \sin\theta\hat{x}\right]. \end{aligned} \tag{3.80}$$

Thus, for example, the rotation of the particular tensor $(T_{xx} - T_{yy})(\hat{x}\hat{x} - \hat{y}\hat{y})$, involving two sets of two directions, is rotated to

$$
\begin{aligned}
R_{\hat{z}}(\theta)(T_{xx} - T_{yy})(\hat{x}\hat{x} - \hat{y}\hat{y}) &= (T_{xx} - T_{yy})\left[\cos^2\theta\hat{x}\hat{x} + \sin\theta\cos\theta(\hat{y}\hat{x} + \hat{x}\hat{y}) + \sin^2\theta\hat{y}\hat{y}\right. \\
&\qquad \left. - \cos^2\theta\hat{y}\hat{y} + \cos\theta\sin\theta(\hat{x}\hat{y} + \hat{y}\hat{x}) - \sin^2\theta\hat{x}\hat{x}\right] \\
&= (T_{xx} - T_{yy})\left[(\cos^2\theta - \sin^2\theta)(\hat{x}\hat{x} - \hat{y}\hat{y}) + 2\cos\theta\sin\theta(\hat{x}\hat{y} + \hat{y}\hat{x})\right]. \qquad (3.81)
\end{aligned}
$$

Similar calculations can be made for tensors associated with the other components of $\mathbf{T}$. As a consequence, the 5×5 matrix representing the rotation is then

$$
\begin{pmatrix}
c^2-s^2 & -2sc & 0 & 0 & 0 \\
2sc & c^2-s^2 & 0 & 0 & 0 \\
0 & 0 & c & -s & 0 \\
0 & 0 & s & c & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix}
\begin{matrix}
T_{xx}-T_{yy} \\
T_{xy}+T_{yx} \\
T_{xz}+T_{zx} \\
T_{yz}+T_{zy} \\
T_{zz}
\end{matrix} \qquad (3.82)
$$

The trace of this matrix is clearly the same as that for the 9×9 matrix.

A purely tensor calculation of the trace is also possible, namely

$$
\Gamma(\theta) = \mathbf{E}^{(2)} \odot^4 \mathbf{R}^{(2)}_{\hat{n}}(\theta) = \mathbf{E}^{(2)} \odot^4 \left[\lfloor \mathbf{R}_{\hat{n}}(\theta) \rfloor \cdot \mathbf{R}_{\hat{n}}(\theta) \right]. \qquad (3.83)
$$

The details of carrying out this calculation is

$$
\begin{aligned}
\Gamma(\theta) &= \frac{1}{2}\left[\lfloor \cdot\mathbf{R}_{\hat{n}}(\theta)\cdot \rfloor \lfloor \cdot\mathbf{R}_{\hat{n}}(\theta)\cdot \rfloor + \lfloor \cdot\mathbf{R}_{\hat{n}}(\theta)\cdot\mathbf{R}_{\hat{n}}(\theta)\cdot \rfloor \right] \\
&\qquad - \frac{1}{3} \lfloor \cdot\mathbf{R}_{\hat{n}}(\theta)\cdot \rfloor\lfloor \cdot\mathbf{R}_{\hat{n}}(\theta)\cdot \rfloor \\
&= \frac{1}{2}\left[(1 + 2\cos\theta)^2 + 1 + 2\cos 2\theta\right] - 1 \\
&= 1 + 2\cos\theta + 2\cos 2\theta. \qquad (3.84)
\end{aligned}
$$

In this calculation, the product of two rotation tensors has been recognized as the rotation tensor for 2θ and for the last term, the transpose of the rotation tensor as the inverse.

Each of these calculations involve a fair amount of detail and are neither simple or immediately obvious. A more direct calculation of characters is obtained when the tensor is represented in a basis formed by the eigenvevtors of the generator of the corresponding rotation. This is what is done in the standard spherical tensor treatment, and connections to that is made in Chap. 5.

Chapter 4

Tensors of r

This short chapter provides some properties of tensors of a vector $\mathbf{r}$. First is a definition of the natural tensors of the vector and to show that the associated contraction between two such natural tensors is proportional to a Legendre polynomial. Second is a classification of the integrals over the unit vector $\hat{r}$ of tensors of $\hat{r}$.

As to integrating over all possible values of the position vector $\mathbf{r}$, including its magnitude, the functions need to vanish sufficiently rapidly at infinity that the integral converges. Since tensors of $\mathbf{r}$ are usually polynomials in $\mathbf{r}$, an appropriate weight factor needs to appear in any such integration. An obvious choice is a gaussian weighting function. The third section of this chapter describes a set of functions of $\mathbf{r}$ that belong to irreducible representations of the rotation group and are orthonormal with a Gaussian weighting. Kumar's [19] generating function for these functions is also discussed. Such functions are particularly useful in certain aspects of gas kinetic theory.

4.1 Natural Tensors of r

The p-fold tensor product $\mathbf{rr}\cdots\mathbf{r}$ of $\mathbf{r}$ with itself forms a tensor (or polyad) of order p. This is clearly symmetric to the interchange of any pair of indices. If terms are subtracted from this combination to make it traceless in all pairs of indices, then a natural tensor of weight p is formed. The result is expressed here as

$$[\mathbf{rr}\cdots\mathbf{r}]^{(p)} = [\mathbf{r}]^{(p)}. \tag{4.1}$$

The square bracket with supercript (p) for Cartesian tensors in what is referred to here as natural form was introduced by Kagan and Maximov [12]. For a natural tensor formed from one vector it is deemed unnecessary to repeat the vector the required number of times, hence the second, shortened, form which is adapted in later use. One way of forming the correct linear combination of tensor product and relevant contractions is to project with $\mathsf{E}^{(p)}$, namely

$$[\mathbf{r}]^{(p)} = \mathsf{E}^{(p)}\odot^p\mathbf{rr}\cdots\mathbf{r}. \tag{4.2}$$

Before proceeding it should also be stated that natural tensors formed from two or more vectors, such as

$$[\mathbf{rp}]^{(2)} = \mathsf{E}^{(2)}\odot^2\mathbf{rp}, \tag{4.3}$$

can clearly be devised, but then the number of times that each vector appears must be indicated, for example

$$[(\mathbf{r})^3(\mathbf{p})^2]^{(5)} = \mathbf{E}^{(5)}\odot^5\mathbf{rrrpp} \tag{4.4}$$

indicates the natural tensor of weight (and order) 5 formed from 3 **r**'s and 2 **p**'s.

Since natural tensors of weight p are associated with the irreducible representation of the 3-dimensional rotation group of maximum weight p, it is reasonable that the p-fold dot product of $[\mathbf{r}]^{(p)}$ and $[\mathbf{u}]^{(p)}$ be proportional to that function of the scalar invariant $\mathbf{r}\cdot\mathbf{u}$ which is associated to the pth irreducible representation of the rotation group, namely the Legendre polynomial of order p. A detailed calculation that this is indeed the case only involves the expansion properties, Eq. (3.49), of $\mathbf{E}^{(p)}$, which is now discussed. In fact, the calculation of this tensor product is

$$\begin{aligned}[\mathbf{r}]^{(p)}\odot^p[\mathbf{u}]^{(p)} &= (\mathbf{r})^p\odot^p\mathbf{E}^{(p)}\odot^p(\mathbf{u})^p \\ &= \sum_{t=0}^{[\frac{1}{2}p]} c_t^{(p)} r^{2t}(\mathbf{r}\cdot\mathbf{u})^{p-2t}u^{2t}.\end{aligned} \tag{4.5}$$

Taking out the magnitudes $(ru)^p$ and introducing the corresponding unit vectors $\hat{r}$ and $\hat{u}$, the tensor product becomes

$$\begin{aligned}\overline{P}_p(\hat{r}\cdot\hat{u}) &\equiv [\hat{r}]^{(p)}\odot^p[\hat{u}]^{(p)} \\ &= \sum_{t=0}^{[\frac{1}{2}p]} c_t^{(p)}(\hat{r}\cdot\hat{u})^{p-2t} = \frac{2^p(p!)^2}{(2p)!}P_p(\hat{r}\cdot\hat{u}).\end{aligned} \tag{4.6}$$

Here the series expansion is recognized as that of the Legendre polynomial $P_p(x)$, see e.g. Eq. (2.5.13) of Ref. [1], this requiring the explicit form for the $\mathbf{E}^{(p)}$ expansion coefficients, Eq. (3.52). If $\hat{r} = \hat{u}$, then $P_p(1) = 1$ and the normalization factor that arises can be recognized as the value of

$$\overline{P}_p(1) = \frac{2^p(p!)^2}{(2p)!} = \sum_{t=0}^{[\frac{1}{2}p]} c_t^{(p)}. \tag{4.7}$$

A natural and useful normalization of $[\hat{r}]^{(p)}$ is in terms of a quantity whose square, when averaged over $\hat{r}$, yields the appropriate identity. Thus the tensor valued function of $\hat{r}$

$$\boldsymbol{\mathcal{Y}}^{(p)}(\hat{r}) \equiv \left(\frac{2p+1}{\overline{P}_p(1)}\right)^{1/2}[\hat{r}]^{(p)} \tag{4.8}$$

is introduced, whose prefactor is chosen so that

$$\frac{1}{4\pi}\int d\hat{r}\boldsymbol{\mathcal{Y}}^{(p)}(\hat{r})\boldsymbol{\mathcal{Y}}^{(p')}(\hat{r}) = \delta_{pp'}\mathbf{E}^{(p)}. \tag{4.9}$$

Note that, after integrating over $\hat{r}$, the integral is independent of any direction and so must be a rotational invariant. As a rotationally invariant tensor, the integral must be expressible in terms of $\mathbf{U}$ and $\boldsymbol{\varepsilon}$. But since the integrand is symmetric and traceless in two sets of indices, the only possible result is to be proportional to $\mathbf{E}^{(p)}$, with $p' = p$, which is the identity for symmetric traceless tensors of order (and weight) p. An alternate way of looking at this result is to note that this is the integral over the product of functions belonging to two irreducible representations of the rotation group, which can be non-zero only if the two functions belong to the same irreducible representation. A further check on Eq. (4.9), in particular that this is the proper normalization, can be made by noting that

$$\mathcal{Y}^{(p)}(\hat{r})\odot^{p}\mathcal{Y}^{(p')}(\hat{r}) = M_{pp'}[\hat{r}]^{(|p-p'|)} \tag{4.10}$$

for some number $M_{pp'}$ and symmetric traceless tensor in $\hat{r}$ of weight $|p-p'|$. If $|p-p'| \neq 0$, then the integral over $\mathbf{r}$ will vanish, while if $p = p'$, it follows from Eqs. (4.6) and (4.8) that $M_{pp} = 2p+1$. Thus if a p-fold contraction of Eq. (4.9) is made, then the integral is trivial and with the help of Eq. (3.58) both sides of the equation have the value $2p+1$. A contraction similar to that of Eq. (4.10) is

$$\mathcal{Y}^{(p)}(\hat{r})\odot^{p}\mathcal{Y}^{(p)}(\hat{u}) = (2p+1)P_p(\hat{r}\cdot\hat{u}), \tag{4.11}$$

involving the Legendre polynomial. This is related to the expansion of the Legendre polynomial in terms of spherical harmonics, a connection that is made in Chap. 5. Likewise, $\mathsf{E}^{(p)}$ projects onto the space covered by all $2p+1$ components of the corresponding irreducible representation, so the normalization condition for $\mathcal{Y}^{(p)}$, namely Eq. (4.9), contains all the orthonormality conditions of the spherical harmonics, see Chap. 5. A related subject is the expansion of a general product of $\mathcal{Y}^{(p)}(\hat{r})$'s in terms of $\mathcal{Y}^{(p'')}(\hat{r})$'s, this is given by Eq. (7.26).

The reduction of a product of $\hat{r}$'s into irreducible representations is now discussed. Since the product of n $\hat{r}$'s is already symmetric, the reduction involves only the division of the product into traceless and trace parts. Retaining the tensor symmetry. this reduction can be written formally as

$$(\hat{r})^n = \sum_{m=0}^{[n/2]} a_{nm}\left\{(\mathsf{U})^m\mathcal{Y}^{(n-2m)}(\hat{r})\right\}^{(n)}. \tag{4.12}$$

The upper limit $[n/2]$ of the sum is the largest integer less than $n/2$ while the tensor is the symmetrized product of m U's and one $\mathcal{Y}^{(n-2m)}(\hat{r})$. Special cases of this are

$$\hat{r}\hat{r} = \sqrt{\frac{15}{2}}\mathcal{Y}^{(2)}(\hat{r}) + \frac{1}{3}\mathsf{U} \tag{4.13}$$

and

$$\hat{r}\hat{r}\hat{r} = \sqrt{\frac{2}{35}}\mathcal{Y}^{(3)}(\hat{r}) + \frac{1}{5\sqrt{3}}\left[\mathsf{U}\mathcal{Y}^{(1)}(\hat{r}) + \underbrace{\mathcal{Y}^{(1)}(\hat{r})\mathsf{U}} + \mathcal{Y}^{(1)}(\hat{r})\mathsf{U}\right]. \tag{4.14}$$

A calculation of the general expansion coefficient a_{nm} is accomplished using the orthogonalization of the symmetrized tensors. This begins with the calculation of the double dot contraction

$$\mathsf{U}\mathbf{:}\left\{(\mathsf{U})^m\mathcal{Y}^{(n-2m)}(\hat{r})\right\}^{(n)} = \frac{2m(2n-2m+1)}{n(n-1)}\left\{(\mathsf{U})^{m-1}\mathcal{Y}^{(n-2m)}(\hat{r})\right\}^{(n-2)}. \tag{4.15}$$

The numerical factor accounts for the number of ways the $n(n-1)/2$ ways of dotting the U into the tensor gives the resulting tensor, with a factor of 3 from the permutation that has the contraction $\mathsf{U}\mathbf{:}\mathsf{U}$. Iterating this result q times with a final contraction with $\mathcal{Y}^{(n-2q)}(\hat{r})$ gives

$$\mathcal{Y}^{(n-2q)}(\hat{r})(\mathsf{U})^q\odot^n\left\{(\mathsf{U})^m\mathcal{Y}^{(n-2m)}(\hat{r})\right\}^{(n)} = \delta_{qm}\frac{m!(2n-2m+1)!(n-2m)!(n-2m)!}{n!(2n-4m)!(n-m)!}. \tag{4.16}$$

This shows the orthogonality of these tensors. The contraction of the same tensor into Eq. (4.12) gives an equation for a single a_{nm} expansion coefficient, thus

$$a_{nm} = \frac{n!(n-m)!}{m!(2n-2m+1)!(n-2m)!}\sqrt{2^{n-2m}(2n-4m+1)!}. \tag{4.17}$$

A check on this expansion is the evaluation of

$$\begin{aligned}(\hat{r})^n \odot^n (\hat{r})^n = 1 &= \sum_{m=0}^{[n/2]} a_{nm}\sqrt{(2n-4m+1)\overline{P}_{n-2m}(1)} \\ &= \sum_{m=0}^{[n/2]} \frac{n!(n-m)!2^{n-2m}(2n-4m+1)}{m!(2n-2m+1)!}.\end{aligned} \tag{4.18}$$

It is easy to carry out the numerical calculation of this sum to verify that it sums to 1.

4.2 Integrals of Products of $\hat{r}$

The calculation of the integral over all directions of a product of $\hat{r}$ can be carried out componentwise, that is, for a product of n $\hat{r}$'s, there are 3^n sets of components and 3^n different integrals to examine. Each such integral reduces to an integral over some product of sines and cosines and the integral can then be carried out. On the other hand, if the integral of a product of $\hat{r}$ is looked at from a tensorial point of view, it is noticed that the integral is a rotational invariant and thus the integral must be expressible in terms of the available rotational invariants. These notions are exemplified by

$$\int \hat{r}\hat{r}d\hat{r} = \frac{4\pi}{3}\mathbf{U}. \tag{4.19}$$

First of all, the integral is a second order rotationally invariant tensor. Since there is only one such tensor, namely $\mathbf{U}$, the integral must be proportional to $\mathbf{U}$. The numerical factor of $4\pi/3$ can be deduced by contracting both sides of the equation with $\mathbf{U}$, namely

$$\int \mathbf{U}{:}\hat{r}\hat{r}d\hat{r} = \int d\hat{r} = 4\pi = \frac{4\pi}{3}\mathbf{U}{:}\mathbf{U} = 4\pi, \tag{4.20}$$

confirming the magnitude of both sides of Eq. (4.19). In contrast, a typical component of Eq. (4.19) is

$$\begin{aligned}\int xx d\hat{r} &= \int_0^{2\pi}\int_0^{\pi} \sin^2\theta\cos^2\phi\sin\theta d\theta d\phi \\ &= \int_{-1}^{1}(1-\cos^2\theta)d\cos\theta\int_0^{2\pi}\frac{1}{2}\left(1+\cos(2\phi)\right)d\phi = \frac{4\pi}{3}.\end{aligned} \tag{4.21}$$

This agrees immediately with the $\hat{x}\hat{x}$ component of Eq. (4.19), but it is stressed that the tensorial form of calculation is faster and moreover, contains more information. Thus the $\hat{x}\hat{y}$ component of Eq. (4.19) is immediately seen to vanish, whereas the calculation using angles needs a separate calculation. In fact, all of the components of Eq. (4.19) are calculated at the same time and easily read off of the integrated result. If the number of $\hat{r}$'s increases, the computation using angles increases enormously, but the tensorial calculation is relatively easy, as is to be shown.

The tensor of third order vanishes by symmetry. This can be seen either from the fact that $\hat{r}\hat{r}\hat{r}$ is antisymmetric to an inversion of $\hat{r}$ and so the integral over all directions must vanish since the integral must be even to spatial inversion (parity), or by the fact that the only rotationally invariant third order tensor is $\boldsymbol{\varepsilon}$, but this is odd to a permutation of the tensorial directions while the tensor $\hat{r}\hat{r}\hat{r}$ in the integrand is symmetric to such a permutation. By similar arguments, the integral of any odd power of $\hat{r}$ vanishes.

For even n, the integral of $(\hat{r})^n$ is a rotational invariant of n directions and thus expressible in terms of combinations of products of $\mathbf{U}$. Moreover, since the integrand is a tensor symmetric to the interchange of any pair of the n directions, the integral must also be a completely symmetric tensor, thus

$$\int (\hat{r})^n d\hat{r} = A_n \left\{ (\mathbf{U})^{n/2} \right\}^{(n)} . \tag{4.22}$$

Here the quantity in braces is to be interpreted as the symmetrized tensor formed from $n/2$ $\mathbf{U}$'s, this being the average of

$$\frac{n!}{2^{n/2}(n/2)!}$$

permutations of the $n/2$ $\mathbf{U}$'s. The calculation of the constant A_n can be accomplished by evaluating one particular component of this integral. Choosing the $(\hat{z})^n$ component likely gives the easiest computation, namely

$$\int (z)^n d\hat{r} = 2\pi \int_{-1}^{1} (\cos\theta)^n d\cos\theta = \frac{4\pi}{n+1} = A_n \tag{4.23}$$

As a consequence of this and the vanishing of A_n for odd n, this constant is in general given by

$$A_n = \begin{cases} 0 & n \text{ odd}, \\ \frac{4\pi}{n+1} & n \text{ even}. \end{cases} \tag{4.24}$$

Besides Eq. (4.19), this result is exemplified by

$$\int \hat{r}\hat{r}\hat{r}\hat{r} d\hat{r} = \frac{4\pi}{5} \{\mathbf{UU}\}^{(4)} = \frac{4\pi}{15} \left[\mathbf{UU} + \mathbf{W} + \mathbf{W} \right] . \tag{4.25}$$

This is equivalent to the evaluation of 81 (scalar) integrals, most of which are zero, but the value of each scalar integral can be read off of the tensorial equation. From the nature of the righthand side, it is clear that a nonzero result occurs (not unexpectedly) only if the numbers of each of the $\hat{x}$, $\hat{y}$ and $\hat{z}$ components are even. The cases of Eq. (4.22) up to n=4 were previously reported in [13].

Finally it might be noted that if there are other vectors in the integrand that are independent of $\hat{r}$, the integral ignores these, for example

$$\int \hat{r}\mathbf{g}\hat{r} d\hat{r} = \frac{4\pi}{3} \mathbf{U}_{\mathbf{g}} \tag{4.26}$$

No end of other possibilities can also be envisaged.

4.3 Orthogonal functions of r associated with a Gaussian weight function

Tensor functions $\mathsf{L}^{\ell n}(\mathbf{r})$ are to be defined [18] that belong to the weight ℓ irreducible representation of the rotation group and are also orthonormal according to

$$\pi^{-3/2}\int e^{-r^2}\mathsf{L}^{\ell n}(\mathbf{r})\mathsf{L}^{\ell' n'}(\mathbf{r})d\mathbf{r} = \delta_{\ell\ell'}\delta_{nn'}\mathsf{E}^{(\ell)}. \tag{4.27}$$

Kumar [19] discovered a generating function for a set of functions that satisfy these conditions, namely

$$G(\mathbf{a},\mathbf{r}) \equiv e^{-a^2+2\mathbf{a}\cdot\mathbf{r}} = \left(\frac{1}{2}\pi^{1/2}\right)^{1/2}\sum_{\ell n}\frac{(-1)^n a^{2n+\ell}\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{a})\odot^{\ell}\mathsf{L}^{\ell n}(\mathbf{r})}{[\Gamma(n+1)\Gamma(\ell+n+\frac{3}{2})]^{1/2}}. \tag{4.28}$$

Orthonormality is proven from the identity

$$\begin{aligned}\pi^{-3/2}\int e^{-r^2}G(\mathbf{a},\mathbf{r})G(\mathbf{b},\mathbf{r})d\mathbf{r} = e^{2\mathbf{a}\cdot\mathbf{b}} &= \frac{1}{2}\pi^{1/2}\sum_{\ell n}\frac{(ab)^{2n+\ell}\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{a})\odot^{\ell}\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{b})}{\Gamma(n+1)\Gamma(\ell+n+\frac{3}{2})} \\ = \quad \frac{1}{2}\pi^{1/2}\sum_{\ell n\ell' n'}&\frac{(-1)^{n+n'}a^{2n+\ell}b^{2n'+\ell'}\boldsymbol{\mathcal{Y}}^{(\ell')}(\hat{a})\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{b})}{[\Gamma(n+1)\Gamma(\ell+n+\frac{3}{2})\Gamma(n'+1)\Gamma(\ell'+n'+\frac{3}{2})]^{1/2}} \\ &\times\odot^{\ell+\ell'}\pi^{-3/2}\int e^{-r^2}\mathsf{L}^{\ell n}(\mathbf{r})\mathsf{L}^{\ell' n'}(\mathbf{r})d\mathbf{r}.\end{aligned} \tag{4.29}$$

On expanding the Kumar generating function relation, Eq. (4.28), and equating powers of a and coefficients of $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{a})$, the tensor functions $\mathsf{L}^{\ell n}(\mathbf{r})$ can be identified in terms of the associated (or generalized) Laguerre polynomials $L_n^{\ell+1/2}(r^2)$ [20] of r^2 as

$$\mathsf{L}^{\ell n}(\mathbf{r}) = \left[\frac{\pi^{1/2}\Gamma(n+1)}{2\Gamma(n+\ell+\frac{3}{2})}\right]^{1/2} r^{\ell}L_n^{\ell+1/2}(r^2)\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}). \tag{4.30}$$

Of course other sets of orthonormal functions of $\mathbf{r}$ could be found to satisfy the rotation group property and Eq. (4.27). Clearly these would also have to be proportional to the $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ since that is the group property, but the dependence on the magnitude r could be different. The set given here might be considered as the natural set of orthogonal polynomials related to the Gaussian weight function.

Chapter 5

Spherical Vectors and Tensors

The essential feature of Cartesian tensor analysis is the emphasis of the directional properties of the tensor. Fundamentally there is no preferred coordinate system used for the description of the tensor. Rather, a pth order Cartesian tensor involves its own inherent p directions. For some computational purposes it is useful to write such a Cartesian tensor in component form. This is accomplished only by introducing a reference set of directions, usually the axes of a right-handed coordinate system. But then the components are dependent not only on the tensor, but also on the coordinate system that has been chosen. For example, the vector $\mathbf{r}$ can be written in the $\hat{x},\ \hat{y},\ \hat{z}$ coordinate system, see Eq. (2.1), whose components $x,\ y,\ z$ depend on the both $\mathbf{r}$ and the chosen coordinate system, but $\mathbf{r}$ itself is inherently independent of any coordinate system. To stress the point again, fundamentally there is no inherent preferred coordinate system in Cartesian tensor analysis. In contrast, spherical tensors are standardly defined [1, 6] in terms of a set of components, assigned according to their behaviour under a rotation about a particular axis. Thus one direction is, and must be, singled out for preferential treatment. We find the lack of emphasis in many treatments of spherical tensors, of this inherently subjective choice of a coordinate system, both troublesome and confusing to students, who end up with some kind of feeling that there is something mystically special about the $\hat{z}$-axis, which is the direction usually assigned for the axis of rotation used for labelling the components of the spherical tensor.

Notwithstanding the ranting in the previous paragraph, we shall use the $\hat{x},\ \hat{y},\ \hat{z}$ coordinate system with the $\hat{z}$-axis as the selected axis for cataloging the rotational properties of tensorial components since the resulting equations can be compared to those standardly found in the literature. But we do wish to stress that this is a choice, and that any axis could be used for this purpose, but of course then the spherical components of a given tensor would be different. Namely again, the tensor has its own identity beyond how it has been chosen to be described in component form.

This chapter starts out by reviewing the commutation properties of the generators of the 3-dimensional rotation group, demonstrating that only the rotations about one axis at a time can be used for classifying the components of an irreducible representation. A classification of the irreducible representations is also given. This is of course exactly analogous to the quantization rules of angular momentum, but again it is stressed that here one is dealing with the symmetry properties of objects (in particular tensors) that do not necessarily have anything to do with angular velocities, moments of inertia, or other physical processes. The chapter proceeds to express, first vectors, and then tensors in spherical tensor form, with an emphasis on the relation between irreducible Cartesian tensors and spherical tensors. The standard functions arising when using spherical coordinates, namely the Legendre functions and the spherical harmonics, arise naturally in this analysis.

5.1 Group Generator Properties

Whether they are the abstract group generators for the 3-dimensional rotation group A.1, the generators for rotating vectors, Eq. (2.103), or the generators for pth order tensors, Eq. (3.3), the three generators satisfy the same set of commutation relations. Expressed in abstract form, and using the $\hat{x}$, $\hat{y}$, $\hat{z}$ coordinate system, this is

$$G_{\hat{x}}G_{\hat{y}} - G_{\hat{y}}G_{\hat{x}} = iG_{\hat{z}} \tag{5.1}$$

and its cyclic analogs. Clearly, these commutation relations mean that any eigenvector of one generator is not simultaneously an eigenvector of either of the other two generators. Thus a classification of any object according to the rotational properties about specific axes can only be done about one axis. This will be chosen as the $\hat{z}$-axis. A further consequence of the commutation properties is that $G^2 \equiv G_{\hat{x}}^2 + G_{\hat{y}}^2 + G_{\hat{z}}^2$ commutes with all rotation generators. As a consequence, the classification of objects according to their possible rotational properties can include their behaviour under G^2 as well as $G_{\hat{z}}$. The detailed consequences of these commutation relations are reviewed here. Since these are exactly the same as the properties of the angular momentum commutation relations in quantum mechanics, the reader familiar with the algebra of angular momentum in quantum mechanics may wish to skim the remainder of this section, looking only at the choice of notation that is to be used in the rest of the book.

Consider an element v_m of some vector space V over the complex numbers which is an eigenvector of $G_{\hat{z}}$ with eigenvalue m, called the *weight*, namely

$$G_{\hat{z}}v_m = mv_m. \tag{5.2}$$

Now the generators can be rearranged in terms of raising and lowering operators

$$G_\pm \equiv G_{\hat{x}} \pm iG_{\hat{y}}, \tag{5.3}$$

which have the commutation relations

$$G_{\hat{z}}G_\pm = G_\pm(G_{\hat{z}} \pm 1). \tag{5.4}$$

As a consequence $G_\pm v_m$ is either an eigenvector of $G_{\hat{z}}$ with eigenvalue (weight) $m \pm 1$, or zero. This implies that sets of eigenvalues of $G_{\hat{z}}$ differ by integer values.

Provided that v_m is also an eigenvector of G^2 with eigenvalue $\ell(\ell+1)$ [the choice of writing the eigenvalue in this way will soon become apparent], then v_m and those eigenvectors formed from v_m by successive raising and lowering operators form the basis for a vector space (a subspace of V) which is irreducible under the 3-dimensional rotation group that is parameterized by ℓ. That is, ℓ classifies the irreducible representations of the 3-dimensional rotation group. By examining their normalizations it is moreover possible and useful to define a normalized basis (which is also orthogonal) which has a convenient phase relation between the basis elements. This phase convention was established by Condon and Shortley [21] for angular momentum, but is adaptable to all irreducible representations of the 3-dimensional rotation group.

Assume that v_m is a normalized vector, namely $\langle v_m|v_m\rangle = 1$, where $\langle v|v\rangle$ denotes the inner product for V as a Euclidean space *over the complex numbers.* Then the normalization of $G_\pm v_m$ is given by

$$\begin{aligned}
\langle G_\pm v_m|G_\pm v_m\rangle &= \langle v_m|(G_{\hat{x}} \mp iG_{\hat{y}})(G_{\hat{x}} \pm iG_{\hat{y}})|v_m\rangle \\
&= \langle v_m|G_{\hat{x}}G_{\hat{x}} + G_{\hat{y}}G_{\hat{y}} \mp G_{\hat{z}}|v_m\rangle \\
&= \langle v_m|G^2 - G_{\hat{z}}G_{\hat{z}} \mp G_{\hat{z}}|v_m\rangle \\
&= \ell(\ell+1) - m^2 \mp m, \qquad (5.5)
\end{aligned}$$

on the basis that v_m is also an eigenvector of G^2 with eigenvalue $\ell(\ell+1)$. If the processes of raising and lowering are to end, then $\ell(\ell+1) - m(m \pm 1)$ must vanish for the largest and smallest allowed values of m. Clearly this occurs when $m = \ell$ and $m = -\ell$ [ℓ positive]. Moreover, since the different values of m differ by an integer, then 2ℓ must be an integer. This leads to the two possibilities, either ℓ is an integer or a half-integer, with the added consequences that integer ℓ has associated with it an odd number, namely $2\ell + 1$, of m values, whereas half-integer ℓ has an even number of m numbers, which is again given by $2\ell + 1$. The set of vectors associated with ℓ constitute an irreducible representation of the group, that is, all $2\ell + 1$ vectors arise via some group action from one another, and the set of vectors cannot be partitioned into a smaller set that is still closed under group action. Thus the irreducible representations of the 3-dimensional rotation group are specified by integer or half-integer ℓ, which is the maximum weight of the irreducible representation having dimension $2\ell + 1$.

The difference between integer and half-integer maximum weight irreducible represention is obtained by examining the angle dependence of any one of their components. Necessarily the eigenvalues of $G_{\hat{z}}$ are either all integer or all half-integer. Since a finite rotation about the $\hat{z}$-axis is found by exponentiating $G_{\hat{z}}$, namely

$$R_{\hat{z}}(\phi) = e^{-iG_{\hat{z}}\phi}, \qquad (5.6)$$

see Eq. (2.91), it follows that a finite rotation of a $G_{\hat{z}}$ eigenvector is given by

$$R_{\hat{z}}(\phi)v_m = e^{-im\phi}v_m. \qquad (5.7)$$

A rotation by 2π then has the effect of either being the identity, if m (and ℓ) is an integer, whereas it changes sign if m is half-integer. In terms of the discussion of the parameterization of the 3-dimensional rotation group, Sec. 2.5.1, the integer ℓ irreducible representations belong to the first homotopy class, while the half-integer ℓ irreducible representations belong to the second homotopy class and need a rotation of 4π to return to the identity. On reduction of the vector and tensor representations of the 3-dimensional rotation group, only integer irreducible representations are obtained, whereas both integer and half-integer irreducible representations are obtained in the reduction of spinors, see Chap. 10.

The Condon and Shortley phase convention is that the different eigenvectors v_m of $G_{\hat{z}}$ are related according to

$$\begin{aligned}
v_{m\pm 1} &= \frac{1}{\sqrt{\ell(\ell+1) - m(m \pm 1)}} G_\pm v_m \\
&= \frac{1}{\sqrt{(\ell \mp m)(\ell \pm m + 1)}} G_\pm v_m. \qquad (5.8)
\end{aligned}$$

Thus the phase factor relating the different eigenvectors is real, while the magnitudes are defined so that all eigenvectors are normalized. These properties simplify all rotation calculations using these eigenvectors and is standardly adopted. They play a central role in the remainder of this chapter as well as everywhere else in this book that eigenvectors of $G_{\hat{z}}$ appear.

A way of distinguishing one irreducible representation from another is via its character. This is a function of the group, which in the case of the 3-dimensional rotation group depends only on the angle of rotation ϕ. Specifically, the character $\chi_\ell(\phi)$ is defined as the trace of the matrix of the group element in the ℓ<u>th</u> irreducible representation, thus

$$\chi_\ell(\phi) \equiv \sum_m \langle v_m | R_{\hat{n}}(\phi) | v_m \rangle \tag{5.9}$$

is the character for the rotation by angle ϕ about the $\hat{n}$ axis. Since the transformation from one axis to another is just a similarity transformation and the trace is unchanged by such a transformation, the character depends only on the angle of rotation. Picking the rotation about the $\hat{z}$ direction for calculating $\chi_\ell(\phi)$, and consequently using the eigenvectors of G_z for carrying out the trace, the character is

$$\chi_\ell(\phi) = \sum_{m=-\ell}^{\ell} e^{-im\phi} = 1 + 2\sum_m \cos(m\phi) = \frac{\sin\left[\left(\ell + \frac{1}{2}\right)\phi\right]}{\sin(\phi/2)}. \tag{5.10}$$

It needs to be emphasized that the vector spaces for the discussion of the eigenvectors of $G_{\hat{z}}$ are naturally over the complex numbers. In particular the normalization condition $\langle v_m | v_m \rangle$. But in ordinary 3-dimensional vector space and its tensorial generalizations, the physical quantities are inherently real and the natural way of getting a scalar is via the appropriate number of dot products. This means that a dual type of structure arises as the tensor analysis over the real numbers and the dot products compete with the inherent complex number properties of the rotational eigenvectors. The usual treatment of spherical vectors and tensors emphasizes the rotational eigenvectors with the disadvantage that the directional properties of the vectors and tensors get lost. In the method presented here, it is the directional properties of the vectors and tensors that are emphasized. It has been shown that the classification according to which irreducible representation a tensor belongs, can be accomplished entirely in real space, namely whether a tensor is in natural form (or is a tensor in which a natural form tensor has been embedded). But when it comes to the further analysis of their properties to a rotation about a given axis, the tensorial description becomes more complicated. If only the dot product is used, which is the natural inner product for vectors and tensors, then the eigenvectors of $G_{\hat{z}}$ are not normalized. The result is that any spherical vector and/or tensor analysis based on the dot product naturally involves a biorthonormal system of basis elements. This complication is a standard problem in tensor analysis and is discussed in this chapter.

5.2 The Components of a Spherical Vector

By a spherical vector is meant the expansion of a 3-dimensional vector in terms of the eigenvectors of $G_{\hat{z}}$. This is to be contrasted with the expression of the vector in spherical coordinates, as in Eq. (2.4). Of course any 3-dimensional vector belongs to the maximum weight 1 (ℓ=1) irreducible representation of the 3-dimensional rotation group, as deduced by the fact that the tensorial form of the Casimir invariant G^2, see Eq. (3.10), is 2 times the identity.

There are two different phase conventions in common use for a spherical vector, with a greater emphasis on the analogous spherical tensors. Both satisfy the Condon and Shortley phase convention, so the only difference is a common phase factor, specifically a factor of $i = \sqrt{-1}$. Since the introduction of an i seems like a silly thing to do and seemingly makes everything more complicated, if only spherical vectors are to be used, then leaving out the extra i is the natural, and most often used, convention. But if different spherical vectors and tensors are coupled together, the unit vectors containing i combine more simply. Here most of the discussion involves the first convention since it is the one commonly used in the physics and chemistry literature, with a few added comments made about the second convention. But it is shown in Chapter 7 that the second convention is natural for defining the 3-j symbols, and in Chapter 10 when dealing with spinors.

The tensorial form for $G_{\hat{z}}$ is $\mathsf{G}_{\hat{z}} = -i\hat{z}\boldsymbol{\cdot}\boldsymbol{\mathcal{E}}$, see Eq. (2.92). Clearly an eigenvector with zero eigenvalue is $\hat{z}$. Setting one basis vector to be this eigenvector, namely

$$\mathbf{e}^{(1)0} = \hat{z}, \tag{5.11}$$

then to be consistent with the Condon Shortley phase conventions, Eq. (5.8), the other basis vectors are given by

$$\begin{aligned} \mathbf{e}^{(1)1} &= \frac{1}{\sqrt{2}}\mathsf{G}_{+}\boldsymbol{\cdot}\mathbf{e}^{(1)0} = -\frac{\hat{x}+i\hat{y}}{\sqrt{2}} \\ \mathbf{e}^{(1)-1} &= \frac{1}{\sqrt{2}}\mathsf{G}_{-}\boldsymbol{\cdot}\mathbf{e}^{(1)0} = \frac{\hat{x}-i\hat{y}}{\sqrt{2}}. \end{aligned} \tag{5.12}$$

Now it is noted that $\mathbf{e}^{(1)1}$ dotted into itself vanishes. Actually all the possible dot products between these basis vectors is summarized by

$$g^{mm'} \equiv \mathbf{e}^{(1)m}\boldsymbol{\cdot}\mathbf{e}^{(1)m'} = (-1)^m \delta_{m,-m'}, \tag{5.13}$$

for $m,\ m' = 1,\ 0,\ -1$. Thus the standard formation of a scalar by taking the dot product is different from the normalization condition of Eq. (5.5). This is because Eq. (5.5) explicitly involves complex numbers, specifically it takes the complex conjugate of the lefthand vector in the inner product, whereas the dot product essentially is for real numbers and has no built in complex conjugation. A *linear* extension to complex numbers then leads to results that are different in principle from when the vectors are purely real.

For a basis that is not orthonormal, a dual basis arises naturally. This is the basis set $\mathbf{e}^{(1)}_m$ defined so that

$$\mathbf{e}^{(1)}_m\boldsymbol{\cdot}\mathbf{e}^{(1)m'} = \delta^{m'}_m, \tag{5.14}$$

where $\delta^{m'}_m$ is the Kronecker delta for mixed subscript and superscript indices. The $\mathbf{e}^{(1)m}$ basis is called the contravariant basis set, which determines the contravariant components of a vector, e.g. $\mathbf{r}$, according to

$$r^m = \mathbf{e}^{(1)m}\boldsymbol{\cdot}\mathbf{r}, \tag{5.15}$$

whereas the covariant basis set $\mathbf{e}^{(1)}_m$ determines the covariant components

$$r_m = \mathbf{e}^{(1)}_m\boldsymbol{\cdot}\mathbf{r}. \tag{5.16}$$

It easily follows that the covariant basis set is

$$\mathbf{e}^{(1)}_1 = -\frac{\hat{x}-i\hat{y}}{\sqrt{2}}; \qquad \mathbf{e}^{(1)}_0 = \hat{z}; \qquad \mathbf{e}^{(1)}_{-1} = \frac{\hat{x}+i\hat{y}}{\sqrt{2}}. \tag{5.17}$$

For **r** given by Eqs. (2.1) and (2.4), the spherical components of **r** are

$$r^1 = -\frac{x+iy}{\sqrt{2}} = -r\frac{\sin\theta e^{im\phi}}{\sqrt{2}}; \qquad r^0 = z = r\cos\theta; \qquad r^{-1} = \frac{x-iy}{\sqrt{2}} = r\frac{\sin\theta e^{-im\phi}}{\sqrt{2}} \tag{5.18}$$

and

$$r_1 = -\frac{x-iy}{\sqrt{2}} = -r\frac{\sin\theta e^{-im\phi}}{\sqrt{2}}; \qquad r_0 = z = r\cos\theta; \qquad r_{-1} = \frac{x+iy}{\sqrt{2}} = r\frac{\sin\theta e^{im\phi}}{\sqrt{2}}. \tag{5.19}$$

From the biorthogonality of the basis sets, a vector **r** can be expanded in terms of either its contravariant or covariant components

$$\mathbf{r} = r^m \mathbf{e}^{(1)}_m = r_m \mathbf{e}^{(1)m}. \tag{5.20}$$

Here the summation convention is used, namely that when the same index appears as both a covariant and a contravariant index, it is implied that a summation over that index is to be performed. Another consequence of the biorthogonality of the basis sets is that the identity U can be expanded as

$$\mathsf{U} = \mathbf{e}^{(1)m}\mathbf{e}^{(1)}_m = \mathbf{e}^{(1)}_m \mathbf{e}^{(1)m}, \tag{5.21}$$

again using the summation convention.

Since the covariant and contravariant basis elements are the complex conjugates of each other, it is noticed that the raising and lowering operators for the covariant basis set are the complex conjugates of the contravariant raising and lowering operators, namely

$$\mathsf{G}^*_+ \mathbf{e}^{(1)}_m = \sqrt{2}\mathbf{e}^{(1)}_{m+1} \qquad \mathsf{G}^*_- \mathbf{e}^{(1)}_m = \sqrt{2}\mathbf{e}^{(1)}_{m-1}. \tag{5.22}$$

Of course these operators are also related to the original raising and lowering operators by

$$\mathsf{G}^*_+ = -\mathsf{G}_- \qquad \mathsf{G}^*_- = -\mathsf{G}_+. \tag{5.23}$$

The function $g^{mm'}$ can be interpreted as a contravariant metric, while

$$g_{mm'} \equiv \mathbf{e}^{(1)}_m \cdot \mathbf{e}^{(1)}_{m'} = (-1)^m \delta_{m,-m'} \tag{5.24}$$

is the analogous, and numerically equal covariant metric. Transformations from one basis to the other, as well as between the components of a vector expressed in contravariant and/or covariant forms, are carried out using these metrics (and the summation convention), namely

$$\mathbf{e}^{(1)}_m = g_{mm'}\mathbf{e}^{(1)m'}; \qquad \mathbf{e}^{(1)m} = g^{mm'}\mathbf{e}^{(1)}_{m'}; \tag{5.25}$$

$$r_m = g_{mm'} r^{m'}; \qquad r^m = g^{mm'} r_{m'}. \tag{5.26}$$

The bases can also be related by complex conjugation, so there are a number of different relationships between these bases, in particular

$$\mathbf{e}^{(1)}_m = \mathbf{e}^{(1)m*} = (-1)^m \mathbf{e}^{(1)-m} = (-1)^m \mathbf{e}^{(1)*}_{-m}. \tag{5.27}$$

The basis vectors $\mathbf{e}^{(1)m}$ are associated with taking $\mathbf{e}^{(1)0} = \hat{z}$ and using the Condon and Shortley phase conventions to obtain the other two basis vectors. But there is also the possibility of starting with a different phase for $\mathbf{e}^{(1)0}$. In particular, the other common choice is to define the basis in terms of $\mathfrak{e}^{(1)0} \equiv i\hat{z}$. Here this basis set and components are written in Euler font in order to distinguish it and its corresponding components and metrics from the set previously introduced. Some of the relations between the two conventions are listed below:

$$\begin{aligned} \mathfrak{e}^{(1)m} &= i\mathbf{e}^{(1)m}; \qquad\qquad \mathfrak{r}^m = ir^m; \\ \mathfrak{e}^{(1)}_m &= -i\mathbf{e}^{(1)}_m; \qquad\qquad \mathfrak{r}_m = -ir_m; \\ \mathfrak{g}^{mm'} &= -g^{mm'} = \mathfrak{g}_{mm'} = -g_{mm'} = (-1)^{1+m}\delta_{m,-m'}. \end{aligned} \tag{5.28}$$

These allow the explicit form for these basis elements and components to be obtained.

5.3 Rotation of a spherical vector

The object of this short section is to draw attention to the differences between how the various basis vectors transform under rotation and how the components of a vector $\mathbf{r}$ transforms under the same rotation. Only a rotation about the $\hat{z}$ axis is discussed since that adequately illustrates the points which are to be emphasized, without the added complexity of worrying about the interplay between rotations about different axes.

The rotation of $\mathbf{r}$ expressed in Cartesian form is reviewed. Consider first how a vector lying along the $\hat{x}$ axis is rotated by an angle θ about the $\hat{z}$ axis. This gives the unit vector

$$\hat{x}' = \mathbf{R}_{\hat{z}}(\theta)\cdot\hat{x} = \cos\theta\hat{x} + \sin\theta\hat{y}, \tag{5.29}$$

or in column vector form (with the components of the column vector being respectively the $\hat{x}$, $\hat{y}$ and $\hat{z}$ components of the associated vector)

$$\hat{x}' \iff \begin{pmatrix} \cos\theta \\ \sin\theta \\ 0 \end{pmatrix} = R_{\hat{z}}(\theta) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{5.30}$$

In analogous form, the rotation of the unit vector along $\hat{y}$ is

$$\hat{y}' = \mathbf{R}_{\hat{z}}(\theta)\cdot\hat{y} = \cos\theta\hat{y} - \sin\theta\hat{x}, \tag{5.31}$$

or in column vector form

$$\hat{y}' \iff \begin{pmatrix} -\sin\theta \\ \cos\theta \\ 0 \end{pmatrix} = R_{\hat{z}}(\theta) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \tag{5.32}$$

A combination of these two results leads to the rotation matrix which describes how the components of a general 3-dimensional vector transforms under this rotation, namely

$$\begin{aligned} \mathbf{r}' &= (x'\hat{x} + y'\hat{y} + z'\hat{z}) \\ &= \mathbf{R}_{\hat{z}}(\theta)\cdot(x\hat{x} + y\hat{y} + z\hat{z}) = (x\cos\theta - y\sin\theta)\hat{x} + (y\cos\theta + x\sin\theta)\hat{y} + z\hat{z} \end{aligned} \tag{5.33}$$

and in component form

$$\vec{r'} = \begin{pmatrix} x\cos\theta - y\sin\theta \\ y\cos\theta + x\sin\theta \\ z \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{5.34}$$

It is to noted how the x and y components of the original vector contribute to the rotated vector $\vec{r'}$.

Now consider expressing the same transformation in terms of spherical vector components. An expansion of the initial vector is

$$\mathbf{r} = \sum_m r_m \mathbf{e}^{(1)m} = -\frac{x - iy}{\sqrt{2}}\mathbf{e}^{(1)1} + z\mathbf{e}^{(1)0} + \frac{x + iy}{\sqrt{2}}\mathbf{e}^{(1)-1}. \tag{5.35}$$

It is noted that it is the covariant components of $\mathbf{r}$ that appear in this expansion. The rotation is generated by $\mathsf{G}_{\hat{z}}$, namely by $\mathsf{R}_{\hat{z}}(\theta) = \exp(-i\theta\mathsf{G}_{\hat{z}})$, Thus the rotated vector is

$$\begin{aligned} \mathbf{r}' &= \mathsf{R}_{\hat{z}}(\theta)\cdot\mathbf{r} = \sum_m r_m e^{-im\theta}\mathbf{e}^{(1)m} \\ &= -\frac{x - iy}{\sqrt{2}}e^{-i\theta}\mathbf{e}^{(1)1} + z\mathbf{e}^{(1)0} + \frac{x + iy}{\sqrt{2}}e^{i\theta}\mathbf{e}^{(1)-1}. \end{aligned} \tag{5.36}$$

Thus the spherical vector components of the rotated vector are

$$r'_m = e^{-im\theta} r_m. \tag{5.37}$$

A Cartesian expansion of the spherical basis vectors in Eq. (5.36) in terms of $\hat{x}$, $\hat{y}$ and $\hat{z}$ is identical to Eq. (5.33). It is noted that this method of carrying out the rotation makes contact with the transformation of the covariant components of the vector. An alternative that emphasizes the contravariant components of the vector (and these are what usually appears in the literature) is to take the contravariant components of the rotated vector, namely

$$r'^n = \mathbf{e}^{(1)n}\cdot\mathbf{r}' = \mathbf{e}^{(1)n}\cdot e^{-i\mathsf{G}_{\hat{z}}}\cdot\mathbf{r}. \tag{5.38}$$

Now on inserting the contravariant component expansion of $\mathbf{r}$,

$$\mathbf{r} = \sum_m r^m \mathbf{e}^{(1)}_m \tag{5.39}$$

into this equation, it is noted that the covariant basis elements are also eigenvectors of $\mathsf{G}_{\hat{z}}$, but with the opposite sign to the contravariant basis set, and that only the $\mathbf{e}^{(1)}_n$ element contributes to the contraction in Eq. (5.38). As a consequence,

$$r'^n = e^{in\theta} r^n. \tag{5.40}$$

In particular for $n = 1$, this relation is

$$r'^1 = -\frac{x' + iy'}{\sqrt{2}} = -(\cos\theta + i\sin\theta)\frac{x + iy}{\sqrt{2}}, \tag{5.41}$$

from which the x and y components of the rotated vector are

$$x' = x\cos\theta - y\sin\theta \qquad y' = y\cos\theta + x\sin\theta. \tag{5.42}$$

These are the same as the relations obtained via Eqs. (5.33) and/or (5.36).

There are clearly other ways of carrying out the calculation of the result of rotating a vector, but the methods presented here illustrate some of the possibilities, as well as some of the care that needs to be exercised in order to get the correct sense of rotation.

5.4 Spherical Tensors

Spherical tensors inherently refer to the representation of an irreducible tensor in a basis associated with the eigenvalues of $G_{\hat{z}}$. As always, any axis of rotation could have been chosen, but the $\hat{z}$-axis is the standard one used in the literature, so this is what is used here. An irreducible Cartesian tensor of weight ℓ can always be reduced in order so that its simplest descriptiosn is when its order and weight are both ℓ, in which case the tensor is necessarily symmetric and traceless in all pairs of indices. This property must arise in a natural way for the spherical basis of the irreducible tensor. Moreover, since a tensor of order ℓ is just a linear combination of polyads, the basis elements must be linear combinations of the products of ℓ vector basis elements. The question of which linear combination of which products is then to be determined. But the simplest case is when there is only one combination of vector basis elements that can form a given tensor basis element, from which all other tensor basis elements can be found by raising and/or lowering operations. The simple cases are those that form the basis elements of maximum and minimum weight. It is the maximum weight basis element that is used as the starting point in the following discussion.

For an irreducible tensor of maximum weight ℓ, the basis element of maximum weight must be the ℓ-fold product of the weight 1 vector basis elements, namely

$$\mathbf{e}^{(\ell)\ell} = \mathbf{e}^{(1)1}\mathbf{e}^{(1)1}\cdots\mathbf{e}^{(1)1}\mathbf{e}^{(1)1}, \tag{5.43}$$

since this is the only way to get an eigenvector of $G_{\hat{z}}$ with eigenvalue ℓ from ℓ vector basis elements. Of course this could be multiplied by any normalization and/or phase factor, but is not. It is immediately obvious that, as a tensor, this basis element is both symmetric and traceless. The other elements of the basis are now obtained by repeated use of the tensorial lowering operator $\mathsf{G}_-^{(\ell)}$, Eq. (3.18), thus the basis element of weight m is given by

$$\mathbf{e}^{(\ell)m} = \sqrt{\frac{(\ell+m)!}{(2\ell)!(\ell-m)!}}\left(\mathsf{G}_-^{(\ell)}\odot^{\ell}\right)^{\ell-m}\mathbf{e}^{(\ell)\ell} \tag{5.44}$$

with the prefactor determined by repeated use of Eq. (5.8). Carrying out the repeated lowering operations gives a weighted sum of terms, each some combination of $\mathbf{e}^{(1)1}$, $\mathbf{e}^{(1)0}$ and $\mathbf{e}^{(1)-1}$ for the ℓ indices of the ℓth order tensor, with the combinations distributed in a symmetric and traceless way among all the indices. These can be classified by the number n of $\mathbf{e}^{(1)-1}$'s, which requires there to be $m+n$ $\mathbf{e}^{(1)1}$'s and $\ell-m-2n$ $\mathbf{e}^{(1)0}$'s. Such a term arises by applying two lowering operators to n $\mathbf{e}^{(1)1}$'s and single lowerings to $\ell-m-2n$ $\mathbf{e}^{(1)1}$'s. The number of ways of successively applying the $\ell-m$ lowering operations to get this term is

$$(\ell-m)!\frac{\ell!}{(m+n)!n!(\ell-m-2n)!2^n}.$$

This includes the number of possible orderings $(\ell - m)!$ of carrying out the lowerings as well as the reduction $1/(2n)!$ for the double lowering to the n $\mathbf{e}^{(1)1}$'s. Together with a $\sqrt{2}$ for each lowering, this gives the mth basis element as

$$\mathbf{e}^{(\ell)m} = \sqrt{\frac{(\ell+m)!(\ell-m)!2^{\ell-m}}{(2\ell)!}} \sum_n \frac{\ell!}{(m+n)!n!(\ell-m-2n)!2^n} \left\{ \left(\mathbf{e}^{(1)1}\right)^{m+n} \left(\mathbf{e}^{(1)-1}\right)^{n} \left(\mathbf{e}^{(1)0}\right)^{\ell-m-2n} \right\}^{(\ell)}. \quad (5.45)$$

In particular, the minimal weight basis element is the simple product

$$\mathbf{e}^{(\ell)-\ell} = \mathbf{e}^{(1)-1}\mathbf{e}^{(1)-1}\cdots\mathbf{e}^{(1)-1}\mathbf{e}^{(1)-1}, \quad (5.46)$$

so that if the process had started with this basis element and successively used the raising operator $\mathbf{G}_+^{(\ell)}$, exactly the same basis would have been obtained.

Actually, as far as the expansion of the $\mathbf{e}^{(\ell)m}$ is concerned, since

$$\mathbf{e}^{(1)-1}\mathbf{e}^{(1)1} = -\frac{1}{2}[\hat{x}\hat{x} + \hat{y}\hat{y} + i(\hat{x}\hat{y} - \hat{y}\hat{x})] = -\frac{1}{2}[\mathbf{U} - \hat{z}\hat{z} + i\boldsymbol{\mathcal{E}}\cdot\hat{z}], \quad (5.47)$$

combined with the requirement that $\mathbf{e}^{(\ell)m}$ be symmetric traceless, it immediately follows that if both $\mathbf{e}^{(1)-1}$ and $\mathbf{e}^{(1)1}$ appear together in an exansion term of $\mathbf{e}^{(\ell)m}$, then this can be simplified to involve only $(\mathbf{e}^{(1)0})^2$. Thus, if $m \geq 0$, the basis element $\mathbf{e}^{(\ell)m}$ can be written with m $\mathbf{e}^{(1)1}$'s in each term in the expansion, and the remaining indices occupied by $\mathbf{e}^{(1)0}$'s and $\mathbf{U}$'s. Actually, the $\mathbf{U}$ terms only arise to make the tensor traceless, so the general basis can be expressed as

$$\mathbf{e}^{(\ell)m} = \begin{cases} N_{\ell m}\left[\left(\mathbf{e}^{(1)1}\right)^m \left(\mathbf{e}^{(1)0}\right)^{\ell-m}\right]^{(\ell)}, & m \geq 0 \\ N_{\ell m}\left[\left(\mathbf{e}^{(1)-1}\right)^{-m} \left(\mathbf{e}^{(1)0}\right)^{\ell+m}\right]^{(\ell)}, & m \leq 0 \end{cases} \quad (5.48)$$

with $N_{\ell m}$ a normalization constant, given in Eq. (5.55). In greater detail, so as to make explicit all the trace conditions, this can be expanded, for $m \geq 0$, to

$$\mathbf{e}^{(\ell)m} = N_{\ell m}\sum_t a_t^{\ell m}\{[\mathbf{e}^{(1)1}]^m[\mathbf{e}^{(1)0}]^{\ell-m-2t}[\mathbf{U}]^t\}^{(\ell)}, \quad (5.49)$$

with $\{\}^{(\ell)}$ designating the symmetrized form of the enclosed tensor. It remains to calculate the expansion coefficients $a_t^{\ell m}$ and the normalization factor $N_{\ell m}$. The former can be accomplished by imposing the condition of being traceless on the sum. If $a_0^{\ell m} = 1$ is taken to define the scaling for the $a_t^{\ell m}$, then on iterating the recursion relation arising from the traceless condition, the expansion coefficients are found to be

$$a_t^{\ell m} = \frac{(-1)^t\ell!(\ell-|m|)!(2\ell-2t)!}{(2\ell)!t!(\ell-|m|-2t)!(\ell-t)!}. \quad (5.50)$$

This has been written in terms of the absolute value $|m|$ of m, since the same argument applies when $m < 0$. These expansion coefficients can be recognized as being proportional to the expansion coeffients for the polynomial related to the associated Legendre functions [that is, the polynomial obtained after taking out a factor of $(\sin\theta)^m$ from an associated Legendre function].

There remains the evaluation of the normalization factor. Since the spherical vector basis elements satisfy certain complex conjugate relations, Eq. (5.27), and the spherical tensor basis elements are products of the spherical vector basis elements, the spherical tensor basis elements satisfy analogous complex conjugate relations, in particular,

$$\mathbf{e}^{(\ell)m*} = (-1)^m \mathbf{e}^{(\ell)-m}. \tag{5.51}$$

It follows from the complex vector space inner product and the above complex conjugation property, that the normalization factor $N_{\ell m}$ is determined by [the calculation done here assumes $m \geq 0$, but really m should be replaced by $|m|$]

$$\begin{aligned}
1 &= \mathbf{e}^{(\ell)m*} \odot^{\ell} \mathbf{e}^{(\ell)m} = (-1)^m \mathbf{e}^{(\ell)-m} \odot^{\ell} \mathbf{e}^{(\ell)m} \\
&= (-1)^m N_{\ell m}^2 \sum_{t'} a_{t'}^{\ell m} \{[\mathbf{e}^{(1)-1}]^m [\mathbf{e}^{(1)0}]^{\ell-m-2t'} [\mathbf{U}]^{t'}\}^{(\ell)} \odot^{\ell} \\
&\qquad\qquad \sum_t a_t^{\ell m} \{[\mathbf{e}^{(1)1}]^m [\mathbf{e}^{(1)0}]^{\ell-m-2t} [\mathbf{U}]^t\}^{(\ell)} \\
&= (-1)^m N_{\ell m}^2 a_0^{\ell m} \{[\mathbf{e}^{(1)-1}]^m [\mathbf{e}^{(1)0}]^{\ell-m}\}^{(\ell)} \odot^{\ell} \sum_t a_t^{\ell m} \{[\mathbf{e}^{(1)1}]^m [\mathbf{e}^{(1)0}]^{\ell-m-2t} [\mathbf{U}]^t\}^{(\ell)} \\
&= (-1)^m N_{\ell m}^2 \sum_t a_t^{\ell m} \frac{(-1)^m}{\binom{\ell}{m}} \\
&= N_{\ell m}^2 \frac{(\ell-m)!(\ell+m)!}{(2\ell)!\binom{\ell}{m}} \sum_t (-1)^t \binom{\ell}{t} \binom{2\ell-2t}{\ell+m}.
\end{aligned} \tag{5.52}$$

In the above, the sum over t' reduced to the single term with $t' = 0$ on the basis that any $\mathbf{U}$ dotted into the sum over t vanishes since this sum is required to be traceless. The remaining tensor contractions each involved the contraction of two symmetric tensors, so one of these does not need to be symmetrized. It is convenient to take the unsymmetrized tensors as those in the sum over t. For each tensor contraction, there are $\binom{\ell}{m}$ ways according to which indices are dotted into $\mathbf{e}^{(1)-1}$ or $\mathbf{e}^{(1)0}$. Since the contraction vanished unless all the $\mathbf{e}^{(1)-1}$'s are dotted into the $\mathbf{e}^{(1)1}$'s, only one of these $\binom{\ell}{m}$ ways is nonzero. This tensor contraction gives the value $(-1)^m$, coming from the m $\mathbf{e}^{(1)-1} \cdot \mathbf{e}^{(1)1}$ contractions. The result of these calculations is the second last form in the above equation. The last form was obtained by inserting the explicit form for $a_t^{\ell m}$ and rewriting the result in terms of combinatorial factors. The final sum can be determined by expanding the following identity in different ways and equating coefficients of u in the result:

$$\begin{aligned}
\left[(1+u)^2 - 1\right]^{\ell} &= (1+u)^{2\ell} \left[1 - \frac{1}{(1+u)^2}\right]^{\ell} \\
u^{\ell}(2+u)^{\ell} &= \sum_t (-1)^t \binom{\ell}{t} (1+u)^{2\ell-2t} \\
\sum_m \binom{\ell}{m} 2^{\ell-m} u^{\ell+m} &= \sum_t (-1)^t \binom{\ell}{t} \sum_n \binom{2\ell-2t}{n} u^n.
\end{aligned} \tag{5.53}$$

Specifically the equality of the $u^{\ell+m}$ term implies that

$$2^{\ell-m} \binom{\ell}{m} = \sum_t (-1)^t \binom{\ell}{t} \binom{2\ell-2t}{\ell+m}. \tag{5.54}$$

It follows that the normalization factor for the spherical tensor basis element is [m is here replaced by $|m|$ wherever it is important to make the difference]

$$N_{\ell m} = \left[\frac{2^{|m|-\ell}(2\ell)!}{(\ell+m)!(\ell-m)!} \right]^{1/2} . \tag{5.55}$$

The basis element

$$\mathbf{e}^{(\ell)0} = N_{\ell 0}[\hat{z}]^{(\ell)} = \left(\frac{1}{\overline{P}_\ell(1)} \right)^{1/2} [\hat{z}]^{(\ell)} \tag{5.56}$$

illustrates the structural nature of these basis elements. Contrast this normalization with that of Eq. (4.8).

Just as for vectors, this basis is not orthonormal and has a contravariant metric that is similar to that for vectors, see Eq. (5.13),

$$g^{mm'} \equiv \mathbf{e}^{(\ell)m} \odot^\ell \mathbf{e}^{(\ell)m'} = (-1)^m \delta_{m,-m'}, \tag{5.57}$$

but extended to $m,\ m' = \ell, \cdots, -\ell$. Thus again a dual basis arises naturally. This is defined as the generalization of Eq. (5.14), namely

$$\mathbf{e}_m^{(\ell)} \odot^\ell \mathbf{e}^{(1)m'} = \delta_m^{m'} . \tag{5.58}$$

As expected this basis is just the tensorial analog of the vector dual basis, for example the maximum weight basis element is

$$\mathbf{e}_\ell^{(\ell)} = \mathbf{e}_1^{(1)} \mathbf{e}_1^{(1)} \cdots \mathbf{e}_1^{(1)} \mathbf{e}_1^{(1)} . \tag{5.59}$$

The covariant basis elements can also be related to the contravariant basis elements by complex conjugation, namely

$$\mathbf{e}_m^{(\ell)} = \left(\mathbf{e}^{(\ell)m} \right)^* . \tag{5.60}$$

These give the covariant metric

$$g_{mm'} \equiv \mathbf{e}_m^{(\ell)} \odot^\ell \mathbf{e}_{m'}^{(\ell)} = (-1)^m \delta_{m,-m'}, \tag{5.61}$$

which can also be used to obtain the dual basis according to

$$\mathbf{e}_m^{(\ell)} = g_{mm'} \mathbf{e}^{(\ell)m'}, \tag{5.62}$$

again using the summation convention. Finally there is also the basis set with the alternate phase convention

$$\mathfrak{e}^{(\ell)m} \equiv (i)^\ell \mathbf{e}^{(\ell)m}, \tag{5.63}$$

which is useful for general theoretical developments, see in particular, Secs. 7.3 and 11.3. Their covariant analogs satisfy the relations

$$\mathfrak{e}_m^{(\ell)} = \left(\mathfrak{e}^{(\ell)m} \right)^* = (-1)^{\ell+m} \mathfrak{e}^{(\ell)-m} \tag{5.64}$$

with the metric

$$\mathfrak{g}_{mm'}^{(\ell)} \equiv \mathfrak{e}_m^{(\ell)} \odot \mathfrak{e}_{m'}^{(\ell)} = (-1)^{\ell+m'} \delta_{m,-m'} . \tag{5.65}$$

Since ℓ and m are integers, the power of (-1) appearing in the last two equations could be written in different ways, for example, as $(-1)^{\ell-m}$, rather than as it appears above. The particular choice in Eq. (5.65) is consistent with the choice used for spinors, see Eqs. (10.92).

For a given natural tensor $\mathbf{T}^{(\ell)}$ of order ℓ, the contravariant and covariant components are obtained by the ℓ-fold dot product of the corresponding basis elements and the Cartesian tensor

$$T^{(\ell)m} = \mathbf{e}^{(\ell)m} \odot^{\ell} \mathbf{T}^{(\ell)}; \qquad T^{(\ell)}_m = \mathbf{e}^{(\ell)}_m \odot^{\ell} \mathbf{T}^{(\ell)}. \tag{5.66}$$

These are related by the metrics according to

$$T^{(\ell)}_m = g_{mm'} T^{(\ell)m'}; \qquad T^{(\ell)m} = g^{mm'} T^{(\ell)}_{m'}. \tag{5.67}$$

It follows from the biorthogonality of the dual basis sets that the natural tensor $\mathbf{T}^{(\ell)}$ can be expanded in terms of its components as

$$\mathbf{T}^{(\ell)} = T^{(\ell)m} \mathbf{e}^{(\ell)}_m = T^{(\ell)}_m \mathbf{e}^{(\ell)m}. \tag{5.68}$$

Since the basis elements are all symmetric and traceless in the ℓ indices, the projector $\mathbf{E}^{(\ell)}$ has no effect when acting on them, namely

$$\mathbf{E}^{(\ell)} \odot^{\ell} \mathbf{e}^{(\ell)m} = \mathbf{e}^{(\ell)m}; \qquad \mathbf{E}^{(\ell)} \odot^{\ell} \mathbf{e}^{(\ell)}_m = \mathbf{e}^{(\ell)}_m. \tag{5.69}$$

This projector, being the identity for the space of natural tensors of weight ℓ, can be expanded in terms of the basis sets,

$$\mathbf{E}^{(\ell)} = \mathbf{e}^{(\ell)}_m \mathbf{e}^{(\ell)m} = \mathbf{e}^{(\ell)m} \mathbf{e}^{(\ell)}_m = \mathbf{e}^{(\ell)m} g_{mm'} \mathbf{e}^{(\ell)m'}, \tag{5.70}$$

and obviously in other combinations. For theoretical developments, it is also important to write this in the $\mathfrak{e}^{(\ell)m}$ basis set, namely

$$\mathbf{E}^{(\ell)} = \sum_m \mathfrak{e}^{(\ell)m} (-1)^{\ell-m} \mathfrak{e}^{(\ell)-m}. \tag{5.71}$$

The ℓ-fold contraction of two natural tensors $\mathbf{T}^{(\ell)}$ and $\mathbf{S}^{(\ell)}$ of common weight ℓ can be expressed in terms of their spherical components as

$$\mathbf{T}^{(\ell)} \odot^{\ell} \mathbf{S}^{(\ell)} = T^{(\ell)}_m S^{(\ell)m} = \sum_m T^{(\ell)-m} (-1)^m S^{(\ell)m}, \tag{5.72}$$

with alternate ways also possible. For the last form given, the sum over m has been written explicitly since m appears in three places, otherwise the summation convention has been assumed. A particular case of tensorial contraction is the formation of the absolute square of the tensor (assuming the Cartesian tensor, in natural form, is real)

$$|\mathbf{T}|^2 \equiv \mathbf{T}^{(\ell)} \odot^{\ell} \mathbf{T}^{(\ell)} = T^{(\ell)}_m T^{(\ell)m} = \sum_m (-1)^m T^{(\ell)-m} T^{(\ell)m}. \tag{5.73}$$

For a real Cartesian tensor this contraction is positive, so the norm of the tensor $|\mathbf{T}|$ can be defined in terms of it, but it is noted that the spherical components are complex numbers. Finally, it should be noted that the contraction between any pth order tensor $\mathbf{V}^{(p)}$ and a natural tensor $\mathbf{T}^{(\ell)}$ immediately selects out only that weight ℓ part of $\mathbf{V}^{(p)}$ into which $\mathbf{T}^{(\ell)}$ is contracted, assuming $p > \ell$. On the other hand, the contraction between a tensor $\mathsf{V}^{(p)}$ and $\mathsf{T}^{(\ell)}$, whose order p is smaller than ℓ, produces a tensor of order and weight $\ell - p$,

$$\mathsf{V}^{(p)} \odot^p \mathsf{T}^{(\ell)} = \mathsf{W}^{(\ell-p)}. \tag{5.74}$$

This has inherited the property of being symmetric and traceless in the $\ell - p$ indices from $\mathsf{T}^{(\ell)}$, so is a natural tensor of weight $\ell - p$. Clearly many other relations could be mentioned, but they all follow from the basic properties of natural tensors and/or their spherical tensor components.

5.5 Spherical Harmonics

Chapter 4 discussed the normalized irreducible tensors $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ of $\hat{r}$, see Eq. (4.8). The $\mathbf{e}^{(\ell)m}$ components of these tensors are also eigenvectors to a rotation about a preferred axis, which by standard usage is labelled the $\hat{z}$-axis. Since the resulting functions satisfy the same group properties as the spherical harmonics, $Y_{(\ell)m}(\hat{r})$, see for example Ref. [1], they must be identical to them, except for possible normalization and phase factors. This section discusses these connections and lists some of the properties of these functions.

The $\mathbf{e}^{(\ell)m}$ component of $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ is denoted by

$$\mathcal{Y}^{(\ell)m}(\hat{r}) \equiv \mathbf{e}^{(\ell)m} \odot^\ell \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}). \tag{5.75}$$

From Eq. (4.9), these functions satisfy the orthonormalization conditions

$$\frac{1}{4\pi} \int d\hat{r} \mathcal{Y}^{(\ell)m}(\hat{r}) \mathcal{Y}^{(\ell')m'}(\hat{r}) = \delta_{\ell\ell'} \mathbf{e}^{(\ell)m} \odot^\ell \mathbf{e}^{(\ell)m'} = (-1)^m \delta_{m,-m'} \delta_{\ell\ell'}. \tag{5.76}$$

An alternate way of writing this orthogonality relation is

$$\frac{1}{4\pi} \int d\hat{r} \mathcal{Y}^{(\ell)m*}(\hat{r}) \mathcal{Y}^{(\ell')m'}(\hat{r}) = \frac{(-1)^m}{4\pi} \int d\hat{r} \mathcal{Y}^{(\ell)-m}(\hat{r}) \mathcal{Y}^{(\ell')m'}(\hat{r}) = \delta_{m,m'} \delta_{\ell\ell'}. \tag{5.77}$$

The contraction of two $\boldsymbol{\mathcal{Y}}^{(\ell)}$ functions, Eq. (4.11), and the expansion of $\mathsf{E}^{(\ell)}$, Eq. (5.70), combine to give the expansion of the Legendre polynomial of $\hat{r}\cdot\hat{u}$ as

$$\begin{aligned} (2\ell+1) P_\ell(\hat{r}\cdot\hat{u}) &= \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) \odot^\ell \mathsf{E}^{(\ell)} \odot^\ell \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{u}) \\ &= \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) \odot^\ell \sum_m \mathbf{e}^{(\ell)m} (-1)^m \mathbf{e}^{(\ell)-m} \odot^\ell \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{u}) \\ &= \sum_m \mathcal{Y}^{(\ell)m}(\hat{r}) (-1)^m \mathcal{Y}^{(\ell)-m}(\hat{u}). \end{aligned} \tag{5.78}$$

Since $\mathbf{e}^{(\ell)m}$ is symmetric and traceless, the detailed form of the $\mathcal{Y}^{(\ell)m}(\hat{r})$ does not require the symmetric traceless property of $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$, but only the normalization factor. Writing $\hat{r}$ in spherical coordinates,

$$\hat{r} = \sin\theta(\hat{x}\cos\phi + \hat{y}\sin\phi) + \hat{z}\cos\theta, \tag{5.79}$$

for $m \geq 0$ this function is

$$\begin{aligned}
\mathcal{Y}^{(\ell)m}(\hat{r}) &= \left(\frac{2\ell+1}{\overline{P}_\ell(1)}\right)^{1/2} \mathbf{e}^{(\ell)m} \odot^\ell (\hat{r})^\ell \\
&= \left(\frac{(2\ell+1)!}{2^\ell(\ell!)^2} \frac{2^{m-\ell}(2\ell)!}{(\ell+m)!(\ell-m)!}\right)^{1/2} \frac{(\ell-m)!(\ell+m)!}{(2\ell)!} \\
&\qquad \times \sum_t (-1)^t \binom{\ell}{t} \binom{2\ell-2t}{\ell+m} \left(\frac{-\sin\theta e^{i\phi}}{\sqrt{2}}\right)^m (\cos\theta)^{\ell-m-2t} \\
&= \frac{(-1)^m}{2^\ell \ell!} \left(\frac{(2\ell+1)(\ell-m)!}{(\ell+m)!}\right)^{1/2} \sin^m\theta e^{im\phi} \\
&\qquad \times \sum_t (-1)^t \binom{\ell}{t} \frac{(2\ell-2t)!}{(\ell-m-2t)!} (\cos\theta)^{\ell-m-2t}. \qquad (5.80)
\end{aligned}$$

For $m < 0$ there is a difference of a factor $(-1)^m$ as well as the obvious change in sign of the ϕ dependence. Both of these differences arise from the difference between the spherical components r^1 and r^{-1} of a vector, see Eq. (5.18). In detail the $m < 0$ component of $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ is

$$\begin{aligned}
\mathcal{Y}^{(\ell)m}(\hat{r}) &= \frac{1}{2^\ell \ell!} \left(\frac{(2\ell+1)(\ell-|m|)!}{(\ell+|m|)!}\right)^{1/2} \sin^{|m|}\theta e^{im\phi} \\
&\qquad \times \sum_t (-1)^t \binom{\ell}{t} \frac{(2\ell-2t)!}{(\ell-|m|-2t)!} (\cos\theta)^{\ell-|m|-2t}. \qquad (5.81)
\end{aligned}$$

This difference is equivalent to the relation

$$\mathcal{Y}^{(\ell)-m}(\hat{r}) = (-1)^m \mathcal{Y}^{(\ell)m*}(\hat{r}), \qquad (5.82)$$

which arises from the analogous relation of the basis vectors, namely Eq. (5.51). The combinatorial and other factors in $\mathcal{Y}^{(\ell)m}(\hat{r})$ are independent of the sign of m, which is explicitly indicated here by writing the absolute value, $|m|$.

The sum over t can be recognized as the polynomial in $\cos\theta$ that appears in the associated Legendre function. This is usually written as a multiple derivative, for u, which is to be equated to $\cos\theta$,

$$\begin{aligned}
\frac{d^{|m|}}{du^{|m|}} P_\ell(u) &= \frac{1}{2^\ell \ell!} \frac{d^{\ell+|m|}}{du^{\ell+|m|}} (u^2-1)^\ell \\
&= \frac{1}{2^\ell \ell!} \frac{d^{\ell+|m|}}{du^{\ell+|m|}} \sum_t (-1)^t \binom{\ell}{t} u^{2\ell-2t} \\
&= \frac{1}{2^\ell \ell!} \sum_t (-1)^t \binom{\ell}{t} \frac{(2\ell-2t)!}{(\ell-|m|-2t)!} u^{\ell-|m|-2t}. \qquad (5.83)
\end{aligned}$$

In this way $\mathcal{Y}^{(\ell)m}(\hat{r})$ can be expressed in terms of the associated Legendre function

$$P_\ell^{|m|}(\cos\theta) \equiv \sin^{|m|}\theta \frac{d^{|m|}}{d\cos\theta^{|m|}} P_\ell(\cos\theta), \qquad (5.84)$$

as

$$\mathcal{Y}^{(\ell)m}(\hat{r}) = (-1)^m \left(\frac{(2\ell+1)(\ell-|m|)!}{(\ell+|m|)!} \right)^{1/2} P_\ell^{|m|}(\cos\theta) e^{im\phi} \tag{5.85}$$

for $m \geq 0$, and without the $(-1)^m$ factor for $m < 0$. These are the forms which can be compared with the spherical harmonics. The definition given by Edmonds [1] corresponds to

$$Y_{\ell m}(\hat{r}) = \frac{1}{\sqrt{4\pi}} \mathcal{Y}^{(\ell)m}(\hat{r}). \tag{5.86}$$

This corresponds to the difference in normalization used here, namely to take the angular average, Eq. (4.9), whereas the surface area of a unit sphere (4π) is usually incorporated into the normalization of the spherical harmonics. Other phase conventions for the spherical harmonics are present in the literature, see Edmonds, page 21, for some comment on this. In particular, the other convention for the basis vectors, Eq. (5.28), if incorporated into the analogous tensors, give rise to the spherical harmonics

$$\mathfrak{Y}_{\ell m}(\hat{r}) \equiv \frac{1}{\sqrt{4\pi}} \mathfrak{e}^{(\ell)m} \odot^\ell \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) = (i)^\ell Y_{\ell m}(\hat{r}) \tag{5.87}$$

with a different overall phase factor. These are also mentioned explicitly by Edmonds.

Chapter 6

3-j Coupling Tensors

The expansion of a product of two irreducible representations into a sum of irreducible representations is known as the Clebsch-Gordan reduction. From the point of view of irreducible Cartesian tensors in natural form, the product of two irreducible representations is the tensor product of two symmetric traceless tensors, whose reduction into irreducible parts is equivalent to expressing the tensor product as a linear combination of symmetric traceless tensors, suitably embedded in the tensor space of order equal to the sum of the weights of the two irreducible representations constituting the product. The embedding tensors, which are by nature rotational invariants, as well as the tensors carrying out the reduction, are necessarily tensors that are symmetric and traceless in three sets of directions. These are the Clebsch-Gordan coupling tensors. As described above, their essential nature is very simple and it is to be shown that the property of being an invariant tensor that is traceless and symmetric in three sets of directions determines the coupling tensor up to a multiplicative constant. The multiplicative constant can be chosen in a number of different ways. While the Clebsch-Gordan reduction treats the three irreducible representations asymmetrically, in that two irreducible representations form the product and the third is associated with the expansion series, Wigner [22] suggested a symmetrical treatment, leading to his 3-j symbols. The tensor analog of that, which is followed here and in Ref. [17], is to treat all three sets of symmetric traceless directions equivalently and the multiplicative constant chosen so that the complete tensor contraction of the 3-j tensor with itself has a magnitude of 1. In this way their spherical tensor representation conforms exactly to the standard 3-j symbols. It is for this reason that the coupling tensors are referred to as 3-j tensors. These were first presented in Ref. [17]. The first section describes the basic structure of the coupling tensors, being labelled as the tensors $\mathbf{T}(\ell_1, \ell_2, \ell_3)$. Then their proper normalization is presented, to give the 3-j tensors $\mathbf{V}(\ell_1, \ell_2, \ell_3)$. The next section deals with the fundamental expansion of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ in terms of $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$. There follows the calculation of the normalization factors. The chapter ends with sections on contraction and recursion relations between different $\mathbf{T}(\ell_1, \ell_2, \ell_3)$. Except for the section on definitions, this chapter is highly technical and might be skipped in a first reading. It is the following chapter that discusses the utilitarian properties of the 3-j tensors, in particular their orthogonality and expansion properties, as well as their connection to Wigner's 3-j symbols. Chapter 8 describes some of the properties of the other n-j symbols.

The Cartesian form of the Clebsch-Gordan reduction was first described, to the author's knowledge, by Barsella and Fabri [23]. They get all the natural form tensors that can be obtained by reduction of a product of two irreducible Cartesian tensors, including also the tensors of 1/2-integral weights. But they do not separate the reduction process from the initial tensor product, so they do not express the result in terms of Clebsch-Gordan tensors, or their 3-j form. Also missing in their presentation is the consequent inverse problem of expressing the tensor product as a sum of its irreducible tensor components. Having 3-j tensors provides a means of describing both of these processes, and has the further advantage of being (cyclically) symmetric in the three weights involved in the tensor.

6.1 Definitions

Given the two irreducible tensors $\mathbf{A}^{(\ell_1)}$ and $\mathbf{B}^{(\ell_2)}$, each in natural form and of respective weights ℓ_1 and ℓ_2, it is desired to express their tensor product as the sum

$$\mathbf{A}^{(\ell_1)}\mathbf{B}^{(\ell_2)} = \sum_{\ell_3} \mathbf{V}(\ell_1,\ell_2,\ell_3) \odot^{\ell_3} \mathbf{W}^{(\ell_3)} \tag{6.1}$$

of irreducible tensors $\mathbf{W}^{(\ell_3)}$, each expressed in natural form. That this can be done is a property of the completeness of the irreducible representations, together with the fact that each irreducible representation can be expressed in natural form. The 3-j tensors $\mathbf{V}(\ell_1,\ell_2,\ell_3)$ are then symmetric and traceless in each of the ℓ_1, ℓ_2 and ℓ_3 sets of directions. Since all rotational properties are to be described by the irreducible tensors, the 3-j tensors must be rotational invariants. The first objective of this chapter is then to first find a rotationally invariant tensor $\mathbf{T}(\ell_1,\ell_2,\ell_3)$ that is symmetric and traceless in the three sets of directions ℓ_1, ℓ_2 and ℓ_3. By construction it is shown that such tensors are unique up to a multiplicative constant. A subsequent choice of normalization converts this to a 3-j tensor.

Any invariant tensor is a linear combination of products of $\mathbf{U}$ and $\boldsymbol{\varepsilon}$. Moreover, the requirement that it is symmetric and traceless in, e.g., ℓ_1 directions is satisfied by taking the appropriate dot product with the projector $\mathbf{E}^{(\ell_1)}$, and the same for the other sets of directions. Thus $\mathbf{T}(\ell_1,\ell_2,\ell_3)$ must satisfy

$$\mathbf{T}(\ell_1,\ell_2,\ell_3) = \mathbf{E}^{(\ell_1)} \odot^{\ell_1} \underbrace{(\mathbf{U})^{\ell_1}\mathbf{E}^{(\ell_2)}(\mathbf{U})}^{\ell_1} \odot^{\ell_1+\ell_2} \mathbf{T}(\ell_1,\ell_2,\ell_3) \odot^{\ell_3} \mathbf{E}^{(\ell_3)}. \tag{6.2}$$

But now the tensor $\mathbf{T}(\ell_1,\ell_2,\ell_3)$ on the right hand side can be replaced by any set of $\mathbf{U}$'s and $\boldsymbol{\varepsilon}$'s that connect the projectors. Clearly, neither both directions of a $\mathbf{U}$ nor two directions of $\boldsymbol{\varepsilon}$ can be dotted into the same projector. Moreover, as proven in Eq. (2.84), at most only one $\boldsymbol{\varepsilon}$ needs to be used to connect the $L \equiv \ell_1 + \ell_2 + \ell_3$ directions. Again, a $\mathbf{U}$ connects (uses up) two directions, while a $\boldsymbol{\varepsilon}$ connects three. It follows that if L is even, only $\mathbf{U}$'s appear whereas if L is odd, one $\boldsymbol{\varepsilon}$ must appear.

For even L, define γ as the number of $\mathbf{U}$'s connecting the ℓ_1 and ℓ_2 directions, β as the number connecting the ℓ_1 and ℓ_3, and α as the number connecting ℓ_2 and ℓ_3. Then the sums

$$\begin{aligned} \beta + \gamma &= \ell_1, \\ \gamma + \alpha &= \ell_2, \\ \alpha + \beta &= \ell_3 \end{aligned} \tag{6.3}$$

are the conditions required to use up all the directions in $\mathbf{T}(\ell_1,\ell_2,\ell_3)$. The solution of these three equations is

$$\alpha = \frac{1}{2}L - \ell_1,$$
$$\beta = \frac{1}{2}L - \ell_2,$$
$$\gamma = \frac{1}{2}L - \ell_3. \tag{6.4}$$

These integers are nonnegative only if

$$|\ell_1 - \ell_2| \leq \ell_3 \leq \ell_1 + \ell_2 \tag{6.5}$$

and its cyclic permutations are satisfied. The condition on ℓ_3 determines which irreducible representations contribute to the sum expressed in Eq. (6.1), while the other conditions are appropriate if the various roles of the irreducible representations are interchanged. But the fact that there is only one solution to the conditions of Eqs. (6.3) implies that a tensor that is traceless and symmetric in three sets of directions is unique up to a multiplicative factor, here proven for even L while the L odd case is now to be discussed.

For odd L there must be one $\boldsymbol{\varepsilon}$, with one direction of $\boldsymbol{\varepsilon}$ dotted into each of the three projectors. That leaves $L-3$ directions to be connected by $\mathbf{U}$'s. If these are labelled as α, β and γ, similar to the L even case, then the number of $\mathbf{U}$'s connecting ℓ_2 and ℓ_3 is

$$\alpha = \frac{1}{2}(L-1) - \ell_1, \tag{6.6}$$

with corresponding formulas for β and γ. Thus any tensor that is symmetric and traceless in three sets of directions is proportional to

$$\mathbf{T}(\ell_1,\ell_2,\ell_3) = \mathbf{E}^{(\ell_1)}\odot^{\ell_1}(\mathbf{U})^{\beta}(\mathbf{U})^{\gamma}\mathbf{E}^{(\ell_2)}\odot^{\ell_2}(\mathbf{U})^{\gamma}(\mathbf{U})^{\alpha}(\mathbf{U})^{\beta}\odot^{\ell_3}\mathbf{E}^{(\ell_3)} \tag{6.7}$$

for even L and

$$\mathbf{T}(\ell_1,\ell_2,\ell_3) = \mathbf{E}^{(\ell_1)}\odot^{\ell_1}(\mathbf{U})^{\beta}(\mathbf{U})^{\gamma}\boldsymbol{\varepsilon}(\mathbf{U})^{\gamma}(\mathbf{U})^{\alpha}\odot^{(\ell_2)}\mathbf{E}^{(\ell_2)}(\mathbf{U})^{\alpha}(\mathbf{U})^{\beta}\odot^{\ell_3}\mathbf{E}^{(\ell_3)} \tag{6.8}$$

for odd L.

The 3-j tensor is proportional to the corresponding tensor $\mathbf{T}(\ell_1,\ell_2,\ell_3)$, with proportionality constant $\Omega(\ell_1,\ell_2,\ell_3)^{-1/2}$, thus

$$\mathbf{V}(\ell_1,\ell_2,\ell_3) \equiv \Omega(\ell_1,\ell_2,\ell_3)^{-1/2}\mathbf{T}(\ell_1,\ell_2,\ell_3). \tag{6.9}$$

It remains to find an appropriate normalization for the 3-j tensors so as to define $\Omega(\ell_1,\ell_2,\ell_3)$. By analogy with the 3-$j$ symbols, all three sets of symmetric traceless tensors are to be treated the same. Thus the chosen normalization is

$$\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{L}\mathbf{V}(\ell_3,\ell_2,\ell_1) = (-1)^{L}. \tag{6.10}$$

The interchange of order of the weights is so that the tensorial contraction of "dotting nearest directions first" leads to the dotting of equal irreducible representations into each other. For even L the contractions in Eq. (6.7) can be interchanged in any order without any effect, as long as the same sets of directions are dotted together. But for odd L, a change in order may imply a change in order of dotting into the $\boldsymbol{\mathcal{E}}$, with an associated sign change. The essential feature is whether the change in order is cyclic or anticyclic. In particular, the normalization condition involves one $\mathbf{V}$ in anticyclic order to the other $\mathbf{V}$, so the normalization condition of Eq. (6.10) is $(-1)^L$. The normalization constant is thus defined as

$$\Omega(\ell_1, \ell_2, \ell_3) = (-1)^L \mathbf{T}(\ell_1, \ell_2, \ell_3) \odot^L \mathbf{T}(\ell_3, \ell_2, \ell_1). \tag{6.11}$$

It is shown in Sec. 6.3 that this normalization constant is given by

$$\Omega(\ell_1, \ell_2, \ell_3) = \frac{(L+1)!(L-2\ell_1)!(L-2\ell_2)!(L-2\ell_3)!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!} \times \begin{cases} 1 & \text{L even,} \\ 2 & \text{L odd.} \end{cases} \tag{6.12}$$

Equations (6.7) and (6.8) give the essential tensorial features of the 3-j tensors while Eqs. (6.9) and (6.10) define their appropriate normalization. These properties are all that are generally needed in order to use the 3-j tensors for most purposes. However their detailed structure in terms of the elementary invariants $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$ are sometimes needed. This calculation as well as the derivation of the normalization constant formula involve a fair amount of algebra which is presented in the following sections. The usage of the 3-j tensors and the relation to the higher n-j symbols are presented in the next chapter.

6.2 Detailed Calculation of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$

The detailed calculation of the tensorial form of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ in terms of the elementary invariants $\mathbf{U}$ and $\boldsymbol{\mathcal{E}}$ are presented in this section. This follows Coope's [17] original derivation. There is some difference in the calculation depending on whether L is even or odd. The even case is treated first.

6.2.1 $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ for L even

One could insert the expansion, Eq. (3.49) for each of the $\mathbf{E}$'s in Eq. (6.7) and carry out the contractions to get an expression for $\mathbf{T}(\ell_1, \ell_2, \ell_3)$. But essentially the result will be of the form

$$\mathbf{T}(\ell_1, \ell_2, \ell_3) = \sum_{a,b,c} x_{a,b,c} \mathbf{T}^{a,b,c,\alpha',\beta',\gamma'} \tag{6.13}$$

where the tensor

$$\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'} \equiv \left\{ (\,|\,)^{\beta'} (\mathbf{U})^a (\,|\,)^{\gamma'} \right\}^{(\ell_1)} \left\{ (\,|\,)^{\gamma'} (\mathbf{U})^b (\,|\,)^{\alpha'} \right\}^{(\ell_2)} \left\{ (\,|\,)^{\alpha'} (\mathbf{U})^c (\,|\,)^{\beta'} \right\}^{(\ell_3)} \tag{6.14}$$

is symmetric in the three sets of ℓ_1, ℓ_2 and ℓ_3 directions, with a, b and c $\mathbf{U}$'s, equivalently traces, in each respective symmetric set. In the expansion of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ there are

$$\alpha' = \frac{1}{2}L - \ell_1 + a - b - c = \alpha + a - b - c \tag{6.15}$$

directions connecting the ℓ_2 and ℓ_3 sets of directions. Similarly, the other numbers of $\mathbf{U}$'s connecting the other sets of directions are

$$\begin{aligned} \beta' &= \frac{1}{2}L - \ell_2 + b - c - a = \beta + b - c - a \\ \gamma' &= \frac{1}{2}L - \ell_3 + c - a - b = \gamma + c - a - b. \end{aligned} \tag{6.16}$$

Thus, in the expansion of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$, α', β' and γ' are determined by ℓ_1, ℓ_2, ℓ_3 and a, b and c. Clearly, if $a = b = c = 0$, then $\alpha' = \alpha$, etc., which is consistent with the definition of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ in terms of the $\mathbf{E}$'s, Eq. (6.7). On setting $x_{0,0,0} = 1$, this equates the leading terms in this association. It is also worth noting that the form of Eq. (6.13) follows from the symmetry requirements of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ so, on the basis of this, Eq. (6.13) could have been written down immediately.

But $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ is also traceless in each of the ℓ_1, ℓ_2 and ℓ_3 sets of directions. This leads to the study of the trace properties of the tensor $\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'}$. Specifically, a $\mathbf{U}$ double dotted into the ℓ_1 set of directions has $\ell_1(\ell_1 - 1)/2$ possible ways of contracting, and leads to a variety of results corresponding to whether the $\mathbf{U}$ is dotted into the a, β' and/or γ' directions. The detailed result is

$$\begin{aligned} \frac{\ell_1(\ell_1-1)}{2}\mathbf{U}\mathbf{:}\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'} &= a(2a+1)\mathbf{T}^{a-1,b,c,\alpha',\beta',\gamma'} + 2a\beta'\mathbf{T}^{a-1,b,c,\alpha',\beta',\gamma'} \\ &+2a\gamma'\mathbf{T}^{a-1,b,c,\alpha',\beta',\gamma'} + \beta'\gamma'\mathbf{T}^{a,b,c,\alpha'+1,\beta'-1,\gamma'-1} \\ &+\frac{\beta'(\beta'-1)}{2}\mathbf{T}^{a,b,c+1,\alpha',\beta'-2,\gamma'} + \frac{\gamma'(\gamma'-1)}{2}\mathbf{T}^{a,b+1,c,\alpha',\beta',\gamma'-2}. \end{aligned} \tag{6.17}$$

Applying this to the expansion of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ and relabelling the terms so as to have a common form for the expansion tensors, namely $\mathbf{T}^{a-1,b,c,\alpha',\beta',\gamma'}$, leads to

$$\begin{aligned} \mathbf{0} = \frac{\ell_1(\ell_1-1)}{2}\mathbf{U}\mathbf{:}\mathbf{T}(\ell_1,\ell_2,\ell_3) &= \sum_{a,b,c}\mathbf{T}^{a-1,b,c,\alpha',\beta',\gamma'}\Bigg[a(2\ell_1-2a+1)x_{a,b,c} \\ &+(\beta'+1)(\gamma'+1)x_{a-1,b,c} + \frac{(\beta'+2)(\beta'+1)}{2}x_{a-1,b,c-1} \\ &+\frac{(\gamma'+2)(\gamma'+1)}{2}x_{a-1,b-1,c}\Bigg]. \end{aligned} \tag{6.18}$$

Since the $\mathbf{T}^{a-1,b,c,\alpha',\beta',\gamma'}$ are linearly independent, it follows that the $x_{a,b,c}$ expansion coefficients must satisfy the recursion relation

$$\begin{aligned} &a(2\ell_1-2a+1)x_{a,b,c} + (\beta'+1)(\gamma'+1)x_{a-1,b,c} + \frac{(\beta'+2)(\beta'+1)}{2}x_{a-1,b,c-1} \\ &+\frac{(\gamma'+2)(\gamma'+1)}{2}x_{a-1,b-1,c} = 0. \end{aligned} \tag{6.19}$$

By symmetry, the recursion relations arising from the doubledot contraction with $\mathbf{U}$ on the two other sets of directions on $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ can be obtained by relabelling, namely

$$\begin{aligned} &b(2\ell_2-2b+1)x_{a,b,c} + (\alpha'+1)(\gamma'+1)x_{a,b-1,c} + \frac{(\alpha'+2)(\alpha'+1)}{2}x_{a,b-1,c-1} \\ &+\frac{(\gamma'+2)(\gamma'+1)}{2}x_{a-1,b-1,c} = 0 \end{aligned} \tag{6.20}$$

and

$$c(2\ell_3 - 2c + 1)x_{a,b,c} + (\beta' + 1)(\alpha' + 1)x_{a,b,c-1} + \frac{(\beta' + 2)(\beta' + 1)}{2}x_{a-1,b,c-1} + \frac{(\alpha' + 2)(\alpha' + 1)}{2}x_{a,b-1,c-1} = 0. \tag{6.21}$$

The solution of these three recursion relations should lead to an explicit equation for $x_{a,b,c}$. While certain special cases of these recursion relations are discussed below, it is difficult to see how to solve the general case. Thus an indirect procedure is given for finding the general formula for $x_{a,b,c}$.

Special cases of the first recursion relation are:

1. if $\ell_3 = 0$, then $\alpha' = \beta' = c = 0$ since each of these must be ≥ 0. Likewise, since $\alpha,\ \beta \geq 0$, it follows that $\ell_2 = \ell_1$, and since then $\alpha' = a - b$, necessarily $b = a$. Any $x_{a,b,c}$ coefficients that do not conform to these conditions must vanish. Under these conditions the first recursion relation becomes

$$a(2\ell_1 - 2a + 1)x_{a,a,0} + \frac{1}{2}(\ell_1 - 2a + 2)(\ell_1 - 2a + 1)x_{a-1,a-1,0} = 0. \tag{6.22}$$

This is recognized as the recursion relation for the $c_a^{(\ell_1)}$ for the expansion of $\mathbf{E}^{(\ell_1)}$, Eq. (3.51), and shows that $\mathbf{T}(\ell_1, \ell_1, 0) = \mathbf{E}^{(\ell_1)}$, which is consistent with the definition of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$.

2. if $b = c = 0$, then the first recursion relation becomes

$$a(2\ell_1 - 2a + 1)x_{a,0,0} + (\beta - a + 1)(\gamma - a + 1)x_{a-1,0,0} = 0. \tag{6.23}$$

This can be rewritten as

$$x_{a,0,0} = -\frac{(\beta - a + 1)(\gamma - a + 1)}{a(2\ell_1 - 2a + 1)}x_{a-1,0,0}, \tag{6.24}$$

which can be easily iterated to give

$$x_{a,0,0} = \frac{(-1)^a 2^a \beta!\gamma!\ell_1!(2\ell_1 - 2a)!}{a!(\beta - a)!(\gamma - a)!(\ell_1 - a)!(2\ell_1)!} \tag{6.25}$$

on the basis that $x_{0,0,0} = 1$. Up to a difference in normalization, this result is equivalent to the set of coefficients that Barsella and Fabri [23] used to obtain the possible irreducible Cartesian tensors arising from the reduction of a product of irreducible Cartesian tensors.

The calculation of the general case is carried out as a sequence of two steps, first, an analysis is made of the special case when $\ell_1 + \ell_2 = \ell_3$ and second, this result is used to rewrite the tensorial expansion of the general coupling tensor.

6.2.2 The special case that $\ell_1 + \ell_2 = \ell_3$

Provided that $\ell_1 + \ell_2 = \ell_3$, then the coupling tensor $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ is equal to $\mathbf{E}^{(\ell_3)}$, essentially having the first (lefthand) two sets of traceless symmetric directions being a special way of writing the first (lefthand) ℓ_3 directions of $\mathbf{E}^{(\ell_3)}$. This follows from the uniqueness of both tensors. On equating the expansion of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ according to Eq.(6.13) and $\mathbf{E}^{(\ell_3)}$ according to Eq. (3.49), namely

$$\sum_{a,b,c} x_{a,b,c} \mathbf{T}^{a,b,c,\alpha',\beta',\gamma'} = \sum_{t=0}^{[\frac{1}{2}\ell_3]} c_t^{(\ell_3)} \Big\{ (\mathbf{U})^t (\mathbf{U})^{\ell_3-2t} \Big\}^{(\ell_3)} \Big\{ (\mathbf{U})^{\ell_3-2t} (\mathbf{U})^t \Big\}^{(\ell_3)}, \tag{6.26}$$

it is possible, on the basis of the number of $\mathbf{U}$'s in $\{\ \}^{(\ell_3)}$, to equate the terms for $t = c$, thus

$$\sum_{a,b} x_{a,b,c} \mathbf{T}^{a,b,c,\alpha',\beta',\gamma'} = c_c^{(\ell_3)} \Big\{ (\mathbf{U})^c (\mathbf{U})^{\ell_3-2c} \Big\}^{(\ell_3)} \Big\{ (\mathbf{U})^{\ell_3-2c} (\mathbf{U})^c \Big\}^{(\ell_3)}. \tag{6.27}$$

The further identification of the terms in the sum is equivalent to partitioning the lefthand set of c $\mathbf{U}$'s from $\mathbf{E}^{(\ell_3)}$ into the sets of a and b $\mathbf{U}$'s respectively within the ℓ_1 and ℓ_2 sets of directions and a set of γ' $\mathbf{U}$'s between these sets of directions. At the same time, the lefthand $\ell_3 - 2c$ directions of $\mathbf{E}^{(\ell_3)}$ connected to the righthand set has to be partitioned into a β' set in ℓ_1 and an α' set in ℓ_2. Since all orders of the ℓ_3 directions on the lefthand side of $\mathbf{E}^{(\ell_3)}$ are equally allowed, the number of terms for each partioning is governed entirely by combinatorics. The calculation of this count is now carried out.

Counting the Partitioning of Pairs

The number of ways of selecting a pairs of directions from ℓ_1 directions can be found by first calculating the number of ways of selecting $2a$ directions and then calculating the number of ways these $2a$ directions can be paired. This is the product of a combinatorial factor for the selection process and the number of ways of ordering the $2a$ directions into unordered pairs, thus

$$M(\ell_1, a) = \binom{\ell_1}{2a} \times \frac{(2a)!}{a!2^a} = \frac{\ell_1!}{2^a a!(\ell_1 - 2a)!}. \tag{6.28}$$

In contrast, the number of ways of placing γ' pairs with one index in each of $\ell_1 - 2a$ and $\ell_2 - 2b$ directions is the product of the combinatorial factors for selecting γ' directions from each set, times the number of ways of pairing the γ' directions, namely

$$M(\ell_1 - 2a, \ell_2 - 2b, \gamma') = \binom{\ell_1 - 2a}{\gamma'} \binom{\ell_2 - 2b}{\gamma'} \gamma'!. \tag{6.29}$$

It follows that the fraction of ways of selecting a pairs from ℓ_1, b pairs from ℓ_2 and $\gamma' = c - a - b$ shared pairs from the number of pairs in $\ell_1 + \ell_2 = \ell_3$ is

$$\begin{aligned} N_{a,b}(\ell_1 \ell_2 | c) &= \frac{M(\ell_1, a) M(\ell_2, b) M(\ell_1 - 2a, \ell_2 - 2b, \gamma')}{M(\ell_1 + \ell_2, c)} \\ &= \frac{2^{c-a-b} \ell_1! \ell_2! c! (\ell_1 + \ell_2 - 2c)!}{a! b! \gamma'! (\ell_1 + \ell_2)! (\ell_1 - 2a - \gamma')! (\ell_2 - 2b - \gamma')!}. \end{aligned} \tag{6.30}$$

Necessarily c is the total number of pairs ($\mathbf{U}$'s) within and between the ℓ_1 and ℓ_2 sets of directions. As a fraction, the sum over a and b must be 1, specifically

$$\sum_{ab} N_{ab}(\ell_1 \ell_2 | c) = 1. \tag{6.31}$$

A direct proof of this is equivalent to the calculation given in Sec. 6.6.1.

It follows from Eq. (6.27) that $x_{a,b,c}$ for $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ with $\ell_1 + \ell_2 = \ell_3$ is given by

$$\begin{aligned} x_{a,b,c} &= c_c^{(\ell_3)} N_{a,b}(\ell_1, \ell_2 | c) \\ &= \frac{(-1)^c 2^{c-a-b} \ell_1! \ell_2! \ell_3! (2\ell_3 - 2c)!}{a! b! (2\ell_3)! (\ell_3 - c)! (c-a-b)! (\ell_1 + b - a - c)! (\ell_2 + a - b - c)!}. \end{aligned} \tag{6.32}$$

The general case for even L is now presented.

6.2.3 The general case for L even

The method of approach is to use the above expansion of $\mathbf{E}^{(\ell_3)}$ to arrive, first at a formula for $x_{a,b,0}$, and then at a general formula for $x_{a,b,c}$. For this purpose the expansion, Eq. (6.13), of the coupling tensor is written in the modified form

$$\begin{aligned} \mathbf{T}(\ell_1, \ell_2, \ell_3) &= \mathbf{T}(\ell_1, \ell_2, \ell_3) \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \\ &= \sum_{\lambda,\mu} x_{\lambda,\mu,0} \mathbf{T}^{\lambda,\mu,0,\alpha'',\beta'',\gamma''} \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \\ &= \sum_{\lambda,\mu} x_{\lambda,\mu,0} \mathbf{T}^{\lambda,\mu,0,\alpha'',\beta'',\gamma''}_{\alpha''\beta'' \ \text{ordered}} \odot^{\ell_3} \mathbf{T}(\beta'', \alpha'', \ell_3) \end{aligned} \tag{6.33}$$

where

$$\mathbf{T}^{a,b,0,\alpha'',\beta'',\gamma''}_{\alpha''\beta'' \ \text{ordered}} \equiv \left\{ (\vert)^{\beta''} (\mathbf{U})^a (\vert)^{\gamma''} \right\}^{(\ell_1)} \left\{ (\vert)^{\gamma''} (\mathbf{U})^b (\vert)^{\alpha''} \right\}^{(\ell_2)} (\vert)^{\alpha''} (\vert)^{\beta''}. \tag{6.34}$$

A relabelling of the expansion parameters is such that $\alpha'' = \alpha + \lambda - \mu$, $\beta'' = \beta + \mu - \lambda$ and $\gamma'' = \gamma - \lambda - \mu$, with α, β, γ retaining their original meanings as given in Eq. (6.3). By including an explicit $\mathbf{E}^{(\ell_3)}$ dotted into the last set of directions, it is recognized that any $c \neq 0$ component of the expansion vanishes. This is the first modification. Second, since the α'' and β'' directions are both dotted into the same symmetric traceless set of ℓ_3 directions on $\mathbf{E}^{(\ell_3)}$, the symmetrization of these directions in the expansion is unnecessary and they can be given a specific order. On recognizing this order, the expansion of Eq. (6.26) can be applied to each respective term in Eq. (6.33) with ℓ_1 and ℓ_2 chosen in Eq. (6.26) as the corresponding β'' and α'' in the term in the sum of Eq. (6.33), noting that $\alpha'' + \beta'' = \ell_3$. Thus Eq. (6.33) becomes

$$\begin{aligned} \mathbf{T}(\ell_1, \ell_2, \ell_3) = & \sum_{\lambda,\mu,p,q,c} x_{\lambda,\mu,0} c_c^{(\ell_3)} N_{p,q}(\beta'', \alpha'' | c) \\ & \times \mathbf{T}^{\lambda,\mu,0,\alpha'',\beta'',\gamma''}_{\alpha''\beta'' \ \text{ordered}} \odot^{\ell_3} \mathbf{T}^{p,q,c,\alpha''',\beta''',\gamma'''}, \end{aligned} \tag{6.35}$$

with parameters

$$\begin{aligned}\alpha''' &= \ell_3 - \beta'' + p - q - c \\ \beta''' &= \ell_3 - \alpha'' + q - p - c \\ \gamma''' &= c - p - q \end{aligned} \tag{6.36}$$

defined according to Eq. (6.26). The tensorial contraction in Eq. (6.35) can be carried out,

$$\mathbf{T}^{\lambda,\mu,0,\alpha'',\beta'',\gamma''}_{\alpha''\beta'' \ \text{ordered}} \odot^{\ell_3} \mathbf{T}^{p,q,c,\alpha''',\beta''',\gamma'''} = \mathbf{T}^{\lambda+p,\mu+q,c,\alpha''',\beta''',\gamma''+\gamma'''}. \tag{6.37}$$

On identifying the respective expansion parameters, it follows that the expansion coefficient for the general $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ is given by

$$x_{a,b,c} = c_c^{(\ell_3)} \sum_{\lambda,\mu} x_{\lambda,\mu,0} N_{a-\lambda,b-\mu}(\beta + \mu - \lambda, \alpha + \lambda - \mu | c). \tag{6.38}$$

It is still necessary to calculate $x_{a,b,0}$, but this can be accomplished as a special case of the above formula. Setting $b = 0$ it follows that

$$x_{a,0,c} = c_c^{(\ell_3)} \sum_{\lambda} x_{\lambda,0,0} N_{a-\lambda,0}(\beta - \lambda, \alpha + \lambda | c) \tag{6.39}$$

since, for $b = 0$, the summation index μ must also be 0. Interchanging the order of parameters and simultaneously interchanging c with b and ℓ_3 with ℓ_2, the formula for $x_{a,b,0}$ is then

$$\begin{aligned} x_{a,b,0} &= c_b^{(\ell_2)} \sum_{\lambda} x_{\lambda,0,0} N_{a-\lambda,0}(\gamma - \lambda, \alpha + \lambda | b) \\ &= \frac{(-1)^b 2^{b-a} \ell_1! \ell_2! \beta! \gamma! (2\ell_2 - 2b)!}{(2\ell_1)!(2\ell_2)!(\ell_2 - b)!(\alpha + a - b)!(\gamma - a - b)!} \\ &\quad \times \sum_{\lambda} \frac{(-1)^{\lambda} 2^{2\lambda} (2\ell_1 - 2\lambda)!(\alpha + \lambda)!}{\lambda!(\ell_1 - \lambda)!(a - \lambda)!(\beta - \lambda)!(b - a + \lambda)!}. \end{aligned} \tag{6.40}$$

Finally, putting this into the general expression for $x_{a,b,c}$ gives

$$\begin{aligned} x_{a,b,c} &= \frac{(-1)^c 2^{c-a-b} \ell_1! \ell_2! \ell_3! \beta! \gamma! (2\ell_3 - 2c)!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!(\ell_3 - c)!(\beta + b - a - c)!(\alpha + a - b - c)!} \\ &\quad \times \sum_{\lambda,\mu} \left[\frac{(-1)^{\mu} 2^{2\mu} (2\ell_2 - 2\mu)!(\beta - \lambda + \mu)!}{(a - \lambda)!(b - \mu)!(\ell_2 - \mu)!(\gamma - \lambda - \mu)!(c - a - b + \lambda + \mu)!} \right. \\ &\quad \left. \times \sum_{\nu} \frac{(-1)^{\nu} 2^{2\nu} (2\ell_1 - 2\nu)!(\alpha + \nu)!}{\nu!(\lambda - \nu)!(\ell_1 - \nu)!(\beta - \nu)!(\mu - \lambda + \nu)!} \right]. \end{aligned} \tag{6.41}$$

This completes the evaluation of the expansion coefficients for even L. The L odd case is presented next.

6.2.4 $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ for L odd

This treatment follows the same procedure as for the even case. The analogous expansion to Eq. (6.13) is the expansion

$$\mathbf{T}(\ell_1, \ell_2, \ell_3) = \sum_{a,b,c} x_{a,b,c} \mathbf{S}^{a,b,c,\alpha',\beta',\gamma'}, \tag{6.42}$$

where the tensor

$$\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'} \equiv$$
$$\left\{ (|)^{\beta'} (\mathbf{U})^a (|)^{\gamma'} | \right\}^{(\ell_1)} | \cdot \boldsymbol{\mathcal{E}} \cdot | \left\{ (|)^{\gamma'} (\mathbf{U})^b (|)^{\alpha'} \right\}^{(\ell_2)} \left\{ (|)^{\alpha'} (\mathbf{U})^c (|)^{\beta'} \right\}^{(\ell_3)} \tag{6.43}$$

has a, b and c $\mathbf{U}$'s associated with each respective symmetric set of ℓ_1, ℓ_2 and ℓ_3 directions and α', β' and γ' sets of connections between the ℓ_1, ℓ_2 and ℓ_3 sets of directions. These numbers are similar to those of the even case, in fact

$$\begin{aligned} \alpha' &= \alpha + a - b - c \\ \beta' &= \beta + b - c - a \\ \gamma' &= \gamma + c - a - b \end{aligned} \tag{6.44}$$

are exactly the same, but it must be remembered that now

$$\begin{aligned} \alpha &= \frac{1}{2}(L-1) - \ell_1 \\ \beta &= \frac{1}{2}(L-1) - \ell_2 \\ \gamma &= \frac{1}{2}(L-1) - \ell_3, \end{aligned} \tag{6.45}$$

for the odd L case, rather than Eq. (6.4) for even L. The expansion coefficients can again be determined from the required trace properties of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$.

The doubledot contraction of $\mathbf{U}$ with the lefthand symmetric traceless set of a typical expansion tensor $\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'}$, results in

$$\begin{aligned} \frac{\ell_1(\ell_1-1)}{2} \mathbf{U}{:}\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'} &= a(2a+3+2\beta'+2\gamma')\mathbf{S}^{a-1,b,c,\alpha',\beta',\gamma'} \\ &\quad + \beta'\gamma'\mathbf{S}^{a,b,c,\alpha'+1,\beta'-1,\gamma'-1} \\ + \frac{\beta'(\beta'-1)}{2}\mathbf{S}^{a,b,c+1,\alpha',\beta'-2,\gamma'} &+ \frac{\gamma'(\gamma'-1)}{2}\mathbf{S}^{a,b+1,c,\alpha',\beta',\gamma'-2}, \end{aligned} \tag{6.46}$$

with the contractions between either one of the β' or γ' directions and that connected to $\boldsymbol{\mathcal{E}}$ vanishing since it leads to a doubledot contraction of $\boldsymbol{\mathcal{E}}$ with either the ℓ_2 or ℓ_3 symmetric traceless sets. From the definitions of β', γ', β and γ, the factor in the first terms simplifies, namely $2a+3+2\beta'+2\gamma' = \ell_1 - 2a + 1$. Now using the above result for the contraction of $\mathbf{U}$ with a typical expansion tensor, $\mathbf{U}$ contracted into the first two directions of $\mathbf{S}(\ell_1, \ell_2, \ell_3)$ together with a relabelling of the terms to have a common form for the expansion tensors $\mathbf{S}^{a-1,b,c,\alpha',\beta',\gamma'}$ gives

$$\mathbf{0} = \frac{\ell_1(\ell_1-1)}{2}\mathbf{U}\mathbf{:}\mathbf{T}(\ell_1,\ell_2,\ell_3) = \sum_{a,b,c} \mathbf{S}^{a-1,b,c,\alpha',\beta',\gamma'} \Bigg[a(2\ell_1 - 2a + 1)x_{a,b,c} + (\beta'+1)(\gamma'+1)x_{a-1,b,c} + \frac{(\beta'+2)(\beta'+1)}{2}x_{a-1,b,c-1} + \frac{(\gamma'+2)(\gamma'+1)}{2}x_{a-1,b-1,c}\Bigg]. \tag{6.47}$$

On the basis that the $\mathbf{S}^{a-1,b,c,\alpha',\beta',\gamma'}$ are linearly independent, it follows that the $x_{a,b,c}$ expansion coefficients satisfy the recursion relation

$$a(2\ell_1 - 2a + 1)x_{a,b,c} + (\beta'+1)(\gamma'+1)x_{a-1,b,c} + \frac{(\beta'+2)(\beta'+1)}{2}x_{a-1,b,c-1} + \frac{(\gamma'+2)(\gamma'+1)}{2}x_{a-1,b-1,c} = 0. \tag{6.48}$$

This is exactly the same recursion relation as for the even L case, so $x_{a,b,c}$ is again given by Eq. (6.41).

Care must be exercised in applying this equality of expansion coefficients between even and odd L. Eq. (6.41) is written both in terms of α, β, γ and ℓ_1, ℓ_2, ℓ_3, yet these sets of parameters determine each other. Similarly, the recursion relations depend explicitly on both sets. Thus Eq. (6.41) is valid for both even and odd L according to the way it is written, but for even L, α, β and γ are determined from ℓ_1, ℓ_2 and ℓ_3 by Eq. (6.4), whereas for odd L, the relation is given by Eq. (6.45).

6.3 Detailed Calculation of $\Omega(\ell_1, \ell_2, \ell_3)$

The normalization constant $\Omega(\ell_1,\ell_2,\ell_3)$ of $\mathbf{T}(\ell_1,\ell_2,\ell_3)$ is defined by Eq. (6.11). Since each $\mathbf{T}(\ell_1,\ell_2,\ell_3)$ in this definition involves a set of $\mathbf{E}^{(\ell)}$ projectors for each ℓ and since these are dotted into each other, one set of projectors can be ignored. Thus, for L even, $\Omega(\ell_1,\ell_2,\ell_3)$ is given by

$$\Omega(\ell_1,\ell_2,\ell_3) = (\lfloor)^\beta(\mathbf{U})^\alpha(\mathbf{U})^\gamma(\rfloor)^\beta \odot^L \mathbf{T}(\ell_1,\ell_2,\ell_3) \tag{6.49}$$

while for L odd

$$\Omega(\ell_1,\ell_2,\ell_3) = -(\lfloor)^\beta(\lfloor)^\alpha\lfloor(\rfloor)^\alpha(\lfloor)^\gamma\rfloor\cdot\boldsymbol{\varepsilon}\,(\rfloor)^\gamma(\rfloor)^\beta \odot^L \mathbf{T}(\ell_1,\ell_2,\ell_3) \tag{6.50}$$

An obvious way of calculating these quantities is to substitute in the respective detailed expansions for $\mathbf{T}(\ell_1,\ell_2,\ell_3)$, Eqs. (6.13) and (6.42). But a simpler way is to use recursion relations, which are now described.

It is clear that if a single contraction between the ℓ_1 and ℓ_2 sets of directions is made in $\mathbf{T}(\ell_1,\ell_2,\ell_3)$, the result is proportional to $\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3)$, unless the contraction vanishes. This is because the contracted tensor is symmetric and traceless in sets of ℓ_1-1, ℓ_2-1 and ℓ_3 directions and such a tensor is unique up to a multiplicative constant. From the definition of the norm of the coupling tensors, it follows that the proportionality constant is determined by the ratio of the norms of the two tensors, namely

$$(\underbrace{\cup^{\ell_1-1}\mathbf{U}\cup)^{\ell_1-1}}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3)=\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\ell_1-1,\ell_2-1,\ell_3)}\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3). \tag{6.51}$$

It is this relation that is used in the following to deduce an equation for $\Omega(\ell_1,\ell_2,\ell_3)$. There are two steps to this procedure, one involves the computation of the ratio from the detailed knowledge, Eqs. (6.13) and (6.42), of the tensors, and the other is the iteration of this recursion relation to involve a tensor with as small an L as possible. The limitations of the iteration step are easiest to describe, so this is done first.

In application, the contraction can be applied to any pair of ℓ's. Here this is taken as ℓ_1 and ℓ_2, and successive application of this simple recursion relation stops when a subsequent contraction vanishes. This occurs when the ℓ values satisfy the conditions: $\ell_1+\ell_2=\ell_3$ for even L; and $\ell_1+\ell_2=\ell_3+1$ for odd L. In either case there are γ contractions from the original coupling tensor to get to this case. Thus repeated application of the recursion relation to the same pair of ℓ directions leads to

$$(\underbrace{\cup^{\ell_1-\gamma}(\mathbf{U})^{\gamma}\cup)^{\ell_1-\gamma}}\odot^{\ell_1+\gamma}\mathbf{T}(\ell_1,\ell_2,\ell_3)=\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\ell_1-\gamma,\ell_2-\gamma,\ell_3)}\mathbf{T}(\ell_1-\gamma,\ell_2-\gamma,\ell_3). \tag{6.52}$$

These coupling tensors with smallest L have relatively simple structures. In particular, for L even, $\ell_1+\ell_2-2\gamma=\ell_3$ and $\mathbf{T}(\ell_1-\gamma,\ell_2-\gamma,\ell_3)=\mathbf{E}^{(\ell_3)}$ is just the projector. As a consequence $\Omega(\ell_1-\gamma,\ell_2-\gamma,\ell_3)=2\ell_3+1$. For odd L, a further calculation must be done, mainly using the same recursion relation above, but applied to different ℓ's. Specifically, contractions are first made between the last two (righthand) sets of symmetric traceless directions until the middle ℓ value is 1. This requires α contractions. In detail this is

$$\begin{aligned}\mathbf{T}(\ell_1-\gamma,\ell_2-\gamma,\ell_3)\odot^{\ell_3+\alpha}&(\underbrace{\cup^{\ell_3-\alpha}(\mathbf{U})^{\alpha}\cup)^{\ell_3-\alpha}}\\ &=\frac{\Omega(\ell_1-\gamma,\ell_2-\gamma,\ell_3)}{\Omega(\beta+1,1,\beta+1)}\mathbf{T}(\beta+1,1,\beta+1).\end{aligned} \tag{6.53}$$

Last is a β-fold contraction between the first and last directions. This gives

$$(\underbrace{\cup^{\beta}\odot^{\beta}\mathbf{T}(\beta+1,1,\beta+1)\odot^{\beta}\cup)^{\beta}}=\frac{\Omega(\beta+1,1,\beta+1)}{\Omega(1,1,1)}\boldsymbol{\mathcal{E}}\,, \tag{6.54}$$

since $\mathbf{T}(1,1,1)=\boldsymbol{\mathcal{E}}$. Moreover, $\Omega(1,1,1)=-\boldsymbol{\mathcal{E}}\odot^3\boldsymbol{\mathcal{E}}=6$, so the general $\Omega(\ell_1,\ell_2,\ell_3)$ for odd L can also be found using the recursion relation, Eq. (6.51), but now applied to three different sets of directions. In order to carry this out, it is still necessary to evaluate the ratios of Ω's in Eq. (6.51), both for even and odd L and interpret the iterations of these ratios.

6.3.1 $\Omega(\ell_1,\ell_2,\ell_3)$ for L even

The ratio of Ω's in Eq. (6.51) is determined from the contraction of the related coupling tensor. This necessitates a detailed examination of how the terms in the tensor, namely Eqs. (6.13) and (6.42), behave under contraction. For even L the coupling tensor can be expanded in terms of $\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'}$, so the contraction of this, between a pair of directions belonging to the ℓ_1 and ℓ_2 symmetric traceless sets needs to be examined. There are three different types of directions (connected to different things) in each symmetric traceless set, so there are nine types of results arising from such a contraction, thus

$$\begin{aligned}
\underbrace{(\mathsf{U})^{\ell_1-1}\mathsf{U}(\mathsf{U})}^{\ell_1-1}\odot^{\ell_1+1}\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'} &= \beta'\gamma'\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'-1} \\
&+2b\beta'\mathbf{T}^{a,b-1,c,\alpha'+1,\beta'-1,\gamma'} + \beta'\alpha'\mathbf{T}^{a,b,c+1,\alpha'-1,\beta'-1,\gamma'} \\
&+2a\gamma'\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'-1} + 4ab\mathbf{T}^{a-1,b-1,c,\alpha',\beta',\gamma'+1} \\
&+2a\alpha'\mathbf{T}^{a-1,b,c,\alpha'-1,\beta'+1,\gamma'} + \gamma'(\gamma'+2)\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'-1} \\
&+2b\gamma'\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'-1} + \alpha'\gamma'\mathbf{T}^{a,b,c,\alpha',\beta',\gamma'-1}.
\end{aligned} \tag{6.55}$$

This could be put in for each term in the expansion, Eq. (6.13), but since each term in the resulting tensor must be related to the others by the symmetry and traceless properties of the tensor, it is sufficient to examine only one such term. It seems that the leading term is the simplest, so all terms that can contribute to $\mathbf{T}^{0,0,0,\alpha,\beta,\gamma-1}$ as the leading term in $\mathbf{T}(\ell_1-1, \ell_2-1, \ell_3)$ resulting from the contraction of $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ are examined. Since a, b and c change by at most 1 in the above contraction, it is sufficient to examine only those terms in which a, b, c are either 0 or 1. Note that α', β' and γ' are determined by Eqs. (6.15) and (6.16). Of the $\ell_1\ell_2$ ways of contracting between the first two sets of symmetric directions, the coefficients in Eq. (6.55) give the number of ways associated with a particular result of the contraction. Taking into account the different possibilities, the ratio of Ω's is given by

$$\begin{aligned}
&\frac{\Omega(\ell_1, \ell_2, \ell_3)}{\Omega(\ell_1-1, \ell_2-1, \ell_3)} \\
&= \frac{\gamma(\gamma+2+\alpha+\beta)x_{0,0,0} + 2(\alpha+1)x_{1,0,0} + 2(\beta+1)x_{0,1,0} + 4x_{1,1,0}}{\ell_1\ell_2}.
\end{aligned} \tag{6.56}$$

Equations for the $x_{a,b,0}$ are required for the further evaluation of this ratio. From Eq. (6.25) it follows that

$$\begin{aligned}
x_{0,0,0} &= 1 \\
x_{1,0,0} &= \frac{-\beta\gamma}{2\ell_1 - 1}
\end{aligned} \tag{6.57}$$

and by label permutation

$$x_{0,1,0} = \frac{-\alpha\gamma}{2\ell_2 - 1}. \tag{6.58}$$

From Eq. (6.40) it follows, after carrying out the summation, that

$$x_{1,1,0} = \frac{\gamma(\gamma-1)(2\alpha\beta + 2\beta + 1 - 2\ell_1)}{2(2\ell_1-1)(2\ell_2-1)}. \tag{6.59}$$

With some careful algebra involving conversions between the various parameters, the Ω ratio can be written in the relatively simple form

$$\frac{\Omega(\ell_1, \ell_2, \ell_3)}{\Omega(\ell_1-1, \ell_2-1, \ell_3)} = \frac{L(L+1)(2\gamma)(2\gamma-1)}{(2\ell_1)(2\ell_1-1)(2\ell_2)(2\ell_2-1)}. \tag{6.60}$$

Iteration of this gives

$$\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\beta,\alpha,\ell_3)} = \frac{(L+1)!}{(2\ell_3+1)!}\,\frac{(2\gamma)!(2\alpha)!(2\beta)!}{(2\ell_1)!(2\ell_2)!}. \tag{6.61}$$

Together with the fact that $\Omega(\beta,\alpha,\ell_3) = 2\ell_3+1$, this gives the formula in Eq. (6.12) for even L.

6.3.2 $\Omega(\ell_1,\ell_2,\ell_3)$ for L odd

It is first necessary to consider the result of performing a contraction between the ℓ_1 and ℓ_2 sets of directions on a typical expansion tensor $\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'}$. The result is slightly different from that for even L, Eq. (6.55), since contractions involved with $\boldsymbol{\varepsilon}$ are possible. In fact, these give a nonzero result only when dotted into a γ' index, which has the net effect of keeping the $\boldsymbol{\varepsilon}$ unchanged, but reducing the order of γ'. There are $2\gamma'$ ways of doing this. The net result is

$$\begin{aligned}
\underbrace{(\bigcup)^{\ell_1-1}\mathbf{U}(\bigcup)^{\ell_1-1}}\odot^{\ell_1+1}\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'} &= (\beta'+2)\gamma'\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'-1}\\
&+2b\beta'\mathbf{S}^{a,b-1,c,\alpha'+1,\beta'-1,\gamma'} + \beta'\alpha'\mathbf{S}^{a,b,c+1,\alpha'-1,\beta'-1,\gamma'}\\
&+2a\gamma'\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'-1} + 4ab\mathbf{S}^{a-1,b-1,c,\alpha',\beta',\gamma'+1}\\
&+2a\alpha'\mathbf{S}^{a-1,b,c,\alpha'-1,\beta'+1,\gamma'} + \gamma'(\gamma'+2)\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'-1}\\
&+2b\gamma'\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'-1} + \alpha'\gamma'\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'-1}.
\end{aligned} \tag{6.62}$$

It follows that the ratio of Ω's differs from the even case only in the coefficient of $x_{0,0,0}$, namely

$$\begin{aligned}
&\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\ell_1-1,\ell_2-1,\ell_3)}\\
&= \frac{\gamma(\gamma+4+\alpha+\beta)x_{0,0,0} + 2(\alpha+1)x_{1,0,0} + 2(\beta+1)x_{0,1,0} + 4x_{1,1,0}}{\ell_1\ell_2}.
\end{aligned} \tag{6.63}$$

Since the expansion coefficients $x_{a,b,c}$ are the same for odd and even L, but the relation between the $\ell_1,\ \ell_2,\ \ell_3$ and $\alpha,\ \beta,\ \gamma$ is different, the net result for the ratio of Ω's is

$$\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\ell_1-1,\ell_2-1,\ell_3)} = \frac{L(L+1)(2\gamma)(2\gamma+1)}{(2\ell_1)(2\ell_1-1)(2\ell_2)(2\ell_2-1)}. \tag{6.64}$$

Iteration of this gives

$$\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\ell_1-\gamma,\ell_2-\gamma,\ell_3)} = \frac{(L+1)!}{(L-2\gamma+1)!}\,\frac{(2\gamma+1)!(2\ell_1-2\gamma)!(2\ell_2-2\gamma)!}{(2\ell_1)!(2\ell_2)!}. \tag{6.65}$$

This has been written in a different form from its even L analog, Eq. (6.61), since, for example $\ell_1-\gamma = \beta+1$, and moreover, because further reduction is needed. As suggested earlier in this section, a further simplification can be made by repeating the procedure, but now applied to the $\ell_2-\gamma$ and ℓ_3 parameters. A relabelling of Eq. (6.65) leads to the ratio

$$\begin{aligned}
&\frac{\Omega(\ell_1-\gamma,\ell_2-\gamma,\ell_3)}{\Omega(\ell_1-\gamma,\ell_2-\gamma-\alpha,\ell_3-\alpha)}\\
&= \frac{(L-2\gamma+1)!}{(L-2\gamma-2\alpha+1)!}\,\frac{(2\alpha+1)!(2\ell_2-2\gamma-2\alpha)!(2\ell_3-2\alpha)!}{(2\ell_2-2\gamma)!(2\ell_3)!}.
\end{aligned} \tag{6.66}$$

A third application, but now to the $\ell_1-\gamma$ and $\ell_3-\beta$ parameters in the last formula gives

$$\frac{\Omega(\ell_1-\gamma,\ell_2-\gamma-\alpha,\ell_3-\alpha)}{\Omega(\ell_1-\gamma-\beta,\ell_2-\gamma-\alpha,\ell_3-\alpha-\beta)} = \frac{(L-2\gamma-2\alpha+1)!}{(L-2\gamma-2\alpha-2\beta+1)!}\,\frac{(2\beta+1)!(2\ell_1-2\gamma-2\beta)!(2\ell_3-2\alpha-2\beta)!}{(2\ell_1-2\gamma)!(2\ell_3-2\alpha)!}. \tag{6.67}$$

Inserting the values of $\alpha,\ \beta$ and γ in terms of $\ell_1,\ \ell_2$ and ℓ_3, the product of these three ratios is

$$\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(1,1,1)} = \frac{(L+1)!(L-2\ell_1)!(L-2\ell_2)!(L-2\ell_3)!}{3(2\ell_1)!(2\ell_2)!(2\ell_3)!}. \tag{6.68}$$

On the basis that $\Omega(1,1,1)=6$, this gives Eq. (6.12) for odd L.

6.4 Three Basic Contractions

This section studies certain transformations of a 3-j tensor that give again a 3-j tensor. These are based on contractions with the three tensors $\mathbf{U}$, $\boldsymbol{\varepsilon}$ and $\mathbf{E}^{(\ell_1+1)}$. Throughout this section $L=\ell_1+\ell_2+\ell_3$ is based on the weights $\ell_1,\ \ell_2$ and ℓ_3, while $\alpha,\ \beta$ and γ are defined for even L by Eq. (6.4) and by Eq. (6.45) for odd L.

Contraction with U

This has already been discussed in the previous section and used there for calculating $\Omega(\ell_1,\ell_2,\ell_3)$. Obviously a double dot contraction of $\mathbf{U}$ with a pair of directions associated with one of the symmetric traceless sets of directions vanishes, while a single dot contraction with any index has no effect. But contracting between different symmetric traceless sets must lead to a decrease in the weight of each. The result of this contraction, valid for both odd and even L is

$$(\,)^{\ell_1-1}\mathbf{U}(\,)^{\ell_1-1}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) = \frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\ell_1-1,\ell_2-1,\ell_3)}\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3)$$
$$= \frac{(L+1)L(\ell_1+\ell_2-\ell_3)(\ell_1+\ell_2-\ell_3-1)}{(2\ell_1)(2\ell_1-1)(2\ell_2)(2\ell_2-1)}\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3). \tag{6.69}$$

It is also obvious that this procedure could be repeated and/or applied to any pair of index sets, provided the appropriate changes in the coefficient are made.

Contraction with ε

Here the contraction will have one index of $\boldsymbol{\varepsilon}$ contracted to each of the symmetric traceless sets of directions in a 3-j tensor. This results in each weight of the 3-j tensor being reduced by 1, so the structural result of such a contraction is

$$(\,)^{\ell_1}\boldsymbol{\varepsilon}(\,)^{\ell_1}\odot^{\ell_1+2}\mathbf{T}(\ell_1+1,\ell_2+1,\ell_3+1)\odot = B\mathbf{T}(\ell_1,\ell_2,\ell_3). \tag{6.70}$$

It remains to evaluate the coefficient B. Note that in the following L and $\alpha,\ \beta$ and γ all relate to $\ell_1,\ \ell_2$ and ℓ_3. Note also the order of contraction with $\boldsymbol{\varepsilon}$ presented in the above formula.

For L even, the calculation is straightforward. Contract both sides of Eq. (6.70) with $\mathbf{T}(\ell_1, \ell_2, \ell_3)$. Then on recognizing that, on the lefthand side of the equation, this contraction together with the contraction with $\boldsymbol{\mathcal{E}}$ is also equivalent to a complete contraction of the 3-j tensor, both contractions give the appropriate Ω, so for even L

$$B = (-)\frac{\Omega(\ell_1+1, \ell_2+1, \ell_3+1)}{\Omega(\ell_1, \ell_2, \ell_3)}. \tag{6.71}$$

The calculation for odd L is a bit more complicated. Essentially there is an $\boldsymbol{\mathcal{E}}$ on each side of Eq. (6.70) so contracting with $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ would put two $\boldsymbol{\mathcal{E}}$'s on the lefthand side, which would have to be sorted out before reducing the contraction to a standard form. The approach presented here is an alternative. That is, to contract Eq. (6.70) with as many $\mathbf{U}$s as possible, using Eq. (6.69), and then to sort out the remainder. Such a contraction is

$$\begin{aligned}
&(\cup)^{\beta}(\mathbf{U})^{\alpha}(\mathbf{U})^{\gamma}(\cup)^{\beta}\odot^{L-3}(\cup)^{\ell_1}\boldsymbol{\mathcal{E}}(\cup)^{\ell_1}\odot^{\ell_1+2}\mathbf{T}(\ell_1+1,\ell_2+1,\ell_3+1)\odot \\
&= \frac{\Omega(\ell_1+1,\ell_2+1,\ell_3+1)}{\Omega(2,2,2)}\,\boldsymbol{\mathcal{E}}\odot^{3}\mathbf{T}(2,2,2)\odot \\
&= B(\cup)^{\beta}(\mathbf{U})^{\alpha}(\mathbf{U})^{\gamma}(\cup)^{\beta}\odot^{L-3}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&= B\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(1,1,1)}\mathbf{T}(1,1,1).
\end{aligned} \tag{6.72}$$

This reduces the computation to the special case of the contraction of $\boldsymbol{\mathcal{E}}$ with $\mathbf{T}(2,2,2)$.

From Eq. (6.13), $\mathbf{T}(2,2,2)$ can be expanded as

$$\begin{aligned}
\mathbf{T}(2,2,2) &= \left\{\left\{\cup\right\}^{(2)}\left\{\cup\right\}^{(2)}\left\{\cup\right\}\right\}^{(2)} + x_{1,1,1}\mathbf{UUU} \\
&+x_{1,0,0}\left[\mathbf{U}\left\{\left\{\cup\right\}^{(2)}\left\{\cup\right\}\right\}^{(2)} + \left\{\left\{\cup\right\}^{(2)}\mathbf{U}\left\{\cup\right\}\right\}^{(2)} + \left\{\left\{\cup\right\}^{(2)}\left\{\cup\right\}\right\}^{(2)}\mathbf{U}\right].
\end{aligned} \tag{6.73}$$

Use has been made of the equality, for $\ell_1 = \ell_2 = \ell_3 = 2$, that $x_{1,0,0} = x_{0,1,0} = x_{0,0,1}$ and the fact that $x_{1,1,0} = x_{1,0,1} = x_{0,1,1} = 0$. The appropriate contraction of this with $\boldsymbol{\mathcal{E}}$ gives

$$\boldsymbol{\mathcal{E}}\odot^{3}\mathbf{T}(2,2,2)\odot = -\frac{1}{4}\boldsymbol{\mathcal{E}} + \frac{3}{2}x_{1,0,0}\boldsymbol{\mathcal{E}} - x_{1,1,1}\boldsymbol{\mathcal{E}} = -\frac{35}{36}\boldsymbol{\mathcal{E}}. \tag{6.74}$$

Recognizing that $\mathbf{T}(1,1,1) = \boldsymbol{\mathcal{E}}$ means that the tensorial parts on both sides of Eq. (6.72) are equal. Then taking into account that $\Omega(1,1,1) = 6$ and $\Omega(2,2,2) = 35/12$, it follows that

$$B = (-)\frac{\Omega(\ell_1+1,\ell_2+1,\ell_3+1)}{\Omega(\ell_1,\ell_2,\ell_3)} \times \begin{cases} 1 & \text{L even} \\ 2 & \text{L odd} \end{cases} \tag{6.75}$$

combining the results of both even and odd L in the same formula.

Contraction with $\mathbf{E}^{(\ell_1+1)}$

Clearly, from the symmetry properties of the tensors, this contraction has the form

$$\mathbf{E}^{(\ell_1+1)}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) = C\mathbf{T}(\ell_1+1,\ell_2-1,\ell_3) \tag{6.76}$$

and it remains to evaluate the coefficient C. Different ways of calculating the coefficient C can be envisaged, one of which is the use of Eq. (3.60) applied to the $p = \ell_2$ set of directions. But likely the easiest way is to use the explicit expansions, Eqs. (6.13) and (6.42), of the 3-j tensors. The expansion tensors can be limited to those that do not vanish when fully contracted into $\mathbf{E}^{(\ell_1+1)}$ on the lefthand side and into $\mathbf{E}^{(\ell_3)}$ on the right, that is, with $a = c = 0$. Thus for even L it is sufficient for the present purpose to expand the starting tensor as

$$\mathbf{T}(\ell_1, \ell_2, \ell_3) = \sum_b x_{0,b,0} \mathbf{E}^{(\ell_1)} \odot^{\ell_1} \mathbf{T}^{0,b,0,\alpha',\beta',\gamma'} \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \tag{6.77}$$

Then the contraction becomes, for even L,

$$\begin{aligned}
&\mathbf{E}^{(\ell_1+1)} \odot^{\ell_1+1} \mathbf{T}^{0,b,0,\alpha',\beta',\gamma'} \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \\
&= \mathbf{E}^{(\ell_1+1)} \odot^{\ell_1+1} \Big\{ \underbrace{(\lfloor)^{\beta'} \big(\underbrace{\lfloor)^{\gamma'} \big\}^{(\ell_1)} \big\{ (\rfloor}\big)^{\gamma'} (\mathbf{U})^b \big(\underbrace{\lfloor)^{\alpha'} \big\}^{(\ell_2)} \big\{ (\rfloor}\big)^{\alpha'} (\rfloor)^{\beta'}} \Big\}^{(\ell_3)} \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \\
&= \frac{2b}{\ell_2} \mathbf{E}^{(\ell_1+1)} \odot^{\ell_1+1} \underbrace{(\lfloor)^{\beta'} \big(\underbrace{\lfloor)^{\gamma'+1} \big\{ (\rfloor}\big)^{\gamma'+1} (\mathbf{U})^{b-1} \big(\underbrace{\lfloor)^{\alpha'} \big\}^{(\ell_2-1)} (\rfloor}\big)^{\alpha'} (\rfloor)^{\beta'}} \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \\
&+ \frac{\alpha'}{\ell_2} \mathbf{E}^{(\ell_1+1)} \odot^{\ell_1+1} \underbrace{(\lfloor)^{\beta'+1} \big(\underbrace{\lfloor)^{\gamma'} \big\{ (\rfloor}\big)^{\gamma'} (\mathbf{U})^b \big(\underbrace{\lfloor)^{\alpha'-1} \big\}^{(\ell_2-1)} (\rfloor}\big)^{\alpha'-1} (\rfloor)^{\beta'+1}} \odot^{\ell_3} \mathbf{E}^{(\ell_3)}.
\end{aligned} \tag{6.78}$$

Since the resulting tensor will have the middle set of directions symmetric and traceless in $\ell_2 - 1$ directions, it is appropriate to contract the above equation with the projector for that as well, to give

$$\begin{aligned}
&\mathbf{E}^{\ell_1+1)} \odot^{\ell_1+1} \mathbf{T}^{0,b,0,\alpha',\beta',\gamma'} \odot^{\ell_3+\ell_2-1} \big(\underbrace{\lfloor)^{\ell_3} \mathbf{E}^{(\ell_2-1)} (\rfloor}\big)^{\ell_3} \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \\
&= \left[\frac{2}{\ell_2} \delta_{b1} + \frac{\alpha}{\ell_2} \delta_{b0} \right] \mathbf{T}(\ell_1 + 1, \ell_2 - 1, \ell_3).
\end{aligned} \tag{6.79}$$

A similar calculation for odd L gives the same result, namely

$$\begin{aligned}
&\mathbf{E}^{\ell_1+1)} \odot^{\ell_1+1} \mathbf{S}^{0,b,0,\alpha',\beta',\gamma'} \odot^{\ell_3+\ell_2-1} \big(\underbrace{\lfloor)^{\ell_3} \mathbf{E}^{(\ell_2-1)} (\rfloor}\big)^{\ell_3} \odot^{\ell_3} \mathbf{E}^{(\ell_3)} \\
&= \left[\frac{2}{\ell_2} \delta_{b1} + \frac{\alpha}{\ell_2} \delta_{b0} \right] \mathbf{T}(\ell_1 + 1, \ell_2 - 1, \ell_3).
\end{aligned} \tag{6.80}$$

In consequence, the coefficient C in Eq. (6.76) is

$$\begin{aligned}
C &= \frac{2}{\ell_2} x_{0,1,0} + \frac{\alpha}{\ell_2} x_{0,0,0} = \frac{\alpha(2\ell_2 - 2\gamma - 1)}{\ell_2(2\ell_2 - 1)} \\
&= \frac{(\ell_2 + \ell_3 - \ell_1)(\ell_2 + \ell_3 - \ell_1 - 1)}{2\ell_2(2\ell_2 - 1)}.
\end{aligned} \tag{6.81}$$

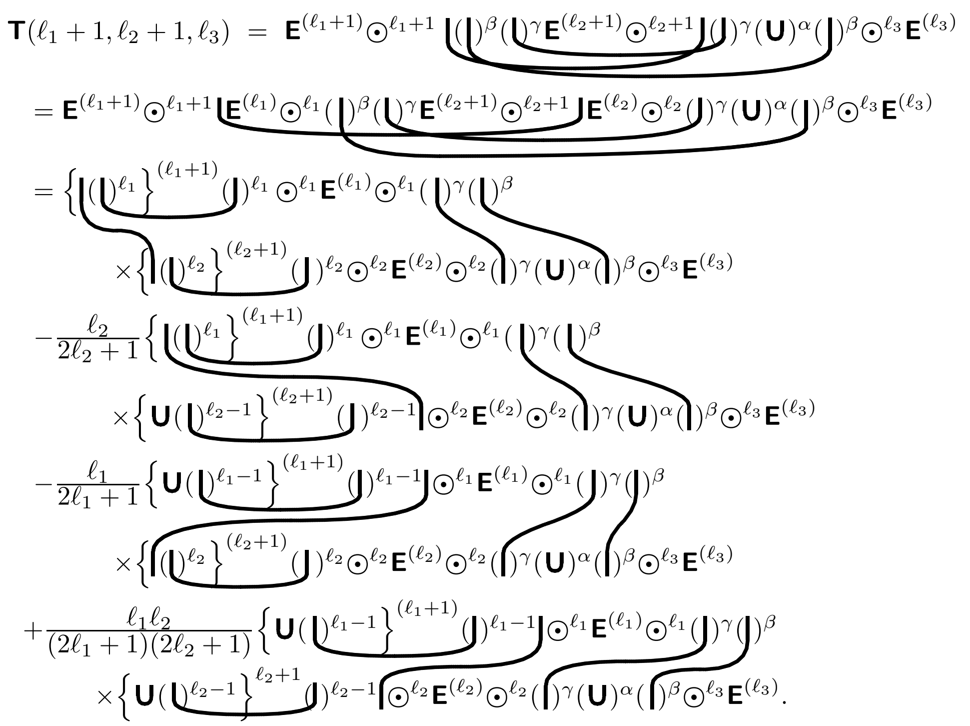
Again, this result is valid for both odd and even L.

6.5 Recursion Relations

The objective of a recursion relation is to express one 3-j tensor in terms of other 3-j tensors, the most useful of such being those relations which express one 3-j tensor in terms of those with smaller total order L. Four such recursion relations are presented. None of the recursion relations listed here involve cross products, equivalently use $\boldsymbol{\varepsilon}$. Such relations appear to be more easily evaluated using n-j symbols to calculate the scalar expansion coefficients that arise in such relations, see Chap. 8.

1.

The first recursion relation gives the relation of 3-j tensors on simultaneously raising two of the weights by 1. It is obtained by using Eq. (3.60), actually its transpose, on both of the related sets of symmetric traceless sets of directions to select out a direction for special consideration. It is convenient to start with weights $\ell_1 + 1,\ \ell_2 + 1$ and ℓ_3 while $\alpha,\ \beta$ and γ are associated with $\ell_1,\ \ell_2$ and ℓ_3. Thus, for even L,



(6.82)

Finally, the various combinations of projectors can be written in terms of $\mathbf{T}$ tensors, so that

$$
\begin{aligned}
&\mathbf{T}(\ell_1+1,\ell_2+1,\ell_3) \\
&= \Big\{(\big\lfloor)^{\ell_1}\big\lfloor\Big\}^{(\ell_1+1)}\Big\{\big\rfloor(\big\lfloor)^{\ell_2}\Big\}^{(\ell_2+1)}(\big\rfloor)^{\ell_2}(\big\rfloor)^{\ell_1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&-\frac{\ell_2}{2\ell_2+1}\Big\{(\big\lfloor)^{\ell_1+1}\Big\}^{(\ell_1+1)}\Big\{\mathbf{U}(\big\lfloor)^{\ell_2-1}\Big\}^{(\ell_2+1)}(\big\rfloor)^{\ell_2-1}(\big\rfloor)^{\ell_1+1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&-\frac{\ell_1}{2\ell_1+1}\Big\{\mathbf{U}(\big\lfloor)^{\ell_1-1}\Big\}^{(\ell_1+1)}\Big\{(\big\lfloor)^{\ell_2+1}\Big\}^{(\ell_2+1)}(\big\rfloor)^{\ell_2+1}(\big\rfloor)^{\ell_1-1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&+\frac{L(L+1)(L-2\ell_3)(L-2\ell_3-1)}{4(2\ell_1+1)(2\ell_1-1)(2\ell_2+1)(2\ell_2-1)}\Big\{\mathbf{U}(\big\rfloor)^{\ell_1-1}\Big\}^{(\ell_1+1)}\Big\{\mathbf{U}(\big\rfloor)^{\ell_2-1}\Big\}^{(\ell_2+1)} \\
&\qquad\qquad\times(\big\lceil)^{\ell_2-1}(\big\lceil)^{\ell_1-1}\odot^{\ell_1+\ell_2-1}\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3).
\end{aligned}
\tag{6.83}
$$

The last term has been simplified with the help of the contraction, Eq. (6.69). Finally it needs to be noted that the final result is the same for odd L since all calculations depend only on selecting a direction from $\mathbf{E}$, Eq. (3.60), and the contractions resulting from those reorganizations.

2.

This recursion relation relates 3-j tensors in which one weight is increased by 1 and another decreased by 1. It arises by a contraction with $\mathbf{E}^{(\ell_1+1)}$ and the result of selecting an direction, Eq. (3.60), from that set. Eq. (6.76) gives one method of calculating the contraction, while the selection process gives an alternate method. Starting with the selection process,

$$
\begin{aligned}
&\mathbf{E}^{(\ell_1+1)}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&= \mathbf{E}^{(\ell_1+1)}\odot^{\ell_1+1}\big\lfloor\mathbf{E}^{(\ell_1)}\odot^{\ell_1}(\big\lfloor)^{\ell_1}\big\rfloor(\big\rfloor)^{\ell_1}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&= \Big\{\big\lfloor(\big\lfloor)^{\ell_1}\Big\}^{(\ell_1+1)}(\big\rfloor)^{\ell_1}\odot^{\ell_1}\mathbf{E}^{(\ell_1)}\odot^{\ell_1}(\big\lfloor)^{\ell_1}\big\rfloor(\big\rfloor)^{\ell_1}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&-\frac{\ell_1}{2\ell_1+1}\Big\{\mathbf{U}(\big\lfloor)^{\ell_1-1}\Big\}^{(\ell_1+1)}(\big\rfloor)^{\ell_1-1}\big\lfloor\odot^{\ell_1}\mathbf{E}^{(\ell_1)}\odot^{\ell_1}(\big\lfloor)^{\ell_1}\big\rfloor(\big\rfloor)^{\ell_1}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&= \Big\{(\big\lfloor)^{\ell_1+1}\Big\}^{(\ell_1+1)}(\big\rfloor)^{\ell_1+1}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&-\frac{L(L+1)(L-2\ell_3)(L-2\ell_3-1)}{4\ell_2(2\ell_1+1)(2\ell_1-1)(2\ell_2-1)} \\
&\qquad\qquad\times\Big\{\mathbf{U}(\big\lfloor)^{\ell_1-1}\Big\}^{(\ell_1+1)}(\big\rfloor)^{\ell_1-1}\odot^{\ell_1-1}\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3).
\end{aligned}
\tag{6.84}
$$

Since the original contraction is proportional to $\mathbf{T}(\ell_1+1,\ell_2-1,\ell_3)$ with coefficient given by Eq. (6.76), it follows that this recursion relation can be expressed as

$$
\begin{aligned}
&\mathbf{T}(\ell_1+1,\ell_2-1,\ell_3) = \\
&= \frac{2\ell_2(2\ell_2-1)}{(L-2\ell_1)(L-2\ell_1-1)}\Big\{(\bigcup^{\ell_1+1}\Big\}^{(\ell_1+1)}(\bigcup)^{\ell_1+1}\odot^{\ell_1+1}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&-\frac{L(L+1)(L-2\ell_3)(L-2\ell_3-1)}{2(2\ell_1+1)(2\ell_1-1)(L-2\ell_1)(L-2\ell_1-1)} \\
&\qquad\times\Big\{\mathbf{U}(\bigcup^{\ell_1-1}\Big\}^{(\ell_1+1)}(\bigcup)^{\ell_1-1}\odot^{\ell_1-1}\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3).
\end{aligned}
\tag{6.85}
$$

3.

The second and third terms of the first recursion relation, Eq. (6.82), mix the directions associated with the ℓ_1 or ℓ_2 sets of directions in $\mathbf{T}(\ell_1,\ell_2,\ell_3)$, when forming either the ℓ_1+1 or ℓ_2+1 symmetric traceless sets. Such cross coupling of sets of directions can be removed by using the second recursion relation. The result is

$$
\begin{aligned}
&\mathbf{T}(\ell_1+1,\ell_2+1,\ell_3) \\
&= \Big\{(\bigcup)^{\ell_1}\bigcup\Big\}^{(\ell_1+1)}\bigcup(\bigcup^{\ell_2}\Big\}^{(\ell_2+1)}(\bigcup)^{\ell_2}(\bigcup)^{\ell_1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1,\ell_2,\ell_3) \\
&-\frac{(L-2\ell_1)(L-2\ell_1-1)}{2(2\ell_2-1)(2\ell_2+1)} \\
&\qquad\times(\bigcup)^{\ell_1+1}\Big\{\mathbf{U}(\bigcup^{\ell_2-1}\Big\}^{(\ell_2+1)}(\bigcup)^{\ell_2-1}(\bigcup)^{\ell_1+1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1+1,\ell_2-1,\ell_3) \\
&-\frac{(L-2\ell_2)(L-2\ell_2-1)}{2(2\ell_1-1)(2\ell_1+1)}\Big\{\mathbf{U}(\bigcup^{\ell_1-1}\Big\}^{(\ell_1+1)}(\bigcup)^{\ell_1-1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1-1,\ell_2+1,\ell_3) \\
&-\frac{L(L+1)(L-2\ell_3)(L-2\ell_3-1)}{4(2\ell_1+1)(2\ell_1-1)(2\ell_2+1)(2\ell_2-1)}\Big\{\mathbf{U}(\bigcup)^{\ell_1-1}\Big\}^{(\ell_1+1)}\Big\{\mathbf{U}(\bigcup)^{\ell_2-1}\Big\}^{(\ell_2+1)} \\
&\qquad\times(\bigcup)^{\ell_1-1}(\bigcup)^{\ell_2-1}\odot^{\ell_1+\ell_2-1}\mathbf{T}(\ell_1-1,\ell_2-1,\ell_3).
\end{aligned}
\tag{6.86}
$$

This separation of the role of different sets of directions is useful when evaluating 3-j invariant functions, see Sec. 7.5.

4.

A different kind of recursion relation is obtained by selecting one direction for special consideration. In the following that is the first direction of the first symmetric traceless set, essentially based on using Eq. (3.60) as it is written, rather than as the transpose as used in Eq. (6.82). For even L the explicit calculation is,

$$
\begin{aligned}
&\mathbf{T}(\ell_1+1,\ell_2+1,\ell_3)\\
&\quad= \mathbf{E}^{(\ell_1+1)}\odot^{\ell_1+1}(\lfloor)^{\beta}(\lfloor)^{\gamma+1}\mathbf{E}^{(\ell_2+1)}\odot^{\ell_2+1}(\rfloor)^{\gamma+1}(\mathbf{U})^{\alpha}(\rfloor)^{\beta}\odot^{\ell_3}\mathbf{E}^{(\ell_3)}\\
&\quad= \Big\lfloor \mathbf{E}^{(\ell_1)}\odot^{\ell_1}(\lfloor)^{\ell_1}\big\{(\rfloor)^{\ell_1}\Big\rfloor\Big\}^{(\ell_1+1)}\\
&\qquad\qquad \odot^{\ell_1+1}(\lfloor)^{\beta}(\lfloor)^{\gamma+1}\mathbf{E}^{(\ell_2+1)}\odot^{\ell_2+1}(\rfloor)^{\gamma+1}(\mathbf{U})^{\alpha}(\rfloor)^{\beta}\odot^{\ell_3}\mathbf{E}^{(\ell_3)}\\
&\qquad -\frac{\ell_1}{2\ell_1+1}\lfloor\mathbf{E}^{(\ell_1)}\odot^{\ell_1}\rfloor(\lfloor)^{\ell_1-1}\{(\rfloor)^{\ell_1-1}\mathbf{U}\Big\}^{(\ell_1+1)}\\
&\qquad\qquad \odot^{\ell_1+1}(\lfloor)^{\beta}(\lfloor)^{\gamma+1}\mathbf{E}^{(\ell_2+1)}\odot^{\ell_2+1}(\rfloor)^{\gamma+1}(\mathbf{U})^{\alpha}(\rfloor)^{\beta}\odot^{\ell_3}\mathbf{E}^{(\ell_3)}\\
&\quad= \frac{\beta}{\ell_1+1}\lfloor\mathbf{T}(\ell_1,\ell_2+1,\ell_3-1)\rfloor\odot^{\ell_3}\mathbf{E}^{(\ell_3)}\\
&\qquad +\frac{\gamma+1}{\ell_1+1}\lfloor(\lfloor)^{\ell_1}\mathbf{E}^{(\ell_2+1)}\odot^{\ell_2+1}\rfloor\Big[(\rfloor)^{\ell_1}\odot^{\ell_1}\mathbf{T}(\ell_1,\ell_2,\ell_3)\Big]\\
&\qquad -\frac{2\beta(\gamma+1)}{(2\ell_1+1)(\ell_1+1)}\lfloor\mathbf{E}^{(\ell_1)}\odot^{\ell_1}\rfloor\mathbf{T}(\ell_1-1,\ell_2+1,\ell_3).
\end{aligned}
\tag{6.87}
$$

The analogous calculation with odd L gives the same result, with the same expansion coefficients, provided the numerators are expressed in terms of β and γ. There is a certain symmetry of this formula in that the first direction is distributed to each symmetric traceless set in the $\mathbf{T}$ tensor. The extra $\mathbf{E}^{(\ell)}$'s can be eliminated by a further use of Eq. (3.60) to each term. The result is

$$
\begin{aligned}
&\mathbf{T}(\ell_1+1,\ell_2+1,\ell_3)\\
&\quad= \frac{\beta}{\ell_1+1}\Big\lfloor\mathbf{T}(\ell_1,\ell_2+1,\ell_3-1)\odot^{\ell_3-1}(\lfloor)^{\ell_3-1}\big\{(\rfloor)^{\ell_3-1}\Big\rfloor\Big\}^{(\ell_3)}\\
&\qquad -\frac{\beta(\ell_3-1)}{(\ell_1+1)(2\ell_3-1)}\lfloor\mathbf{T}(\ell_1,\ell_2+1,\ell_3-1)\odot^{\ell_3-1}\rfloor(\lfloor)^{\ell_3-2}\big\{(\rfloor)^{\ell_3-2}\mathbf{U}\Big\}^{(\ell_3)}\\
&\qquad +\frac{\gamma+1}{\ell_1+1}\lfloor(\lfloor)^{\ell_1}\rfloor(\lfloor)^{\ell_2}\Big\}^{\ell_2+1}(\rfloor)^{\ell_2}(\rfloor)^{\ell_1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1,\ell_2,\ell_3)\\
&\qquad -\frac{(\gamma+1)\ell_2}{(\ell_1+1)(2\ell_2+1)}\lfloor(\lfloor)^{\ell_1}\Big\{\mathbf{U}(\lfloor)^{\ell_2-1}\Big\}^{\ell_2+1)}(\rfloor)^{\ell_2-1}\rfloor(\rfloor)^{\ell_1}\odot^{\ell_1+\ell_2}\mathbf{T}(\ell_1,\ell_2,\ell_3)\\
&\qquad -\frac{2\beta(\gamma+1)}{(2\ell_1+1)(\ell_1+1)}\lfloor\Big\{\rfloor(\lfloor)^{\ell_1-1}\Big\}^{\ell_1)}(\rfloor)^{\ell_1-1}\odot^{\ell_1-1}\mathbf{T}(\ell_1-1,\ell_2+1,\ell_3).\\
&\qquad +\frac{2\beta(\gamma+1)(\ell_1-1)}{(2\ell_1+1)(\ell_1+1)(2\ell_1-1)}\Big\lfloor\Big\{\mathbf{U}(\lfloor)^{\ell_1-2}\Big\}^{\ell_1)}(\rfloor)^{\ell_1-2}\Big\rfloor\\
&\qquad\qquad\qquad \odot^{\ell_1-1}\mathbf{T}(\ell_1-1,\ell_2+1,\ell_3).
\end{aligned}
\tag{6.88}
$$

6.6 Calculation of $\sum_{abc} x_{a,b,c}$

For even L the sum of $x_{a,b,c}$ over all values of a, b and c arises in the calculation of the integral of the product of three $\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{r})$'s and is proportional to a particular 3-j symbol. For odd L, the same sum is proportional to another 3-j symbol. This section is devoted to calculating the sum over $x_{a,b,c}$ for both odd and even L, there being no difference in the procedure as long as all six variables ℓ_1, ℓ_2, ℓ_3, α, β, γ are treated as independent. It is only at the end of the calculation that the relations (6.4) and (6.45) between ℓ_1, ℓ_2, ℓ_3 and α, β, γ are used to simplify the general expression for the sum for even or odd L. The method used here for the summation is based on recognizing that for the six-fold sum arising from summing Eq. (6.41), doing the sum over a and b first allows a separation of the sum over c from the remaining three sums over λ, μ and ν. The latter are then summed essentially in the sequence: μ, ν, λ, but with the help of some change of variables.

The sum is first rewritten in order to isolate the sums over a and b, thus

$$\begin{aligned}\sum_{abc} x_{a,b,c} &= \frac{\ell_1!\ell_2!\ell_3!\beta!\gamma!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!}\sum_c \frac{(-1)^c 2^c (2\ell_3-2c)!}{(\ell_3-c)!} \\ &\times \sum_{\lambda\mu} \frac{(-1)^\mu 2^{\mu-\lambda}(2\ell_2-2\mu)!(\beta-\lambda+\mu)!}{(\ell_2-\mu)!(\gamma-\lambda-\mu)!} \\ &\times \sum_\nu \frac{(-1)^\nu 2^{2\nu}(2\ell_1-2\nu)!(\alpha+\nu)!}{\nu!(\lambda-\nu)!(\ell_1-\nu)!(\beta-\nu)!(\mu-\lambda+\nu)!} \\ \times \sum_{ab} & \frac{2^{\mu+\lambda-a-b}}{(a-\lambda)!(b-\mu)!(c-a-b+\lambda+\mu)!(\beta+b-a-c)!(\alpha+a-b-c)!}. \end{aligned} \tag{6.89}$$

The first subsection calculates the above sum over a and b.

6.6.1 Sum over a and b

Displacing the summation variables according to $a \to a+\lambda$ and $b \to b+\mu$, with the temporary notation $x \equiv \beta+\mu-\lambda-c$ and $y \equiv \alpha+\lambda-\mu-c$, the above sum over a and b can be expressed as

$$\begin{aligned} A &\equiv \sum_{ab} \frac{2^{-a-b}}{a!b!(c-a-b)!(x-a+b)!(y+a-b)!} \\ &= \frac{1}{c!(x+y)!}\sum_{ab} 2^{-a-b}\binom{a+b}{a}\binom{c}{a+b}\binom{x+y}{x-a+b}. \end{aligned} \tag{6.90}$$

Now the following identities are valid:

$$\begin{aligned} (1+u)^{x+y+2c} &= (1+u)^{2c}(1+u)^{x+y} = (1+2u+u^2)^c(1+u)^{x+y} \\ &= \sum_p \binom{c}{p}(1+u^2)^p(2u)^{c-p}\sum_q \binom{x+y}{q}u^q \\ = \sum_r \binom{x+y+2c}{r}u^r &= \sum_{paq}\binom{c}{p}\binom{p}{a}u^{2a}(2u)^{c-p}\binom{x+y}{q}u^q. \end{aligned} \tag{6.91}$$

On equating the rth power of u, the double sum over p and a has the value

$$\binom{x+y+2c}{r} = \sum_{pa} \binom{c}{p}\binom{p}{a}(2)^{c-p}\binom{x+y}{r-2a-c+p}. \tag{6.92}$$

Replacing r by $x+c$ and p by $a+b$, implies that A is given by

$$\begin{aligned} A &= \frac{2^{-c}}{c!(x+y)!}\binom{x+y+2c}{x+c} \\ &= \frac{(\alpha+\beta)!}{2^c c!(\alpha+\beta-2c)!(\beta+\mu-\lambda)!(\alpha+\lambda-\mu)!}, \end{aligned} \tag{6.93}$$

having substituted back the values of the temporary parameters x and y. As a consequence, the x_{abc} sum reduces to

$$\begin{aligned} \sum_{abc} x_{a,b,c} &= \frac{\ell_1!\ell_2!\ell_3!\beta!\gamma!(\alpha+\beta)!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!} \sum_c \frac{(-1)^c(2\ell_3-2c)!}{c!(\ell_3-c)!(\alpha+\beta-2c)!} \\ &\times \sum_{\lambda\mu} \frac{(-1)^\mu 2^{\mu-\lambda}(2\ell_2-2\mu)!}{(\ell_2-\mu)!(\gamma-\lambda-\mu)!(\alpha+\lambda-\mu)!} \\ &\times \sum_\nu \frac{(-1)^\nu 2^{2\nu}(2\ell_1-2\nu)!(\alpha+\nu)!}{\nu!(\lambda-\nu)!(\ell_1-\nu)!(\beta-\nu)!(\mu-\lambda+\nu)!}. \end{aligned} \tag{6.94}$$

It is now seen that the sum over c is completely independent of the other sums, so it can be calculated immediately.

For even L this computation of A is equivalent to proving that the sum over a and b of $N_{ab}(\ell_1\ell_2|c)$, Eq. (6.31), is 1, specifically by setting $x=\ell_1-c$ and $y=\ell_2-c$ in Eq. (6.90).

6.6.2 Sum over c

The sum over c can be rewritten in the form

$$\begin{aligned} \sum_c \frac{(-1)^c(2\ell_3-2c)!}{c!(\ell_3-c)!(\alpha+\beta-2c)!} &= \frac{(2\ell_3-\alpha-\beta)!}{\ell_3!}\sum_c (-1)^c\binom{\ell_3}{c}\binom{2\ell_3-2c}{2\ell_3-\alpha-\beta} \\ &= \frac{(2\ell_3-\alpha-\beta)!}{\ell_3!}\binom{\ell_3}{\ell_3-\alpha-\beta}2^{\alpha+\beta} \\ &= \frac{(2\ell_3-\alpha-\beta)!2^{\alpha+\beta}}{(\ell_3-\alpha-\beta)!(\alpha+\beta)!}. \end{aligned} \tag{6.95}$$

Here the summation follows from Eq. (5.54).

As a result of the a, b and c sums, the $x_{a,b,c}$ sum can be simplified to

$$\sum_{abc} x_{a,b,c} = \frac{\ell_3!(2\ell_3-\alpha-\beta)!2^{\alpha+\beta}}{(2\ell_3)!(\ell_3-\alpha-\beta)!}\sum_{ab} x_{a,b,0}. \tag{6.96}$$

In this, the general term in the remaining triple sum in Eq. (6.94) has been recognized as $x_{a,b,0}$, Eq. (6.40), if λ and μ are replaced by a and b.

6.6.3 Calculation of $\sum_{ab} x_{a,b,0}$

The sum over $x_{a,b,0}$ can be written

$$\begin{aligned}\sum_{ab} x_{a,b,0} &= \sum_{ab} \frac{(-1)^b 2^{b-a} \ell_1! \ell_2! \beta! \gamma! (2\ell_2 - 2b)!}{(2\ell_1)!(2\ell_2)!(\ell_2 - b)!(\alpha + a - b)!(\gamma - a - b)!} \\ &\quad \times \sum_{\lambda} \frac{(-1)^\lambda 2^{2\lambda}(2\ell_1 - 2\lambda)!(\alpha + \lambda)!}{\lambda!(\ell_1 - \lambda)!(a - \lambda)!(\beta - \lambda)!(b - a + \lambda)!} \\ &= \frac{\ell_1! \ell_2! \beta! \gamma!}{(2\ell_1)!(2\ell_2)!} \sum_{c\lambda} \frac{(-1)^\lambda 2^{2\lambda + c}(2\ell_1 - 2\lambda)!(\alpha + \lambda)!(2\ell_2 - \gamma - c)!}{\lambda!(\ell_1 - \lambda)!(\beta - \lambda)!(c + \lambda)!(\alpha - c)!(\ell_2 - \lambda - c)!} \\ &\quad \times \sum_b (-1)^b \binom{2\ell_2 - 2b}{\gamma + c - 2b} \binom{\ell_2 - \lambda - c}{\ell_2 - b}, \end{aligned} \tag{6.97}$$

where, in the last form, the sum over a has been replaced by a sum over $c \equiv b - a$ and a reorganization of the terms has been carried out. Now the sum over b can be explicitly carried out. Specifically, if b is replaced by $t \equiv b - c - \lambda$, then this sum is

$$\begin{aligned}&\sum_b (-1)^b \binom{2\ell_2 - 2b}{\gamma + c - 2b} \binom{\ell_2 - \lambda - c}{\ell_2 - b} \\ &= (-1)^{\lambda + c} \sum_t (-1)^t \binom{M}{t} \binom{2M - 2t}{M + \ell_2 + \lambda - \gamma} \\ &= (-1)^{\lambda + c} \binom{M}{\ell_2 + \lambda - \gamma} 2^{M - \ell_2 - \lambda + \gamma} = (-1)^{\lambda + c} \binom{\ell_2 - \lambda - c}{\ell_2 + \lambda - \gamma} 2^{-2\lambda - c + \gamma}. \end{aligned} \tag{6.98}$$

Here $M = \ell_2 - \lambda - c$ has been used as a temporary label so as to more easily identify the sum as a special case of Eq. (5.54). As a consequence, the sum over $x_{a,b,0}$ has been reduced to a double sum, which can be written in the form

$$\begin{aligned}\sum_{ab} x_{a,b,0} &= \frac{2^\gamma \ell_1! \ell_2! \beta! \gamma!}{(2\ell_1)!(2\ell_2)!} \sum_\lambda \frac{(2\ell_1 - 2\lambda)!(2\ell_2 + 2\lambda - 2\gamma)!}{\lambda!(\ell_1 - \lambda)!(\beta - \lambda)!(\ell_2 + \lambda - \gamma)!} \\ &\quad \times \sum_c (-1)^c \binom{\alpha + \lambda}{\alpha - c} \binom{2\ell_2 - \gamma - c}{2\ell_2 + 2\lambda - 2\gamma}. \end{aligned} \tag{6.99}$$

Now the sum over c can be carried out. Replace c by $u \equiv \lambda + c$, so that the sum over c becomes

$$\begin{aligned}&\sum_c (-1)^c \binom{\alpha + \lambda}{\alpha - c} \binom{2\ell_2 - \gamma - c}{2\ell_2 + 2\lambda - 2\gamma} \\ &= \sum_u (-1)^{\lambda + u} \binom{\alpha + \lambda}{u} \binom{2\ell_2 + \lambda - \gamma - u}{\gamma - \lambda - u} \\ &= (-1)^\lambda \binom{2\ell_2 - \alpha - \gamma}{\gamma - \lambda}. \end{aligned} \tag{6.100}$$

This sum is a special case of Eq. (A1.2) of Ref. [1], or better the equation before (A1.2). Thus the sum over $x_{a,b,0}$ has been reduced to the single sum

$$\sum_{ab} x_{a,b,0} = \frac{2^\gamma \ell_1!\ell_2!\beta!\gamma!(2\ell_2-\alpha-\gamma)!}{(2\ell_1)!(2\ell_2)!} S \tag{6.101}$$

where

$$S \equiv \sum_\lambda \frac{(-1^\lambda(2\ell_1-2\lambda)!(2\ell_2+2\lambda-2\gamma)!}{\lambda!(\ell_1-\lambda)!(\beta-\lambda)!(\gamma-\lambda)!(\ell_2+\lambda-\gamma)!(2\ell_2-\alpha-2\gamma+\lambda)!} \tag{6.102}$$

The λ sum in S requires a number of rearrangements before it can be recognized in terms of standard functions, specifically the generalized hypergeometric function ${}_3F_2$, Ref. [24]. These rearrangements and the subsequent calculation of the sum are carried out with the help of equations in that reference, which are denoted by, for example, Eq. HTF(1.2.15).

It is first necessary to reduce the factorials involving 2λ using Eq. HTF(1.2.15). This also means that the factorials need to be written in terms of Gamma functions, thus

$$\begin{aligned} S &= 4\sum_\lambda \frac{(-1)^\lambda\Gamma(2\ell_1-2\lambda)\Gamma(2\ell_2-2\gamma+2\lambda)}{\lambda!\Gamma(\ell_1-\lambda)\Gamma(\beta+1-\lambda)\Gamma(\gamma+1-\lambda)\Gamma(\ell_2-\gamma+\lambda)\Gamma(2\ell_2-\alpha-2\gamma+1+\lambda)} \\ &= \frac{2^{2\ell_1+2\ell_2-2\gamma}}{\pi}\sum_\lambda \frac{(-1)^\lambda\Gamma(\ell_1-\lambda+\frac{1}{2})\Gamma(\ell_2-\gamma+\lambda+\frac{1}{2})}{\lambda!\Gamma(\beta+1-\lambda)\Gamma(\gamma+1-\lambda)\Gamma(2\ell_2-\alpha-2\gamma+1+\lambda)}. \end{aligned} \tag{6.103}$$

This sum has contributions only for λ between 0 and the minimum of $\gamma+1$ and $\beta+1$. In order to identify with a hypergeometric function, and/or related functions, the factors depending on the summation index, λ, must appear in the form of

$$(A)_\lambda \equiv \frac{\Gamma(A+\lambda)}{\Gamma(A)}. \tag{6.104}$$

This rewrite is straightforward for the those Γ functions in which λ appears with a positive sign, but when $-\lambda$ appears, this is accomplished according to

$$\begin{aligned} \Gamma(A-\lambda) &= \frac{\Gamma(A)}{(A-1)(A-2)\cdots(A-\lambda)} \\ &= \frac{(-1)^\lambda\Gamma(A)}{(1-A)(2-A)\cdots(\lambda-A)} = \frac{(-1)^\lambda\Gamma(A)}{(1-A)_\lambda}. \end{aligned} \tag{6.105}$$

In terms of these quantities, S has the form

$$\begin{aligned} S &= \frac{2^{2\ell_1+2\ell_2-2\gamma}}{\pi}\frac{\Gamma(\ell_1+\frac{1}{2})\Gamma(\ell_2-\gamma+\frac{1}{2})}{\beta!\gamma!\Gamma(2\ell_2-\alpha-2\gamma+1)} \\ &\quad\times\sum_\lambda \frac{(-\beta)_\lambda(-\gamma)_\lambda(\ell_2-\gamma+\frac{1}{2})_\lambda}{\lambda!(\frac{1}{2}-\ell_1)_\lambda(2\ell_2-\alpha-2\gamma+1)_\lambda}. \end{aligned} \tag{6.106}$$

This λ sum can be recognized as the generalized hypergeometric function ${}_3F_2(-\beta,-\gamma,\ell_2-\gamma+1/2;1/2-\ell_1,2\ell_2-\alpha-2\gamma+1;1)$, see e.g. Eq. HTF(4.1.1). But for its evaluation in terms of Gamma functions, the relevant equation is Saalschütz's formula, Eq. HTF(2.1.30). This evaluation of the sum over λ requires that 1 plus the sum of the first three indices minus the fourth index be the fifth index, together with the condition that one of the first three indices be a negative integer. Here $-\gamma$ is taken as the negative integer while the combination of indices that appears here is

$$1-\beta-\gamma+\ell_2-\gamma+\frac{1}{2}-(\frac{1}{2}-\ell_1)=\ell_1+\ell_2-\beta-2\gamma+1. \tag{6.107}$$

This is to be equal to

$$2\ell_2-\alpha-2\gamma+1. \tag{6.108}$$

It is not obvious that this is a valid relation, but if the identities,

$$\ell_1=\beta+\gamma \qquad\qquad \ell_2=\alpha+\gamma, \tag{6.109}$$

valid for even L are inserted, the equality is satisfied. For odd L, the identities

$$\ell_1=\beta+\gamma+1 \qquad\qquad \ell_2=\alpha+\gamma+1 \tag{6.110}$$

show that the equality is again satisfied. Thus Saalschütz's formula can be applied in either case with the result that

$$\begin{aligned} S &= \frac{2^{2\ell_1+2\ell_2-2\gamma}}{\pi}\frac{\Gamma(\ell_1+\frac{1}{2})\Gamma(\ell_2-\gamma+\frac{1}{2})}{\beta!\gamma!\Gamma(2\ell_2-\alpha-2\gamma+1)} \\ &\quad\times\frac{(\beta+\frac{1}{2}-\ell_1)_\gamma(\gamma-\ell_1-\ell_2)_\gamma}{(\frac{1}{2}-\ell_1)_\gamma(\beta+\gamma-\ell_1-\ell_2)_\gamma}. \end{aligned} \tag{6.111}$$

Since α, β and γ are dominated by ℓ_1, ℓ_2 and ℓ_3, it is best if the factors are written in such a way that the factors are positive. This is accomplished by the identity

$$\begin{aligned} (-A)_\lambda &= (\lambda-1-A)(\lambda-2-A)\cdots(1-A)(-A) \\ &= (-1)^\lambda(A-\lambda+1)(A-\lambda+2)\cdots(A-1)(A) \\ &= (-1)^\lambda(A-\lambda+1)_\lambda=\frac{\Gamma(A+1)}{\Gamma(A-\lambda+1)}. \end{aligned} \tag{6.112}$$

With the aid of this identity, S can be written as

$$\begin{aligned} S &= \frac{2^{2\ell_1+2\ell_2-2\gamma}}{\pi}\frac{\Gamma(\ell_1+\frac{1}{2})\Gamma(\ell_2-\gamma+\frac{1}{2})\Gamma(\ell_1-\beta+\frac{1}{2})}{\beta!\gamma!\Gamma(2\ell_2-\alpha-2\gamma+1)\Gamma(\ell_1-\beta-\gamma+\frac{1}{2})} \\ &\quad\times\frac{\Gamma(\ell_1-\gamma+\frac{1}{2})\Gamma(\ell_1+\ell_2-\gamma+1)\Gamma(\ell_1+\ell_2-\beta-2\gamma+1)}{\Gamma(\ell_1+\frac{1}{2})\Gamma(\ell_1+\ell_2-2\gamma+1)\Gamma(\ell_1+\ell_2-\beta-\gamma+1)}. \end{aligned} \tag{6.113}$$

Finally Eq. HTF(1.2.15) is used to rid the equation of Gamma functions of half integer variables. After converting again to factorials, S becomes

$$\begin{aligned} S &= \frac{(\ell_1+\ell_2-\gamma)!(\ell_1+\ell_2-\beta-2\gamma)!(2\ell_2-2\gamma)!}{\beta!\gamma!(\ell_1+\ell_2-2\gamma)!(\ell_1+\ell_2-\beta-\gamma)!(\ell_2-\gamma)!} \\ &\quad\times\frac{(2\ell_1-2\beta)!(\ell_1-\beta-\gamma)!(2\ell_1-2\gamma)!}{(2\ell_2-\alpha-2\gamma)!(\ell_1-\beta)!(2\ell_1-2\beta-2\gamma)!(\ell_1-\gamma)!}. \end{aligned} \tag{6.114}$$

As a consequence, the $x_{a,b,c}$ sum can be written in general as

$$\begin{aligned}\sum_{abc} x_{a,b,c} &= \frac{2^{\alpha+\beta+\gamma}\ell_1!\ell_2!\ell_3!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!}\frac{(2\ell_3-\alpha-\beta)!(2\ell_2-\alpha-\gamma)!(2\ell_2-2\gamma)!}{(\ell_3-\alpha-\beta)!(2\ell_2-\alpha-2\gamma)!(\ell_2-\gamma)!} \\ &\times\frac{(2\ell_1-2\beta)!(2\ell_1-2\gamma)!(\ell_1-\beta-\gamma)!}{(\ell_1-\beta)!(\ell_1-\gamma)!(2\ell_1-2\beta-2\gamma)!}\frac{(\ell_1+\ell_2-\gamma)!(\ell_1+\ell_2-\beta-2\gamma)!}{(\ell_1+\ell_2-2\gamma)!(\ell_1+\ell_2-\beta-\gamma)!}. \qquad (6.115)\end{aligned}$$

The L even and odd cases of this result are written out in the last subsection.

6.6.4 $\sum_{abc} x_{a,b,c}$ for even and odd L

These results have been previously reported in tables III and IV of Ref. [17]. They follow from the general expression, Eq. (6.115).

For even L, the relations of Eq. (6.109) as well as

$$2\alpha+2\beta+2\gamma = L \qquad \ell_3 = \alpha+\beta \qquad (6.116)$$

are valid. With these relations the sum over $x_{a,b,c}$ becomes

$$\sum_{abc} x_{a,b,c} = 2^{L/2}(L/2)!\frac{\ell_1!\ell_2!\ell_3!(L-2\ell_1)!(L-2\ell_2)!(L-2\ell_3)!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!(L/2-\ell_1)!(L/2-\ell_2)!(L/2-\ell_3)!}. \qquad (6.117)$$

This quantity, for even L, is needed in Chap. 7 for the evaluation of $C_{\ell_1\ell_2\ell_3}$, Eq. (7.24), and determines the value of a particular 3-j symbol, Eq. (7.38).

For odd L, it is the relations of Eq. (6.110) and the relations

$$2\alpha+2\beta+2\gamma = L-3 \qquad \ell_3 = \alpha+\beta+1 \qquad (6.118)$$

that are required to simplify the sum over $x_{a,b,c}$ to

$$\sum_{abc} x_{a,b,c} = 2^{\frac{L+1}{2}}\left(\frac{L+1}{2}\right)!\frac{\ell_1!\ell_2!\ell_3!(L-2\ell_1)!(L-2\ell_2)!(L-2\ell_3)!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!(\frac{L-1}{2}-\ell_1)!(\frac{L-1}{2}-\ell_2)!(\frac{L-1}{2}-\ell_3)!}. \qquad (6.119)$$

Some cancellation of factors has been used to get this final form. This sum determines the value of another particular 3-j symbol, see Eq. (7.66).

Chapter 7

Properties of 3-j Tensors

The 3-j tensors $\mathbf{V}(\ell_1, \ell_2, \ell_3)$ were defined in Chap. 6 as tensors symmetric and traceless in three sets of indices, of respective order ℓ_1, ℓ_2 and ℓ_3, with the normalization, Eq. (6.10),

$$\mathbf{V}(\ell_1, \ell_2, \ell_3) \odot^L \mathbf{V}(\ell_3, \ell_2, \ell_1) = (-1)^L. \tag{7.1}$$

It was shown there that these conditions make these tensors unique except for a possible sign. The latter is determined by the condition that the coefficient of the prenormalized version $\mathbf{T}(\ell_1, \ell_2, \ell_3)$ of the 3-j tensor, as written in Eq. (6.7) or (6.8), has a positive coefficient. These defining properties, together with the normalization constant, Eq. (6.12), are sufficient for discussing most of the properties of 3-j tensors. The exceptions are those properties that depend on detailed numerical values and/or functional properties of related functions. These need some of the information contained in the remainder of Chap. 6.

For the special case that ℓ_3 is zero, $\mathbf{V}$ reduces to

$$\mathbf{V}(\ell_1, \ell_2, 0) = \frac{\delta_{\ell_1 \ell_2}}{\sqrt{2\ell_1 + 1}} \mathbf{E}^{(\ell_1)}, \tag{7.2}$$

which is consistent with the normalization of Eq. (7.1). A permutation of the ℓ's gives similar results if one the other ℓ's is zero.

This chapter is devoted to examining many of the properties of the 3-j tensors. The first topic that is dealt with is the completeness relation associated with the reduction of a product of irreducible tensors. This is then applied to the properties of integrating over $\hat{r}$ of products of natural tensors of $\hat{r}$. The second major topic is the connection to the 3-j symbols that are commonly used throughout spherical tensor theory. It is shown how the properties of the 3-j symbols arise naturally from this connection. Finally there are the properties of invariant functions defined by contracting a $\mathbf{V}(\ell_1, \ell_2, \ell_3)$ with three sets of $\boldsymbol{\mathcal{Y}}^{(\ell)}$'s. The chapter ends with the technical evaluation of the simplest 3-j symbols for even and odd L.

7.1 Completeness Relation

If two sets of symmetric traceless indices are contracted in the product of two 3-j tensors, then the result is a tensor that is symmetric and traceless in the remaining two sets of indices, specifically

$$\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_2+\ell_3}\mathbf{V}(\ell_3,\ell_2,\ell_1') = \delta_{\ell_1,\ell_1'}\frac{(-1)^L}{2\ell_1+1}\mathbf{E}^{(\ell_1)}. \tag{7.3}$$

The evaluation of this contraction, as given on the right-hand side, is true since: 1) the left-hand side is an isotropic tensor that is symmetric and traceless in ℓ_1 and ℓ_1' sets of indices; 2) such a tensor can be nonzero only if ℓ_1 and ℓ_1' are equal, and then is a multiple of the weight ℓ_1 identity $\mathbf{E}^{(\ell_1)}$; 3) the coefficient is consistent with the normalizations, Eqs. (3.58) and (6.10), of $\mathbf{E}$ and $\mathbf{V}$.

The motivation for introducing the 3-j tensors is that they carry out the Clebsch-Gordan reduction of a direct product of irreducible tensors $\mathbf{A}^{(\ell_1)}\otimes\mathbf{B}^{(\ell_2)}$ into their irreducible components, Eq. (6.1),

$$\mathbf{A}^{(\ell_1)}\mathbf{B}^{(\ell_2)} = \sum_{\ell_3}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{W}^{(\ell_3)}, \tag{7.4}$$

in the case that all irreducible tensors are written in natural form. According to Eq. (7.3), it follows that the weight ℓ_3 component of this reduction is given by

$$\mathbf{W}^{(\ell_3)} = (-1)^L(2\ell_3+1)\mathbf{V}(\ell_3,\ell_2,\ell_1)\odot^{\ell_1+\ell_2}\mathbf{A}^{(\ell_1)}\mathbf{B}^{(\ell_2)}. \tag{7.5}$$

Substitution of this evaluation of the expansion tensor $\mathbf{W}^{(\ell_3)}$ back into the Clebsch-Gordan reduction, Eq. (7.4), gives

$$\mathbf{A}^{(\ell_1)}\mathbf{B}^{(\ell_2)} = \sum_{\ell_3}(-1)^L(2\ell_3+1)\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,\ell_2,\ell_1)\odot^{\ell_1+\ell_2}\mathbf{A}^{(\ell_1)}\mathbf{B}^{(\ell_2)}. \tag{7.6}$$

Since this is an identity in the product $\mathbf{A}^{(\ell_1)}\mathbf{B}^{(\ell_2)}$, it follows that the 3-$j$ tensors satisfy the completeness relation

$$\sum_{\ell_3}(-1)^L(2\ell_3+1)\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,\ell_2,\ell_1) = \mathbf{E}^{(\ell_1)}\odot^{\ell_1}(\underbrace{\cup^{\ell_1}\mathbf{E}^{(\ell_2)}\cup})^{\ell_1}. \tag{7.7}$$

It is this pair of properties of the 3-j tensors, namely Eqs. (7.3) and (7.7), that are useful for reducing and combining tensors having different weights.

7.2 Integrals over functions of $\hat{r}$

A common procedure in much of the physics and chemistry literature is to expand any function of $\mathbf{r}$ in terms of spherical harmonics. These are, as discussed in Chap. 5, just particular components of the natural tensors $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$. The emphasis in this presentation is on the properties of expanding a function of $\mathbf{r}$ in terms of these tensors, which describe the dependence on the orientation of $\mathbf{r}$. The connection with the standard method of expansion in spherical harmonics is also discussed. In this discussion, any dependence of a function on the magnitude of the vector $\mathbf{r}$ is downplayed since that has nothing to do with the rotational properties of the function.

Given a function $f(\mathbf{r})$ of the vector $\mathbf{r}$, the completeness of the irreducible representations of the rotation group imply that this function can be expanded as a linear combination of the irreducible Cartesian tensors $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$, namely

$$f(\mathbf{r}) = \sum_{\ell} \mathbf{f}^{(\ell)}(r) \odot^{\ell} \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}). \tag{7.8}$$

From the orthonormality properties of the $\boldsymbol{\mathcal{Y}}^{(\ell)}$, Eq. (4.9), it follows that the expansion tensors are

$$\mathbf{f}^{(\ell)}(r) = \frac{1}{4\pi} \int d\hat{r} \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) f(\mathbf{r}). \tag{7.9}$$

Necessarily these expansion tensors are symmetric and traceless tensors, which are also functions of the magnitude r of the vector $\mathbf{r}$. Clearly the orientational dependence of the $\mathbf{f}^{(\ell)}(r)$ must be determined by some direction and/or directions other than those of $\hat{r}$. To make a connection with the more standard expansions, it is merely necessary to further expand $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ in terms of its spherical components, see Eqs. (5.68) and (5.75),

$$\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) = \sum_{m} \mathbf{e}_{m}^{(\ell)} \mathcal{Y}^{(\ell)m}(\hat{r}) = \sqrt{4\pi} \sum_{m} \mathbf{e}_{m}^{(\ell)} Y_{\ell m}(\hat{r}), \tag{7.10}$$

so that Eq. (7.8) can be further expanded as

$$f(\mathbf{r}) = \sum_{\ell m} f_{\ell m}(r) Y_{\ell m}(\hat{r}), \tag{7.11}$$

with expansion coefficient

$$f_{\ell m}(r) = \sqrt{4\pi}\, \mathbf{f}^{(\ell)}(r) \odot^{\ell} \mathbf{e}_{m}^{(\ell)}. \tag{7.12}$$

This has incorporated the factor of $\sqrt{4\pi}$ to account for the difference in normalization of the $\mathcal{Y}^{(\ell)m}$ and the $Y_{\ell m}$. Finally, the expansion tensor $\mathbf{f}^{(\ell)}(r)$ can be expanded,

$$\mathbf{f}^{(\ell)}(r) = \frac{1}{\sqrt{4\pi}} \sum_{m} f_{\ell m} \mathbf{e}^{(\ell)m}. \tag{7.13}$$

This is based on the above relations and the properties of the spherical tensors as given in Chap. 5.

An important example of such an expansion is the expansion of a plane wave,

$$\begin{aligned} e^{i\mathbf{k}\cdot\mathbf{r}} &= \sum_{\ell} i^{\ell}(2\ell+1) j_{\ell}(kr) P_{\ell}(\hat{k}\cdot\hat{r}) \\ &= \sum_{\ell} i^{\ell} j_{\ell}(kr) \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{k}) \odot^{\ell} \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}). \end{aligned} \tag{7.14}$$

$j_{\ell}(kr)$ is a spherical Bessel function, see for example Ref. [25]. The second form has the advantage that the Cartesian directions of $\mathbf{k}$ and $\mathbf{r}$ have been separated, as well as being classified according to the irreducible representations of the rotation group, all with one summation index, but of course with tensorial contractions. From the point of view of the previous discussion, the expansion of the plane wave in terms of the $\boldsymbol{\mathcal{Y}}(\hat{r})$ has the expansion tensor

$$i^{\ell} j_{\ell}(kr) \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{k}), \tag{7.15}$$

whose orientation is determined by the orientation, $\hat{k}$, of the wavevector. While a further expansion in terms of spherical harmonics is possible, as is usually done, most often it is only the separation of the dependence on the different vector directions that is important. The Cartesian tensor forms provide this separation, while avoiding the extra phase factors and angle calculations that usually arise when using spherical harmonics.

Since the integral of one $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$,

$$\int d\hat{r}\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) = 4\pi\delta_{\ell 0} \tag{7.16}$$

is just a special case of the orthonormality relation, Eq. (4.9), the integral of the $f(\mathbf{r})$ of Eq. (7.8),

$$\int f(\mathbf{r})d\hat{r} = 4\pi\mathsf{f}^{(0)}(r), \tag{7.17}$$

is proportional to the weight 0 component of its expansion in terms of the $\boldsymbol{\mathcal{Y}}$'s. This can also be recognized as $\sqrt{4\pi}\ f_{00}(r)$, in terms of the spherical harmonic expansion. The integral of the product of two functions, $f_1(\mathbf{r})$ and $f_2(\mathbf{r})$ can be expressed in terms of their $\boldsymbol{\mathcal{Y}}$ expansion coefficients according to

$$\int f_1\mathbf{r})f_2(\mathbf{r})d\hat{r} = 4\pi\sum_\ell \mathsf{f}_1^{(\ell)}(r)\odot^\ell\mathsf{f}_2^{\ell)}(r). \tag{7.18}$$

If, moreover, the orientation dependence of these expansion coefficients are determined respectively by vectors $\mathbf{k}_1$ and $\mathbf{k}_2$, namely

$$\mathsf{f}_j^{(\ell)}(r) = f_j^{(\ell)}(r,k_j)\boldsymbol{\mathcal{Y}}_j^{(\ell)}(\hat{k}_j), \tag{7.19}$$

then the above integral reduces to

$$\int f_1\mathbf{r})f_2(\mathbf{r})d\hat{r} = 4\pi\sum_\ell(2\ell+1)f_1^{(\ell)}(r,k_1)f_2^{\ell)}(r,k_2)P_\ell(\hat{k}_1\cdot\hat{k}_2). \tag{7.20}$$

It is noted that no "m" indices of spherical tensor analysis is needed to carry out these calculations, nor is any complex conjugation of one of the functions required to use the orthogonality of the angle dependent functions. Integrals for three or more functions can be calculated in an analogous way, but require the reduction of products of irreducible tensors. The basic feature for carrying out such calculations is the integral of three $\boldsymbol{\mathcal{Y}}^{(\ell)}$ functions. This is now considered.

For three $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$'s, the integral is symmetric and traceless in three sets of indices, and isotropic, since the integral is over all orientations of $\hat{r}$, so the result must be proportional to the corresponding 3-j tensor, namely

$$\int d\hat{r}\boldsymbol{\mathcal{Y}}^{(\ell_1)}(\hat{r})\boldsymbol{\mathcal{Y}}^{(\ell_2)}(\hat{r})\boldsymbol{\mathcal{Y}}^{(\ell_3)}(\hat{r}) = 4\pi C_{\ell_1\ell_2\ell_3}\mathsf{V}(\ell_1,\ell_2,\ell_3). \tag{7.21}$$

By fully contracting both sides of this equation with $\mathsf{V}(\ell_3,\ell_2,\ell_1)$, the integration constant follows from the normalization condition for the 3-j tensors, Eq. (6.10), as

$$\begin{aligned} C_{\ell_1\ell_2\ell_3} &= (-1)^{\ell_1+\ell_2+\ell_3}\boldsymbol{\mathcal{Y}}^{(\ell_1)}(\hat{r})\boldsymbol{\mathcal{Y}}^{(\ell_2)}(\hat{r})\boldsymbol{\mathcal{Y}}^{(\ell_3)}(\hat{r})\odot^{\ell_1+\ell_2+\ell_3}\mathsf{V}(\ell_3,\ell_2,\ell_1) \\ &= \left(\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{\overline{P}_{\ell_1}(1)\overline{P}_{\ell_2}(1)\overline{P}_{\ell_3}(1)}\right)^{1/2}(\hat{r})^{\ell_1+\ell_2+\ell_3}\odot^{\ell_1+\ell_2+\ell_3}\mathsf{V}(\ell_1,\ell_2,\ell_3), \end{aligned} \tag{7.22}$$

noting in passing that $\ell_1 + \ell_2 + \ell_3$ must be even for such an integral to be nonzero, or else an inversion of $\hat{r}$ would change the sign of the integral [since all directions are integrated over, such a result vanishes]. The further evaluation of this result requires a detailed knowledge of the 3-j tensors, specifically the expansion of the unnormalized $\mathbf{T}$ tensor, Eq. (6.13). Since all indices of the $\mathbf{U}$'s in that expansion are dotted into $\hat{r}$, it follows that

$$(\hat{r})^{\ell_1+\ell_2+\ell_3} \odot^{\ell_1+\ell_2+\ell_3} \mathbf{V}(\ell_1, \ell_2, \ell_3) = \Omega(\ell_1, \ell_2, \ell_3)^{-1/2} \sum_{abc} x_{a,b,c}. \tag{7.23}$$

The combination of these calculations shows that $C_{\ell_1\ell_2\ell_3}$ is given by

$$C_{\ell_1\ell_2\ell_3} = \left(\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{\overline{P}_{\ell_1}(1)\overline{P}_{\ell_2}(1)\overline{P}_{\ell_3}(1)\Omega(\ell_1,\ell_2,\ell_3)} \right)^{1/2} \sum_{abc} x_{a,b,c}, \tag{7.24}$$

again noting that $\ell_1 + \ell_2 + \ell_3$ is even. An alternative which is equivalent to how the integral of three spherical harmonics is expressed in the spherical tensor literature, is that this is equal to

$$C_{\ell_1\ell_2\ell_3} = i^{\ell_1+\ell_2+\ell_3} \left[(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)\right]^{1/2} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}, \tag{7.25}$$

involving a 3-j symbol. This relation is discussed in section 7.4.

A property of the $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$'s that is related to the last integral is the expansion of a product of two $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$'s in terms of these functions. Essentially this is the Clebsch-Gordan expansion. The expansion coefficients follow immediately from the above integrals, so that

$$\boldsymbol{\mathcal{Y}}^{(\ell_1)}(\hat{r})\boldsymbol{\mathcal{Y}}^{(\ell_2)}(\hat{r}) = \sum_{\ell_3} C_{\ell_1\ell_2\ell_3} \mathbf{V}(\ell_1, \ell_2, \ell_3) \odot^{\ell_3} \boldsymbol{\mathcal{Y}}^{(\ell_3)}(\hat{r}). \tag{7.26}$$

The result of an integral involving more than three $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$'s can be expressed in many different ways. It is necessary to expand products of two $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$'s according to Eq. (7.26) until the sum involves at most three $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$'s in the integral, from which that integral follows from above. But the choice of how to pair the $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$'s is responsible for the multitude of ways in which the result may be expressed.

7.3 3-j symbols

The spherical tensor analog of a 3-j Cartesian tensor is a 3-j symbol. These are obtained by contraction with the spherical tensor basis elements, thus

$$\begin{aligned} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \mathfrak{e}^{(\ell_3)m_3} \mathfrak{e}^{(\ell_2)m_2} \mathfrak{e}^{(\ell_1)m_1} \odot^{\ell_1+\ell_2+\ell_3} \mathbf{V}(\ell_1, \ell_2, \ell_3) \\ &= i^{\ell_1+\ell_2+\ell_3} \mathbf{e}^{(\ell_3)m_3} \mathbf{e}^{(\ell_2)m_2} \mathbf{e}^{(\ell_1)m_1} \odot^{\ell_1+\ell_2+\ell_3} \mathbf{V}(\ell_1, \ell_2, \ell_3). \end{aligned} \tag{7.27}$$

Note that it is the spherical basis set $\mathfrak{e}^{(\ell)m}$ that is used for the definition of the 3-j symbols although it is the $\mathbf{e}^{(\ell)m}$ basis set that is standardly used for most calculations in the physics and chemistry literature. The reason the former basis set is chosen has to do with making the 3-j symbols, and historically the Clebsch-Gordan coefficients, real.

First of all, it is noted that the 3-j tensor is real, while the elements of the basis set are in general complex, essentially involving powers of $\hat{x} \pm i\hat{y}$ according to whether each non-zero m_ℓ is positive or negative. Reality then implies that there must be equal numbers of $\hat{x} + i\hat{y}$ factors and its complex conjugate, $\hat{x} - i\hat{y}$, factors, which in turn requires that $m_1 + m_2 + m_3 = 0$. This is also a requirement of rotational invariance about the $\hat{z}$ axis, associated with the fact that a 3-j symbol has no preferred direction and must be a rotational invariant. That is, a 3-j symbol is a function only of the ℓ's and m's. While all the m's are eigenvalues associated with a rotation about the same particular axis, which physical direction that axis refers to is irrelevant as far as the 3-j symbol is concerned. Thus the 3-j symbols are scalar quantities, equivalently, they are rotational invariants.

Finally, a factor of i^L, where $L \equiv \ell_1 + \ell_2 + \ell_3$, is real for even L, so either basis would give a real 3-j symbol, but for odd L, there is an $\boldsymbol{\varepsilon}$ in the 3-j tensor so a cross product must occur in the evaluation of the scalar 3-j symbol. Such a term gives a factor of i. To make the 3-j symbol real, this is compensated for by the factor of i^L. This is exemplified by the simplest case, namely the case for which $\ell_1 = \ell_2 = \ell_3 = 1$. The only nonzero 3-$j$ symbol with these ℓ values is, except for permutations,

$$\begin{aligned} \begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \end{pmatrix} &= \mathfrak{e}^{(1)1}\mathfrak{e}^{(1)0}\mathfrak{e}^{(1)-1}\odot^3 \mathbf{V}(1,1,1) \\ &= \frac{i^3}{2}(-1)(\hat{x}+i\hat{y})\hat{z}(\hat{x}-i\hat{y})\odot^3 \frac{\boldsymbol{\varepsilon}}{\Omega(1,1,1)^{1/2}} \\ &= \frac{i}{2\sqrt{6}}(\hat{x}+i\hat{y})\cdot[(\hat{x}-i\hat{y})\times\hat{z}] = \frac{1}{\sqrt{6}}. \end{aligned} \tag{7.28}$$

This is real, also compare the sign with that listed, for example, in Edmonds' Table 2, page 125 in Ref. [1].

7.3.1 Basic Properties of 3-j symbols

Consequences of the 3-j symbols being real

Since both the 3-j tensors and symbols are real, it follows that the combination of basis vectors must be real. Now the complex conjugate of a spherical tensor basis element, Eq. (5.64), changes the sign of the corresponding m value, with the consequence that

$$\begin{aligned} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^* \\ &= \left[\mathfrak{e}^{(\ell_3)m_3}\mathfrak{e}^{(\ell_2)m_2}\mathfrak{e}^{(\ell_1)m_1}\odot^{\ell_1+\ell_2+\ell_3}\mathbf{V}(\ell_1,\ell_2,\ell_3)\right]^* \\ &= \left[\mathfrak{e}^{(\ell_3)m_3}\mathfrak{e}^{(\ell_2)m_2}\mathfrak{e}^{(\ell_1)m_1}\right]^*\odot^{\ell_1+\ell_2+\ell_3}\mathbf{V}(\ell_1,\ell_2,\ell_3) \\ &= (-1)^{\ell_1+\ell_2+\ell_3}(-1)^{m_1+m_2+m_3}\mathfrak{e}^{(\ell_3)-m_3}\mathfrak{e}^{(\ell_2)-m_2}\mathfrak{e}^{(\ell_1)-m_1}\odot^{\ell_1+\ell_2+\ell_3}\mathbf{V}(\ell_1,\ell_2,\ell_3) \\ &= (-1)^{\ell_1+\ell_2+\ell_3}\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}. \end{aligned} \tag{7.29}$$

The factor of $(-1)^{m_1+m_2+m_3} = 1$ since $m_1 + m_2 + m_3 = 0$. Thus the reality of the 3-j symbols implies that a change in sign of all the m's leaves the 3-j symbol unchanged except for a possible sign. It is also noticed that the complex conjugate of a (contravariant) spherical tensor basis element is the corresponding covariant basis element, Eq. (5.60). As a consequence, a 3-j symbol can also be defined in terms of the covariant spherical tensor basis elements, namely

$$\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{\ell_1+\ell_2+\ell_3} \boldsymbol{\mathfrak{e}}^{(\ell_3)}_{m_3} \boldsymbol{\mathfrak{e}}^{(\ell_2)}_{m_2} \boldsymbol{\mathfrak{e}}^{(\ell_1)}_{m_1} \odot^{\ell_1+\ell_2+\ell_3} \mathsf{V}(\ell_1, \ell_2, \ell_3). \tag{7.30}$$

In both of these relations, the factor of $(-1)^{\ell_1+\ell_2+\ell_3}$ comes from the fact that it is the basis set $\boldsymbol{\mathfrak{e}}^{(\ell)m}$ rather than the basis set $\mathbf{e}^{(\ell)m}$ that is used for calculating the 3-j symbols. As stressed previously, this choice of basis set was made in order to make the 3-j symbols real.

Permutation symmetries

For even $L \equiv \ell_1 + \ell_2 + \ell_3$, the 3-$j$ tensors $\mathsf{V}(\ell_1, \ell_2, \ell_3)$, $\mathsf{V}(\ell_3, \ell_1, \ell_2)$ and $\mathsf{V}(\ell_2, \ell_1, \ell_3)$ differ only in the order in which the U's are organized, as do the other three ways in which the weights (ℓ's) can be permuted. On the other hand, for odd L, there is also an $\boldsymbol{\varepsilon}$ in the 3-j tensor, so that a cyclic permutation of the weights retains the order of connectivity to the $\boldsymbol{\varepsilon}$, while a transposition of two weights interchanges that connectivity and results in a minus sign. On contracting with a basis set, these symmetries are retained. Thus the 3-j symbols satisfy the permutation symmetries

$$\begin{aligned} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= (-1)^L \begin{pmatrix} \ell_2 & \ell_1 & \ell_3 \\ m_2 & m_1 & m_3 \end{pmatrix} \\ = \begin{pmatrix} \ell_2 & \ell_3 & \ell_1 \\ m_2 & m_3 & m_1 \end{pmatrix} &= (-1)^L \begin{pmatrix} \ell_3 & \ell_2 & \ell_1 \\ m_3 & m_2 & m_1 \end{pmatrix} \\ = \begin{pmatrix} \ell_3 & \ell_1 & \ell_2 \\ m_3 & m_1 & m_2 \end{pmatrix} &= (-1)^L \begin{pmatrix} \ell_1 & \ell_3 & \ell_2 \\ m_1 & m_3 & m_2 \end{pmatrix}. \end{aligned} \tag{7.31}$$

These are the well known permutation properties of the 3-j symbols, here deduced from the symmetry properties of the 3-j tensors.

Orthonormalization properties

The spherical tensor analogs of Eqs. (7.3) and (7.7) immediately give the orthonormalization properties of the 3-j symbols. Replacing the contractions in Eq. (7.3) with the corresponding identities, $\mathsf{E}^{(\ell_2)}$ and $\mathsf{E}^{(\ell_3)}$, and their subsequent expansions in spherical tensor basis elements, as in Eq. (5.71), Eq. (7.3) becomes

$$\begin{aligned} &\sum_{m_2 m_3} \boldsymbol{\mathfrak{e}}^{(\ell_1)m_1} \odot^{\ell_1} \mathsf{V}(\ell_1, \ell_2, \ell_3) \odot^{\ell_2+\ell_3} \boldsymbol{\mathfrak{e}}^{(\ell_3)m_3} \boldsymbol{\mathfrak{e}}^{(\ell_2)m_2} (-1)^{\ell_2+m_2+\ell_3+m_3} \\ &\qquad \times \boldsymbol{\mathfrak{e}}^{(\ell_2)-m_2} \boldsymbol{\mathfrak{e}}^{(\ell_3)-m_3} \odot^{\ell_2+\ell_3} \mathsf{V}(\ell_3, \ell_2, \ell_1) \odot^{\ell_1} \boldsymbol{\mathfrak{e}}^{(\ell_1)-m_1'} \\ = &\sum_{m_2 m_3} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} (-1)^{\ell_2+m_2+\ell_3+m_3} \begin{pmatrix} \ell_3 & \ell_2 & \ell_1' \\ -m_3 & -m_2 & -m_1' \end{pmatrix} \\ = &\ \delta_{\ell_1 \ell_1'} \frac{(-1)^L}{2\ell_1+1} \boldsymbol{\mathfrak{e}}^{(\ell_1)m_1} \odot^{\ell_1} \boldsymbol{\mathfrak{e}}^{(\ell_1')-m_1'} = \frac{(-1)^L}{2\ell_1+1} (-1)^{\ell_1+m_1} \delta_{\ell_1 \ell_1'} \delta_{m_1 m_1'}. \end{aligned} \tag{7.32}$$

Cancelling out the various factors of (-1), noting that $m_1 + m_2 + m_3 = 0$, interchanging the order of the ℓ, m's in the second 3-j symbol as well as changing the signs of the m's in that quantity [two factors of $(-1)^L$ cancel], the result can be written

$$\sum_{m_2 m_3} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} \ell_1' & \ell_2 & \ell_3 \\ m_1' & m_2 & m_3 \end{pmatrix} = \frac{\delta_{\ell_1 \ell_1'} \delta_{m_1 m_1'}}{2\ell_1 + 1}. \tag{7.33}$$

This is a standardly quoted orthogonality relation for 3-j symbols.

A second relation, namely the spherical tensor analog of Eq. (7.7), is obtained in the same manner. The initial calculation of the spherical tensor basis elements is

$$\begin{aligned} & \sum_{\ell_3 m_3} (-1)^L (2\ell_3 + 1) \mathbf{e}^{(\ell_2) m_2} \mathbf{e}^{(\ell_1) m_1} \odot^{\ell_1 + \ell_2} \mathbf{V}(\ell_1, \ell_2, \ell_3) \odot^{\ell_3} \mathbf{e}^{(\ell_3) m_3} (-1)^{\ell_3 + m_3} \\ & \qquad \times \mathbf{e}^{(\ell_3) - m_3} \odot^{\ell_3} \mathbf{V}(\ell_3, \ell_2, \ell_1) \odot^{\ell_1 + \ell_2} \mathbf{e}^{(\ell_1) - m_1'} \mathbf{e}^{(\ell_2) - m_2'} \\ = & \sum_{\ell_3 m_3} (-1)^L (2\ell_3 + 1) \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} (-1)^{\ell_3 + m_3} \begin{pmatrix} \ell_3 & \ell_2 & \ell_1 \\ -m_3 & -m_2' & -m_1' \end{pmatrix} \\ = & (-1)^{\ell_1 + m_1 + \ell_2 + m_2} \delta_{m_1 m_1'} \delta_{m_2 m_2'} \end{aligned} \tag{7.34}$$

Rearranging the order of ℓ, m's and the signs of the m's in the second 3-j symbol gives

$$\sum_{\ell_3 m_3} (2\ell_3 + 1) \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta_{m_1 m_1'} \delta_{m_2 m_2'}. \tag{7.35}$$

This is also a standard relation for 3-j symbols.

7.4 Integrals of Spherical Harmonics

Integrals over $\hat{r}$ of products of $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ have already been discussed in this chapter. The spherical tensor components of these integral relations determine the corresponding integrals of the spherical harmonics. A spherical component of $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ is defined in Eq. (5.75), but an extra $\sqrt{4\pi}$ difference in normalization is needed to get the standardly used spherical harmonic, Eq. (5.86). The simplest integral is for a single spherical harmonic, namely the spherical tensor component of Eq. (7.16),

$$\int d\hat{r} Y_{\ell m}(\hat{r}) = \sqrt{4\pi} \delta_{\ell 0}. \tag{7.36}$$

The corresponding integral of two spherical harmonics follows from Eq. (5.77)

$$\int d\hat{r} Y^*_{\ell_1 m_1}(\hat{r}) Y_{\ell_2 m_2}(\hat{r}) = (-1)^{m_1} \int d\hat{r} Y_{\ell_1, -m_1}(\hat{r}) Y_{\ell_2 m_2}(\hat{r}) = \delta_{\ell_1 \ell_2} \delta_{m_1, m_2}, \tag{7.37}$$

the standard orthonormalization of the spherical harmonics.

For listing the integral of the product of three spherical harmonics, it is first useful to complete the connection between the two ways in which $C_{\ell_1 \ell_2 \ell_3}$, Eqs. (7.24) and (7.25) is expressed. This is a straightforward calculation which follows from the combination of the definitions, Eq. (7.27) for a

3-j symbol, Eq. (5.56) for the special basis elements and Eqs. (6.7-6.9) for the form of a 3-j tensor. For odd L, the following 3-j symbol is zero, while for even L, it follows that

$$\begin{aligned} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} &= \mathfrak{e}^{(\ell_3)0}\mathfrak{e}^{(\ell_2)0}\mathfrak{e}^{(\ell_1)0}\odot^{\ell_1+\ell_2+\ell_3}\mathbf{V}(\ell_1,\ell_2,\ell_3) \\ &= i^L\left[\frac{1}{\overline{P}_{\ell_1}(0)\overline{P}_{\ell_2}(0)\overline{P}_{\ell_3}(0)}\right]^{1/2}(\hat{z})^L\odot^L\mathbf{V}(\ell_1,\ell_2,\ell_3) \\ &= i^L\left[\frac{1}{\overline{P}_{\ell_1}(0)\overline{P}_{\ell_2}(0)\overline{P}_{\ell_3}(0)\Omega(\ell_1,\ell_2,\ell_3)}\right]^{1/2}\sum_{abc} x_{a,b,c}. \end{aligned} \tag{7.38}$$

The detailed calculation of this 3-j is given in Sec. 7.6.

Now the spherical tensor component of Eq. (7.21) gives

$$\begin{aligned} \int d\hat{r} Y_{\ell_1 m_1}(\hat{r})Y_{\ell_2 m_2}(\hat{r})Y_{\ell_3 m_3}(\hat{r}) &= \frac{1}{\sqrt{4\pi}}(-i)^{\ell_1+\ell_2+\ell_3}C_{\ell_1\ell_2\ell_3}\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ = \left[\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{4\pi}\right]^{1/2} & \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \end{aligned} \tag{7.39}$$

This is a standard result. The related reduction of the product of two spherical harmonics to a sum of spherical harmonics follows from Eq. (7.26),

$$\begin{aligned} Y_{\ell_1 m_1}(\hat{r})Y_{\ell_2 m_2}(\hat{r}) &= \frac{1}{\sqrt{4\pi}}\sum_{\ell_3 m_3}(-i)^{\ell_1+\ell_2+\ell_3}C_{\ell_1\ell_2\ell_3}\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix}Y^*_{\ell_3 m_3}(\hat{r}) \\ = \sum_{\ell_3 m_3}\left[\frac{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}{4\pi}\right]^{1/2} & \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix}Y^*_{\ell_3 m_3}(\hat{r}). \end{aligned} \tag{7.40}$$

This completes the discussion of the 3-j symbols, their basic properties, and their connection to the 3-j tensors.

7.5 Invariant Functions of Three Vectors

An invariant function is defined as one that is invariant to any rotation. The simplest case is a function $f(\mathbf{r})$ dependent on only one vector. If this is to be invariant it must be a function of the rotational invariants of $\mathbf{r}$, which consists only of the magnitude $r = \sqrt{\mathbf{r}\cdot\mathbf{r}}$ of the vector. Thus, in this case, $f(\mathbf{r})$ must be a function only of r, that is $f(\mathbf{r}) = f(r)$. For an invariant function $f(\mathbf{r}_1, \mathbf{r}_2)$ of the two vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, there are three invariants, the magnitudes r_1, r_2 and the scalar product $\mathbf{r}_1\cdot\mathbf{r}_2$. From a rotation group theory viewpoint, only the dependence on the scalar product is of interest, and then with the thought of separating the dependence on the two unit vectors $\hat{r}_1$ and $\hat{r}_2$. Thus an expansion in irreducible representations based on $\hat{r}_1$ and $\hat{r}_2$ would be appropriate. Such an expansion necessarily has the form

$$\begin{aligned} f(\mathbf{r}_1,\mathbf{r}_2) &= \sum_\ell f_\ell(r_1,r_2)\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}_1)\odot^\ell\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}_2) \\ &= \sum_\ell \frac{(2\ell+1)!}{2^\ell(\ell!)^2}f_\ell(r_1,r_2)[\hat{r}_1]^{(\ell)}\odot^\ell[\hat{r}_2]^{(\ell)}, \end{aligned} \tag{7.41}$$

because of the (rotational) invariance of $f(\mathbf{r}_1, \mathbf{r}_2)$. Other ways of writing this expansion, in the presumably more familiar notation of Legendre polynomials or spherical harmonics, are

$$\begin{aligned} f(\mathbf{r}_1, \mathbf{r}_2) &= \sum_\ell (2\ell+1) f_\ell(r_1, r_2) P_\ell(\hat{r}_1 \cdot \hat{r}_2) \\ &= 4\pi \sum_{\ell m} f_\ell(r_1, r_2) Y^*_{\ell m}(\hat{r}_1) Y_{\ell m}(\hat{r}_2). \end{aligned} \tag{7.42}$$

Note that the sum over the m index involves only the spherical harmonics, there being no dependence of the expansion coefficient $f_\ell(r_1, r_2)$ on m. Thus the Cartesian tensor form of the expansion is more efficient in that there is only one summation index, but a separation of the dependence on the directions of the two vectors is still attained. Of course the payment for this is the presence of the ℓ-fold contraction, but added advantages are that there are no phase factors to remember nor is there a requirement to convert to angles in order to calculate the spherical harmonics.

Invariant functions of three or more vectors are of importance in many applications, as are the tensor valued functions of several vectors. A discussion of invariant functions of several vectors with an emphasis on the Cartesian point of view has been given by Lehman and Parke [26], but they do not explicitly use 3-j tensors. In this book, the discussion is limited to the invariant functions of three vectors and this is the content of the remainder of this section. Clearly the approach can be generalized to both invariant and tensorial functions of several vectors.

An invariant function $f(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ can have its dependence on the angles of the three vectors $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{r}_3$ expanded in the form

$$f(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \sum_{\ell_1 \ell_2 \ell_3} f_{\ell_1 \ell_2 \ell_3}(r_1, r_2, r_3) \boldsymbol{\mathcal{Y}}^{(\ell_3)}(\hat{r}_3) \boldsymbol{\mathcal{Y}}^{(\ell_2)}(\hat{r}_2) \boldsymbol{\mathcal{Y}}^{(\ell_1)}(\hat{r}_1) \odot^L \mathbf{V}(\ell_1, \ell_2, \ell_3), \tag{7.43}$$

Here again L is defined as $L = \ell_1 + \ell_2 + \ell_3$. The possible invariants formed from three vectors consist of the three magnitudes r_1, r_2, r_3 and the four scalars $\hat{r}_1 \cdot \hat{r}_2$, $\hat{r}_2 \cdot \hat{r}_3$, $\hat{r}_3 \cdot \hat{r}_1$ and $\hat{r}_1 \cdot (\hat{r}_2 \times \hat{r}_3)$. The dependence of $f(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ on these last four scalars is contained in the invariant contraction of three $\boldsymbol{\mathcal{Y}}^{(\ell)}$'s with the appropriate 3-j tensor. The contraction in Eq. (7.43) is convenient in that the dependence of each vector's direction is explicitly displayed and separated from the dependence on the directions of the other vectors. Alternate ways of expressing the tensorial contraction is to expand it in terms of spherical harmonics,

$$\begin{aligned} P_{\ell_1 \ell_2 \ell_3}(\hat{r}_1, \hat{r}_2, \hat{r}_3) &\equiv \boldsymbol{\mathcal{Y}}^{(\ell_3)}(\hat{r}_3) \boldsymbol{\mathcal{Y}}^{(\ell_2)}(\hat{r}_2) \boldsymbol{\mathcal{Y}}^{(\ell_1)}(\hat{r}_1) \odot^L \mathbf{V}(\ell_1, \ell_2, \ell_3) \\ = (4\pi)^{3/2} (-i)^{\ell_1+\ell_2+\ell_3} &\sum_{m_1 m_2 m_3} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} Y_{\ell_1 m_1}(\hat{r}_1) Y_{\ell_2 m_2}(\hat{r}_2) Y_{\ell_3 m_3}(\hat{r}_3) \\ = (4\pi)^{3/2} (i)^{\ell_1+\ell_2+\ell_3} &\sum_{m_1 m_2 m_3} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} Y_{\ell_1 m_1}(\hat{r}_1) Y_{\ell_2 m_2}(\hat{r}_2) Y_{\ell_3 m_3}(\hat{r}_3). \end{aligned} \tag{7.44}$$

These functions have appeared in the literature, but with a variety of normalizations. For even L, McCourt et al [11] define functions with the same notation, here denoted with a subscript "M", but with an added factor, thus

$$P_{\ell_1 \ell_2 \ell_3}(\hat{r}_1, \hat{r}_2, \hat{r}_3)\big|_{\mathrm{M}} = \frac{(-i)^{\ell_1+\ell_2+\ell_3}}{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} P_{\ell_1 \ell_2 \ell_3}(\hat{r}_1, \hat{r}_2, \hat{r}_3). \tag{7.45}$$

That book refers to an article by Köhler et al [27], who refer to similar functions, again restricted to even L, as "generalized Legendre functions". There the coupling coefficients are the Clebsch-Gordan coefficients rather than the 3-j's, so their functions, denoted by a subscript "K", differ from those defined by McCourt et al according to

$$P_{\ell_1\ell_2\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\big|_K = (2\ell_3+1)P_{\ell_1\ell_2\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\big|_M. \tag{7.46}$$

Blum and Torruella [28] define more general invariant functions, specifically replacing two of the $Y_{\ell m}$'s by rotation $\mathcal{D}^{(\ell)}_{mn}$ matrices, see Chap. 9. This is appropriate for the description of a pair of symmetric top molecules. But reduced to the spherical harmonic case, their invariant functions are related to the present ones according to

$$\begin{aligned}\Phi^{\ell_1\ell_2\ell_3}_{00}(\hat{r}_1,\hat{r}_2,\hat{r}_3) &= \sum_{m_1m_2m_3}\frac{(4\pi)^{3/2}}{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}\begin{pmatrix}\ell_1 & \ell_2 & \ell_3\\ m_1 & m_2 & m_3\end{pmatrix}\\ &\qquad\times Y_{\ell_1m_1}(\hat{r}_1)Y_{\ell_2m_2}(\hat{r}_2)Y_{\ell_3m_3}(\hat{r}_3)\\ &= \frac{(-i)^L}{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}P_{\ell_1\ell_2\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3).\end{aligned} \tag{7.47}$$

Köhler et al [27], see also McCourt et al [11] discuss a number of properties of these functions. One such relation is the reduction to a multiple of a Legendre polynomial when one of the ℓ's is zero. For the particular case that $\ell_3=0$, this is

$$P_{\ell_1\ell_2 0}(\hat{r}_1,\hat{r}_2,\hat{r}_3) = \delta_{\ell_1\ell_2}\sqrt{2\ell_1+1}P_{\ell_1}(\hat{r}_1\cdot\hat{r}_2). \tag{7.48}$$

Other properties are obtained by contracting Eq. (7.21) with the appropriate $\boldsymbol{\mathcal{Y}}^{(\ell)}$'s, to give

$$\int d\hat{u}P_{\ell_1}(\hat{r}_1\cdot\hat{u})P_{\ell_2}(\hat{r}_2\cdot\hat{u})P_{\ell_3}(\hat{r}_3\cdot\hat{u}) = \frac{4\pi C_{\ell_1\ell_2\ell_3}}{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}P_{\ell_1\ell_2\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3), \tag{7.49}$$

and of Eq. (7.26), to give

$$P_{\ell_1}(\hat{r}_1\cdot\hat{r}_3)P_{\ell_2}(\hat{r}_2\cdot\hat{r}_3) = [(2\ell_1+1)(2\ell_2+1)]^{-1}\sum_{\ell_3}C_{\ell_1\ell_2\ell_3}P_{\ell_1\ell_2\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3). \tag{7.50}$$

Finally the orthonormalization property of the $\boldsymbol{\mathcal{Y}}^{(\ell)}$'s, Eq. (4.9), and the normalization of the 3-j tensors, Eq. (7.1), gives

$$\iiint d\hat{r}_1d\hat{r}_2d\hat{r}_3P_{\ell_1\ell_2\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3)P_{\ell_1'\ell_2'\ell_3'}(\hat{r}_1,\hat{r}_2,\hat{r}_3) = (4\pi)^3\delta_{\ell_1\ell_1'}\delta_{\ell_2\ell_2'}\delta_{\ell_3\ell_3'}. \tag{7.51}$$

While most of these identities are restricted to even L, the last equation is also valid for odd L.

Clearly these invariant functions can be calculated using the 3-j symbols but a more direct way is to use the expansions, Eqs. (6.13) and (6.42), for the $\mathbf{T}(\ell_1,\ell_2,\ell_3)$ tensors. The result is

$$\begin{aligned}P_{\ell_1'\ell_2'\ell_3'}(\hat{r}_1,\hat{r}_2,\hat{r}_3) &= \left[\frac{(2\ell_1+1)!(2\ell_2+1)!(2\ell_3+1)!}{2^L(\ell_1!\ell_2!\ell_3!)^2\Omega(\ell_1,\ell_2,\ell_3)}\right]^{1/2}\\ &\quad\times\sum_{a,b,c}x_{a,b,c}(\hat{r}_2\cdot\hat{r}_3)^{\alpha'}(\hat{r}_1\cdot\hat{r}_3)^{\beta'}(\hat{r}_1\cdot\hat{r}_2)^{\gamma'}\begin{cases}1 & \text{L even}\\ \hat{r}_1\cdot(\hat{r}_2\times\hat{r}_3) & \text{L odd.}\end{cases}\end{aligned} \tag{7.52}$$

The $x_{a,b,c}$ are the same for even and odd L, provided it is expressed precisely as in Eq. (6.41), with α, β and γ calculated according to Eq. (6.4) for even L or Eq. (6.45) for odd L. The powers α', β' and γ' are given by Eqs. (6.44) for both even and odd L.

It is also possible to calculate these invariant functions from a recursion relation for the 3-j tensors, specifically the third recursion relation, Eq. (6.86). Such possibilities were suggested by Coope [17]. Expressed in terms of the invariant functions, this recursion relation is

$$\begin{aligned}
&P_{\ell_1+1\ell_2+1\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\\
&= 2\hat{r}_1\cdot\hat{r}_2\left[\frac{(2\ell_1+3)(2\ell_1+1)(2\ell_2+3)(2\ell_2+1)}{(L+3)(L+2)(L+2-2\ell_3)(L+1-2\ell_3)}\right]^{1/2} P_{\ell_1\ell_2\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\\
&\quad-\left[\frac{(2\ell_2+3)(L-2\ell_1)(L-1-2\ell_1)(L+2-2\ell_2)(L+1-2\ell_2)}{(2\ell_2-1)(L+3)(L+2)(L+2-2\ell_3)(L+1-2\ell_3)}\right]^{1/2} P_{\ell_1+1\ell_2-1\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\\
&\quad-\left[\frac{(2\ell_1+3)(L-2\ell_2)(L-1-2\ell_2)(L+2-2\ell_1)(L+1-2\ell_1)}{(2\ell_1-1)(L+3)(L+2)(L+2-2\ell_3)(L+1-2\ell_3)}\right]^{1/2} P_{\ell_1-1\ell_2+1\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\\
&\quad-\left[\frac{(2\ell_1+3)(2\ell_2+3)(L+1)L(L-2\ell_3)(L-1-2\ell_3)}{(2\ell_1-1)(2\ell_2-1)(L+3)(L+2)(L+2-2\ell_3)(L+1-2\ell_3)}\right]^{1/2} P_{\ell_1-1\ell_2-1\ell_3}(\hat{r}_1,\hat{r}_2,\hat{r}_3). \qquad (7.53)
\end{aligned}$$

It is the nature of this recursion relation that it calculates the invariant function for $L+2$ from the values of the invariant function for L and $L-2$. In particular, the recursion relation involves only even L, or odd L, which is reasonable according to the condition that the odd L functions involve the cross product $\hat{r}_1\cdot(\hat{r}_2\times\hat{r}_3)$, while the even L functions are independent of this quantity. As written, the recursion relation is assymmetric to the interchange of ℓ_1, ℓ_2 and ℓ_3 because it involves a stepping up of ℓ_1 and ℓ_2 for fixed ℓ_3. The symmetry of the invariant function to a simultaneous permutation of the ℓ's and the $\hat{r}$'s means that similar recursion relations can be written stepping up any other pair of ℓ's.

Notes on implementation of this recursion relation

For even L, the evaluation of the invariant functions for a given set of $\hat{r}$'s can be based on Eq. (7.53). This first needs the initializations

$$\begin{aligned}
P_{000} &= 1 & P_{110} &= \sqrt{3}\hat{r}_1\cdot\hat{r}_2\\
P_{101} &= \sqrt{3}\hat{r}_1\cdot\hat{r}_3 & P_{011} &= \sqrt{3}\hat{r}_2\cdot\hat{r}_3. \qquad (7.54)
\end{aligned}$$

But note that as written, the recursion relation does not include stepping up ℓ_3. A permutation of Eq. (7.53) can accomplish this. In fact, it is sufficient to calculate only those invariant functions with $\ell_1+\ell_2=\ell_3$ and use Eq. (7.53) to cover the other cases. One way to do this is by stepping up ℓ_1 and ℓ_3 with the restriction $\ell_1+\ell_2=\ell_3$. Eq. (7.53), as modified for these conditions, becomes

$$\begin{aligned}
P_{\ell_1+1\ell_2\ell_1+\ell_2+1}(\hat{r}_1,\hat{r}_2,\hat{r}_3) &= \hat{r}_1\cdot\hat{r}_3\left[\frac{2(L+1)(2\ell_1+3)}{(L+2)(\ell_1+1)}\right]^{1/2} P_{\ell_1\ell_2\ell_1+\ell_2}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\\
&\quad-\left[\frac{2\ell_2(2\ell_2-1)}{(L-1)(L+2)(\ell_1+1)(2\ell_1+1)}\right]^{1/2} P_{\ell_1+1\ell_2\ell_1+\ell_2-1}(\hat{r}_1,\hat{r}_2,\hat{r}_3)\\
&\quad-\left[\frac{L(L+1)\ell_1(2\ell_1+3)}{(L-1)(L+2)(\ell_1+1)(2\ell_1+1)}\right]^{1/2} P_{\ell_1-1\ell_2\ell_1+\ell_2-1}(\hat{r}_1,\hat{r}_2,\hat{r}_3). \qquad (7.55)
\end{aligned}$$

What is still missing are the cases where $\ell_1 = 0$. Another permutation of Eq. (7.53), or a permutation of Eq. (7.55), and the subsequent restriction to $\ell_1 = 0$, gives

$$\begin{aligned} P_{0\ell_2+1\ell_2+1}(\hat{r}_1, \hat{r}_2, \hat{r}_3) &= \hat{r}_2 \cdot \hat{r}_3 \frac{\left[(2\ell_2+1)(2\ell_2+3)\right]^{1/2}}{(\ell_2+1)} P_{0\ell_2\ell_2}(\hat{r}_1, \hat{r}_2, \hat{r}_3) \\ &- \frac{\ell_2}{\ell_2+1} \left[\frac{(2\ell_2+3)}{(2\ell_2-1)}\right]^{1/2} P_{0\ell_2-1\ell_2-1}(\hat{r}_1, \hat{r}_2, \hat{r}_3). \end{aligned} \tag{7.56}$$

This is equivalent to the recursion relation for the Legendre polynomials, compare Eq. (7.48) for the reduction of the invariant function for the analogous case in which $\ell_3 = 0$. It is the combination of these three recursion relations, used for successive values of L, that enable the calculation of all the invariant functions for even L up to a selected maximum L.

The odd L case is similar. Now only the initialization that

$$P_{111}(\hat{r}_1, \hat{r}_2, \hat{r}_3) = \frac{3}{2}\sqrt{2}\; \hat{r}_1 \cdot (\hat{r}_2 \times \hat{r}_3) \tag{7.57}$$

is needed. Eq. (7.53) can again be used as the main recursion relation, while the stepping up of ℓ_3 can be accomplished with ℓ_2 fixed and $\ell_3 = \ell_1 + \ell_2 - 1$, according to

$$\begin{aligned} P_{\ell_1+1\ell_2\ell_1+\ell_2}(\hat{r}_1, \hat{r}_2, \hat{r}_3) &= \hat{r}_1 \cdot \hat{r}_3 \left[\frac{2L(2\ell_1+3)}{(L+3)\ell_1}\right]^{1/2} P_{\ell_1\ell_2\ell_1+\ell_2-1}(\hat{r}_1, \hat{r}_2, \hat{r}_3) \\ &- \left[\frac{6(\ell_2-1)(2\ell_2-1)}{(L-2)(L+3)\ell_1(2\ell_1+1)}\right]^{1/2} P_{\ell_1+1\ell_2\ell_1+\ell_2-2}(\hat{r}_1, \hat{r}_2, \hat{r}_3) \\ &- \left[\frac{L(L+1)(\ell_1-1)(2\ell_1+3)}{(L-2)(L+3)\ell_1(2\ell_1+1)}\right]^{1/2} P_{\ell_1-1\ell_2\ell_1+\ell_2-2}(\hat{r}_1, \hat{r}_2, \hat{r}_3). \end{aligned} \tag{7.58}$$

Finally the values of the $\ell_1 = 1$ invariant functions can be obtained by

$$\begin{aligned} P_{1\ell_2+1\ell_2+1}(\hat{r}_1, \hat{r}_2, \hat{r}_3) &= \hat{r}_2 \cdot \hat{r}_3 \left[\frac{4L(L+2)}{(L-1)(L+3)}\right]^{1/2} P_{1\ell_2\ell_2}(\hat{r}_1, \hat{r}_2, \hat{r}_3) \\ &- \left[\frac{(L+1)(L+2)(L-3)}{(L-1)(L-2)(L+3)}\right]^{1/2} P_{1\ell_2-1\ell_2-1}(\hat{r}_1, \hat{r}_2, \hat{r}_3). \end{aligned} \tag{7.59}$$

The use of these three recursion relations for successive L values is a means of calculating all invariant functions, for odd L, up to a selected maximum L value.

7.6 Calculation of two particular sets of 3-j symbols

The detailed structure of a 3-j tensor is governed by the expansion coefficients $x_{a,b,c}$ according to Eqs. (6.13) or (6.42), respectively for even or odd L. Since the 3-j symbols are components of these, Eq. (7.27), the 3-j symbols are also determined by these coefficients. A particular combination of the $x_{a,b,c}$ is the sum over all a, b and c. This combination determines two particular sets of 3-j symbols, according to whether L is even or odd.

For even L, the relation between the $x_{a,b,c}$ sum and a 3-j symbol has already been given, Eq. (7.38). It remains to insert the evaluation of the different factors in order to complete its evaluation. This needs Eq. (6.117) as well as the values for $\Omega(\ell_1, \ell_2, \ell_3)$ and $\overline{P}_\ell(1)$, Eqs. (6.12) and (4.7). It is easy to show that

$$\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix} = \frac{(i)^L (L/2)!}{(\frac{L}{2}-\ell_1)!(\frac{L}{2}-\ell_2)!(\frac{L}{2}-\ell_3)!}\sqrt{\frac{L-2\ell_1)!(L-2\ell_2)!(L-2\ell_3)!}{(L+1)!}}. \tag{7.60}$$

This is a well known result for this particular set of 3-j symbols.

For odd L, the calculation of the $x_{a,b,c}$ sum is given by Eq. (6.119). It remains to find which 3-j symbol this is related to and then to evaluate the 3-j symbol from this relation. Since this combination is the simplest sum of $x_{a,b,c}$'s for an odd L, it should also be related to the simplest 3-j for odd L. Clearly this is the 3-j symbol

$$\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ -1 & 0 & 1 \end{pmatrix} = (i)^L \mathbf{e}^{(\ell_3)1}\mathbf{e}^{(\ell_2)0}\mathbf{e}^{(\ell_1)-1}\odot^L \mathbf{V}(\ell_1, \ell_2, \ell_3). \tag{7.61}$$

Now $\mathbf{e}^{(\ell_3)1}$ is a symmetric traceless tensor based on the product of $\mathbf{e}^{(1)0} = \hat{z}$'s and one $\mathbf{e}^{(1)1} = -(\hat{x}+i\hat{y})/\sqrt{2}$, with an analogous structure for $\mathbf{e}^{(\ell_1)-1}$. The L-fold contraction is thus equivalent to

$$\begin{aligned} &\mathbf{e}^{(\ell_3)1}\mathbf{e}^{(\ell_2)0}\mathbf{e}^{(\ell_1)-1}\odot^L \mathbf{V}(\ell_1, \ell_2, \ell_3) \\ &= \quad N_{\ell_3 1}N_{\ell_2 0}N_{\ell_1 -1}\mathbf{e}^{(1)1}[\mathbf{e}^{(1)0}]^{L-2}\mathbf{e}^{(1)-1}\odot^L \mathbf{V}(\ell_1, \ell_2, \ell_3). \end{aligned} \tag{7.62}$$

Tensorially, the product

$$\begin{aligned} \mathbf{e}^{(1)1}\mathbf{e}^{(1)-1} &= (-1/2)(\hat{x}+i\hat{y})(\hat{x}-i\hat{y}) \\ &= (-1/2)[\hat{x}\hat{x}+\hat{y}\hat{y}-i(\hat{x}\hat{y}-\hat{y}\hat{x})] \\ &= (-1/2)[\mathbf{U}-\hat{z}\hat{z}-i\boldsymbol{\varepsilon}\cdot\hat{z}] \end{aligned} \tag{7.63}$$

involves only the direction $\hat{z}$ and invariant tensors. Since $\mathbf{e}^{(1)0} = \hat{z}$, and since, for odd L, the 3-j tensor involves one $\boldsymbol{\varepsilon}$, it follows that only the part of the above product that involves $\boldsymbol{\varepsilon}$ contributes to the evaluation of the 3-j symbol.

From the expansion of the 3-j coupling tensor, Eq. (6.42), it follows that the contraction of a typical term with L-2 $\hat{z}$'s and one $\hat{z}\cdot\boldsymbol{\varepsilon}$ (appropriately ordered) is

$$\hat{z}\cdot\boldsymbol{\varepsilon}\,(\hat{z})^{L-2}\odot^L \mathbf{S}^{a,b,c,\alpha',\beta',\gamma'} \;=\; \frac{1}{\ell_1\ell_3}\hat{z}\cdot\boldsymbol{\varepsilon}:(\boldsymbol{\varepsilon}\cdot\hat{z}) \;=\; \frac{2}{\ell_1\ell_3}. \tag{7.64}$$

This has recognized that $\hat{z}$ is dotted into everything except one of the ℓ_1 and one of the ℓ_3 indices and the contraction with $\boldsymbol{\varepsilon}$ is nonvanishing only if it is dotted into the $\boldsymbol{\varepsilon}$ indices of $\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'}$. There are $\ell_1\ell_3$ ways in which the $\boldsymbol{\varepsilon}$ indices can be placed in the latter quantity, so it is this selection that gives the factor of $1/\ell_1\ell_3$. Since the contraction is the same for all $\mathbf{S}^{a,b,c,\alpha',\beta',\gamma'}$, it follows that

$$\hat{z}\cdot\boldsymbol{\varepsilon}\,(\hat{z})^{L-2}\odot^L \mathbf{T}(\ell_1, \ell_2, \ell_3) \;=\; \frac{2}{\ell_1\ell_3}\sum_{abc} x_{a,b,c} \tag{7.65}$$

and

$$\begin{aligned} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ -1 & 0 & 1 \end{pmatrix} &= \frac{(i)^{L+1}}{\ell_1\ell_3}\frac{N_{\ell_3 1}N_{\ell_2 0}N_{\ell_1 -1}}{[\Omega(\ell_1, \ell_2, \ell_3)]^{1/2}}\sum_{abc} x_{a,b,c} \\ &= \frac{2(i)^{L+1}(\frac{L+1}{2})!}{(\frac{L-1}{2}-\ell_1)!(\frac{L-1}{2}-\ell_2)!(\frac{L-1}{2}-\ell_3)!}\left[\frac{(L-2\ell_1)!(L-2\ell_2)!(L-2\ell_3)!}{(L+1)!\ell_1(\ell_1+1)\ell_3(\ell_3+1)}\right]^{1/2}. \end{aligned} \tag{7.66}$$

This completes the identification of the two sets of 3-j symbols that are related to $\sum_{abc} x_{a,b,c}$, together with their explicit expression in terms of factorials.

Chapter 8

The 6-j and other n-j Symbols

The n-j symbols for n greater than 3 are rotational invariants formed by combinations of 3-j tensors. The basic scalar invariant is the 6-j, formed by contracting four 3-j's, equivalently involving six irreducible representations of the rotation group. Contractions involving more 3-j's (and irreducible representations) can always be expressed in terms of the 6-j's, usually as a sum of products of 6-j's. Except in the case when such a contraction can be reduced to a simple product of 6-j's, the contraction is standardly thought of as a separate entity, such as the 9-j, 12-j, etc. symbols. The main application of n-j symbols has been to the algebra of angular momentum in quantum mechanics, where the 6-j and higher n-j symbols reflect the relation between the various ways in which angular momentum states can be coupled. This chapter covers the definitions and properties of 6-j symbols as they relate to irreducible Cartesian tensors whereas only the 9-j of the higher ordered recoupling coefficients are discussed, and then only sufficiently for their definition.

n-j symbols standardly have n a multiple of 3 and as stated above, are associated with multiples of 3-j tensors, equivalently 3-j symbols, whose importance is that of providing the transformations between different orders of carrying out the Clebsch-Gordan reduction of a product of several irreducible representations of the rotation group. Another kind of n-j symbol is the spherical metric $\mathfrak{g}^{(\ell)}_{mm'}$, which can be considered [17,29] as a 1-j symbol. This can also be recognized as a special case of a 3-j symbol, specifically the contravariant form is

$$\mathfrak{g}^{(\ell)mm'} = \begin{pmatrix} \ell \\ mm' \end{pmatrix} = \sqrt{2\ell+1} \begin{pmatrix} \ell & 0 & \ell \\ m & 0 & m' \end{pmatrix} = (-1)^{\ell+m}\delta_{m',-m}. \tag{8.1}$$

This might also be thought of as a 2-j symbol, since this involves two weights, which must be equal in order to be a rotational invariant, but such a designation does not seem to be in the literature. Since the metric is just a representation of the identity, it does not provide a new property to the tensor analysis, especially when emphasizing Cartesian tensors, whereas the n-j symbols with n a multiple of 3 provide all the properties of the Clebsch-Gordan reduction and its repeated application. It is for this reason that only these symbols are emphasized when dealing with the rotation group. But for more general groups, other symbols can be important.

8.1 The 6-j Symbol

If three 3-j tensors are contracted in the following way

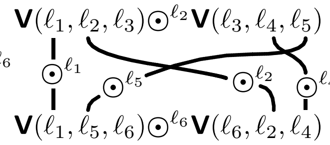
$$\underbrace{(\llcorner^{\ell_1}\odot^{\ell_1}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_2}\mathbf{V}(\ell_3,\ell_4,\ell_5)\odot^{\ell_5}\mathbf{V}(\ell_5,\ell_6,\ell_1)\odot^{\ell_1}(\lrcorner)}^{\ell_1}, \tag{8.2}$$

then the resulting tensor, being a rotational invariant and symmetric traceless in the three sets of indices $\ell_2,\ \ell_4$ and ℓ_6, must be proportional to the 3-j tensor $\mathbf{V}(\ell_2,\ell_4,\ell_6)$, thus

$$\begin{aligned}&\underbrace{(\llcorner^{\ell_1}\odot^{\ell_1}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_2}\mathbf{V}(\ell_3,\ell_4,\ell_5)\odot^{\ell_5}\mathbf{V}(\ell_5,\ell_6,\ell_1)\odot^{\ell_1}(\lrcorner)}^{\ell_1}\\ &= (-1)^{\ell_2+\ell_4+\ell_6}\left\{\begin{matrix}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{matrix}\right\}\mathbf{V}(\ell_2,\ell_4,\ell_6)\end{aligned} \tag{8.3}$$

The coefficient of expansion depends on six sets of indices and is equal to the 6-j symbol usually defined by contraction of the m-indices of four 3-j symbols. This connection is made as follows. From the normalization of the 3-j tensors, Eq. (7.1), the contraction of Eq. (8.3) gives

$$\left\{\begin{matrix}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{matrix}\right\} = (-1)^{\ell_2+\ell_4+\ell_6}$$



(8.4)

with the factor of $(-1)^{\ell_2+\ell_4+\ell_6}$ due to the interchange of the order for writing the 3-j with the same indices, which order is useful for the graphical representation of the contractions. Since any multifold dot contraction over a set of symmetric traceless indices is equivalent, in spherical tensor terms, to the sum over m index

$$\mathbf{E}^{(\ell)} = \sum_m \mathfrak{e}^{(\ell)m}(-1)^{\ell+m}\mathfrak{e}^{(\ell)-m}, \tag{8.5}$$

see Eq. (5.71), it follows that the 6-j symbol can be expressed as the sum of products of four 3-j symbols,

$$\begin{aligned}\left\{\begin{matrix}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{matrix}\right\} &= (-1)^{\ell_1+\ell_2+\ell_3+\ell_4+\ell_5+\ell_6}\sum_{\substack{m_1m_2m_3\\ m_4m_5m_6}}\begin{pmatrix}\ell_1 & \ell_2 & \ell_3\\ m_1 & m_2 & m_3\end{pmatrix}\begin{pmatrix}\ell_1 & \ell_5 & \ell_6\\ -m_1 & m_5 & -m_6\end{pmatrix}\\ &\times(-1)^{m_1+m_2+m_3+m_4+m_5+m_6}\begin{pmatrix}\ell_4 & \ell_2 & \ell_6\\ -m_4 & -m_2 & m_6\end{pmatrix}\begin{pmatrix}\ell_4 & \ell_5 & \ell_3\\ m_4 & -m_5 & -m_3\end{pmatrix}.\end{aligned} \tag{8.6}$$

All the (-1) factors have been retained for symmetry of presentation while certain combinations could be eliminated by making use of the symetry properties of the 3-j symbols. The choice as to which m's are positive and which are negative has been made to conform to Edmond's Eq.(6.2.4) [1]. Eq. (8.6) is the standard way in which the 6-j is defined. It is important to recognize the order in which the different ℓ's appear in the 6-j and the associated 3-j's. In the 6-j, the 3-j's are associated graphically according to the four combinations shown in Fig. 8.1.

Figure 8.1: The 3-j combinations of j's in a 6-j

The 6-j can be written in a number of different ways, just as long as each 3-j preserves its cyclic order, or two 3-j's have their order inverted, and the connectivity of the 3-j's, essentially which tensors are contracted together, are preserved. Specifically the value of a 6-j is unchanged under any permutation of the columns, or if two elements in the rows are interchanged. It is easy to see that the latter is just an equivalent way of expressing the contractions of the 3-j tensors, as they are expressed in Eq. (8.4), while interchanging a pair of columns inverts the cyclic order of all 3-j's.

One way of representing the symmetry of the 6-j is to represent it by a tetrahedron, Fig. 8.2.

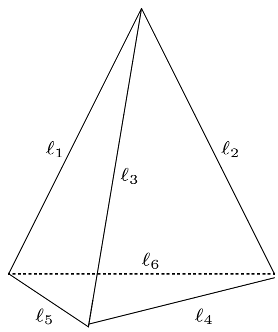


Figure 8.2: The tetrahedron representing a 6-j

Each line is labelled by an ℓ and each vertex represents a 3-j, with here the order of the ℓ values being consistent with a righthand rule having the thumb pointing towards the tetrahedron, the dotted line horizontal line (labelled ℓ_6 being behind the line labelled ℓ_3. Thus for the apex, the order is ℓ_1, ℓ_2, ℓ_3, as appears in the 6-j. This is a fairly common geometrical representation of a 6-j. An alternative, which emphasizes the connections between the $\mathbf{E}^{(\ell)}$'s, is the bipyramid, Fig. 8.3.

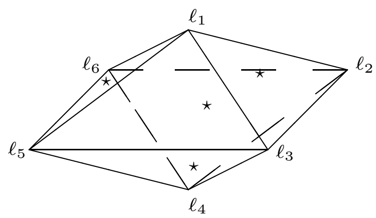


Figure 8.3: The bipyramid representing a 6-j

Now each vertex is labelled by an ℓ and represents an $\mathbf{E}^{(\ell)}$ while the four faces labelled by $\star$'s designate the 3-j's. This shows the connectivity between the different $\mathbf{E}^{(\ell)}$, there being four such connections for each $\mathbf{E}^{(\ell)}$, two for each 3-j to which it is associated. The order of ℓ's in a 3-j is chosen

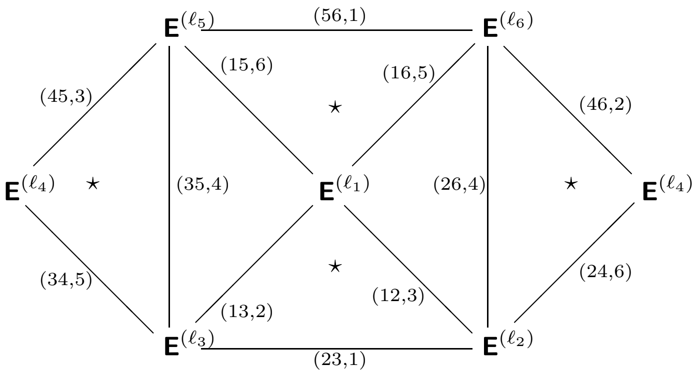


Figure 8.4: The opened bipyramid representing a 6-j

here to be consistent with a righthand rule with the thumb pointing into the bipyramid. Clearly the four unstarred faces do NOT represent 3-j's. If the bipyramid is opened up by cutting at the ℓ_4 vertex, then the structure can be written in two dimensions, see Fig. 8.4. This gives the oportunity to express the $\mathbf{E}^{(\ell)}$ projectors and to indicate the number of $\mathbf{U}$'s conecting each of the $\mathbf{E}^{(\ell)}$'s. The abbreviation

$$(mn,p) \equiv \begin{cases} \frac{1}{2}(\ell_m + \ell_n - \ell_p) & \text{for } \ell_m + \ell_n + \ell_p \text{ even} \\ \frac{1}{2}(\ell_m + \ell_n - \ell_p - 1) & \text{for } \ell_m + \ell_n + \ell_p \text{ odd} \end{cases} \tag{8.7}$$

is used for this number. Again the faces with stars are associated with the 3-j tensors with the order of the ℓ's consistent with a righthand rule with the thumb pointing into the paper. What are not explicitly indicated are the $\boldsymbol{\varepsilon}$'s associated with the three ℓ's of a 3-j when the corresponding sum of ℓ's is odd. The star in that case may be interpreted as carrying such an $\boldsymbol{\varepsilon}$.

8.2 6-j Symbol properties

Equation (8.3) shows how three interlinked 3-j's are related to a 6-j. A similar result is available for two linked 3-j's. Starting with two 3-j's having one set of symmetric traceless indices contracted

$$\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,\ell_4,\ell_5) \tag{8.8}$$

this invariant tensor with four sets of symmetric traceless indices can be expanded in terms of another pair of 3-j's having a different association of ℓ values in each 3-j. A particular choice is

$$\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,\ell_4,\ell_5) = \sum_{\ell_6} a_{\ell_6}\mathbf{V}(\ell_1,\ell_5,\ell_6)\odot^{\ell_6}\mathbf{V}(\ell_6,\ell_4,\ell_2). \tag{8.9}$$

The expansion coefficient a_{ℓ_6} can be calculated by contracting the sets ℓ_1 and ℓ_5 on both sides with $\mathbf{V}(\ell_1,\ell_5,\ell)$, and then comparing results. Essentially this reduces the lefthand side to being of the same form as the lefthand side of Eq. (8.3) while the contraction on the righthand side gives the factor

$$\frac{\delta_{\ell_6\ell}}{(2\ell+1)}\mathbf{V}(\ell_6,\ell_4,\ell_2).$$

On comparison with Eq. (8.3), the coefficient a_{ℓ_6} is identified as being proportional to a 6-j and the above relation written as

$$\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,\ell_4,\ell_5) = \sum_{\ell_6}(2\ell_6+1)\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{array}\right\}\mathbf{V}(\ell_1,\ell_5,\ell_6)\odot^{\ell_6}\mathbf{V}(\ell_6,\ell_4,\ell_2). \tag{8.10}$$

This expansion can be repeated. Specifically if ℓ_1 and ℓ_2 are chosen in the same 3-j, then

$$\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,\ell_4,\ell_5) = \sum_{\ell_6\ell_7}(2\ell_6+1)(2\ell_7+1) \times\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{array}\right\}\left\{\begin{array}{ccc}\ell_1 & \ell_5 & \ell_6\\ \ell_4 & \ell_2 & \ell_7\end{array}\right\}\mathbf{V}(\ell_1,\ell_2,\ell_7)\odot^{\ell_7}\mathbf{V}(\ell_7,\ell_4,\ell_5). \tag{8.11}$$

Clearly the tensors on the two sides of this equation are of the same form, except for the ℓ_3 and ℓ_7 labels. Since the four sets of symmetric traceless indices are the same on both sides of the equation are the same, it follows that ℓ_7 must equal ℓ_3. Formally this can be proved by contracting ℓ_1 and ℓ_2 on both sides of the equation with $\mathbf{V}(\ell_1,\ell_2,\ell_8)$. The resulting Kronecker delta functions from applying Eq. (7.3), implies that the 6-j's satisfy the orthonormality condition

$$\sum_{\ell_6}(2\ell_6+1)(2\ell_7+1)\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{array}\right\}\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_7\\ \ell_4 & \ell_5 & \ell_6\end{array}\right\} = \delta_{\ell_3\ell_7}. \tag{8.12}$$

Some symmetry properties of the 6-j have been used to express this result in this way. This is a well known property of the 6-j's.

The contraction of Eq. (8.10) with $\mathbf{V}(\ell_1,\ell_4,\ell_7)\odot^{\ell_7}\mathbf{V}(\ell_7,\ell_2,\ell_5)$ with labelled sets of indices contracted, gives a result that can be written in the form

$$\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_3\\ \ell_5 & \ell_4 & \ell_7\end{array}\right\} = \sum_{\ell_6}(-1)^{\ell_6+\ell_3+\ell_7}(2\ell_6+1)\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{array}\right\}\left\{\begin{array}{ccc}\ell_1 & \ell_5 & \ell_6\\ \ell_2 & \ell_4 & \ell_7\end{array}\right\}. \tag{8.13}$$

The factor involving (-1) arises from permuting the ℓ's in 3-j tensors so as to write the combinations as 6-j's. Another relation is obtained by contracting Eq. (8.10) with

$$\underbrace{\mathbf{V}(\ell_1,\ell_7,\ell_8)\odot^{\ell_8}\mathbf{V}(\ell_8,\ell_2,\ell_9)\odot^{\ell_9}\mathbf{V}(\ell_9,\ell_4,\ell_{10})\odot^{\ell_{10}}\mathbf{V}(\ell_{10},\ell_7,\ell_5)}_{\odot^{\ell_7}}$$

In the contraction of the lefthand side it is noticed that the ℓ_3, ℓ_9 and ℓ_7 sets of indices separate the $\mathbf{V}$'s into two parts. If one part is recognized as being invariant and thus proportional to $\mathbf{V}(\ell_3,\ell_9,\ell_7)$, then the parts can each be recognized as a 6-j. A similar argument is valid for the tensors on the righthand side so that the identity

$$\left\{\begin{array}{ccc}\ell_7 & \ell_8 & \ell_1\\ \ell_2 & \ell_3 & \ell_9\end{array}\right\}\left\{\begin{array}{ccc}\ell_3 & \ell_4 & \ell_5\\ \ell_{10} & \ell_7 & \ell_9\end{array}\right\} = \sum_{\ell_6}(2\ell_6+1)(-1)^{\ell_1+\ell_2+\ell_3+\ell_4+\ell_5+\ell_6+\ell_7+\ell_8+\ell_9+\ell_{10}} \times\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_3\\ \ell_4 & \ell_5 & \ell_6\end{array}\right\}\left\{\begin{array}{ccc}\ell_1 & \ell_5 & \ell_6\\ \ell_{10} & \ell_8 & \ell_7\end{array}\right\}\left\{\begin{array}{ccc}\ell_6 & \ell_4 & \ell_2\\ \ell_9 & \ell_8 & \ell_{10}\end{array}\right\} \tag{8.14}$$

results. Equations (8.13) and (8.14) are equivalent to (i.e. different labellings) Eqs. (6.2.11) and (6.2.12) of Edmonds [1], where the latter is referred to as the sum rule of Biedenharn and Elliot. Other relations can be found but no catalog of all the possibilities is attempted.

8.3 Evaluation of certain 6-j Symbols

8.3.1 The cases when ℓ=0 and 1

If one of the ℓ's is 0, then the 6-j is especially simple. Specifically, two of the 3-j tensors become proportional to $\mathbf{E}^{(\ell)}$'s so the contraction is

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & \ell_5 & \ell_6 \end{Bmatrix} = \frac{\delta_{\ell_5\ell_3}\delta_{\ell_6\ell_2}}{\sqrt{(2\ell_2+1)(2\ell_3+1)}}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^L\mathbf{V}(\ell_3,\ell_2,\ell_1)$$
$$= (-1)^{\ell_1+\ell_2+\ell_3}\frac{\delta_{\ell_5\ell_3}\delta_{\ell_6\ell_2}}{\sqrt{(2\ell_2+1)(2\ell_3+1)}}. \tag{8.15}$$

Here the square root terms are due to the normalization of those $\mathbf{V}$'s containing a 0.

If one of the ℓ's is 1, then there are essentially four types of 6-j's, namely

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ 1 & \ell_3+a & \ell_2+b \end{Bmatrix},$$

with $a=b=0$ or with $a=-1$ and $b=\pm1$ or 0. Other possible cases having one $\ell=1$ can be obtained from these by relabelling and applying the symmetries of the 6-j symbol.

For the case with $a=-1$, at least one of the 3-j tensors containing 1 again reduces to being proportional to an $\mathbf{E}^{(\ell)}$, but the resulting contractions are a bit more complicated than when one of the ℓ's was 0. The calculation when b is also equal to -1 is

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ 1 & \ell_3-1 & \ell_2-1 \end{Bmatrix}$$
$$= \overbrace{\mathbf{V}(\ell_1,\underbrace{\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,1}_{\odot^{\ell_2}\ \mathbf{V}(\ell_2,1,\ell_2-1)},\ell_3-1)\odot^{\ell_3-1}\mathbf{V}(\ell_3-1,\underbrace{\ell_2-1,\ell_1}_{\odot^{\ell_2-1}})}^{\odot^{\ell_1}}$$
$$= \frac{1}{\sqrt{(2\ell_2+1)(2\ell_3+1)}}\mathbf{V}(\ell_3\underbrace{-1,\ell_2-1,\ell_1)\odot^{\ell_1+\ell_2-1}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3+1}(\ )}_{\odot^{\ell_3-1}}{}^{\ell_3-1}\mathbf{U}$$
$$= \sqrt{\frac{\Omega(\ell_1,\ell_2,\ell_3)}{\Omega(\ell_1,\ell_2-1,\ell_3-1)}}\frac{(-1)^{\ell_1+\ell_2+\ell_3}}{\sqrt{(2\ell_2+1)(2\ell_3+1)}}$$
$$= (-1)^{\ell_1+\ell_2+\ell_3}\left[\frac{(L+1)L(L-2\ell_1)(L-2\ell_1-1)}{(2\ell_2+1)(2\ell_2)(2\ell_2-1)(2\ell_3+1)(2\ell_3)(2\ell_3-1)}\right]^{1/2}. \tag{8.16}$$

The root of the Omega factors arise from the $\mathbf{U}$ contraction of $\mathbf{T}(\ell_1,\ell_2,\ell_3)$, Eq. (6.69) coupled with the change in normalization factors between $\mathbf{T}$ and $\mathbf{V}$, Eq. (6.9).

When $b=1$, the tensor algebra is simpler, with the $\mathbf{E}^{(\ell)}$ contractions leading to

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ 1 & \ell_3-1 & \ell_2+1 \end{Bmatrix}$$
$$= \frac{1}{\sqrt{(2\ell_3+1)(2\ell_2+3)}}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_1+\ell_2+\ell_3}\mathbf{V}(\ell_3-1,\ell_2+1,\ell_1)$$

$$= \sqrt{\frac{\Omega(\ell_3,\ell_2,\ell_1)}{(2\ell_3+1)(2\ell_2+3)\Omega(\ell_3-1,\ell_2+1,\ell_1)}}\,\frac{(L-2\ell_3+2)(L-2\ell_3+1)}{(2\ell_2+2)(2\ell_2+1)}(-1)^L$$

$$= (-1)^L\sqrt{\frac{(L-2\ell_2)(L-2\ell_2-1)(L-2\ell_3+2)(L-2\ell_3+1)}{(2\ell_3+1)(2\ell_3)(2\ell_3-1)(2\ell_2+3)(2\ell_2+2)(2\ell_2+1)}}. \tag{8.17}$$

Here the essential contraction is of the type described in Eq. (6.76).

Finally, for $b = 0$, the 6-j can easily be reduced to the contraction

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ 1 & \ell_3-1 & \ell_2 \end{Bmatrix} = \frac{1}{\sqrt{(2\ell_3+1)\Omega(\ell_2,1,\ell_2)}}$$

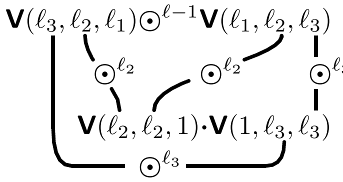
$$\times\left[\underbrace{(\,)\odot^{\ell_3-1}\mathbf{V}(\ell_3-1,\ell_2,\ell_1)\odot^{\ell_1+\ell_2-1}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3-1}(\,)}\,{}^{\ell_3-1}\right]\odot^3\boldsymbol{\varepsilon}\,. \tag{8.18}$$

The subsequent evaluation requires the expansion of at least one of the 3-j's. If the expansion according to Eq. (6.7) or (6.8) [corresponding to whether $L = \ell_1+\ell_2+\ell_3$ is odd or even] is applied to the 3-j having the $\ell_3 - 1$, with a further expansion of $\mathbf{E}^{(\ell_2)}$ made according to Eq. (3.60), the contractions can be simplified. The end result is

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ 1 & \ell_3-1 & \ell_2 \end{Bmatrix} = (-1)^L\sqrt{\frac{2(L+1)(L-2\ell_1)(L-2\ell_2)(L-2\ell_3+1)}{(2\ell_3-1)(2\ell_3)(2\ell_3+1)(2\ell_2)(2\ell_2+1)(2\ell_2+2)}}. \tag{8.19}$$

The evaluation of the 6-j for the $a = b = 0$ case is more involved because two, and possibly four, of the 3-j's involve an $\boldsymbol{\varepsilon}$, thus

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ 1 & \ell_3 & \ell_2 \end{Bmatrix} = (-1)$$



$$= \frac{1}{\sqrt{\Omega(\ell_2,1,\ell_2)\Omega(\ell_3,1,\ell_3)}}$$

$$\times\Big[\underbrace{(\,)^{\ell_3-1}\odot^{\ell_3+1}\mathbf{V}(\ell_3,\ell_2,\ell_1)\odot^{\ell_1+\ell_2-1}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3+1}(\,)^{\ell_3-1}}$$

$$-\mathbf{U}\underbrace{(\,)^{\ell_3-1}\odot^{\ell_3+1}\mathbf{V}(\ell_3,\ell_2,\ell_1)\odot^{\ell_1+\ell_2-1}\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3+1}(\,)^{\ell_3-1}}\mathbf{U}\Big], \tag{8.20}$$

where the factor $\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}$ arising from $\mathbf{V}(\ell_2,\ell_2,1)\cdot\mathbf{V}(1,\ell_3,\ell_3)$ has been evaluated from Eq. (2.81) to give rise to the combination of contractions of the two remaining 3-j tensors. The -1 comes from reordering the indices in $\mathbf{V}(\ell_2,\ell_2,1)$. Now the second contraction involves reducing the values of two of the indices of a 3-j, this follows Eq. (6.69), and the subsequent evaluation of the norm of the result leads to the net value of $[L = \ell_1 + \ell_2 + \ell_3]$

$$(-1)^L \Omega(\ell_1, \ell_2, \ell_3)/\Omega(\ell_1, \ell_2 - 1, \ell_3 - 1). \tag{8.21}$$

The first contraction involves two cases of transposing one vector direction from one symmetric traceless set to another. In the case that L is odd, it is noticed that the transpositions must either not involve the $\boldsymbol{\varepsilon}$'s in the 3-j's, or else both must act to exchange the order of the contractions. The presence of the latter possibility means that the intermediary calculation for even and odd L is different. An expansion of one of the 3-j's according to Eqs. (6.13) or (6.42) results in the contraction being given by

$$\left[(\beta\gamma + \alpha)x_{0,0,0} + 2(\beta+1)x_{0,1,0} + 2(\gamma+1)x_{0,0,1} + 4x_{0,1,1}\right]/(\ell_2\ell_3) \tag{8.22}$$

for L even and

$$-\left[(\beta\gamma + \alpha - 1)x_{0,0,0} + 2(\beta+1)x_{0,1,0} + 2(\gamma+1)x_{0,0,1} + 4x_{0,1,1}\right]/(\ell_2\ell_3) \tag{8.23}$$

for L odd. On putting these intermediary results together and after lengthy simplifications, the 6-j can be written, for both even and odd L, in the form

$$\left\{\begin{array}{ccc} \ell_1 & \ell_2 & \ell_3 \\ 1 & \ell_3 & \ell_2 \end{array}\right\} = \frac{2(-1)^L[\ell_1(\ell_1+1) - \ell_2(\ell_2+1) - \ell_3(\ell_3+1)]}{\sqrt{(2\ell_2)(2\ell_2+1)(2\ell_2+2)(2\ell_3)(2\ell_3+1)(2\ell_3+2)}}. \tag{8.24}$$

8.3.2 The case when $\ell_3 = \ell_1 + \ell_2$

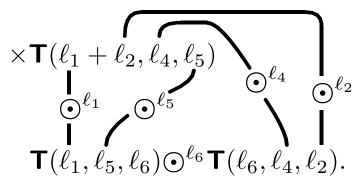
The computation of such 6-j's requires the consideration of three different possibilities. First is the case in which all 3-j tensors are even ordered, while if two 3-j's are of odd order, it is necessary to consider separately whether the 3-j having the traceless symmetric set of order $\ell_1 + \ell_2$ is not or is of odd order. In fact, in all cases, the result can be written in the common form

$$\left\{\begin{array}{ccc} \ell_1 & \ell_2 & \ell_1+\ell_2 \\ \ell_4 & \ell_5 & \ell_6 \end{array}\right\} = (-1)^{\ell_1+\ell_2+\ell_4+\ell_5} \times\sqrt{\frac{(2\ell_1)!(2\ell_2)!(\ell_1+\ell_2+\ell_4+\ell_5+1)!(\ell_1+\ell_2+\ell_5-\ell_4)!(\ell_1+\ell_2+\ell_4-\ell_5)!(\ell_5+\ell_6-\ell_1)!(\ell_4+\ell_6-\ell_2)!}{(2\ell_1+2\ell_2+1)!(\ell_4+\ell_5-\ell_1-\ell_2)!(\ell_1+\ell_5+\ell_6+1)!(\ell_4+\ell_2+\ell_6+1)!(\ell_1+\ell_6-\ell_5)!(\ell_1+\ell_5-\ell_6)!(\ell_2+\ell_4-\ell_6)!(\ell_2+\ell_6-\ell_4)!}}. \tag{8.25}$$

The deduction of this result is considered in detail for the case in which all 3-j tensors are of even order, while comments on the calculation for the other two cases are sketched.

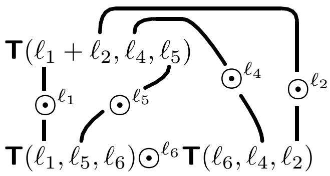
In all cases the 3-j involving ℓ_1 and ℓ_2 is governed by $\mathbf{E}^{(\ell_1+\ell_2)}$ so, after taking out the normalizations of the various 3-j tensors, the 6-j can be written in terms of the contraction of three $\mathbf{T}$ tensors,

$$\left\{\begin{array}{ccc} \ell_1 & \ell_2 & \ell_1+\ell_2 \\ \ell_4 & \ell_5 & \ell_6 \end{array}\right\} = \frac{1}{\sqrt{(2\ell_1+2\ell_2+1)\Omega(\ell_1,\ell_5,\ell_6)\Omega(\ell_4,\ell_5,\ell_1+\ell_2)\Omega(\ell_4,\ell_2,\ell_6)}}$$



(8.26)

For the case that all 3-j tensors have even order, the structure of $\mathbf{T}(\ell_1,\ell_5,\ell_6)$ as given by Eq. (6.7) has $\gamma \equiv (\ell_1+\ell_5-\ell_6)/2$ $\mathbf{U}$'s connecting $\mathbf{E}^{(\ell_1)}$ and $\mathbf{E}^{(\ell_5)}$. These can be used to contract the dominant $\mathbf{T}$ in Eq. (8.26), namely $\mathbf{T}(\ell_1+\ell_2,\ell_4,\ell_5)$, reducing $\mathbf{T}(\ell_1,\ell_5,\ell_6)$ to $\mathbf{E}^{(\ell_6)}$. The same procedure can be applied to $\mathbf{T}(\ell_6,\ell_4,\ell_2)$, since there are $v \equiv (\ell_2+\ell_4-\ell_6)/2$ $\mathbf{U}$'s connecting $\mathbf{E}^{(\ell_4)}$ and $\mathbf{E}^{(\ell_2)}$. Thus the tensor in Eq. (8.26) reduces to



$$= \frac{\Omega(\ell_1+\ell_2,\ell_4,\ell_5)}{\Omega(\ell_1+\ell_2-\gamma-v,\ell_4-v,\ell_5-\gamma)} \;\mathbf{T}(\ell_1-\gamma+\ell_2-v,\ell_4-v,\ell_5-\gamma)\;\odot^{\ell_1-\gamma}\;\odot^{\ell_2-v}\;\odot^{\ell_4-v}\;(\,)^{\ell_1-\gamma}(\,)^{\ell_5-\gamma}\odot^{\ell_6}\mathbf{E}^{\ell_6}\odot^{\ell_6}(\,)^{\ell_2-v}(\,)^{\ell_4-v}\;\odot^{\ell_5-\gamma} \tag{8.27}$$

Here $\mathbf{E}^{(\ell_6)}$ is contracted on the left into the tensor product of orders $\ell_1-\gamma$ and $\ell_5-\gamma$, and on the right into tensors of order ℓ_2-v and ℓ_4-v. To proceed further, the expansion of $\mathbf{E}^{(\ell_6)}$, Eq. (3.49), is used. For the tth term there are t $\mathbf{U}$'s that are available for contraction between the $\ell_1-\gamma$ and $\ell_5-\gamma$ directions. Any other use of these $\mathbf{U}$'s gives a vanishing contribution to the 6-j. A count of the fraction of ways that these contractions contribute is needed. For the first $\mathbf{U}$ the fraction of ways is

$$2\frac{(\ell_1-\gamma)(\ell_5-\gamma)}{\ell_6(\ell_6-1)}, \tag{8.28}$$

with the 2 associated with whether the first or second index of $\mathbf{U}$ is dotted into $\ell_1-\gamma$. For the t $\mathbf{U}$'s, the successive application of this gives the fraction

$$\frac{2^t(\ell_1-\gamma)!(\ell_5-\gamma)!(\ell_6-2t)!}{(\ell_1-\gamma-t)!(\ell_5-\gamma-t)!\ell_6!} \tag{8.29}$$

of ways the t $\mathbf{U}$'s on the lefthand side of $\mathbf{E}^{(\ell_6)}$ contribute to the evaluation of the 6-j. A similar calculation is made for the righthand side. The net result for the tensor in Eq. (8.27) is the product of the fractions associated with the $\mathbf{U}$ contractions, an appropriate Ω ratio and the tensor contraction

$$\mathbf{T}(\ell_1-\gamma-t+\ell_2-v-t,\ell_4-v-t,\ell_5-\gamma-t)\;\odot^{\ell_1-\gamma-t}\;\odot^{\ell_2-v-t}\;\odot^{\ell_4-v-t}\;\odot^{\ell_5-\gamma-t}\;(\,)^{\ell_1-\gamma-t}\odot^{\ell_1-\gamma-t}\{(\,)^{\ell_2-v-t}(\,)^{\ell_4-v-t}\}^{(\ell_6-2t)}\odot^{\ell_5-\gamma-t}(\,)^{\ell_5-\gamma-t}. \tag{8.30}$$

In order to assess the number of possible ways in which the $\ell_1-\gamma-t$ and $\ell_5-\gamma-t$ sets of directions can be contracted with the ℓ_2-v-t and ℓ_4-v-t sets, it is initially assumed that $\ell_1-\gamma-t$ is less than ℓ_2-v-t. It is also noted that a contraction between a $\ell_1-\gamma-t$ and ℓ_2-v-t direction gives a null result because of the traceless nature of the set of directions of $\mathbf{T}(\cdots)$ into which both are contracted. Thus all the $\ell_1-\gamma-t$ directions must be contracted into the ℓ_4-v-t directions, which corresponds to the fraction

$$\frac{(\ell_4-v-t)!(\ell_5-\gamma-t)!}{(\ell_4-v-\ell_1+\gamma)!(\ell_6-2t)!} \tag{8.31}$$

of the possible ways in which all possible contractions could occur. The contraction of the $\mathbf{T}(\cdots)$ gives the corresponding Ω normalization factor. Collecting these results together implies that the 6-j with all even ordered 3-j tensors is equal to

$$\begin{aligned}\left\{\begin{array}{ccc}\ell_1 & \ell_2 & \ell_1+\ell_2\\ \ell_4 & \ell_5 & \ell_6\end{array}\right\} &= \sqrt{\frac{\Omega(\ell_1+\ell_2,\ell_4,\ell_5)}{(2\ell_1+2\ell_2+1)\Omega(\ell_1,\ell_5,\ell_6)\Omega(\ell_4,\ell_2,\ell_6)}}\\ &\times\frac{(\ell_5-\gamma)!(\ell_4-v)!}{(2\ell_6)!(\ell_4-v-\ell_1+\gamma)!}Y(\ell_1-\gamma,\ell_2-v,\ell_6),\end{aligned} \tag{8.32}$$

where

$$\begin{aligned}Y(a,b,\ell) &\equiv \frac{a!b!(2\ell)!}{(\ell!)^2}\sum_t c_t^{(\ell)}\frac{2^{2t}(\ell-2t)!}{(a-t)!(b-t)!}\\ &= \sum_t\frac{(-1)^t2^{2t}(2\ell-2t)!a!b!}{t!(\ell-t)!(a-t)!(b-t)!}.\end{aligned} \tag{8.33}$$

It is possible to identify $Y(a,b,\ell)$ in terms of the hypergeometric function,

$$Y(a,b,\ell)=\frac{2^{2\ell}\Gamma(\ell+1/2)}{\sqrt{\pi}}F(-a,-b;-\ell+1/2;1), \tag{8.34}$$

but the standard evaluation of this hypergeometric function, Eq. HTF(2.1.14), requires a condition on its parameters which may not be satisfied. An alternative calculation of $Y(a,b,\ell)$ is as follows. First get rid of the factorial involving $2t$ by use of the formula for $\Gamma(2z)$, Eq. HTF(1.2.15), and re-express the terms in the sum as combinatorial factors [the choice of basing this on a or b is arbitrary]

$$Y(a,b,\ell)=\frac{b!2^{2\ell}}{\sqrt{\pi}}(\ell-b-1/2)!\sum_t(-1)^t\binom{a}{t}\binom{\ell-t-1/2}{b-t}. \tag{8.35}$$

This sum can be recognized as fitting the form of one of the formulas of Edmonds [1] Appendix 1, or equivalently can be identified as the coefficient of u^b in the identity

$$\begin{aligned}(1+u)^{\ell-a-1/2} &= \sum_m\binom{\ell-a-1/2}{m}u^m\\ &= (1+u)^{\ell-1/2}\left[1-\frac{u}{1+u}\right]^a=\sum_t(-1)^t\binom{a}{t}u^t(1+u)^{\ell-t-1/2}\\ &= \sum_t(-1)^t\binom{a}{t}\sum_n\binom{\ell-t-1/2}{n}u^{n+t}.\end{aligned} \tag{8.36}$$

The result is that

$$Y(a,b,\ell) = \frac{2^{2\ell}}{\sqrt{\pi}} \frac{(\ell-a-1/2)!(\ell-b-1/2)!}{(\ell-a-b-1/2)!}. \tag{8.37}$$

Applying this to Eq. (8.32), together with various rewritings of the factorials gives Eq. (8.25) for the evaluation of the 6-j with all 3-j's being even ordered tensors. It is noticed that this expression is symmetric to the interchange of the first two columns of the 6-j, so the assumption that $\ell_1 - \gamma$ is less than $\ell_2 - v$ can be repeated with the opposite assumption to yield the same result.

For the case in which $\ell_1 + \ell_5 + \ell_6$ and $\ell_1 + \ell_2 + \ell_4 + \ell_5$ are both odd, Eq. (8.27) is modified by the addition of an $\boldsymbol{\mathcal{E}}$ on the left hand side of $\mathbf{E}^{(\ell_6)}$, γ is now given by $\gamma = (\ell_1 + \ell_5 - \ell_6 - 1)/2$ while v is still given by $(\ell_2 + \ell_4 - \ell_6)/2$. The other two directions of $\boldsymbol{\mathcal{E}}$ are dotted respectively into the $\ell_1 - v$ and $\ell_5 - \gamma$ sets of directions of the $\mathbf{T}$ tensor. On expansion of $\mathbf{E}^{(\ell_6)}$, the structure of the tth term of that line of Eq. (8.27) becomes

$$\boldsymbol{\mathcal{E}}\,(\mathbf{I})^{\ell_1-\gamma-1}(\mathbf{I})^{\ell_5-\gamma-1}\odot^{\ell_6}\{(\mathbf{U})^t(\underbrace{\mathbf{|})^{\ell_6-2t}\}^{(\ell_6)}\{(\mathbf{|}}\,)^{\ell_6-2t}(\mathbf{U})^t\}^{\ell_6}\odot^{\ell_6}(\mathbf{I})^{\ell_2-v}(\mathbf{I})^{\ell_4-v}. \tag{8.38}$$

The only nonvanishing contribution comes from having the third direction of $\boldsymbol{\mathcal{E}}$ dotted into the $\ell_4 - v$ set of directions of the $\mathbf{T}$. The fraction of the possible ways in which this can be done is

$$\frac{(\ell_6 - 2t)(\ell_4 - v)}{(\ell_6)^2}.$$

As a result, the $\mathbf{T}$ tensor is contracted with a normalization ratio as follows

$$\begin{aligned} \mathbf{T}(\ell_1+\ell_2-\gamma-v,\ell_4-v,\ell_5-\gamma) \rightarrow \\ \frac{-\Omega(\ell_1+\ell_2-\gamma-v,\ell_4-v,\ell_5-\gamma)}{\Omega(\ell_1+\ell_2-\gamma-v-1,\ell_4-v-1,\ell_5-\gamma-1)} \\ \times\mathbf{T}(\ell_1+\ell_2-\gamma-v-1,\ell_4-v-1,\ell_5-\gamma-1). \end{aligned}$$

The sign comes because of the order in which $\boldsymbol{\mathcal{E}}$ is dotted into the three sets of directions of $\mathbf{T}$. The remaining contractions can be calculated in a manner similar to those leading to Eq. (8.32) with the factor multiplying the root Ω ratio being

$$\frac{\ell_5-\gamma-1)!(\ell_4-v)!}{(2\ell_6)!(\ell_4-v-\ell_1+\gamma)!}Y(\ell_6,\ell_1-\gamma-1,\ell_2-v). \tag{8.39}$$

Evaluation of this with the appropriate γ and v leads to Eq. (8.25) for this case.

Finally, for the case in which $\ell_1 + \ell_5 + \ell_6$ and $\ell_6 + \ell_4 + \ell_2$ odd, Eq. (8.27) is modified by the presence of an $\boldsymbol{\mathcal{E}}$ on both sides of $\mathbf{E}^{(\ell_6)}$. γ is now given by $\gamma = (\ell_1 + \ell_5 - \ell_6 - 1)/2$ while v is given by $(\ell_2 + \ell_4 - \ell_6 - 1)/2$. After an expansion of $\mathbf{E}^{(\ell_6)}$, the nonzero contributions are given only if the $\boldsymbol{\mathcal{E}}$'s are dotted together, with probability $(\ell_6 - 2t)/(\ell_6)^2$, or if each $\boldsymbol{\mathcal{E}}$ is separately contracted into $\mathbf{T}$, with probability

$$\frac{(\ell_6-2t)(\ell_4-v-1)}{(\ell_6)^2}\frac{(\ell_6-2t-1)(\ell_5-\gamma-1)}{(\ell_6-1)^2}. \tag{8.40}$$

The result of the contraction in the first case leads to $\mathbf{T}(\ell_1+\ell_2-\gamma-v-2,\ell_4-v-1,\ell_5-\gamma-1)$ while the second case gives $\mathbf{T}(\ell_1+\ell_2-\gamma-v-2,\ell_4-v-2,\ell_5-\gamma-2)$ with a factor of 2 arising from the first contraction with $\boldsymbol{\varepsilon}$, see Eq. (6.70). The coefficient multiplying the root Ω ratio from this combination of contributions can be written

$$\frac{(\ell_5-\gamma-1)!(\ell_4-v-1)!}{(2\ell_6)!(\ell_4-v-\ell_1+\gamma)!}[1+2(\ell_4-v-\ell_1+\gamma)]Y(\ell_6,\ell_1-\gamma-1,\ell_2-v-1), \tag{8.41}$$

where the two terms in the square bracket are respectively from the first and second $\mathbf{T}$ contractions. Evaluation of the combination of all factors again leads to Eq. (8.25) for this case.

8.3.3 A recursion relation

Equation (8.14) can be used as a basis for formulating a variety of recursion relations for the calculation of the 6-j's. For example, Edmonds [1] uses this relation to get a recursion relation that steps up a set of indices by 1/2. Since irreducible Cartesian tensors do not have 1/2-integral orders, such a recursion relation is not available. But a recursion relation that steps an index by 1 is derived as follows.

Set $\ell_{10}=1$, $\ell_9=\ell_4$ and $\ell_7=\ell_5$ in Eq. (8.14). Also interchange ℓ_6 and ℓ_8 for convenience. After these relabellings, the sum is restricted to ℓ_8 being equal to ℓ_6 and $\ell_6\pm 1$. Since the 6-j symbols having one index equal to 1 have been evaluated, it follows that Eq. (8.14) can be written in the form

$$\left\{\begin{array}{ccc}\ell_1&\ell_2&\ell_3\\ \ell_4&\ell_5&\ell_6\end{array}\right\}=A_{-1}\left\{\begin{array}{ccc}\ell_1&\ell_2&\ell_3\\ \ell_4&\ell_5&\ell_6-1\end{array}\right\}+A_0\left\{\begin{array}{ccc}\ell_1&\ell_2&\ell_3\\ \ell_4&\ell_5&\ell_6\end{array}\right\}+A_{+1}\left\{\begin{array}{ccc}\ell_1&\ell_2&\ell_3\\ \ell_4&\ell_5&\ell_6+1\end{array}\right\} \tag{8.42}$$

with the A_k coefficients given by

$$A_k=\frac{(-1)^{\ell_1+\ell_2+\ell_3+k+1}(2\ell_6+2k+1)}{\left\{\begin{array}{ccc}\ell_3&\ell_4&\ell_5\\ 1&\ell_5&\ell_4\end{array}\right\}}\left\{\begin{array}{ccc}\ell_1&\ell_5&\ell_6+k\\ 1&\ell_6&\ell_5\end{array}\right\}\left\{\begin{array}{ccc}\ell_2&\ell_4&\ell_6+k\\ 1&\ell_6&\ell_4\end{array}\right\}. \tag{8.43}$$

These coefficients can be calculated from previous formulas given in this section. One way of implementing this recursion relation is to rearrange the relation to solve for the 6-j having ℓ_6-1 in terms of the 6-j's having ℓ_6 and ℓ_6+1. An initial starting point for this recursion relation could be for $\ell_6=\min(\ell_1+\ell_5,\ell_4+\ell_2)$ whose 6-j value is given by Eq. (8.25). On the further recognition that any 6-j vanishes that does not satisfy the triangle conditions for any 3-j tensors forming the 6-j, the recursion relation for this maximal value of ℓ_6 determines the value of the 6-j for ℓ_6-1 in terms of the ratio $(1-A_0)/A_{-1}$. Subsequent applications of the recursion relation provides a way to calculate the 6-j symbol for successively smaller values of ℓ_6. Since this recursion relation involves changing only one index, it may be more efficient than the recursion relation given by Edmonds, since that recursion relation apparently involves keeping track of the changes in three indices.

8.4 The 9-j Symbol

A 9-j symbol involves the contraction of six 3-j tensors in such a way that the contraction does not break into two pieces. That is, the contractions between the 3-j's must interlock each other in such a way that an imaginary cutting of the contractions of three of the sets of symmetric traceless sets does not break the contraction of the six 3-j tensors into two pieces. If it does break the contraction in two, the rotational invariance of the combination of 3-j tensors on one side of the break implies that it is proportional to a 3-j tensor. Necessarily the coefficient of proportionality is a 6-j symbol and the calculation of the other part is a second 6-j symbol.

The basic definition of the 9-j symbol together with an expansion in terms of a sum of products of 6-j's can be found in the following way. Start by contracting Eq. (8.10) through the ℓ_5 index with $\mathbf{V}(\ell_5,\ell_6,\ell_7)$ [change the summation index to ℓ_{10} and the order of the indices in one of the 3-j's on the right hand side to make the contracted form simpler] to give

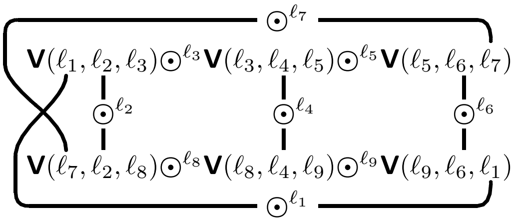
$$\mathbf{V}(\ell_1,\ell_2,\ell_3)\odot^{\ell_3}\mathbf{V}(\ell_3,\ell_4,\ell_5)\odot^{\ell_5}\mathbf{V}(\ell_5,\ell_6,\ell_7) = \sum_{\ell_{10}}(2\ell_{10}+1)\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ \ell_4 & \ell_5 & \ell_{10} \end{Bmatrix}$$
$$\times(-1)^{\ell_1+\ell_5+\ell_{10}}\mathbf{V}(\ell_6,\ell_7,\ell_5)\odot^{\ell_5}\mathbf{V}(\ell_5,\ell_1,\ell_{10})\odot^{\ell_{10}}\mathbf{V}(\ell_{10},\ell_4,\ell_2). \tag{8.44}$$

Copy this with changed indices, such that

$$\mathbf{V}(\ell_7,\ell_2,\ell_8)\odot^{\ell_8}\mathbf{V}(\ell_8,\ell_4,\ell_9)\odot^{\ell_9}\mathbf{V}(\ell_9,\ell_6,\ell_1) = \sum_{\ell_{11}}(2\ell_{11}+1)\begin{Bmatrix} \ell_7 & \ell_2 & \ell_8 \\ \ell_4 & \ell_9 & \ell_{11} \end{Bmatrix}$$
$$\times(-1)^{\ell_7+\ell_9+\ell_{11}}\mathbf{V}(\ell_6,\ell_1,\ell_9)\odot^{\ell_9}\mathbf{V}(\ell_9,\ell_7,\ell_{11})\odot^{\ell_{11}}\mathbf{V}(\ell_{11},\ell_4,\ell_2). \tag{8.45}$$

Now contract the lefthand sides of these equations together to give the 9-j symbol

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ \ell_9 & \ell_8 & \ell_4 \\ \ell_6 & \ell_7 & \ell_5 \end{Bmatrix} \equiv$$



(8.46)

In the contraction of the righthand sides, the presence of ℓ_4 and ℓ_2 in two 3-j tensors implies, according to Eq. (7.3), that $\ell_{11}=\ell_{10}$ with the result that the 9-j is given by the single sum

$$\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ \ell_9 & \ell_8 & \ell_4 \\ \ell_6 & \ell_7 & \ell_5 \end{Bmatrix} = \sum_{\ell_{10}}(2\ell_{10}+1)\begin{Bmatrix} \ell_1 & \ell_2 & \ell_3 \\ \ell_4 & \ell_5 & \ell_{10} \end{Bmatrix}\begin{Bmatrix} \ell_7 & \ell_2 & \ell_8 \\ \ell_4 & \ell_9 & \ell_{10} \end{Bmatrix}\begin{Bmatrix} \ell_1 & \ell_5 & \ell_{10} \\ \ell_7 & \ell_9 & \ell_6 \end{Bmatrix}. \tag{8.47}$$

This expansion is often used for the calculation of 9-j symbols.

A standard graphical representation of a 9-j symbol is given in Fig. 8.5. In this, each apex represents a 3-j tensor and each line an ℓ.

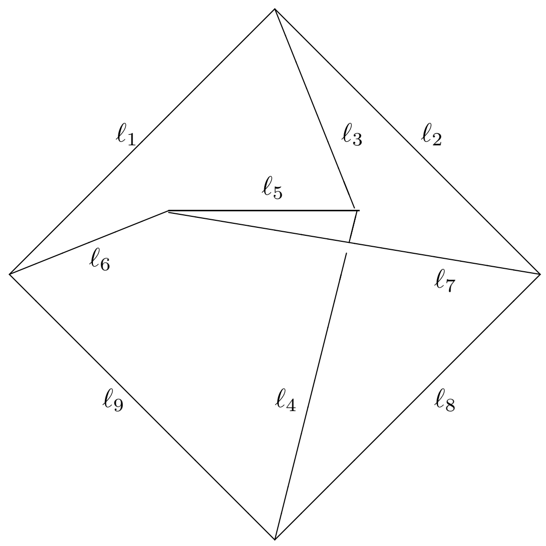


Figure 8.5: The standard figure representing a 9-j

An alternate graphical representation is Fig. 8.6. Now each apex represents an ℓ. Since each ℓ is associated with two 3-j tensors and thus to 4 ℓ's, the four lines joined together at an apex are divided, two to the ℓ's for one 3-j tensor, and two to the ℓ's for the other 3-j tensor.

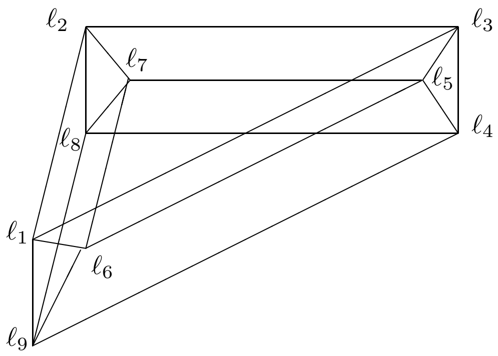


Figure 8.6: The triangular torus representing a 9-j

This triangular torus is to be interpreted as having ℓ_6, ℓ_7 and ℓ_5 as the innermost triangle of the torus. These are the three ℓ's in a 3-j, and in the same cyclic order as in one of the 3-j tensors that appears as a row in the 9-j symbol in Eq. (8.46). The other two rows in the 9-j symbol correspond to the other two triangles parallel to the innermost triangle. On the other hand, the columns of the 9-j correspond to the triangles forming the ring of the torus. As set up, a rotation of the torus by

120° about its symmetry axis interchanges the positions of all ℓ's but retains the cyclic nature of the 3-j tensors of the rows of the 9-j. This is an invariance of the 9-j symbol to a cyclic permutation of the columns of the 9-j. The invariance to a cyclic permutation of the rows corresponds to a rotation, by ±120°, of the ring of the torus. In this way, Fig. 8.6 clearly indicates the cyclic symmetries of the 9-j. The interchange of two rows or two columns of the 9-j inverts the order of the ℓ's in three 3-j tensors. Thus the 9-j symbol changes sign if the sum $\ell_1 + \ell_2 + \ell_3 + \ell_4 + \ell_5 + \ell_6 + \ell_7 + \ell_8 + \ell_9$ of all the ℓ values is odd. In the torus representation of the 9-j, this corresponds to a reflection of the torus, in the plane perpendicular to the symmetry axis for an interchange of two columns, or in a plane containing the symmetry axis for the interchange of two rows.

Invariants formed by the contraction of more 3-j tensors can also be devised, that are moreover not simply decomposable into a product of invariants with fewer 3-j's. Well known are the 12-j and 15-j symbols. Since no attempt is made here to classify all possible invariants, such quantities are not discussed in this book.

Chapter 9

Rotation Matrices

The (active) rotation of a tensor by an angle θ about axis $\hat{n}$ has been discussed in Chap. 3. Essentially this involves rotating each of the p directions of a tensor of order p. This action can be expressed in tensorial form as the contraction of a $2p$ rotation tensor with the initial tensor. While this formal action is simple in principle, calculating the resulting tensor can become complicated. The classic manner in which this is done is to express both initial and final tensors in spherical tensor form with the rotation represented by a matrix. This can clearly be obtained from the rotation tensor with the use of the spherical tensor basis elements $\mathbf{e}^{(\ell)n}$ and/or $\mathbf{e}_n^{(\ell)}$ of Sec. 5.4, but which choice is to be used? The standard result is equivalent to

$$D_{mn}^{(\ell)}(R_{\hat{n}}(\theta)) \equiv \mathbf{e}_m^{(\ell)} \odot^{\ell} \mathsf{R}_{\hat{n}}^{(\ell)}(\theta) \odot^{\ell} \mathbf{e}^{(\ell)n}. \tag{9.1}$$

Another way of interpreting this choice is that this matrix describes the active rotation of the spherical basis tensor $\mathbf{e}^{(\ell)n}$, or more correctly, the above matrix element is the $\mathbf{e}^{(\ell)m}\underline{\text{th}}$ component of the rotated spherical basis tensor, as in the expansion of the rotated tensor

$$\mathsf{R}_{\hat{n}}^{(\ell)}(\theta) \odot^{\ell} \mathbf{e}^{(\ell)n} = \sum_m \mathbf{e}^{(\ell)m} \odot^{\ell} D_{mn}^{(\ell)}(R_{\hat{n}}(\theta)). \tag{9.2}$$

As an active rotation, the coordinate system is unchanged and the expansion functions, the $\mathbf{e}^{(\ell)m}$, are defined in that coordinate system, so the rows and columns of $D(\ )_{mn}$ refer to that fixed coordinate system. It should also be recognized that the rotated spherical basis tensor is an eigenvector of the generator of rotations about the rotated $\hat{z}$-axis, namely $\hat{z}_R \equiv \mathsf{R}_{\hat{n}}(\theta) \cdot \hat{z}$, that is

$$G_{\hat{z}_R} \mathsf{R}_{\hat{n}}^{(\ell)}(\theta) \odot^{\ell} \mathbf{e}^{(\ell)n} = n \mathsf{R}_{\hat{n}}^{(\ell)}(\theta) \odot^{\ell} \mathbf{e}^{(\ell)n}. \tag{9.3}$$

This has assumed that the spherical basis tensors are eigenvectors of the rotation generator $G_{\hat{z}}$. Most discussions of rotation matrices in the literature have the rotation expressed in terms of Euler angles. But the Euler angles appear in different ways according to how the rotation is used, for example, whether the rotation is active or passive, and according to the convention used by different authors. Some comments are made later in this section about various uses and interpretations of the rotation matrix, but first a detailed calculation of a rotation matrix is given in both the axis and angle representation and in terms of the Euler angles.

9.1 Axis-angle representation

This representation was first given in detail by Moses [30]. The derivation given here is an adaptation of that presentation.

With an emphasis on the axis of rotation, a rotation tensor is the exponential of a rotation generator, Eq. (3.6). A differentiation of that result and taking matrix elements is

$$i\frac{\partial D^{(\ell)}_{mn}(R_{\hat{n}}(\theta))}{\partial\theta} = \sum_{m'} G^{(\ell)}_{mm'} D^{(\ell)}_{m'n}(R_{\hat{n}}(\theta)), \tag{9.4}$$

with

$$\begin{aligned} G^{(\ell)}_{mm'} &= \mathbf{e}^{(\ell)}_m \odot^\ell \mathbf{G}^{(\ell)}_{\hat{n}} \odot^\ell \mathbf{e}^{(\ell)m'} \\ &= \mathbf{e}^{(\ell)}_m \odot^\ell \left[n_z \mathbf{G}^{(\ell)}_{\hat{z}} + (1/2)(n_x - in_y)\mathbf{G}^{(\ell)}_{+} + (1/2)(n_x + in_y)\mathbf{G}^{(\ell)}_{-} \right] \odot^\ell \mathbf{e}^{(\ell)m'} \\ &= mn_z\delta_{m,m'} + (1/2)(n_x - in_y)\sqrt{(\ell - m + 1)(\ell + m)}\delta_{m,m'+1} \\ &\quad +(1/2)(n_x + in_y)\sqrt{(\ell + m + 1)(\ell - m)}\delta_{m,m'-1}. \end{aligned} \tag{9.5}$$

Here n_x, n_y and n_z are the direction cosines of the rotation axis $\hat{n}$ and the tensorial form of the rotation generator $\mathbf{G}^{(\ell)}_{\hat{n}}$ is resolved into its components and expressed in terms of raising and lowering tensors, Eq. (3.18), with the subsequent evaluation of their matrix elements, consistant with Eq. (5.8). The derivative (9.4) of an element of the rotation matrix thus reduces to a sum of three terms involving different values of the first index of the matrix. The set of such equations is to be solved subject to the initial condition $D^{(\ell)}_{mn}(R_{\hat{n}}(0)) = \delta_{mn}$.

The square root and $(n_x \pm in_y)$ factors can be eliminated by the transformation

$$D^{(\ell)}_{mn}(R_{\hat{n}}(\theta)) = \sqrt{\frac{(\ell+m)!(\ell-m)!}{(\ell+n)!(\ell-n)!}}(n_x - in_y)^{m-n} f_{mn}(\theta), \tag{9.6}$$

to give the set of coupled differential equations

$$i\frac{\partial f_{mn}}{\partial\theta} = mn_z f_{mn} + (1/2)(\ell - m + 1)f_{m-1,n} + (1/2)(1 - n_z^2)(\ell + m + 1)f_{m+1,n}, \tag{9.7}$$

subject to the initial condition $f_{mn}(0) = \delta_{mn}$. In this, the dependence on the angle θ and the index ℓ is to be understood. A generating function for the set of functions f_{mn} with fixed n is defined as

$$F_n(\theta, u) \equiv \sum_m u^m f_{mn}(\theta). \tag{9.8}$$

The set of coupled differential equations is then equivalent to the partial differential equation

$$i\frac{\partial F_n}{\partial\theta} + \left[\frac{u^2}{2} - un_z - \frac{1}{2}(1 - n_z^2)\right]\frac{\partial F_n}{\partial u} = \frac{\ell}{2}\left(u + \frac{1 - n_z^2}{u}\right)F_n. \tag{9.9}$$

As a first order partial differential equation, this can be solved by the method of characteristics, whose curves

$$\frac{u - n_z - 1}{u - n_z + 1} = e^{-i(\theta-\chi)} \tag{9.10}$$

are parameterized by χ. Along a characteristic curve F_n is given by

$$F_n = C\left[\frac{(u-n_z)^2-1}{u}\right]^\ell. \tag{9.11}$$

On making use of the initial condition $F_n(0,u) = u^n$ to determine the value of the constant C for each characteristic curve, it follows after some rearrangement, that the generating function is

$$F_n(\theta,u) = u^n\left[\cos\frac{\theta}{2} - \left(n_z + \frac{1-n_z^2}{u}\right)i\sin\frac{\theta}{2}\right]^{\ell+n}\left[\cos\frac{\theta}{2} - (u-n_z)i\sin\frac{\theta}{2}\right]^{\ell-n}. \tag{9.12}$$

To get back to the f_{mn}'s, two binomial expansions are required to collect the powers of u, with the result that

$$\begin{aligned} f_{mn}(\theta) &= \sum_r \binom{\ell+n}{r}\binom{\ell-n}{m+r-n}(1-n_z^2)^r\left(-i\sin\frac{\theta}{2}\right)^{m-n+2r} \\ &\times\left(\cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2}\right)^{\ell+n-r}\left(\cos\frac{\theta}{2} + in_z\sin\frac{\theta}{2}\right)^{\ell-m-r}. \end{aligned} \tag{9.13}$$

There are many ways of parameterizing this sum and arranging the factors. To compare with Moses' [30] equation, r is replaced by $q = \ell - m - r$ as a summation index and the factors organized so that

$$\begin{aligned} f_{mn}(\theta) &= \left(-i\sin\frac{\theta}{2}\right)^{m-n}\left(\cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2}\right)^{m+n}\sum_q\binom{\ell+n}{m+n+q} \\ &\times\binom{\ell-n}{q}\left(-(1-n_z^2)\sin^2\frac{\theta}{2}\right)^{\ell-m-q}\left(\cos^2\frac{\theta}{2} + n_z^2\sin^2\frac{\theta}{2}\right)^q. \end{aligned} \tag{9.14}$$

On introducing the quantity $v \equiv (1-n_z^2)\cos\theta + n_z^2$ (Moses uses z), then

$$\begin{aligned} v+1 &= 2\left(\cos^2\frac{\theta}{2} + n_z^2\sin^2\frac{\theta}{2}\right) \\ v-1 &= -2(1-n_z^2)\sin^2\frac{\theta}{2} \end{aligned}$$

and f_{mn} can be simplified to

$$\begin{aligned} f_{mn}(\theta) &= \left(-i\sin\frac{\theta}{2}\right)^{m-n}\left(\cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2}\right)^{m+n} 2^{m-\ell} \\ &\times\sum_q\binom{\ell+n}{m+n+q}\binom{\ell-n}{q}(v-1)^{\ell-m-q}(v+1)^q \\ &= \left(-i\sin\frac{\theta}{2}\right)^{m-n}\left(\cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2}\right)^{m+n} P_{\ell-m}^{m-n,m+n}(v), \end{aligned} \tag{9.15}$$

involving the Jacobi polynomial, Eq. HTF(10.8.12) of Ref. [24]. Combined with the prefactors to get the corresponding rotation matrix, the latter is

$$\begin{aligned} D^{(\ell)}_{mn}(R_{\hat{n}}(\theta)) &= \sqrt{\frac{(\ell+m)!(\ell-m)!}{(\ell+n)!(\ell-n)!}} \left[-i(n_x - in_y)\sin\frac{\theta}{2}\right]^{m-n} \\ &\times \left(\cos\frac{\theta}{2} - in_z \sin\frac{\theta}{2}\right)^{m+n} P^{m-n,m+n}_{\ell-m}((1-n_z^2)\cos\theta + n_z^2). \end{aligned} \tag{9.16}$$

This agrees with Moses quantum equation after taking into account his different phase convention for his bra's and ket's as well as changing the sign of all the components of $\hat{n}$, since his equation is for a rotation about the opposite direction. Possibly a more symmetrical representation is

$$\begin{aligned} D^{(\ell)}_{mn}(R_{\hat{n}}(\theta)) &= \sqrt{\frac{(\ell+m)!(\ell-m)!}{(\ell+n)!(\ell-n)!}} \left[-i(n_x - in_y)\sin\frac{\theta}{2}\right]^{m-n} \\ &\times \sum_q \binom{\ell+n}{m+n+q}\binom{\ell-n}{q} \left[-(1-n_z^2)\sin^2\frac{\theta}{2}\right]^{\ell-m-q} \\ &\times \left(\cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2}\right)^{m+n+q} \left(\cos\frac{\theta}{2} + in_z\sin\frac{\theta}{2}\right)^{q}. \end{aligned} \tag{9.17}$$

This also has all quantities explicitly displayed rather than having to refer to Jacobi polynomials.

9.2 Euler angle representation

Expressed in terms of Euler angles, the rotation matrix is

$$\begin{aligned} D^{(\ell)}_{mn}(\alpha,\beta,\gamma) &= \mathbf{e}^{(\ell)}_m \odot^\ell \mathbf{R}^{(\ell)}_{\hat{z}}(\alpha) \odot^\ell \mathbf{R}^{(\ell)}_{\hat{y}}(\beta) \odot^\ell \mathbf{R}^{(\ell)}_{\hat{z}}(\gamma) \odot^\ell \mathbf{e}^{(\ell)n} \\ &= \sum_{n'n''} D^{(\ell)}_{mn''}(R_{\hat{z}}(\alpha)) D^{(\ell)}_{n''n'}(R_{\hat{y}}(\beta)) D^{(\ell)}_{n'n}(R_{\hat{z}}(\gamma)) \\ &= e^{-im\alpha} D^{(\ell)}_{mn}(R_{\hat{y}}(\beta)) e^{-in\gamma}. \end{aligned} \tag{9.18}$$

Here a listing of the Euler angles in $D^{(\ell)}_{mn}$ has been introduced as a shorthand notation for a full description in terms of the set of rotation operators. The rotation matrix for a rotation about the $\hat{y}$-axis can be obtained directly from Eq. (9.17), namely

$$\begin{aligned} d^{(\ell)}(\beta)_{mn} &\equiv D^{(\ell)}_{mn}(R_{\hat{y}}(\beta)) = \left[\frac{(\ell+m)!(\ell-m)!}{(\ell+n)!(\ell-n)!}\right]^{1/2} \sum_q \binom{\ell+n}{\ell-m-q}\binom{\ell-n}{q} \\ &\times (-1)^{\ell-n-q} (\cos\frac{\beta}{2})^{m+n+2q} (\sin\frac{\beta}{2})^{2\ell-m-n-2q}. \end{aligned} \tag{9.19}$$

This result is equal to Eq. (4.13) of Rose [2], but differs from that given by Edmonds [1] and Wigner [3]. As a summary,

$$D^{(\ell)}_{mn}(0,\beta,0) = d^{(\ell)}_{mn}(\beta)\Big|_{\text{Rose}} = (-1)^{m+n} d^{(\ell)}_{mn}(\beta)\Big|_{\text{Edmonds}}$$

$$\begin{aligned} &= (-1)^{m+n} D^{(\ell)}_{mn}(0,-\beta,0) = (-1)^{m+n} D^{(\ell)}_{-m,-n}(0,\beta,0) \\ &= (-1)^{m+n} D^{(\ell)}_{nm}(0,\beta,0) \end{aligned} \tag{9.20}$$

gives these relations together with the symmetry properties of the $D^{(\ell)}_{mn}(0,\beta,0)$.

Edmonds [1], and Wigner [3], define a rotation matrix

$$\mathcal{D}^{(\ell)}_{mn}(\alpha,\beta,\gamma) = D^{(\ell)}_{mn}(-\alpha,-\beta,-\gamma) = \mathbf{e}^{(\ell)m} \odot^{\ell} \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma) \odot^{\ell} \mathbf{e}^{(\ell)}_{n}. \tag{9.21}$$

The simple reversal of signs of the angles does not fit naturally into the rotation properties of the tensors as presented here, corresponding to neither the inverse rotation (equivalently the passive rotation - possibly related to a left versus righthanded coordinate system) so these matrices are not used in this book. Interestingly, they appear to correspond to the active rotation of the covariant basis set instead of the contravariant basis set.

9.2.1 Alternate formula

The rotation matrix for a rotation about the $\hat{y}$-axis can also be obtained as a product of vector rotation matrices, taking into account all the combinations of vector basis elements required by the symmetric traceless nature of the tensor bases. This provides an alternate method of calculating the rotation matrix. Such a calculation depends on knowing the rotation matrices for the vector case ($\ell = 1$) which is now discussed. In particular, the 11 matrix element is

$$\begin{aligned} D^{(1)}_{11}(0,\beta,0) &= \mathbf{e}^{(1)}_{1} \cdot [\hat{y}\hat{y} + (\mathbf{U} - \hat{y}\hat{y})\cos\beta - \hat{y}\cdot\boldsymbol{\varepsilon}\ \sin\beta] \cdot \mathbf{e}^{(1)1} \\ &= \frac{-1}{\sqrt{2}}(\hat{x} - i\hat{y}) \cdot [\hat{y}\hat{y} + (\mathbf{U} - \hat{y}\hat{y})\cos\beta - \hat{y}\cdot\boldsymbol{\varepsilon}\ \sin\beta] \cdot \frac{-1}{\sqrt{2}}(\hat{x} + i\hat{y}) \\ &= \frac{1}{2}(1 + \cos\beta). \end{aligned} \tag{9.22}$$

Following the same procedure, the matrix $D^{(1)}(0,\beta,0)$ is calculated to be

$m\backslash n$	1	0	-1
1	$\frac{1}{2}(1+\cos\beta)$	$\frac{-1}{\sqrt{2}}\sin\beta$	$\frac{1}{2}(1-\cos\beta)$
0	$\frac{1}{\sqrt{2}}\sin\beta$	$\cos\beta$	$\frac{-1}{\sqrt{2}}\sin\beta$
-1	$\frac{1}{2}(1-\cos\beta)$	$\frac{1}{\sqrt{2}}\sin\beta$	$\frac{1}{2}(1+\cos\beta)$

(9.23)

This corresponds to the matrix given by Rose [2] but differs in the sign of β to that given by Edmonds [1], which is again equivalent to multiplying the matrix elements by $(-1)^{m+n}$. This is attributed to Edmonds' choice of dealing with passive rotations.

A calculation of the general $D^{(\ell)}(0,\beta,0)$ matrix can be accomplished within the Irreducible Cartesian Tensor method and based on the expansion of the $\mathbf{e}^{(\ell)}_{m}$'s and $\mathbf{e}^{(\ell)n}$'s, Eq. (5.49), to give

$$\begin{aligned} D^{(\ell)}_{mn}(0,\beta,0) &= \frac{N_{\ell m}N_{\ell n}}{\binom{\ell}{|m|}} \sum_{tp} a^{\ell|n|}_{t} N^{\ell|n|t}_{|m|;p,|m|-p,0} \left[D^{(1)}_{\mu\nu}(0,\beta,0)\right]^{p} \\ \times \left[D^{(1)}_{0\nu}(0,\beta,0)\right]^{|n|-p} &\left[D^{(1)}_{\mu 0}(0,\beta,0)\right]^{|m|-p} \left[D^{(1)}_{00}(0,\beta,0)\right]^{\ell-|m|-|n|-2t+p}. \end{aligned} \tag{9.24}$$

This is derived in Appendix B. Here μ and ν are defined as being equal to ± 1, corresponding to whether m, respectively n, are positive or negative. Explicitly this reduces to

$$\begin{aligned} D^{(\ell)}_{mn}(0,\beta,0) &= \frac{(-\mu)^m(\nu)^n|m|!|n|!}{2^\ell}\left[\frac{(\ell-|m|)!(\ell-|n|)!}{(\ell+|m|)!(\ell+|n|)!}\right]^{1/2}(\sin\beta)^{|m|+|n|} \\ &\times\sum_{tp}\frac{(-\mu\nu)^p(-1)^{t+p}(2\ell-2t)!(\cos\beta)^{\ell+p-|m|-|n|-2t}}{t!p!(\ell-t)!(|m|-p)!(|n|-p)!(\ell+p-|m|-|n|-2t)!(1-\mu\nu\cos\beta)^p}. \end{aligned} \tag{9.25}$$

This has a different form from Eq. (9.19). Use of various trigonometric relations, see Appendix B, enables this to be written with the same β dependence, but with different coefficients. Computationally, it has been shown that the two expressions are the same, but this author is not aware of an algebraic proof of their equality.

9.3 Connection with Spherical Harmonics

Here the discussion is limited to the 4π normalized versions $\mathcal{Y}^{(\ell)m}(\hat{r}) = \sqrt{4\pi}Y_{\ell m}(\hat{r})$. There are four obvious ways of implementing a rotation of a spherical harmonic, or of any function of a vector, which can be expanded in terms of spherical harmonics. These four way are:

1) Consider the active rotation of a basis tensor, which may be thought of actively rotating the function [indicated here by the subscripts "af" for "active" and "function"] of a parameter $\hat{r}$. Thus, from Eq. (9.2) and using the somewhat obvious abbreviation of a list of the Euler angles for the sequence of rotations,

$$\begin{aligned} R_{af}(\alpha,\beta,\gamma)\mathcal{Y}^{(\ell)n}(\hat{r}) &\equiv \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})\odot^\ell\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)\odot^\ell\mathbf{e}^{(\ell)n} \\ &= \sum_m \mathcal{Y}^{(\ell)m}(\hat{r})D^{(\ell)}_{mn}(\alpha,\beta,\gamma) \end{aligned} \tag{9.26}$$

gives an expansion of the rotated function (spherical harmonic) in terms of the initial set of functions belonging to the same irreducible representation of the rotation group. This relation can be rewritten to interpret the rotation to act on $\hat{r}$, specifically,

$$\begin{aligned} \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})\odot^\ell\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)\odot^\ell\mathbf{e}^{(\ell)n} &= \mathbf{e}^{(\ell)n}\odot^\ell\mathbf{R}^{(\ell)}(-\gamma,-\beta,-\alpha)\odot^\ell\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) \\ &= \sum_m \mathcal{Y}^{(\ell)m}(\hat{r})D^{(\ell)}_{mn}(\alpha,\beta,\gamma). \end{aligned} \tag{9.27}$$

Note that the order in which tensors are contracted to give a scalar is irrelevant so it is easier to write the above contraction in such a way that the rotation tensor is put between the two ℓth order tensors. The rotation acting on $\hat{r}$ is the inverse of the rotation acting on the basis element. If the rotation acting on $\hat{r}$ is considered to act on the components of $\hat{r}$, this rotation can be considered as the effect on those components of a passive rotation. Thus defining the vector

$$\hat{r}''' \equiv x'''\hat{x} + y'''\hat{y} + z'''\hat{z} \tag{9.28}$$

with the passively rotated coordinates $\vec{r}'''$ of $\hat{r}$ [see the "v" analog of this transformation, Eq. (2.146)] and the original vector basis set, then the effect of this passive rotation can be written

$$\mathcal{Y}^{(\ell)n}(\hat{r}''') = \sum_m \mathcal{Y}^{(\ell)m}(\hat{r})D^{(\ell)}_{mn}(\alpha,\beta,\gamma). \tag{9.29}$$

An equivalent way of expressing this result is to consider the spherical harmonics to be functions of the components of a vector, thus

$$\mathcal{Y}^{(\ell)n}(\vec{r}''') = \sum_m \mathcal{Y}^{(\ell)m}(\vec{r}) D^{(\ell)}_{mn}(\alpha,\beta,\gamma). \tag{9.30}$$

Most treatments emphasize the components of a vector (or tensor) rather than its abstract nature, so it is the last form that is commonly presented. In fact this is exactly the form of Eq. (4.28a) of Rose [2], expressed in terms of the usual spherical harmonics, Eq. (5.86).

2) If the vector $\hat{r}$ is rotated actively [subscript v for "variable" replacing f],

$$\begin{aligned} R_{av}(\alpha,\beta,\gamma)\mathcal{Y}^{(\ell)m}(\hat{r}) &\equiv \mathcal{Y}^{(\ell)m}(\mathbf{R}(\alpha,\beta,\gamma)\cdot\hat{r}) = \mathbf{e}^{(\ell)m}\odot^\ell \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)\odot^\ell \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) \\ &= \sum_n \mathbf{e}^{(\ell)m}\odot^\ell \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)\odot^\ell \mathbf{e}^{(\ell)}_n \mathcal{Y}^{(\ell)n}(\hat{r}) \\ &= \sum_n (-1)^{m+n} D^{(\ell)}_{-m,-n}(\alpha,\beta,\gamma)\mathcal{Y}^{(\ell)n}(\hat{r}) \\ &= \sum_n \mathcal{Y}^{(\ell)n}(\hat{r}) D^{(\ell)}_{nm}(-\gamma,-\beta,-\alpha) \end{aligned} \tag{9.31}$$

gives an expansion of the function of the transformed (rotated) variable in terms of functions of the original variable.

3) A third way is to passively [subscript p for "passive"] rotate the function [determined by the tensor $\mathbf{e}^{(\ell)m}$],

$$\begin{aligned} R_{pf}(\alpha,\beta,\gamma)\mathcal{Y}^{(\ell)m}(\hat{r}) &= \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})\odot^\ell \mathbf{R}^{(\ell)}(-\gamma,-\beta,-\alpha)\odot^\ell \mathbf{e}^{(\ell)m} \\ &= \sum_n \mathcal{Y}^{(\ell)n}(\hat{r}) D^{(\ell)}_{nm}(-\gamma,-\beta,-\alpha). \end{aligned} \tag{9.32}$$

Namely the directions determining the function are expressed in terms of the rotated basis vectors, so the detailed nature of the function has been changed. In comparison with 2), it is seen, as it should be, that a passive rotation of a function is equivalent to an active rotation of the variable on which the function depends.

4) Lastly there is the passive rotation of the variable $\hat{r}$,

$$\begin{aligned} R_{pv}(\alpha,\beta,\gamma)\mathcal{Y}^{(\ell)n}(\hat{r}) &= \mathcal{Y}^{(\ell)n}(\mathbf{R}(-\gamma,-\beta,-\alpha)\cdot\hat{r}) \\ &= \mathbf{e}^{(\ell)n}\odot^\ell \mathbf{R}^{(\ell)}(-\gamma,-\beta,-\alpha)\odot^\ell \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r}) \\ &= \sum_m (-1)^{m+n} D^{(\ell)}_{-n,-m}(-\gamma,-\beta,-\alpha)\mathcal{Y}^{(\ell)m}(\hat{r}) \\ &= \sum_m \mathcal{Y}^{(\ell)m}(\hat{r}) D^{(\ell)}_{mn}(\alpha,\beta,\gamma). \end{aligned} \tag{9.33}$$

In this implementation of a rotation, the function of the coordinates of the vector ($\hat{r}$), expressed in terms of the rotated coordinate system, is expanded in terms of functions of the coordinates of the vector expressed in terms of the original coordinate system. This passive rotation of the variable is equivalent to the active rotation of the function, as already stressed in 1).

The rotation properties of the spherical harmonics can also be used to show that the spherical harmonics are special cases of the rotation matrices. If $\hat{r}$ is set to $\hat{z}$, then the corresponding spherical harmonic has only the $m = 0$ component. Thus the active rotation of the spherical harmonic function, af, Eq. (9.30) of 1) above, gives

$$\mathcal{Y}^{(\ell)n}(\vec{z}''') = \sqrt{2\ell+1}D^{(\ell)}_{0n}(\alpha,\beta,\gamma). \tag{9.34}$$

The meaning of $\vec{z}'''$ can be found from Eq. (2.146), namely

$$x''',\ y''',\ z''' = -\sin\beta\cos\gamma,\ \ \sin\beta\sin\gamma,\ \ \cos\beta, \tag{9.35}$$

which implies that the angles in the spherical harmonic are $-\beta$ and $-\gamma$. This can also be obtained by setting $\ell = 1$ in Eq. (9.34) and applying Eq. (9.23). On changing the signs of the angles and expressing everything in terms of angle variables, this can be rewritten

$$\begin{aligned}\mathcal{Y}^{(\ell)n}(\beta,\gamma) &= \sqrt{2\ell+1}D^{(\ell)}_{0n}(0,-\beta,-\gamma)\\ &= (-1)^n\sqrt{2\ell+1}D^{(\ell)}_{-n,0}(\gamma,\beta,0),\end{aligned} \tag{9.36}$$

the latter using the symmetry properties of the $D^{(\ell)}$'s. The last relation can also be written in the form

$$\mathcal{Y}^{(\ell)n*}(\beta,\gamma) = (-1)^n\mathcal{Y}^{(\ell)-n}(\beta,\gamma) = \sqrt{2\ell+1}D^{(\ell)}_{n,0}(\gamma,\beta,0), \tag{9.37}$$

which is the connection reported as Rose's [2] Eq. (4.30). A similar relation can be obtained from the implementation of the active rotation of the variable in the spherical harmonic, namely from Eq. (9.31) by again setting $\hat{r} = \hat{z}$. Now the rotated $\hat{z}$ is the unit vector with angles β and α, compare the third column of the matrix of Eq. (2.118). Then Eq. (9.31) gives

$$\mathcal{Y}^{(\ell)m}(\beta,\alpha) = (-1)^m\sqrt{2\ell+1}D^{(\ell)}_{-m,0}(\alpha,\beta,0), \tag{9.38}$$

which is the same as above except for the replacement of γ by α.

9.4 Properties of the Rotation Matrices

As matrices associated with an irreducible representation of the rotation group, a group multiplication is represented by matrix multiplication. Thus, if R_1 and R_2 are two rotations whose product R_1R_2 is R_3, whose ℓth order rotation tensors are respectively $\mathbf{R}^{(\ell)}_1$, $\mathbf{R}^{(\ell)}_2$ and $\mathbf{R}^{(\ell)}_3$, the rotation matrices satisfy

$$\begin{aligned}D^{(\ell)}_{mn}(R_3) &= \mathbf{e}^{(\ell)}_m\odot^\ell\mathbf{R}^{(\ell)}_3\odot^\ell\mathbf{e}^{(\ell)n} = \mathbf{e}^{(\ell)}_m\odot^\ell\mathbf{R}^{(\ell)}_1\odot^\ell\mathbf{R}^{(\ell)}_2\odot^\ell\mathbf{e}^{(\ell)n}\\ &= \sum_k \mathbf{e}^{(\ell)}_m\odot^\ell\mathbf{R}^{(\ell)}_1\odot\mathbf{e}^{(\ell)k}\mathbf{e}^{(\ell)}_k\odot^\ell\mathbf{R}^{(\ell)}_2\odot^\ell\mathbf{e}^{(\ell)n}\\ &= \sum_k D^{(\ell)}_{mk}(R_1)D^{(\ell)}_{kn}(R_2).\end{aligned} \tag{9.39}$$

In particular, if $R_2 = R_1^{-1}$, the R_3 is the identity and the rotation matrices satisfy

$$\sum_k D^{(\ell)}_{mk}(R_1)D^{(\ell)}_{kn}(R_1^{-1}) = \delta_{mn}. \tag{9.40}$$

Since the rotation matrix of the inverse rotation is the adjoint matrix

$$\begin{aligned} D^{(\ell)}_{kn}(R_1^{-1}) &= \mathbf{e}^{(\ell)}_k \odot^\ell \left[\mathbf{R}^{(\ell)}_1\right]^{-1} \odot^\ell \mathbf{e}^{(\ell)n} \\ &= \mathbf{e}^{(\ell)n} \odot^\ell \mathbf{R}^{(\ell)}_1 \odot^\ell \mathbf{e}^{(\ell)}_k \\ &= (-1)^{n+k} D^{(\ell)}_{-n,-k}(R_1) = D^{(\ell)*}_{nk}(R_1), \end{aligned} \tag{9.41}$$

on the basis of the symmetry properties of the spherical basis elements, this sum becomes an orthonormality relation

$$\sum_k D^{(\ell)}_{mk}(R_1) D^{(\ell)*}_{nk}(R_1) = \delta_{mn}. \tag{9.42}$$

Applying the inverse to the first term rather than to the second gives the other orthonormality relation

$$\sum_k D^{(\ell)*}_{km}(R_1^{-1}) D^{(\ell)}_{kn}(R_1^{-1}) = \delta_{mn}. \tag{9.43}$$

These must be satisfied for all rotations R_1, incidently demonstrating that the rotation matrix is unitary.

A different kind of multiplication formula for the rotation matrices can be obtained from the rotational invariance of the 3-j tensors. Specifically, the rotational invariance of a 3-j tensor can be written

$$\mathbf{R}^{(\ell)} \odot^\ell \mathbf{V}(\ell,\ell_1,\ell_2) = \mathbf{V}(\ell,\ell_1,\ell_2) \odot^{\ell_1+\ell_2} \big[\mathbf{R}^{(\ell_2)} \odot^{\ell_2} \underbrace{(\;)^{\ell_2}\big]\mathbf{R}^{(\ell_1)}(\;)}^{\ell_2}. \tag{9.44}$$

Here the detailed specification of which rotation is considered, i.e., which axis $\hat{n}$ and angle θ or which set of Euler angles, has not been indicated so as to simplify the writing while the tensorial manipulations are emphasized. Now the $\mathbf{e}^{(\ell)}_m \cdots \mathbf{e}^{(\ell_2)n_2}\mathbf{e}^{(\ell_1)n_1}$ matrix element of this symmetry condition, together with the introduction of expansions of the tensor contractions in terms of spherical basis tensors, is

$$\begin{aligned} &\sum_n D^{(\ell)}_{mn} \mathbf{e}^{(\ell)}_n \odot^\ell \mathbf{V}(\ell,\ell_1,\ell_2) \odot^{\ell_1+\ell_2} \mathbf{e}^{(\ell_2)n_2}\mathbf{e}^{(\ell_1)n_1} \\ &\qquad = \sum_{m_1 m_2} \mathbf{e}^{(\ell)}_m \odot^\ell \mathbf{V}(\ell,\ell_1,\ell_2) \odot^{\ell_1+\ell_2} \mathbf{e}^{(\ell_2)m_2}\mathbf{e}^{(\ell_1)m_1} D^{(\ell_1)}_{m_1 n_1} D^{(\ell_2)}_{m_2 n_2} \\ = &\sum_n D^{(\ell)}_{mn} (-1)^n (-i)^{\ell+\ell_1+\ell_2} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -n & n_1 & n_2 \end{pmatrix} \\ &\qquad = \sum_{m_1 m_2} (-1)^m (-i)^{\ell+\ell_1+\ell_2} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -m & m_1 & m_2 \end{pmatrix} D^{(\ell_1)}_{m_1 n_1} D^{(\ell_2)}_{m_2 n_2}, \end{aligned}$$

or on simplifying,

$$\begin{aligned} &D^{(\ell)}_{m,n_1+n_2} (-1)^{n_1+n_2} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -n_1-n_2 & n_1 & n_2 \end{pmatrix} \\ &\qquad = \sum_{m_1} (-1)^m \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -m & m_1 & m-m_1 \end{pmatrix} D^{(\ell_1)}_{m_1 n_1} D^{(\ell_2)}_{m-m_1,n_2}. \end{aligned} \tag{9.45}$$

Use of the orthonormality relations, Eqs. (7.33) and (7.35), of the 3-j symbols allows this relation between rotation matrices to be written in the forms

$$\begin{aligned} D^{(\ell)}_{mn} &= (2\ell+1)(-1)^{m+n} \\ &\times \sum_{m_1 n_1} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -m & m_1 & m-m_1 \end{pmatrix} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -n & n_1 & n-n_1 \end{pmatrix} D^{(\ell_1)}_{m_1 n_1} D^{(\ell_2)}_{m-m_1,n-n_1} \end{aligned} \tag{9.46}$$

and

$$\begin{aligned} D^{(\ell_1)}_{m_1 n_1} D^{(\ell_2)}_{m_2 n_2} &= \sum_{\ell} (2\ell+1)(-1)^{m_1+m_2+n_1+n_2} \\ &\times \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -m_1-m_2 & m_1 & m_2 \end{pmatrix} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -n_1-n_2 & n_1 & n_2 \end{pmatrix} D^{(\ell)}_{m_1+m_2,n_1+n_2}. \end{aligned} \tag{9.47}$$

The first form, which gives an expansion of one rotation matrix in terms of two others, could be used to calculate the rotation matrix for a higher weight in terms of known rotation matrices of lower weight.

Another set of properties is the effect of integrating over all elements of the rotation group. The proper weighting of such an integration has been discussed in Sec. 3.6.1. It is appropriate to start with the integration of the rotation tensor for a single vector, thus from Eq. (2.90),

$$\begin{aligned} & \frac{1}{4\pi^2} \int\!\!\int \mathbf{R}_{\hat{n}}(\theta)(1-\cos\theta) d\hat{n} d\theta \\ =\; & \frac{1}{4\pi^2} \int\!\!\int [\hat{n}\hat{n} + \cos\theta(\mathbf{U} - \hat{n}\hat{n}) - \sin\theta \hat{n}\cdot\boldsymbol{\mathcal{E}}\,](1-\cos\theta) d\theta d\hat{n} = \mathbf{0}. \end{aligned} \tag{9.48}$$

This can be interpreted as the effect on a vector of averaging it by rotating it in all possible ways. Since there is now no direction left after averaging on which the average vector can depend, the average must vanish. The same argument must be valid for averaging any tensor belonging to an irreducible representation of the rotation group whose weight is nozero. Essentially there are no directions left on which the averaged tensor can depend, so the average must vanish, thus

$$\frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} \mathbf{E}^{(\ell)} \odot^{\ell} \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma) \odot^{\ell} \mathbf{E}^{(\ell)} \sin\beta d\beta d\alpha d\gamma = \delta_{\ell,0} \mathbf{E}^{(\ell)}. \tag{9.49}$$

The integration here has been expressed in terms of Euler angles while the $\mathbf{E}^{(\ell)}$'s on each side of the rotation tensor is to ensure that the rotation tensor is restricted to belonging to the weight ℓ irreducible representation of the rotation group. Only for $\ell = 0$ is such an average nonzero since then the tensor is a rotational invariant. In terms of the rotation matrices this averaging is

$$\frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} D^{(\ell)}_{mn}(\alpha,\beta,\gamma) \sin\beta d\beta d\alpha d\gamma = \delta_{\ell,0} \delta_{m0} \delta_{n0}. \tag{9.50}$$

The integration of a product of rotation matrices can be evaluated using the above integral, the expression (9.47) of a product of rotation matrices in terms of a sum of rotation matrices and the values of the 3-j symbols evaluated after integration has been performed, thus

$$\frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} D^{(\ell_1)}_{m_1 n_1}(\alpha,\beta,\gamma) D^{(\ell_2)}_{m_2 n_2}(\alpha,\beta,\gamma) \sin\beta d\beta d\alpha d\gamma$$

$$
\begin{aligned}
&= \sum_\ell (2\ell+1)(-1)^{m_1+m_2+n_1+n_2} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -m_1-m_2 & m_1 & m_2 \end{pmatrix} \begin{pmatrix} \ell & \ell_1 & \ell_2 \\ -n_1-n_2 & n_1 & n_2 \end{pmatrix} \\
&\qquad \times \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} D^{(\ell)}_{m_1+m_2,n_1+n_2}(\alpha,\beta,\gamma) \sin\beta d\beta d\alpha d\gamma \\
&= \frac{(-1)^{m_1+n_1}}{2\ell_1+1} \delta_{\ell_1,\ell_2} \delta_{m_1,-m_2} \delta_{n_1,-n_2}. \qquad (9.51)
\end{aligned}
$$

From the complex conjugate properties of the rotation matrices, Eq. (9.41), the standard way of writing this orthogonality relation is

$$\frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} D^{(\ell_1)}_{m_1 n_1}(\alpha,\beta,\gamma)^* D^{(\ell_2)}_{m_2 n_2}(\alpha,\beta,\gamma) \sin\beta d\beta d\alpha d\gamma = \frac{\delta_{\ell_1,\ell_2}\delta_{m_1,m_2}\delta_{n_1,n_2}}{2\ell_1+1}. \qquad (9.52)$$

The integral of three rotation matrices can be obtained by using the expansion of a pair, Eq. (9.47), and then using the orthogonality of the resulting rotation matrices

$$
\begin{aligned}
&\frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} D^{(\ell_1)}_{m_1 n_1}(\alpha,\beta,\gamma) D^{(\ell_2)}_{m_2 n_2}(\alpha,\beta,\gamma) D^{(\ell_3)}_{m_3 n_3}(\alpha,\beta,\gamma) \sin\beta d\beta d\alpha d\gamma \\
&\qquad = \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ n_1 & n_2 & n_3 \end{pmatrix}. \qquad (9.53)
\end{aligned}
$$

This is a generalization of Eq. (7.39). Integrals involving more than three rotation matrices can be found in a similar way but the result has no unique way of being expressed because of the multitude of different choices as to how Eq. (9.47) can be applied.

9.5 As Eigenvectors of the Rotation Generators

The rotation matrices are the eigenvectors of certain rotation generators, as is to be shown. This is accomplished by first examining the action of the rotation generators on a rotation tensor parameterized by Euler angles, to express the action of a rotation generator in terms of an equivalent differential operator. On application of these differential operators to the angle dependence of the rotation matrices identifies the eigenvalues of the rotation generators to which a rotation matrix belongs.

The simplest of these is the generator for a rotation about the $\hat{z}$ axis, thus

$$
\begin{aligned}
\mathbf{G}^{(\ell)}_{\hat{z}} \odot^\ell \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma) &= \mathbf{G}^{(\ell)}_{\hat{z}} \odot^\ell e^{-i\alpha \mathbf{G}^{(\ell)}_{\hat{z}}} \odot^\ell e^{-i\beta \mathbf{G}^{(\ell)}_{\hat{y}}} \odot^\ell e^{-i\gamma \mathbf{G}^{(\ell)}_{\hat{z}}} \\
&= i\frac{\partial}{\partial\alpha} \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma). \qquad (9.54)
\end{aligned}
$$

From the fact that $\mathbf{G}_{\hat{z}}$ involves only rotationally invariant tensors besides $\hat{z}$, it follows that

$$\mathbf{G}_{\mathbf{R}(\alpha,\beta,\gamma)\cdot\hat{z}} = \mathbf{R}(\alpha,\beta,\gamma)\cdot\mathbf{G}_{\hat{z}}\cdot\mathbf{R}(\alpha,\beta,\gamma)^{-1} \qquad (9.55)$$

is the generator for a rotation about the rotated $\hat{z}$ direction, namely the $\mathbf{R}(\alpha,\beta,\gamma)\cdot\hat{z}$ direction. The action of this generator is given by

$$
\begin{aligned}
\mathbf{G}^{(\ell)}_{\mathbf{R}(\alpha,\beta,\gamma)\cdot\hat{z}} \odot^\ell \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma) &= \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma) \odot^\ell \mathbf{G}^{(\ell)}_{\hat{z}} \odot^\ell \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)^{-1} \odot^\ell \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma) \\
&= \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma) \odot^\ell \mathbf{G}^{(\ell)}_{\hat{z}} = i\frac{\partial}{\partial\gamma} \mathbf{R}^{(\ell)}(\alpha,\beta,\gamma). \qquad (9.56)
\end{aligned}
$$

Application of these differential operators to the rotation matrix $D^{(\ell)}_{mn}(\alpha,\beta,\gamma)$ immediately identifies m and n as eigenvalues of the generators about, respectively, the $\hat{z}$ and rotated $\hat{z}$ axes, namely

$$i\frac{\partial}{\partial\alpha}D^{(\ell)}_{mn}(\alpha,\beta,\gamma)=mD^{(\ell)}_{mn}(\alpha,\beta,\gamma)\qquad i\frac{\partial}{\partial\gamma}D^{(\ell)}_{mn}(\alpha,\beta,\gamma)=nD^{(\ell)}_{mn}(\alpha,\beta,\gamma).\tag{9.57}$$

The action on the rotation tensor $\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)$ of the rotation generators about the $\hat{x}$ and $\hat{y}$ axes are much more elaborate. For $\mathbf{G}^{(\ell)}_{\hat{x}}$, this action can be rewritten as

$$\begin{aligned}
&\mathbf{G}^{(\ell)}_{\hat{x}}\odot^\ell e^{-i\alpha\mathbf{G}^{(\ell)}_{\hat{z}}}\odot^\ell e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}\odot^\ell e^{-i\gamma\mathbf{G}^{(\ell)}_{\hat{z}}}\\
=\;& e^{-i\alpha\mathbf{G}^{(\ell)}_{\hat{z}}}\odot^\ell e^{i\alpha\mathbf{G}^{(\ell)}_{\hat{z}}}\odot^\ell\mathbf{G}^{(\ell)}_{\hat{x}}\odot^\ell e^{-i\alpha\mathbf{G}^{(\ell)}_{\hat{z}}}\odot^\ell e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}\odot^\ell e^{-i\gamma\mathbf{G}^{(\ell)}_{\hat{z}}}\\
=\;& e^{-i\alpha\mathbf{G}^{(\ell)}_{\hat{z}}}\odot^\ell\mathbf{G}^{(\ell)}_{\hat{x}\cos\alpha-\hat{y}\sin\alpha}\odot^\ell e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}\odot^\ell e^{-i\gamma\mathbf{G}^{(\ell)}_{\hat{z}}}\\
=\;& -i\sin\alpha\frac{\partial}{\partial\beta}\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)+\cos\alpha e^{-i\alpha\mathbf{G}^{(\ell)}_{\hat{z}}}\odot^\ell\mathbf{G}^{(\ell)}_{\hat{x}}\odot^\ell e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}\odot^\ell e^{-i\gamma\mathbf{G}^{(\ell)}_{\hat{z}}}.
\end{aligned}\tag{9.58}$$

This has been organized so that the generator is rotated, with the result recognized in terms of the generator of a rotation about the rotated axis. An expansion of the rotated generator leads to the last form, but this still involves the generator $\mathbf{G}^{(\ell)}_{\hat{x}}$. Now the identity

$$e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}\odot^\ell\mathbf{G}^{(\ell)}_{\hat{z}}\odot^\ell e^{i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}=\mathbf{G}^{(\ell)}_{\hat{z}\cos\beta+\hat{x}\sin\beta}=\cos\beta\mathbf{G}^{(\ell)}_{\hat{z}}+\sin\beta\mathbf{G}^{(\ell)}_{x},\tag{9.59}$$

or equivalently

$$e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}\odot^\ell\mathbf{G}^{(\ell)}_{\hat{z}}=\cos\beta\mathbf{G}_{\hat{z}}\odot^\ell e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}}+\sin\beta\mathbf{G}^{(\ell)}_{\hat{x}}\odot^\ell e^{-i\beta\mathbf{G}^{(\ell)}_{\hat{y}}},\tag{9.60}$$

can be used to eliminate $\mathbf{G}^{(\ell)}_{\hat{x}}$ in the last form of Eq. (9.58) to give

$$\mathbf{G}^{(\ell)}_{\hat{x}}\odot^\ell\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)=\left[-i\sin\alpha\frac{\partial}{\partial\beta}+i\frac{\cos\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}-i\cos\alpha\cot\beta\frac{\partial}{\partial\alpha}\right]\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma).\tag{9.61}$$

An analogous calculation gives

$$\mathbf{G}^{(\ell)}_{\hat{y}}\odot^\ell\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)=\left[i\cos\alpha\frac{\partial}{\partial\beta}+i\frac{\sin\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}-i\sin\alpha\cot\beta\frac{\partial}{\partial\alpha}\right]\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma).\tag{9.62}$$

On iterating the differential operators, the action of the Casimir invariant on the rotation operator $\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)$ is equivalent to the differential operator as given by

$$\begin{aligned}
&\mathbf{G}^{(\ell)2}\odot^\ell\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma)\\
=\;&\left[\frac{-1}{\sin\beta}\frac{\partial}{\partial\beta}\left(\sin\beta\frac{\partial}{\partial\beta}\right)-\frac{1}{\sin^2\beta}\left(\frac{\partial^2}{\partial\alpha^2}+\frac{\partial^2}{\partial\gamma^2}\right)+\frac{2\cos\beta}{\sin^2\beta}\frac{\partial^2}{\partial\gamma\partial\alpha}\right]\mathbf{R}^{(\ell)}(\alpha,\beta,\gamma).
\end{aligned}\tag{9.63}$$

It is an exercise to show that a rotation matrix is an eigenvector of this Differential Operator, denoted here by G^2_{DO}, namely

$$G^2_{\mathrm{DO}}D^{(\ell)}_{mn}(\alpha,\beta,\gamma)=\ell(\ell+1)D^{(\ell)}_{mn}(\alpha,\beta,\gamma).\tag{9.64}$$

Thus the three parameters ℓ, m and n labelling a rotation matrix can be associated with the eigenvalues of certain rotation generators. As special cases of the rotation matrices, the spherical harmonics, Eqs. (9.36-9.38), are also eigenvectors of G^2_{DO}. These associations have physical meanings in the quantum mechanical application of the rotation group, see Chap. 11.

Chapter 10

Spinors

While the 1/2-integer represenions of the rotation group cannot be expressed in terms of Cartesian tensors, the methods used for discussing the properties of Cartesian tensors are adapted to discuss these representations. This leads to some novel features. First of all, the representation space is complex, and second, the naturally arising bases are biorthogonal rather than orthogonal. These are written as contravariant and covariant 2-dimensional vectors. The properties of these bases and the components of a spinor expanded in terms of these bases are described. Central to the classification of objects under the rotation group is the presence of rotational invariants. For spinors, it is shown that there is a single invariant $\boldsymbol{\epsilon}$. The consequences of the presence of this invariant are discussed, in particular to imply specific relations between the contravariant and covariant basis sets. With that as a background, the tensor product of spinors and the reduction of the tensor product under the action of the rotation group is presented. Connections to rotation matrices, 3-j symbols and Cartesian tensors are then made. Notationwise, a complex 2-dimensional vector will be here referred to as a spinor, whereas elements of the tensor product space of complex 2-dimensional vectors will be referred to variously as tensors, spinor tensors and/or spinors of order p (the latter for elements of the p-fold tensor product space).

The properties of the generators of the 3-dimensional rotation group have been discussed in Sec. 5.1. According to that discussion, there are irreducible representations of the group having integer as well as half integer maximum weight. Necessarily the dimensionality of the integer weight representations is odd, while the half integer weight representations are of even dimension. Since the Cartesian tensors are built from a space of odd dimension, it follows that all irreducible representations describable by Cartesian tensors are of integral weight .

In contrast, the irreducible representations of half integer weight need to be built from a space of even dimension, starting with the 2-dimensional irreducible representation of weight 1/2. Necessarily, this 2-dimensional space must also be complex and is known as the spinor representation of the rotation group. Mathematically its relation to the 3-dimensional rotation group is described by noting that the covering group of the 3-dimensional rotation group is the special unitary group of two dimensions, SU(2). This is associated with embedding the 3-dimensional rotation group, as for example parameterized by the projected sphere P_3 [see the discussion in Sec. 2.5.1] in a two-sheeted, single valued manifold by identifying the two homotopy classes of P_3 as separate sheets [5].

General 2-dimensional complex vectors are written in this chapter as boldface Greek letters such as $\boldsymbol{\Psi}$ and $\boldsymbol{\Phi}$. There is a natural inner product $\langle\boldsymbol{\Phi}|\boldsymbol{\Psi}\rangle$ in this space, linear in the righthand vector, antilinear in the lefthand vector, with the norm of a vector given in terms of the inner product according to $\|\mathbf{\Psi}\| = \sqrt{\langle \mathbf{\Psi}|\mathbf{\Psi}\rangle}$. This has been written in a notation which is the same as that used in quantum mechanics. But to compare with Cartesian vector notation, which has the notion of dot product, the inner product will also be written in the form

$$\langle \mathbf{\Phi}|\mathbf{\Psi}\rangle = \mathbf{\Phi}^{\dagger}\bullet\mathbf{\Psi}. \tag{10.1}$$

Here $\mathbf{\Phi}^{\dagger}$ designates what is here called the adjoint spinor to $\mathbf{\Phi}$, whose properties are to be elaborated upon after a discussion of basis sets has been given. Suffice it to say at this point that the adjoint includes taking the complex conjugate, which emphasizes the antilinear nature of the lefthand vector in the inner product, while the dot product manner of writing the inner product also introduces the notion of a vector contraction to give a scalar. The notation $\bullet$ is used to contrast the 2-dimensional case with the $\cdot$ of the 3-dimensional case, yet similar enough to carry an association with the same concept. $\mathbf{\Phi}\bullet\mathbf{\Psi}$ is a bilinear mapping [linear in both $\mathbf{\Psi}$ and $\mathbf{\Phi}$] to the scalars (the complex numbers) but must be consistent with the positivity of the inner product when $\mathbf{\Phi} = \mathbf{\Psi}^{\dagger}$. Necessarily, if $\|\mathbf{\Psi}\| = 0$, then $\mathbf{\Psi}$ is the zero spinor, $\mathbf{\Psi} = \mathbf{0}$. The introduction of a basis for the vector space allows these vectors to be written in column and/or row vector form, but a particular basis is emphasized later and used exclusively in this chapter.

In analogy to the 3-dimensional case, a tensor product $\mathbf{\Psi\Phi}$ of two spinors can be considered, as well as sums of such products, the analogs of dyads and dyadics. These can be considered as entities in their own right, but with the use of the dot product, they can be treated as operators on other spinors. A particular second order tensor is the identity operator U, as used for example in

$$\mathbf{\Psi} = \mathsf{U}\bullet\mathbf{\Psi}. \tag{10.2}$$

This square (bolface, sans serif) U is analogous to the real 2-dimensional case U, Eq. (2.35), and is of a form that allows similar overlapping of symbols to be made. Generally, spinor tensors will be written as capital boldface Greek or Euler objects with some feature to distinguish them from the analogous 3-dimensional quantities. Basis spinors are boldface lowercase Euler. An attempt will be made to comment on whether quantities are based on a 2- or 3-dimensional space, but in general the context should make it clear as to which space is involved.

10.1 The standard spinor basis sets

There is no unique association of any 2-dimensional complex vector with a direction in physical (3-dimensional) space. So some particular assignment needs to be made in order to carry out such an association and make a connection with a rotation about a specific physical axis. For this purpose it is standard to introduce as a basis for the spinor space, the two eigenvectors of the rotation generator $G_{\hat{z}}$. Since these are the analogs of the spherical tensors, they will be denoted here by $\mathfrak{e}^{(1/2)1/2}$ and $\mathfrak{e}^{(1/2)-1/2}$, written as contravariant vectors, with a column vector form appropriate for matrix calculations according to

$$\begin{aligned} G_{\hat{z}}\mathfrak{e}^{(1/2)1/2} &= (1/2)\mathfrak{e}^{(1/2)1/2}, & G_{\hat{z}}\mathfrak{e}^{(1/2)-1/2} &= (-1/2)\mathfrak{e}^{(1/2)-1/2} \\ \mathfrak{e}^{(1/2)1/2} &\Longleftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \mathfrak{e}^{(1/2)-1/2} &\Longleftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned} \tag{10.3}$$

The notation "$\mathfrak{e}$" is used in place of "$\mathbf{e}$" for spherical tensor basis elements since, as shown later, the tensors formed from this basis set are related to the Cartesian basis set of Eq. (5.28), denoted by the same symbolism. The dual (covariant) basis vectors are denoted by $\mathbf{e}^{(1/2)}_{\pm 1/2}$ and are defined to satisfy

$$\mathbf{e}^{(1/2)}_{1/2}\bullet\begin{cases}\mathbf{e}^{(1/2)1/2}=1\\ \mathbf{e}^{(1/2)-1/2}=0\end{cases}\qquad \mathbf{e}^{(1/2)}_{-1/2}\bullet\begin{cases}\mathbf{e}^{(1/2)1/2}=0\\ \mathbf{e}^{(1/2)-1/2}=1.\end{cases} \tag{10.4}$$

These correspond to the row vectors

$$\mathbf{e}^{(1/2)}_{1/2}\Longleftrightarrow\begin{pmatrix}1 & 0\end{pmatrix}\qquad \mathbf{e}^{(1/2)}_{-1/2}\Longleftrightarrow\begin{pmatrix}0 & 1\end{pmatrix}, \tag{10.5}$$

which is the matrix form that is consistent with the above orthogonality properties. If the biorthonormality relations (10.4) are recognized as inner product relations, then the identifications

$$\mathbf{e}^{(1/2)}_{\pm 1/2}=\mathbf{e}^{(1/2)\pm 1/2\dagger} \tag{10.6}$$

can be made. This allows the operations of complex conjugation, dot product and inner product to be carried out in a consistent manner. The identity tensor can be identified as the combination

$$\mathbf{U}=\mathbf{e}^{(1/2)1/2}\mathbf{e}^{(1/2)}_{1/2}+\mathbf{e}^{(1/2)-1/2}\mathbf{e}^{(1/2)}_{-1/2} \tag{10.7}$$

of contravariant and covariant basis elements.

The introduction of a basis set enables any (2-dimensional complex) vector $\mathbf{\Psi}$ to be written as

$$\mathbf{\Psi}=\mathbf{e}^{(1/2)1/2}\Psi_{1/2}+\mathbf{e}^{(1/2)-1/2}\Psi_{-1/2}\Longleftrightarrow\begin{pmatrix}\Psi_{1/2}\\ \Psi_{-1/2}\end{pmatrix} \tag{10.8}$$

and its adjoint spinor as

$$\mathbf{\Psi}^\dagger=\Psi^*_{1/2}\mathbf{e}^{(1/2)}_{1/2}+\Psi^*_{-1/2}\mathbf{e}^{(1/2)}_{-1/2}\Longleftrightarrow\begin{pmatrix}\Psi^*_{1/2} & \Psi^*_{-1/2}\end{pmatrix}. \tag{10.9}$$

As a consequence, the inner product of two arbitrary spinors can be calculated in terms of the inner product,

$$\langle\mathbf{\Phi}|\mathbf{\Psi}\rangle=\mathbf{\Phi}^\dagger\bullet\mathbf{\Psi}=\Phi^*_{1/2}\Psi_{1/2}+\Phi^*_{-1/2}\Psi_{-1/2}\Longleftrightarrow\begin{pmatrix}\Phi^*_{1/2} & \Phi^*_{-1/2}\end{pmatrix}\begin{pmatrix}\Psi_{1/2}\\ \Psi_{-1/2}\end{pmatrix}. \tag{10.10}$$

The components of the spinor $\mathbf{\Psi}$ are found by the contractions

$$\Psi_{\pm 1/2}=\mathbf{e}^{(1/2)}_{\pm 1/2}\bullet\mathbf{\Psi}, \tag{10.11}$$

and Eq. (10.8) corresponds to the expansion of the identity

$$\mathbf{\Psi}=\mathbf{U}\bullet\mathbf{\Psi}=\left(\mathbf{e}^{(1/2)1/2}\mathbf{e}^{(1/2)}_{1/2}+\mathbf{e}^{(1/2)-1/2}\mathbf{e}^{(1/2)}_{-1/2}\right)\bullet\mathbf{\Psi}. \tag{10.12}$$

See Eq. (10.56) and the associated discussion for the covariant basis set expansion of $\mathbf{\Psi}$.

An analogous expansion of the adjoint spinor is

$$\mathbf{\Psi}^\dagger=\mathbf{\Psi}^\dagger\bullet\mathbf{U}=\mathbf{\Psi}^\dagger\bullet\left(\mathbf{e}^{(1/2)1/2}\mathbf{e}^{(1/2)}_{1/2}+\mathbf{e}^{(1/2)-1/2}\mathbf{e}^{(1/2)}_{-1/2}\right), \tag{10.13}$$

with the identification of the components according to

$$\Psi^*_{\pm 1/2} = \mathbf{\Psi}^\dagger \bullet \mathfrak{e}^{(1/2)\pm 1/2} = \mathbf{\Psi}^\dagger \bullet \mathfrak{e}^{(1/2)\,\dagger}_{\pm 1/2} = \left(\mathfrak{e}^{(1/2)}_{\pm 1/2} \bullet \mathbf{\Psi}\right)^*. \tag{10.14}$$

Note that for $\mathbf{\Psi}$, the identity is multiplied on the left, while for the adjoint, the identity is multiplied on the right. Note also that the adjoint of a product is the product of the adjoints, but in the opposite order. This asymmetry on contractions needs to be treated with care, and reflects the asymmetry between a spinor and its adjoint.

10.2 Rotation of a spinor

While in many ways unnecessary, it is at times useful to introduce the spinor tensor equivalent to the rotation generator, e.g. $\mathfrak{G}^{(1/2)}_{\hat{z}}$. This serves to emphasize the weight of the irreducible representation, which reflects the order of the tensor space, with weight 1/2 corresponding to the order of the spinor space, namely 2-dimensional. The eigenvector properties of $\mathfrak{G}^{(1/2)}_{\hat{z}}$ are equivalent to Eq. (10.3), but read as

$$\mathfrak{G}^{(1/2)}_{\hat{z}} \bullet \mathfrak{e}^{(1/2)1/2} = (1/2)\mathfrak{e}^{(1/2)1/2}; \qquad \mathfrak{G}^{(1/2)}_{\hat{z}} \bullet \mathfrak{e}^{(1/2)-1/2} = (-1/2)\mathfrak{e}^{(1/2)-1/2}. \tag{10.15}$$

The hermiticity of $\mathfrak{G}^{(1/2)}_{\hat{z}}$ is expressed as

$$\mathbf{\Phi}^\dagger \bullet \mathfrak{G}^{(1/2)}_{\hat{z}} \bullet \mathbf{\Psi} = \left(\mathfrak{G}^{(1/2)}_{\hat{z}} \bullet \mathbf{\Phi}\right)^\dagger \bullet \mathbf{\Psi}. \tag{10.16}$$

From the fact that the raising operator $G_+ = G_{\hat{x}} + iG_{\hat{y}}$ has the action $G_+ \mathfrak{e}^{(1/2)1/2} = \mathbf{0}$, $G_+ \mathfrak{e}^{(1/2)-1/2} = \mathfrak{e}^{(1/2)1/2}$, and analogous relations for G_-, it follows that the matrix representations of the rotation generators are

$$G_{\hat{x}} \iff \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv \frac{1}{2}\sigma_x; \qquad G_{\hat{y}} \iff \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv \frac{1}{2}\sigma_y;$$
$$G_{\hat{z}} \iff \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \frac{1}{2}\sigma_z. \tag{10.17}$$

These are just proportional to the well known Pauli spin matrices σ_x, σ_y, σ_z, as they are designated here. It is also clear that $G_+^2 = 0$ and $G_-^2 = 0$ in a 2-dimensional space and that $G_{\hat{x}} G_{\hat{y}} = (i/2) G_{\hat{z}}$ (and its cyclic permutations). The latter can be proven formally by the action of

$$G_{\hat{x}} G_{\hat{y}} = (-i/4)(G_+ + G_-)(G_+ - G_-) = (-i/4)[-G_+G_- + G_-G_+], \tag{10.18}$$

or more directly by multiplying the equivalent representation matrices. It is also useful to note that in a 2-dimensional space, there are at most 4 independent operators. A convenient choice for these are the identity 1 and the three generators $G_{\hat{x}}$, $G_{\hat{y}}$ and $G_{\hat{z}}$, so any operator can be expressed in terms of these 4 operators.

The corresponding rotation generator about an arbitrary axis $\hat{n}$ has a matrix represention, using the $\mathfrak{e}^{(1/2)1/2}$, $\mathfrak{e}^{(1/2)-1/2}$ basis set which gives a preference to the $\hat{z}$-axis,

$$G_{\hat{n}} = n_x G_{\hat{x}} + n_y G_{\hat{y}} + n_z G_{\hat{z}} \iff \frac{1}{2}\begin{pmatrix} \cos\eta & \sin\eta e^{-i\zeta} \\ \sin\eta e^{i\zeta} & -\cos\eta \end{pmatrix}. \tag{10.19}$$

Here the unit axis vector $\hat{n}$ is given in Cartesian and spherical coordinates according to

$$\hat{n} = n_x\hat{x} + n_y\hat{y} + n_z\hat{z} = \sin\eta(\hat{x}\cos\zeta + \hat{y}\sin\zeta) + \hat{z}\cos\eta. \tag{10.20}$$

It is straightforward to prove that the eigenvectors of $G_{\hat{n}}$ associated with its $+1/2$ and $-1/2$ eigenvalues are respectively the normalized spinors

$$\mathbf{\Psi}_{\hat{n}}^{1/2} \iff \begin{pmatrix} \cos(\eta/2)e^{-i\zeta/2} \\ \sin(\eta/2)e^{+i\zeta/2} \end{pmatrix} \quad \text{and} \quad \mathbf{\Psi}_{\hat{n}}^{-1/2} \iff \begin{pmatrix} -\sin(\eta/2)e^{-i\zeta/2} \\ \cos(\eta/2)e^{i\zeta/2} \end{pmatrix}. \tag{10.21}$$

defined up to arbitrary phase factors. As written, these two eigenvectors reduce to $\mathfrak{e}^{(1/2)\pm 1/2}$, Eq. (10.3), when $\hat{n} = \hat{z}$. Since $G_{\hat{n}}$ has eigenvalues $\pm 1/2$, it follows that $G_{\hat{n}}^2 = 1/4$. The tensor equivalent of the last relation is $\left(\mathfrak{G}_{\hat{n}}^{(1/2)}\right)^2 = 1/4\mathbf{U}$, which emphasizes the operator identity of the "constant" term. Tensor forms for the other generators can be written down in a straightforward manner.

The rotation of a spinor by an angle θ about the $\hat{n}$ axis is determined by $\mathfrak{G}_{\hat{n}}^{(1/2)}$ according to

$$\begin{aligned} \mathfrak{R}_{\hat{n}}^{(1/2)}(\theta) &= e^{-i\theta\mathfrak{G}_{\hat{n}}^{(1/2)}}\bullet\mathbf{U} = \cos(\mathfrak{G}_{\hat{n}}^{(1/2)}\theta) - i\sin(\mathfrak{G}_{\hat{n}}^{(1/2)}\theta) \\ &= \mathbf{U}\cos(\theta/2) - 2i\mathfrak{G}_{\hat{n}}^{(1/2)}\sin(\theta/2). \end{aligned} \tag{10.22}$$

This should be contrasted with the formulas for the corresponding rotation in a real 2-dimensional space, Eq. (2.54), and in 3-dimensions, Eq. (2.96). The matrix form of this rotation, using the $\mathfrak{e}^{(1/2)\pm 1/2}$ basis is

$$\begin{aligned} \mathfrak{R}_{\hat{n}}^{(1/2)}(\theta) &\iff \left(\mathfrak{e}_{\mu}^{(1/2)} \bullet \mathfrak{R}_{\hat{n}}^{(1/2)}(\theta) \bullet \mathfrak{e}^{(1/2)\nu}\right) = \left(R_{\hat{n}}^{(1/2)}(\theta)_{\mu}^{\nu}\right) \\ &\iff \begin{pmatrix} \cos(\theta/2) - i\sin(\theta/2)\cos\eta & -i\sin(\theta/2)\sin\eta e^{-i\zeta} \\ -i\sin(\theta/2)\sin\eta e^{i\zeta} & \cos(\theta/2) + i\sin(\theta/2)\cos\eta \end{pmatrix}. \end{aligned} \tag{10.23}$$

Thus the rotation of a spinor is reflected in the transformation of its covariant components according to

$$\left(\mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)\bullet\mathbf{\Psi}\right)_{\mu} = \sum_{\nu} R_{\hat{n}}^{(1/2)}(\theta)_{\mu}^{\nu}\Psi_{\nu}. \tag{10.24}$$

Special cases are a rotation of angle α about the $\hat{z}$ axis ($\eta = 0$)

$$\mathfrak{R}_{\hat{z}}^{(1/2)}(\alpha) \iff \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix}, \tag{10.25}$$

and a rotation by angle β about the $\hat{y}$ axis ($\eta = \zeta = \pi/2$)

$$\mathfrak{R}_{\hat{y}}^{(1/2)}(\beta) \iff \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix}. \tag{10.26}$$

These correspond to the rotations used in the Euler angle description of a rotation, see Sec. 2.5.2,. In particular, as described in terms of Euler angles, a general rotation is

$$\begin{aligned} \mathfrak{R}^{(1/2)}(\alpha\beta\gamma) &\equiv \mathfrak{R}_{\hat{z}}^{(1/2)}(\alpha)\bullet\mathfrak{R}_{\hat{y}}^{(1/2)}(\beta)\bullet\mathfrak{R}_{\hat{z}}^{(1/2)}(\gamma) \\ &\iff \begin{pmatrix} \cos(\beta/2)e^{-i(\alpha+\gamma)/2} & -\sin(\beta/2)e^{-i(\alpha-\gamma)/2} \\ \sin(\beta/2)e^{i(\alpha-\gamma)/2} & \cos(\beta/2)e^{i(\alpha+\gamma)/2} \end{pmatrix} \\ &= D^{(1/2)}(\alpha\beta\gamma), \end{aligned} \tag{10.27}$$

with the product of the matrices giving the standard rotation matrix listed for an active rotation, compare Rose [2]. Eq. (10.26) is the standard $d^{(1/2)}(\beta)$ rotation matrix. It is also of note that for a rotation by an angle of 2π, the rotation tensor is the negative of the identity, that is

$$\mathfrak{R}^{(1/2)}_{\hat{n}}(2\pi) = -\mathbf{U} \iff \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{10.28}$$

This implies that the representation is double valued, that is, a rotation of 2π is not the identity, but a rotation by 4π is the identity. The columns of the $D^{(1/2)}(\alpha\beta\gamma)$, Eq. (10.27), are the same as the basis spinors in Eq. (10.21) with the identification of β with η and ζ with α, but with extra phase factors of $e^{\mp i\gamma}$. In particular

$$\Psi^{1/2}_{\hat{n}} = \mathfrak{R}^{(1/2)}(\zeta,\eta,0)\bullet\mathfrak{e}^{(1/2)1/2} = \mathfrak{e}^{(1/2)1/2}\cos(\eta/2)e^{-i\zeta/2} + \mathfrak{e}^{(1/2)-1/2}\sin(\eta/2)e^{i\zeta/2} \tag{10.29}$$

and its analog $\Psi^{-1/2}_{\hat{n}}$ can be used as a basis for the spinor space, with $\hat{n}$ replacing $\hat{z}$ as the reference axis for classifying the basis. More generally, the rotation of the standard basis spinors, Eq. (10.3), produces a basis set associated with the rotation generator $G_{\hat{m}}$, where $\hat{m}$ is determined by those spherical coordinates β and α which appear as the Euler angles of the rotation.

10.2.1 Products of Rotations

The product of a rotation θ_1 about axis $\hat{n}_1$ followed by a rotation θ_2 about axis $\hat{n}_2$ is equivalent to some rotation θ about some axis $\hat{n}$. As discussed in Sec. 2.5.1, this is necessary in order that the set of rotations form a multiplicative group. The resulting angle of rotation θ and axis $\hat{n}$ was calculated using the explicit form for a finite rotation in 3-dimensional space. Here this calculation is repeated using spinors [31]. It is seen that this calculation is much simpler than the previous one.

In order to simplify the writing of the matrix calculation, the following short-hand notations are introduced (j=1,2):

$$\begin{aligned} c_j \equiv \cos(\theta_j/2), &\qquad s_j \equiv \sin(\theta_j/2) \\ n_{jz} \equiv \cos(\eta_j), &\qquad n_{j\pm} \equiv n_{jx} \pm i n_{jy} = \sin(\eta_j)e^{\pm i\zeta_j}. \end{aligned} \tag{10.30}$$

Then the product of the rotations is

$$\begin{aligned} \mathfrak{R}^{(1/2)}_{\hat{n}_2}(\theta_2)\bullet\mathfrak{R}^{(1/2)}_{\hat{n}_1}(\theta_1) &\iff \begin{pmatrix} c_2 - is_2n_{2z} & -is_2n_{2-} \\ -is_2n_{2+} & c_2 + is_2n_{2z} \end{pmatrix}\begin{pmatrix} c_1 - is_1n_{1z} & -is_1n_{1-} \\ -is_1n_{1+} & c_1 + is_1n_{1z} \end{pmatrix} \\ &= \begin{pmatrix} c_2c_1 - ic_1s_2n_{2z} - ic_2s_1n_{1z} - s_1s_2(n_{1z}n_{2z} + n_{1+}n_{2-}) & \cdots \\ -ic_1s_2n_{2+} - ic_2s_1n_{1+} + s_1s_2(n_{1+}n_{2z} - n_{2+}n_{1z}) & \cdots \end{pmatrix} \\ = \mathfrak{R}^{(1/2)}_{\hat{n}}(\theta) &\iff \begin{pmatrix} \cos(\theta/2) - i\sin(\theta/2)\cos\eta & -i\sin(\theta/2)\sin\eta e^{-i\zeta} \\ -i\sin(\theta/2)\sin\eta e^{i\zeta} & \cos(\theta/2) + i\sin(\theta/2)\cos\eta \end{pmatrix}, \end{aligned} \tag{10.31}$$

with the missing terms having a form that fits into the structure of $\mathfrak{R}^{(1/2)}_{\hat{n}}(\theta)$. The real and imaginary parts of the 1/2,1/2 matrix element determine

$$\begin{aligned} \cos(\theta/2) &= c_1c_2 - s_1s_2\left[n_{1z}n_{2z} + (1/2)(n_{1+}n_{2-} + n_{1-}n_{2+})\right] \\ &= \cos(\theta_1/2)\cos(\theta_2/2) - \sin(\theta_1/2)\sin(\theta_2/2)\hat{n}_1\cdot\hat{n}_2 \end{aligned} \tag{10.32}$$

and

$$\begin{aligned} \sin(\theta/2)\cos\eta &= c_1 s_2 n_{2z} + c_2 s_1 n_{1z} + s_1 s_2 \sin(\eta_1)\sin(\eta_2)\sin(\zeta_1 - \zeta_2) \\ &= \cos(\theta_1/2)\sin(\theta_2/2) n_{2z} + \cos(\theta_2/2)\sin(\theta_1/2) n_{1z} - \sin(\theta_1/2)\sin(\theta_2/2)(\hat{n}_1 \times \hat{n}_2)_z . \end{aligned} \tag{10.33}$$

These agree with the angle θ and $\hat{z}$ component of the axis $\hat{n}$ calculated in Sec. 2.5.1, see Eqs. 2.99 and 2.101. The $\hat{x}$ and $\hat{y}$ components of $\hat{n}$ follow from examining the $1/2, -1/2$ matrix element. With this identification of the product of two rotations, the multiplicative group properties of these rotation operators are assured.

10.3 The invariant tensor $\boldsymbol{\epsilon}$

Mappings between tensor spaces that preserve the group properties are carried out by invariant tensors. So the identification of all invariant tensors is central to any tensor analysis. If $\mathbf{A}$ is an invariant second order tensor, then the condition

$$\mathfrak{R}_{\hat{n}}^{(1/2)}(\theta) \bullet \lfloor \mathfrak{R}_{\hat{n}}^{(1/2)}(\theta) \rfloor \bullet^2 \mathbf{A} = \mathbf{A} \tag{10.34}$$

for all $\hat{n}$ and all θ describes the rotational invarince of $\mathbf{A}$. Equivalently, the generator of an arbitrary rotation acting on $\mathbf{A}$ must be zero,

$$\mathfrak{G}_{\hat{n}}^{(1/2)} \bullet \mathbf{A} + \lfloor \mathfrak{G}_{\hat{n}}^{(1/2)} \rfloor \bullet^2 \mathbf{A} = \mathbf{0} \tag{10.35}$$

Since any second order tensor can be expanded in the form

$$\mathbf{A} = \sum_{\mu\nu} A_{\mu\nu} \mathfrak{e}^{(1/2)\mu} \mathfrak{e}^{(1/2)\nu}, \tag{10.36}$$

the action of any generator on this tensor is to add the effects of the generator on each of its indices. It is required that the result vanish for rotational invariance. For $G_{\hat{z}}$, the action on $\mathbf{A}$ is as follows,

$$G_{\hat{z}} \mathbf{A} = A_{1/2,1/2} \mathfrak{e}^{(1/2)1/2} \mathfrak{e}^{(1/2)1/2} - A_{-1/2,-1/2} \mathfrak{e}^{(1/2)-1/2} \mathfrak{e}^{(1/2)-1/2}, \tag{10.37}$$

with the other components not contributing. Since $G_{\hat{z}} \mathbf{A}$ must vanish, it follows that $A_{1/2,1/2} = A_{-1/2,-1/2} = 0$. The action of G_+ on the remaining terms is

$$G_+ \mathbf{A} = A_{1/2,-1/2} \mathfrak{e}^{(1/2)1/2} \mathfrak{e}^{(1/2)1/2} + A_{-1/2,1/2} \mathfrak{e}^{(1/2)1/2} \mathfrak{e}^{(1/2)1/2}, \tag{10.38}$$

whose vanishing requires that $A_{-1/2,1/2} = -A_{1/2.-1/2}$. The action of G_- leads to the same condition. Thus the only invariant second order contravariant tensor is (up to a multiplicative constant)

$$\boldsymbol{\epsilon} \equiv \mathfrak{e}^{(1/2)-1/2} \mathfrak{e}^{(1/2)1/2} - \mathfrak{e}^{(1/2)1/2} \mathfrak{e}^{(1/2)-1/2}. \tag{10.39}$$

Since the product of $\boldsymbol{\epsilon}$ with itself is again an invariant, this product must be a multiple of $\boldsymbol{\epsilon}$. A natural choice for this multiplicative factor is 1, whch implies that $\boldsymbol{\epsilon}$ is idempotent,

$$\boldsymbol{\epsilon} \bullet \boldsymbol{\epsilon} = \boldsymbol{\epsilon}. \tag{10.40}$$

As a consequence, the eigenvalues of $\boldsymbol{\epsilon}$, as an operator acting on spinors, are 0 and 1. This choice determines various multiplicative factors relating the properties of the different basis elements, which are now discussed. An obvious alternate choice for the multiplicative constant in Eq. (10.40) is -1, which would lead to the same consequences as defining $\boldsymbol{\epsilon}$ as the negative of how it is defined in Eq. (10.39) and would lead to the relations between contravariant and covariant basis spinors, as obtained below, to have the opposite signs.

The idempotency of $\boldsymbol{\epsilon}$, Eq. (10.40), together with its definition, Eq. (10.39), in terms of the contravariant basis set can be written in the form

$$\begin{aligned}\mathfrak{e}^{(1/2)-1/2}\mathfrak{e}^{(1/2)1/2} - \mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)-1/2} &= \left[\mathfrak{e}^{(1/2)-1/2}\mathfrak{e}^{(1/2)1/2} - \mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)-1/2}\right] \\ &\bullet \left[\mathfrak{e}^{(1/2)-1/2}\mathfrak{e}^{(1/2)1/2} - \mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)-1/2}\right]. \end{aligned} \tag{10.41}$$

For this equality to be valid, the scalar product of the contravariant basis elements must satisfy

$$\mathfrak{g}^{\mu\nu} \equiv \mathfrak{e}^{(1/2)\mu} \bullet \mathfrak{e}^{(1/2)\nu} = (-1)^{1/2+\nu}\delta_{\mu,-\nu}. \tag{10.42}$$

This quantity is taken as the metric for the contravariant basis elements. It seems reasonable to define the inverse of this quantity as the covariant metric $\mathfrak{g}_{\lambda\mu}$,

$$\sum_{\mu} \mathfrak{g}_{\lambda\mu}\mathfrak{g}^{\mu\nu} = \delta_{\lambda}^{\ \nu}. \tag{10.43}$$

Then, as a function of the indices μ and ν, $\mathfrak{g}_{\lambda\mu}$ is the negative of $\mathfrak{g}^{\lambda\mu}$. It will be shown that this metric is given in terms of the covariant basis elements according to

$$\mathfrak{g}_{\lambda\mu} = (-1)^{1/2-\mu}\delta_{\lambda,-\mu} = -\mathfrak{e}^{(1/2)}_{\lambda} \bullet \mathfrak{e}^{(1/2)}_{\mu}. \tag{10.44}$$

Since $\boldsymbol{\epsilon}$ is a rotational invariant, the action of contracting a basis element with $\boldsymbol{\epsilon}$ gives a spinor that must have the same rotational properties as the basis element, so must be a multiple of the original basis element. Stated otherwise, every basis element with a definite rotational symmetry is an eigenvector of $\boldsymbol{\epsilon}$, and since $\boldsymbol{\epsilon}$ is idempotent, the corresponding eigenvalue must be 0 or 1. Applying these considerations to the left multiplication of $\boldsymbol{\epsilon}$ with $\mathfrak{e}^{(1/2)}_{1/2}$ gives

$$\mathfrak{e}^{(1/2)}_{1/2} \bullet \boldsymbol{\epsilon} = \begin{cases} \mathbf{0} & \text{if the eigenvalue is 0;} \\ \mathfrak{e}^{(1/2)}_{1/2} & \text{if the eigenvalue is 1.} \end{cases} \tag{10.45}$$

But from the definitions of $\boldsymbol{\epsilon}$ and $\mathfrak{e}^{(1/2)}_{1/2}$, this product gives $-\mathfrak{e}^{(1/2)-1/2}$, clearly not $\mathbf{0}$. Together with an analogous calculation using $\mathfrak{e}^{(1/2)}_{-1/2}$, the equalities

$$\mathfrak{e}^{(1/2)}_{1/2} = -\mathfrak{e}^{(1/2)-1/2}, \qquad \mathfrak{e}^{(1/2)}_{-1/2} = \mathfrak{e}^{(1/2)1/2} \tag{10.46}$$

are obtained. It is noted that these identifications require losing the row-column associations of covariant-contravariant spinors presented in Eqs. (10.3) and (10.5). These identities imply several other relations. In particular, the nonzero elements of the metric tensors can be written in the following ways

$$
\begin{aligned}
1 = \mathfrak{g}^{1/2,-1/2} &= \mathfrak{e}^{(1/2)1/2} \bullet \mathfrak{e}^{(1/2)-1/2} = \mathfrak{e}^{(1/2)}_{-1/2} \bullet \mathfrak{e}^{(1/2)-1/2} = -\mathfrak{e}^{(1/2)1/2} \bullet \mathfrak{e}^{(1/2)}_{1/2} \\
&= -\mathfrak{e}^{(1/2)}_{-1/2} \bullet \mathfrak{e}^{(1/2)}_{1/2} = \mathfrak{g}_{-1/2,1/2}, \\
-1 = \mathfrak{g}^{-1/2,1/2} &= \mathfrak{e}^{(1/2)-1/2} \bullet \mathfrak{e}^{(1/2)1/2} = \mathfrak{e}^{(1/2)-1/2} \bullet \mathfrak{e}^{(1/2)}_{-1/2} = -\mathfrak{e}^{(1/2)}_{1/2} \bullet \mathfrak{e}^{(1/2)1/2} \\
&= -\mathfrak{e}^{(1/2)}_{1/2} \bullet \mathfrak{e}^{(1/2)}_{-1/2} = \mathfrak{g}_{1/2,-1/2}.
\end{aligned} \tag{10.47}
$$

These equations include the identification of the covariant metric in terms of the covariant basis, compare Eq. (10.44). The relations between contravariant and covariant basis spinors can be written

$$
\mathfrak{e}^{(1/2)\mu} = \sum_{\nu} \mathfrak{g}^{\mu\nu} \mathfrak{e}^{(1/2)}_{\nu} \qquad \text{and} \qquad \mathfrak{e}^{(1/2)}_{\mu} = \sum_{\nu} \mathfrak{g}_{\mu\nu} \mathfrak{e}^{(1/2)\nu}. \tag{10.48}
$$

Another consequence is the various ways of writing ϵ,

$$
\begin{aligned}
\epsilon &= \mathfrak{e}^{(1/2)-1/2}\mathfrak{e}^{(1/2)1/2} - \mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)-1/2} = \sum_{\mu\nu} \mathfrak{e}^{(1/2)\mu}\mathfrak{g}_{\mu\nu}\mathfrak{e}^{(1/2)\nu} \\
&= \mathfrak{e}^{(1/2)-1/2}\mathfrak{e}^{(1/2)}_{-1/2} + \mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)}_{1/2} = \sqcup \\
&= -\mathfrak{e}^{(1/2)}_{1/2}\mathfrak{e}^{(1/2)1/2} - \mathfrak{e}^{(1/2)}_{-1/2}\mathfrak{e}^{(1/2)-1/2} \\
&= -\mathfrak{e}^{(1/2)}_{1/2}\mathfrak{e}^{(1/2)}_{-1/2} + \mathfrak{e}^{(1/2)}_{-1/2}\mathfrak{e}^{(1/2)}_{1/2} = -\sum_{\mu\nu} \mathfrak{e}^{(1/2)}_{\mu}\mathfrak{g}^{\mu\nu}\mathfrak{e}^{(1/2)}_{\nu}.
\end{aligned} \tag{10.49}
$$

In particular, this invariant tensor is seen to be equivalent to the identity tensor. It is only a difference as to whether the tensor is expressed in terms of contravariant or covariant bases, or a combination of the two. A consequence of the antisymmetry of ϵ and the equality of ϵ and $\sqcup$, is that $\sqcup$ is essentially antisymmetric,

$$
(\sqcup)^t = -\sqcup, \tag{10.50}
$$

but this does not appear explicit in the definition of $\sqcup$ since it was defined as a combination of contravariant and covariant basis spinors. But this antisymmetry has the consequence that contractions of $\sqcup$ with itself,

$$
\sqcup\!\bullet\!\sqcup = \sqcup\!\bullet\!\sqcup = -\sqcup \tag{10.51}
$$

have a minus sign due to the contraction of contravariant with contravariant (or covariant with covariant) basis spinors. From the above expressions, it is also noticed that, while the covariant basis set was defined so that $\mathfrak{e}^{(1/2)}_{\mu} \bullet \mathfrak{e}^{(1/2)\nu} = \delta_{\mu\nu}$, the contraction in the opposite order has the opposite sign, namely

$$
\mathfrak{e}^{(1/2)\nu} \bullet \mathfrak{e}^{(1/2)}_{\mu} = -\mathfrak{e}^{(1/2)}_{\mu} \bullet \mathfrak{e}^{(1/2)\nu} = -\delta_{\nu\mu}. \tag{10.52}
$$

This need to be careful about the order of spinors when contracting is similar to the manner in which the components of the adjoint spinor are calculated, see Eq. (10.14).

A related property of ϵ, is that its contraction, or equivalently, the double contraction of ϵ with itself, gives -2, namely

$$
\overset{\bullet}{\epsilon} = \epsilon \bullet^2 \epsilon = \sqcup \bullet^2 \sqcup = -2. \tag{10.53}
$$

This is a straightforward calculation, and not surprising when compared with the triple contraction of the Levi Civita tensor, Eq. (2.83). But that the double contraction of $\boldsymbol{\sqcup}$ is negative is conterintuitive. As the identity for the spinor space, it is a projector onto a 2-dimensional space and so its trace must be 2 (positive). The difference with the above result is that, when calculating the trace, the righthand direction is essentially moved to the lefthand side before taking the contraction, in detail

$$\mathrm{Tr}\boldsymbol{\sqcup} = \sum_{k=\pm 1/2} \mathfrak{e}_k^{(1/2)} \bullet \boldsymbol{\sqcup} \bullet \mathfrak{e}^{(1/2)k} = \sum_{k=\pm 1/2} \mathfrak{e}_k^{(1/2)} \bullet \mathfrak{e}^{(1/2)k} = 2. \tag{10.54}$$

In the straightforward contraction of $\boldsymbol{\sqcup}$, this transfer is not done and the basic antisymmetry of this tensor gives a minus sign.

Another property of $\boldsymbol{\epsilon}$ is that the tensor product of $\boldsymbol{\epsilon}$ with itself can be expressed as a combination of products of the identity, namely

$$\boldsymbol{\epsilon\epsilon} = \boldsymbol{\sqcup\!\!\sqcup} - \boldsymbol{\lfloor\sqcup\rfloor}. \tag{10.55}$$

This identity is like a projection of Eq. (2.84) onto a plane.

The emphasis so far has been on the properties of the basis elements with the presence of the invariant $\boldsymbol{\epsilon}$ implying specific relations between the different contravariant and covariant basis elements. Eq. (10.8) expands $\boldsymbol{\Psi}$ in terms of the contravariant basis set to get the covariant components, Eq. (10.11) of $\boldsymbol{\Psi}$. The analogous expansion

$$\boldsymbol{\Psi} = \Psi^{1/2}\mathfrak{e}_{1/2}^{(1/2)} + \Psi^{-1/2}\mathfrak{e}_{-1/2}^{(1/2)} \tag{10.56}$$

defines the contravariant components of the spinor, and these are calculated from $\boldsymbol{\Psi}$ according to

$$\Psi^{\pm 1/2} = \boldsymbol{\Psi} \bullet \mathfrak{e}^{(1/2)\pm 1/2} = -\mathfrak{e}^{(1/2)\pm 1/2} \bullet \boldsymbol{\Psi}. \tag{10.57}$$

Note the negative sign in the last equality. From the relations, Eqs. (10.46), between the basis elements, it follows that the components are related by

$$\Psi^{1/2} = -\Psi_{-1/2}, \qquad \Psi^{-1/2} = \Psi_{1/2}. \tag{10.58}$$

These component relations can be expressed in matrix form as

$$\begin{pmatrix} \Psi^{1/2} \\ \Psi^{-1/2} \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \Psi_{1/2} \\ \Psi_{-1/2} \end{pmatrix}, \qquad \begin{pmatrix} \Psi_{1/2} \\ \Psi_{-1/2} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \Psi^{1/2} \\ \Psi^{-1/2} \end{pmatrix}, \tag{10.59}$$

or in more standardly expressed spherical tensor form

$$\Psi^m = \sum_{m'} \Psi_{m'}\mathfrak{g}^{m'm} = -\sum_{m'} \mathfrak{g}^{mm'}\Psi_{m'}, \tag{10.60}$$

$$\Psi_m = \sum_{m'} \Psi^{m'}\mathfrak{g}_{m'm} = -\sum_{m'} \mathfrak{g}_{mm'}\Psi^{m'}. \tag{10.61}$$

Wigner [3] writes the metric tensors as $\mathfrak{g}^{mm'} = C_{1/2}^{mm'}$ and $\mathfrak{g}_{mm'} = C_{mm'}^{1/2}$. The negative signs and different way of writing the transformations of the spinor components, compared to Wigner's, is associated with the difference in emphasis of spinor basis sets versus spinor components. The metric as defined here is associated with the transformation to and from the contravariant and covariant basis sets, see Eq. (10.48), rather than of the spinor components. Again, it is the contravariant basis set that is used as a starting point in this presentation, Eq. (10.3). Seemingly, almost all treatments of spinors deal only with the spinor components, and say nothing about basis sets. By emphasizing the latter, the contraction of arbitrary spinors can be defined rather than just via the inner product, Eq. (10.1).

10.4 Spinor Invariants

A large body of literature [32] emphasizes spinor invariants. The basic spinor invariant is exemplified by

$$\boldsymbol{\epsilon} \bullet^2 \boldsymbol{\Psi\Phi} = \Psi^{1/2}\Phi^{-1/2} - \Psi^{-1/2}\Phi^{1/2} = \sum_{\mu\nu} \mathfrak{g}_{\mu\nu}\Psi^{\mu}\Phi^{\nu}. \quad (10.62)$$

Polynomials of such invariants are standardly used for the description of all irreducible representations of the rotation group. In contrast, the subsequent sections introduce some of these properties in what the author considers to be a more direct manner, namely by the same method as that used for deducing the properties of Cartesian tensors. Here some elementary but essential properties of the basic spinor invariant is discussed.

The basic spinor invariant, as exemplified above, is just the spinor dot product $\boldsymbol{\Psi}\bullet\boldsymbol{\Phi}$ of $\boldsymbol{\Psi}$ and $\boldsymbol{\Phi}$. This connection arises because of the various properties of $\boldsymbol{\epsilon}$. Namely, since $\boldsymbol{\epsilon}$ and $\sqcup$ are identical, it follows that

$$\boldsymbol{\epsilon} \bullet \boldsymbol{\Psi} = \boldsymbol{\Psi} \bullet \boldsymbol{\epsilon} = \boldsymbol{\Psi}, \quad (10.63)$$

see Eqs. (10.12) and (10.49), and thus the identity follows. The spinor dot product can be expanded in many ways, specifically in terms of purely contravariant or covariant components

$$\begin{aligned}
\boldsymbol{\epsilon} \bullet^2 \boldsymbol{\Psi\Phi} &= \boldsymbol{\Psi}\bullet\boldsymbol{\Phi} \\
&= \left[\mathfrak{e}^{(1/2)}_{1/2}\Psi^{1/2} + \mathfrak{e}^{(1/2)}_{-1/2}\Psi^{-1/2}\right] \bullet \left[\mathfrak{e}^{(1/2)}_{1/2}\Phi^{1/2} + \mathfrak{e}^{(1/2)}_{-1/2}\Phi^{-1/2}\right] \\
&= \Psi^{1/2}\Phi^{-1/2} - \Psi^{-1/2}\Phi^{1/2} \\
&= \left[\mathfrak{e}^{(1/2)1/2}\Psi_{1/2} + \mathfrak{e}^{(1/2)-1/2}\Psi_{-1/2}\right] \bullet \left[\mathfrak{e}^{(1/2)1/2}\Phi_{1/2} + \mathfrak{e}^{(1/2)-1/2}\Phi_{-1/2}\right] \\
&= \Psi_{1/2}\Phi_{-1/2} - \Psi_{-1/2}\Phi_{1/2},
\end{aligned} \quad (10.64)$$

as well as the mixed expansions

$$\begin{aligned}
\boldsymbol{\Psi}\bullet\boldsymbol{\Phi} &= \Psi^{1/2}\Phi_{1/2} + \Psi^{-1/2}\Phi_{-1/2} \\
&= -\Psi_{1/2}\Phi^{1/2} - \Psi_{-1/2}\Phi^{-1/2}.
\end{aligned} \quad (10.65)$$

All these ways of writing the spinor invariant are equivalent, according to the relations between the spinor components, Eq. (10.58). The negative signs in the these forms result from the essential antisymmetry of the spinor dot product. Another important property of the spinor dot product is that the contraction of a spinor with itself vanishes, that is

$$\boldsymbol{\Psi}\bullet\boldsymbol{\Psi} = 0. \quad (10.66)$$

This follows immediately from the above expansions.

Since the spinor space is 2-dimensional, there are only two independent basis elements. This has been extensively used in the previous section. But more generally, if one has the three spinors $\boldsymbol{\Psi}$, $\boldsymbol{\Phi}$ and $\boldsymbol{\Upsilon}$, these cannot be linearly independent and one spinor, say $\boldsymbol{\Upsilon}$, can be expanded in terms of the other two, thus

$$\boldsymbol{\Upsilon} = a\boldsymbol{\Psi} + b\boldsymbol{\Phi}, \quad (10.67)$$

with expansion coefficients a and b. The latter can be calculated by taking spinor dot products,

$$\begin{aligned}
\boldsymbol{\Psi}\bullet\boldsymbol{\Upsilon} &= b\boldsymbol{\Psi}\bullet\boldsymbol{\Phi} \\
\boldsymbol{\Phi}\bullet\boldsymbol{\Upsilon} &= a\boldsymbol{\Phi}\bullet\boldsymbol{\Psi}.
\end{aligned} \quad (10.68)$$

These results are particularly simple because of the antisymmetry of the spinor dot product. An interesting way of writing the consequences of these calculations is

$$\boldsymbol{\Upsilon}\boldsymbol{\Psi}\bullet\boldsymbol{\Phi} = \boldsymbol{\Psi}\boldsymbol{\Upsilon}\bullet\boldsymbol{\Phi} + \boldsymbol{\Psi}\bullet\boldsymbol{\Upsilon}\boldsymbol{\Phi}. \tag{10.69}$$

This equation keeps the order of $\boldsymbol{\Psi}$ and $\boldsymbol{\Phi}$, with $\boldsymbol{\Upsilon}$ not contracted on the lefthand side of the equation, but successively contracted into each of the other two spinors while being inserted between them. It is a useful exercise for the reader to write this equation out in component form.

Another useful identity arising from the 2-dimensionality of the space of spinors is

$$\boldsymbol{\epsilon}\Psi\bullet\Phi = \Phi\Psi - \Psi\Phi. \tag{10.70}$$

This is an embedding property, namely embedding a scalar product as a second order spinor. It is an application of the identity of Eq. (10.55).

10.5 Reduction of spinor tensors of order p

A spinor tensor of order p is defined here as a quantity with p spinor directions. Such a quantity can be expressed in terms of a sum over the 2^p p-fold products of the standard basis set, with expansion coefficients having p indices. Under a rotation of a given spinor of order p, each of the p spinor directions must be rotated and a classification can be made as to what representation of the rotation group this tensor belongs. In general the representation is reducible and a reduction of the spinor representation into irreducible representations of the rotation group can be made. Even after reduction into irreducible representations, the given tensorial form may not be the simplest way in which the irreducible representations can be presented, specifically an irreducible spinor tensor may be mapped one-to-one into a tensor of lower order, just as were the Cartesian tensors. The objective of this section is to consider the reduction of pth order spinor tensors into irreducible parts and to represent these in the simplest (natural) way.

In order to preserve the rotational properties of a tensor, a reduction in tensorial order can only be accomplished by means of an invariant tensor. For spinors, any rotational invariant is a combination of $\boldsymbol{\epsilon}$'s, so reduction of tensorial order ceases only when all possible contractions with $\boldsymbol{\epsilon}$ vanish. If a spinor tensor is thought of as being described using a contravariant basis set then, since $\boldsymbol{\epsilon}$ is antisymmetric in covariant basis elements, its contraction with the spinor tensor vanishes only when the tensor is symmetric among all its covariant indices. The same is true if the tensor is written in terms of contravariant indices. But if the description is mixed, some contravariant and some covariant indices, then irreducibility requires symmetry between contravariant indices, symmetry between covariant indices, but antisymmetry between covariant and contravariant indices. Equivalently, the mixed indices case requires that any contraction between contravariant and covariant indices must vanish. These various cases arise via the different forms for the invariant $\boldsymbol{\epsilon}$, Eq. (10.49). The advantage of treating a spinor tensor as an abstract entity is that these cases do not have to be considered separately and contractions can be carried out directly without having to worry about which kind of contraction needs to be carried out.

From the above arguments, a spinor tensor that belongs to a particular irreducible representation can have its order decreased by contracting with $\boldsymbol{\epsilon}$ in all possible ways until the spinor is symmetric in all its directions, or it vanishes. Since $\boldsymbol{\epsilon}$ is the only rotational invariant, this is the only way of reducing a spinor tensor and the result, a symmetric spinor tensor, is irreducible. Clearly such a

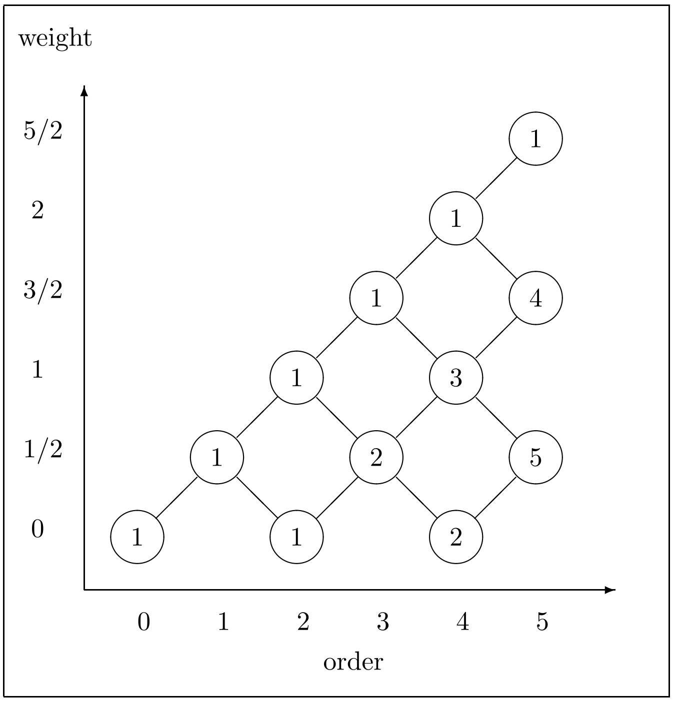


Figure 10.1: Parentage Scheme. The number of linearly independent irreducible representations of weight ℓ in a spinor of order p.

spinor tensor remains symmetric under any rotation so belongs to a representation of the rotation group. Moreover, if its order is p, then it is a linear combination of the $p+1$ symmetric spinor tensors formed according to the number of ways of assigning either $\mathfrak{e}^{(1/2)1/2}$ or $\mathfrak{e}^{(1/2)-1/2}$ to each spinor direction. Again, the spinor tensor of largest possible weight (eigenvalue of $G_{\hat{z}}$) is $\{\mathfrak{e}^{(1/2)1/2}\}^{(p)}$, with weight $p/2$. This verifies that such a spinor tensor belongs to an irreducible representation of weight $\ell = p/2$. Such a spinor tensor will be referred to as a natural spinor. To recap, a natural spinor of order p is symmetric whose maximum possible weight is $p/2$, corresponding to all of the spinor components being $1/2$. Thus the natural form for a spinor of weight ℓ is as a symmetric spinor tensor of order 2ℓ. Such a spinor can be embedded in a tensor space of higher order by taking the tensor product of the natural spinor with multiples of $\boldsymbol{\epsilon}$, with a variety of ways of ordering the tensorial directions. It is noticed that in such a process, the order of the spinor always increases by a multiple of 2. The possible irreducible spinors that can be in a pth order spinor can be deduced by a parentage scheme, similar to that for Cartesian tensors given in Fig. 3.1, but inherently simpler, see Fig. 10.1. This scheme is equivalent to successively building up all spinor tensors of order p by considering the tensor product of a spinor $\boldsymbol{\Phi}$ of order $p-1$ and weight ℓ with a spinor $\boldsymbol{\Psi}$ of order 1 to give a spinor of order p. This tensor product can be taken in such a way that the resulting spinor is symmetric to the interchange of all spinor directions, or the direction of $\boldsymbol{\Psi}$ is antisymmetric with respect to all the other directions. In the first case the resulting tensor is of weight $\ell + 1/2$ while in the second case, the weight is $\ell - 1/2$ and can have its order lowered by two by contracting with $\boldsymbol{\epsilon}$. Equivalently, any pth order spinor tensor can be decomposed into a combination of spinor tensors, each of which is an embedding of a symmetric spinor tensor. In this way, any spinor tensor can be reduced to a combination of irreducible representations of the rotation group.

Two simple examples of such reductions are given here. If $\boldsymbol{\Psi}$ is a spinor tensor of order 2, its reduction is given by

$$\boldsymbol{\Psi} = [\boldsymbol{\Psi}]^{(1)} - \frac{1}{2}\boldsymbol{\epsilon}\,[\boldsymbol{\Psi}]^{(0)} = [\boldsymbol{\Psi}]^{(1)} - \frac{1}{2}\boldsymbol{\epsilon}\boldsymbol{\epsilon} \bullet^2 \boldsymbol{\Psi}. \tag{10.71}$$

This is just the breakdown of $\boldsymbol{\Psi}$ into its symmetric and antisymmetric parts. The manner in which the indices of the spinor tensor occurs when making such an expansion in component form is useful to recognize, thus

$$\begin{aligned} \boldsymbol{\Psi} &= \lfloor\sqcup\rfloor \bullet^2 \boldsymbol{\Psi} \\ &= \sum_{j,k=\{+1/2,-1/2\}} \mathfrak{e}_j^{(1/2)} \mathfrak{e}_k^{(1/2)} \mathfrak{e}^{(1/2)k} \mathfrak{e}^{(1/2)j} \bullet \boldsymbol{\Psi} \\ &= \sum_{j,k=\{+1/2,-1/2\}} \mathfrak{e}_j^{(1/2)} \mathfrak{e}_k^{(1/2)} \Psi^{jk}. \end{aligned} \tag{10.72}$$

The weight 1 part of $\boldsymbol{\Psi}$ is

$$[\boldsymbol{\Psi}]^{(1)} = 1/2\left(\boldsymbol{\Psi} + \boldsymbol{\Psi}^t\right) = \frac{1}{2} \sum_{j,k=\{+1/2,-1/2\}} \mathfrak{e}_j^{(1/2)} \mathfrak{e}_k^{(1/2)} \left(\Psi^{jk} + \Psi^{kj}\right) \tag{10.73}$$

while the scalar (weight 0) part of $\boldsymbol{\Psi}$ is

$$[\boldsymbol{\Psi}]^{(0)} \equiv \boldsymbol{\epsilon} \bullet^2 \boldsymbol{\Psi} = \Psi^{1/2,-1/2} - \Psi^{-1/2,1/2}. \tag{10.74}$$

After the embedding of this into second order spinor tensor space via $(-1/2)\boldsymbol{\epsilon}$ and adding the weight 1 part, this reproduces $\boldsymbol{\Psi}$.

If $\boldsymbol{\Upsilon}$ is an order 3 spinor tensor, this spinor tensor can be written in terms of a weight 3/2 and two independent weight 1/2 spinor tensors. One way of embedding these irreducible representations in the order 3 tensor space is

$$\boldsymbol{\Upsilon} = [\boldsymbol{\Upsilon}]^{(3/2)} + \boldsymbol{\epsilon}\boldsymbol{\Upsilon}_1 + \boldsymbol{\Upsilon}_2\boldsymbol{\epsilon}, \tag{10.75}$$

where $\boldsymbol{\Upsilon}_1$ and $\boldsymbol{\Upsilon}_2$ are order 1, weight 1/2, spinor tensors. Clearly the weight 3/2 spinor tensor part of $\boldsymbol{\Upsilon}$ is obtained by taking the symmetric part of $\boldsymbol{\Upsilon}$, namely

$$[\boldsymbol{\Upsilon}]^{(3/2)} = \frac{1}{6}\Big(\boldsymbol{\Upsilon} + \lfloor\boldsymbol{\Upsilon}\bullet\rfloor + \lfloor\bullet\boldsymbol{\Upsilon}\rfloor + \lfloor\sqcup\!\sqcup\rfloor\bullet^2\boldsymbol{\Upsilon} + \lfloor\lfloor\sqcup\!\sqcup\rfloor\bullet^2\boldsymbol{\Upsilon}\bullet\rfloor + \boldsymbol{\Upsilon}\bullet^2\lfloor\sqcup\!\sqcup\rfloor\Big). \tag{10.76}$$

The two weight 1/2 spinor tensors can be calculated from the contractions

$$\boldsymbol{\epsilon} \bullet^2 \boldsymbol{\Upsilon} = -2\boldsymbol{\Upsilon}_1 + \boldsymbol{\Upsilon}_2 \tag{10.77}$$

and

$$\boldsymbol{\Upsilon} \bullet^2 \boldsymbol{\epsilon} = \boldsymbol{\Upsilon}_1 - 2\boldsymbol{\Upsilon}_2, \tag{10.78}$$

whose solution is

$$\boldsymbol{\Upsilon}_1 = -\frac{1}{3}\left[2\boldsymbol{\epsilon} \bullet^2 \boldsymbol{\Upsilon} + \boldsymbol{\Upsilon} \bullet^2 \boldsymbol{\epsilon}\right] \tag{10.79}$$

and

$$\boldsymbol{\Upsilon}_2 = -\frac{1}{3}\left[\boldsymbol{\epsilon} \bullet^2 \boldsymbol{\Upsilon} + 2\boldsymbol{\Upsilon} \bullet^2 \boldsymbol{\epsilon}\right]. \tag{10.80}$$

Obviously a double contraction using the other pair of directions gives just a linear combination of the above relations determining $\boldsymbol{\Upsilon}_1$ and $\boldsymbol{\Upsilon}_2$, so leads to no new irreducible representation, consistent with the general arguments on the numbers of irreducible representations into which $\boldsymbol{\Upsilon}$ can be decomposed, as given by Fig. 10.1.

This decomposition of a general 3rd order $\boldsymbol{\Upsilon}$ into irreducible representations of the rotation group can be verified by equating components of both sides of Eq. (10.75) with the above expressions for $\boldsymbol{\Upsilon}_1$ and $\boldsymbol{\Upsilon}_2$. A special case of this decomposition is for $\boldsymbol{\Upsilon} = \boldsymbol{\alpha\beta\gamma}$. Then according to the above expressions, the weight 1/2 spinor tensors are

$$\boldsymbol{\Upsilon}_1 = -\frac{1}{3}[2\boldsymbol{\alpha} \bullet \boldsymbol{\beta\gamma} + \boldsymbol{\alpha\beta} \bullet \boldsymbol{\gamma}] \tag{10.81}$$

and

$$\boldsymbol{\Upsilon}_2 = -\frac{1}{3}[\boldsymbol{\alpha} \bullet \boldsymbol{\beta\gamma} + 2\boldsymbol{\alpha\beta} \bullet \boldsymbol{\gamma}]. \tag{10.82}$$

Eq. (10.75) for this decomposition can be verified using purely formal spinor manipulations, including of course the weight 3/2 part given by the completely symmetrized tensor, but it is necessary to use the identity of Eq. (10.69) to complete the proof of the identity.

10.6 Spinor tensors of weight ℓ

It is convenient to introduce the set of projectors $\boldsymbol{\mathcal{E}}^{(\ell)}$, which are spinor tensors of order 4ℓ and project out the natural spinor tensor of order 2ℓ and weight ℓ from an arbitrary spinor tensor of order $p = 2\ell$. Essentially such a projector is just the projector onto the symmetric spinor tensor of order $p = 2\ell$. This can be written in terms of products of the spinor identity $\boldsymbol{\sqcup}$ as

$$\boldsymbol{\mathcal{E}}^{(\ell)} = \{\lfloor \cdots \lfloor\}^{(2\ell)}\{\rfloor \cdots \rfloor\}^{(2\ell)}, \tag{10.83}$$

where $\{\cdots\}^{(2\ell)}$ indicates the symmetric part of the 2ℓ order spinor tensor. It can also be written in terms of indices, namely

$$\mathcal{E}^{(\ell)\mu_1\ldots\mu_{2\ell}}_{\nu_1\ldots\nu_{2\ell}} = \frac{1}{(2\ell)!}\sum_P \prod_{j=1}^{2\ell} \delta^{\mu_{Pj}}_{\nu_j}, \tag{10.84}$$

where the sum is over all permutations P of the indices $1\ldots 2\ell$ with Pj the result of the permutation P acting on index j. The contrast with the Cartesian projector $\mathsf{E}^{(\ell)}$ of Eq. (3.49) is noted, with the later requiring the projected tensor to be traceless as well as symmetric (and of course there is also the difference in vector space dimension and tensorial order for the same integer weight).

The contravariant basis set appropriate to eigenvectors of $G_{\hat{z}}$ with maximum weight ℓ are then the spinor tensors

$$\begin{aligned}
\mathfrak{e}^{(\ell)\mu} &= \begin{pmatrix} 2\ell \\ \ell-\mu \end{pmatrix}^{1/2} \boldsymbol{\mathcal{E}}^{(\ell)} \bullet^{2\ell} \left(\mathfrak{e}^{(1/2)1/2}\right)^{\ell+\mu}\left(\mathfrak{e}^{(1/2)-1/2}\right)^{\ell-\mu} \\
&= \sqrt{\frac{(2\ell)!}{(\ell-\mu)!(\ell+\mu)!}}\left\{\left(\mathfrak{e}^{(1/2)1/2}\right)^{\ell+\mu}\left(\mathfrak{e}^{(1/2)-1/2}\right)^{\ell-\mu}\right\}^{(2\ell)}.
\end{aligned} \tag{10.85}$$

For an eigenvalue of μ, the eigenvector is just the symmetric combination of $\ell+\mu$ factors of $\mathfrak{e}^{(1/2)1/2}$ and $\ell-\mu$ factors of $\mathfrak{e}^{(1/2)-1/2}$. The normalization is chosen so that

$$\mathfrak{e}^{(\ell)}_{\nu} \bullet^{2\ell} \mathfrak{e}^{(\ell)\mu} = \delta^{\mu}_{\nu} \tag{10.86}$$

with the covariant basis set defined in a manner analogous to that for the contravariant basis set. As an example, consider the basis element

$$\begin{aligned} \mathfrak{e}^{(3/2)1/2} &= \binom{3}{1}^{1/2} \left\{ \left(\mathfrak{e}^{(1/2)1/2}\right)^2 \mathfrak{e}^{(1/2)-1/2} \right\}^{(3)} \\ &= \frac{1}{\sqrt{3}} \Big[\mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)-1/2} + \mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)-1/2}\mathfrak{e}^{(1/2)1/2} \\ &\qquad + \mathfrak{e}^{(1/2)-1/2}\mathfrak{e}^{(1/2)1/2}\mathfrak{e}^{(1/2)1/2} \Big]. \end{aligned} \tag{10.87}$$

This illustrates the details of how the number of terms in the symmetrization, namely the combinatorial factor, enters into the normalization prefactor for the sum of products of spinor basis elements. It is easy to show that the contravariant basis satisfies the raising and lowering operations

$$G_{\pm}\mathfrak{e}^{(\ell)\mu} = \sqrt{\ell(\ell+1)-\mu(\mu\pm 1)}\,\mathfrak{e}^{(\ell)\mu\pm 1}. \tag{10.88}$$

An expansion of the projector $\boldsymbol{\mathcal{E}}^{(\ell)}$ in terms of these basis sets is

$$\boldsymbol{\mathcal{E}}^{(\ell)} = \sum_{\mu} \mathfrak{e}^{(\ell)\mu}\mathfrak{e}^{(\ell)}_{\mu}. \tag{10.89}$$

It follows that the trace of $\boldsymbol{\mathcal{E}}^{(\ell)}$ is

$$\mathrm{Tr}\boldsymbol{\mathcal{E}}^{(\ell)} = \sum_{\nu} \mathfrak{e}^{(\ell)}_{\nu} \bullet^{2\ell} \boldsymbol{\mathcal{E}}^{(\ell)} \bullet^{2\ell} \mathfrak{e}^{(\ell)\nu} = \sum_{\nu} \mathfrak{e}^{(\ell)}_{\nu} \bullet^{2\ell} \mathfrak{e}^{(\ell)\nu} = 2\ell+1. \tag{10.90}$$

This is the dimension of the irreducible representation, which is easily obtained from counting the number of basis elements, as in the above equation. It is an interesting exercise to also get it from taking the trace of $\boldsymbol{\mathcal{E}}^{(\ell)}$ in its symmetric product of $\sqcup$ form, Eq. (10.83). Note that, when carrying out the trace, this involves taking the righthand indices over to the left side of the tensor and then contracting. This order is especially important when the order of directions in a contraction matters, as it does in the spinor case. An immediate consequence of the dimensionality of these spinor projectors is that, since the contraction of $\boldsymbol{\mathcal{E}}^{(\ell)}$ must be proportional to $\boldsymbol{\mathcal{E}}^{(\ell-1/2)}$, that the proportionality constant is

$$\lfloor \bullet \boldsymbol{\mathcal{E}}^{(\ell)} \bullet \rfloor = -\left(\frac{2\ell+1}{2\ell}\right) \boldsymbol{\mathcal{E}}^{(\ell-1/2)}. \tag{10.91}$$

The minus sign comes from the change from contravariant to covariant basis elements in order to carry out the contractions. This again points out the difference between carrying out a trace versus carrying out a contraction between left and right hand directions and is associated with the antisymmetry of the identity $\sqcup$.

The contravariant and covariant metrics

$$\begin{aligned} \mathfrak{g}^{(\ell)\mu\nu} &\equiv \mathfrak{e}^{(\ell)\mu} \bullet^{2\ell} \mathfrak{e}^{(\ell)\nu} = (-1)^{\ell+\nu}\delta_{\mu,-\nu} \\ \mathfrak{g}^{(\ell)}_{\mu\nu} &\equiv \mathfrak{e}^{(\ell)}_{\mu} \bullet^{2\ell} \mathfrak{e}^{(\ell)}_{\nu} = (-1)^{\ell-\nu}\delta_{\mu,-\nu} \end{aligned} \tag{10.92}$$

are the generalizations of Eqs. (10.42) and 10.44). For integer ℓ there is no difference between contravariant and covariant metrics and then they also agree with the Cartesian metric $\mathfrak{g}_{\mu\nu}$ of Eq. (5.65), [but not for the $g_{\mu\nu}$ Cartesian metric of Eq. (5.61)]. An immediate consequence of these metrics is the relation between covariant and contravariant spinor tensor basis elements,

$$\mathfrak{e}^{(\ell)\mu} = \sum_{\nu} \mathfrak{g}^{(\ell)\mu\nu} \mathfrak{e}_{\nu}^{(\ell)} = (-1)^{\ell-\mu} \mathfrak{e}_{-\mu}^{(\ell)}. \tag{10.93}$$

This relation is also consistent with the product structure of the contravariant tensor basis elements, Eq. (10.85), and the equivalent formula for the covariant basis elements, together with the relations between the elementary spinor basis elements, Eqs. (10.46).

The pth power $(\mathbf{\Psi})^p$ of a spinor $\mathbf{\Psi} = u\mathfrak{e}^{(1/2)1/2} + v\mathfrak{e}^{(1/2)-1/2}$ of order 1 is reducible. All irreducible spinor tensor representations based on $\mathbf{\Psi}$ are of the form

$$[\mathbf{\Psi}]^{(\ell)} = \mathcal{E}^{(\ell)} \bullet^{2\ell} (\mathbf{\Psi})^{2\ell} = \sum_{\mu} \mathfrak{e}^{(\ell)\mu} [\Psi]_{\mu}^{(\ell)}, \tag{10.94}$$

where the spherical tensor component is

$$[\Psi]_{\mu}^{(\ell)} = \mathfrak{e}_{\mu}^{(\ell)} \bullet^{2\ell} (\mathbf{\Psi})^{2\ell} = \begin{pmatrix} 2\ell \\ \ell+\mu \end{pmatrix}^{1/2} u^{\ell+\mu} v^{\ell-\mu}. \tag{10.95}$$

The notation $[\cdots]^{(\ell)}$ has been borrowed from Cartesian tensor analysis to indicate an irreducible spinor of weight ℓ. Each irreducible spinor may appear several times in the reduction of the product $(\mathbf{\Psi})^p$, the multiplicity being given by the parentage scheme, Fig. 10.1. It is the spinor components, Eq. (10.95), that appear standardly in the literature [3, 32] and that have been used for the calculation of the rotation matrices $D_{mn}^{(\ell)}$ and n-j symbols. Again, the present treatment has inherently considered the general (tensor) product of arbitrary spinors whereas the standard presentations seem to limit the discussion only to those spinor tensors belonging to an irreducible representation of the rotation group.

10.7 3-j spinor tensors

Rotationally invariant spinor tensors that have three sets of directions, with the tensor being symmetric in each set of directions, describes a coupling between three irreducible representations of the rotation group. The natural way of obtaining such a tensor is to contract three projection operators. Since the 3-j symbols have been defined so that they are cyclically invariant and have a particular normalization, the spinor tensors need to be defined so that these properties are retained. On using $\boldsymbol{\mathcal{W}}(\ell_1, \ell_2, \ell_3)$ as the notation for a 3-j spinor tensor, such a tensor is given by

$$\boldsymbol{\mathcal{W}}(\ell_1, \ell_2, \ell_3) = \frac{(-1)^{2\ell_2}}{\sqrt{\omega(\ell_1, \ell_2, \ell_3)}} \boldsymbol{\mathcal{T}}(\ell_1, \ell_2, \ell_3) \tag{10.96}$$

where

$$\begin{aligned} \boldsymbol{\mathcal{T}}(\ell_1, \ell_2, \ell_3) &= \boldsymbol{\mathcal{E}}^{(\ell_1)} \bullet^{2\ell_1} (\,|\,)^{\beta} (\,|\,)^{\gamma} \boldsymbol{\mathcal{E}}^{(\ell_2)} \bullet^{2\ell_2} (\,|\,)^{\gamma} (\,|\,)^{\alpha} \boldsymbol{\mathcal{E}}^{(\ell_3)} \bullet^{2\ell_3} (\,|\,)^{\alpha} (\,|\,)^{\beta} \\ &= \{(\,|\,)^{\beta} (\,|\,)^{\gamma}\}^{(2\ell_1)} \{(\,|\,)^{\gamma} (\,|\,)^{\alpha}\}^{(2\ell_2)} \{(\,|\,)^{\alpha} (\,|\,)^{\beta}\}^{(2\ell_3)} \end{aligned} \tag{10.97}$$

It might be useful to remind the reader that $\sqcup = \epsilon$, so that this is essentially a combination of antisymmetic second order spinors. Here $L \equiv \ell_1 + \ell_2 + \ell_3 = \alpha + \beta + \gamma$ is the sum of the weights and is necessarily an integer. The numbers of contractions between the three projection operators are

$$\alpha = L - 2\ell_1, \qquad \beta = L - 2\ell_2, \qquad \gamma = L - 2\ell_3 \tag{10.98}$$

and the normalization constant (see the following subsection)

$$\omega(\ell_1, \ell_2, \ell_3) = \frac{(L+1)!(L-2\ell_1)!(L-2\ell_2)!(L-2\ell_3)!}{(2\ell_1)!(2\ell_2)!(2\ell_3)!}. \tag{10.99}$$

is chosen so that

$$\boldsymbol{\mathcal{W}}(\ell_3, \ell_2, \ell_1) \bullet^{2L} \boldsymbol{\mathcal{W}}(\ell_1, \ell_2, \ell_3) = (-1)^L. \tag{10.100}$$

It is noticed that the normalization factor is the same as that for the Cartesian 3-j tensors, Eq. (6.11) for L even, but in the spinor case, the formula for the odd L has the same form as that for even L. The $(-1)^L$ factor arises from the product of double contractions between pairs of $\sqcup$'s, Eq. (10.54), (equivalenly, pairs of ϵ's) which is analogous to the Cartesian case involving the contraction of the 3rd order invariant $\boldsymbol{\mathcal{E}}$, Eq. (6.10). To treat all symmetric sets of indices in a similar manner, all the contractions into the projection operators are between the righthand (covariant) indices. Finally, the factor of $(-1)^{2\ell_2}$ in the definition of $\boldsymbol{\mathcal{W}}(\ell_1, \ell_2, \ell_3)$, Eq. (10.96), is introduced so as to make the 3-j have cyclic symmetry. This arises because the contraction between covariant indices is antisymmetric, and can be seen as follows. On cycling the 3-j to $\boldsymbol{\mathcal{W}}(\ell_2, \ell_3, \ell_1)$, the γ contractions between $\boldsymbol{\mathcal{E}}^{(\ell_1)}$ and $\boldsymbol{\mathcal{E}}^{(\ell_2)}$ have their left and right indices interchanged, thus giving a factor of $(-1)^\gamma$. Similarly for the β contractions. As a consequence, to retain cyclic invariance, a factor of $(-1)^{\gamma+\beta} = (-1)^{2\ell_1}$ must be inserted into the ratio of the factors defining the 3-j and its cycled variation. Since L is an integer, $(-1)^{2L} = 1$, and this ratio is equal to $(-1)^{2\ell_2+2\ell_3}$. This is compensated for by the change in the powers of (-1) appearing in the prefactor in the definition of the 3-j and its cycled variation, to retain an overall cyclical property for the 3-j spinor tensor.

10.7.1 Normalization calculation

The normalization factor $\omega(\ell_1, \ell_2, \ell_3)$ can be calculated in a manner analogous to the method used for the Cartesian case, Sec. 6.3, namely by a recursion relation based on a contraction between two of the projectors. For the spinor case, each contraction is associated with a decrease in the ℓ values by 1/2. On the basis of the normalization of the 3-j spinor tensors, a single contraction between the $\boldsymbol{\mathcal{E}}^{(\ell_1)}$ and $\boldsymbol{\mathcal{E}}^{(\ell_2)}$ projectors leads to the equation

$$\begin{aligned}
-(\rfloor)^{2\ell_1-1}\sqcup(\lfloor)^{2\ell_1-1}\bullet^{2\ell_1+1}\boldsymbol{\mathcal{T}}(\ell_1, \ell_2, \ell_3) &= \lfloor\bullet\{(\lfloor)^{\beta}(\lfloor)^{\gamma}\}^{(2\ell_1)}\rfloor\bullet\{(\rfloor)^{\gamma}(\lfloor)^{\alpha}\}^{(2\ell_2)}\{(\rfloor)^{\alpha}(\rfloor)^{\beta}\}^{(2\ell_3)} \\
&= \frac{\omega(\ell_1, \ell_2, \ell_3)}{\omega(\ell_1-1, \ell_2-1, \ell_3)}\boldsymbol{\mathcal{T}}(\ell_1-1, \ell_2-1, \ell_3)
\end{aligned} \tag{10.101}$$

for the ratio of the normalization factors. That the contraction leads to a 3-j spinor tensor results from the fact that the contraction is a rotationally invariant tensor that is symmetric in three sets of spinor directions. The evaluation of the normalization ratio is accomplished by cataloguing the possible different results of the contraction with $\boldsymbol{\sqcup}$. For the lefthand part of $\boldsymbol{\sqcup}$, namely the one contracted into the ℓ_1 set of directions, this is contracted either into one of the set of γ directions with a possibility $\gamma/(2\ell_1)$ or to one of the β directions with possibility $\beta/(2\ell_1)$. Similarly the righthand part of $\boldsymbol{\sqcup}$ is contracted either into a γ direction or an α direction with possibilities $\alpha/(2\ell_2)$ and $\beta/(2\ell_2)$. The results of these four possibilities is considered in turn.

- If both directions of $\boldsymbol{\sqcup}$ involve γ directions, then pick one of the $\gamma/(2\ell_1)$ directions for the lefthand part of $\boldsymbol{\sqcup}$. The righthand side of $\boldsymbol{\sqcup}$ has a possibility $1/(2\ell_2)$ of being contracted with the same $\boldsymbol{\sqcup}$ joining the the two symmetric sets. Since the resulting contraction is 2, the contribution to the normalization ratio is $2\gamma/(4\ell_1\ell_2)$. Otherwise the two sides of $\boldsymbol{\sqcup}$ are contracted into different $\boldsymbol{\sqcup}$'s and two transpositions give a $+1$. There are $\gamma(\gamma-1)/(4\ell_1\ell_2)$ ways in which such a contraction occurs. In either case, in the resulting tensor, the number of contractions between the ℓ_1 and ℓ_2 sets of directions, namely γ, has been reduced by 1, giving the indicated 3-j spinor. Combined, the total contribution to the normalization ratio from having the $\boldsymbol{\sqcup}$ contracted on both sides into the set of γ directions is

$$\frac{\gamma(\gamma+1)}{(2\ell_1)(2\ell_2)}.$$

- If the lefthand side of $\boldsymbol{\sqcup}$ is contracted into a γ direction and the righthand side into an α direction, this rearranges the number of connections so that essentially γ is decreased by 1, just as in the first case. The number of possibilities for this to occur equals the contribution to the normalization ratio, which is

$$\frac{\gamma\alpha}{(2\ell_1)(2\ell_2)}.$$

- If the lefthand side of $\boldsymbol{\sqcup}$ is contracted into a β direction and the righthand side into a γ direction the contribution is

$$\frac{\beta\gamma}{(2\ell_1)(2\ell_2)}.$$

- Finally, if the lefthand side is contracted into a β direction and the righthand side into an α direction, then both end up in the ℓ_3 set and give a vanishing contribution since $\boldsymbol{\sqcup}$ is antisymmetic while the ℓ_3 set must be symmetric.

The normalization ratio is the sum of the various contributions, so

$$\frac{\omega(\ell_1,\ell_2,\ell_3)}{\omega(\ell_1-1/2,\ell_2-1/2,\ell_3)} = \frac{\gamma(\gamma+1+\alpha+\beta)}{(2\ell_1)(2\ell_2)} = \frac{\gamma(L+1)}{(2\ell_1)(2\ell_2)}. \tag{10.102}$$

This can be iterating a times, so that a more general normalization ratio is

$$\frac{\omega(\ell_1,\ell_2,\ell_3)}{\omega(\ell_1-a/2,\ell_2-a/2,\ell_3)} = \frac{(L+1)!\gamma!(2\ell_1-a)!(2\ell_2-a)!}{(L+1-a)!(\gamma-a)!(2\ell_1)!(2\ell_2)!}. \tag{10.103}$$

If a is picked so that $\ell_1+\ell_2$ is reduced to ℓ_3, which is always possible, then the corresponding 3-j spinor is $\boldsymbol{\mathcal{T}}(\ell_1,\ell_2,\ell_3) = \boldsymbol{\mathcal{E}}^{(\ell_3)}$, whose square normalization is $2\ell_3+1$. Sorting out the various factors when $a=\ell_1+\ell_2-\ell_3$ determines $\omega(\ell_1,\ell_2,\ell_3)$ to be given by Eq. (10.99).

10.7.2 3-j symbols

The 3-j symbols are the spherical tensor components of the 3-j spinor tensors and thus can be obtained by contracting the contravariant basis spinor tensors with the 3-j spinor tensors, namely

$$\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ \mu_1 & \mu_2 & \mu_3 \end{pmatrix} = \mathfrak{e}^{(\ell_3)\mu_3}\mathfrak{e}^{(\ell_2)\mu_2}\mathfrak{e}^{(\ell_1)\mu_1} \bullet^{2L} \boldsymbol{\mathcal{W}}(\ell_1,\ell_2,\ell_3). \tag{10.104}$$

Here again the order of contraction is to contract nearest indices. This contraction can be evaluated fairly easily. It should also be noted that $\mu_1+\mu_2+\mu_3=0$ since this is the component of an invariant spinor tensor.

Since the basis spinor tensors are symmetric, the $\boldsymbol{\mathcal{E}}^{(\ell)}$ projectors are redundant and the 3-j symbol reduces to a particular contraction of three basis spinor tensors with a normalization factor. This can be further reduced to a contraction of the symmetrized products of spinor basis elements. These two steps give

$$\begin{aligned} &\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ \mu_1 & \mu_2 & \mu_3 \end{pmatrix} \\ &= \frac{(-1)^{2\ell_2}}{\sqrt{\omega(\ell_1,\ell_2,\ell_3)}}\, \mathfrak{e}^{(\ell_1)\mu_1} \bullet^{2\ell_1} (\sqcup)^{\beta}(\sqcup)^{\gamma}\mathfrak{e}^{(\ell_2)\mu_2} \bullet^{2\ell_2} (\sqcup)^{\gamma}(\sqcup)^{\alpha}\mathfrak{e}^{(\ell_3)\mu_3} \bullet^{2\ell_3} (\sqcup)^{\alpha}(\sqcup)^{\beta} \\ &= \frac{(-1)^{2\ell_2}(2\ell_1)!(2\ell_2)!(2\ell_3)!}{[(L+1)!\alpha!\beta!\gamma!(\ell_1-\mu_1)!(\ell_1+\mu_1)!(\ell_2-\mu_2)!(\ell_2+\mu_2)!(\ell_3-\mu_3)!(\ell_3+\mu_3)!]^{1/2}} \\ &\quad \left\{\left(\mathfrak{e}^{(1/2)1/2}\right)^{\ell_1+\mu_1}\left(\mathfrak{e}^{(1/2)-1/2}\right)^{\ell_1-\mu_1}\right\}^{(2\ell_1)} \bullet^{2\ell_1} (\sqcup)^{\gamma}(\sqcup)^{\beta} \\ &\quad \left\{\left(\mathfrak{e}^{(1/2)1/2}\right)^{\ell_2+\mu_2}\left(\mathfrak{e}^{(1/2)-1/2}\right)^{\ell_2-\mu_2}\right\}^{(2\ell_2)} \bullet^{2\ell_2} (\sqcup)^{\alpha}(\sqcup)^{\gamma} \\ &\quad \left\{\left(\mathfrak{e}^{(1/2)1/2}\right)^{\ell_3+\mu_3}\left(\mathfrak{e}^{(1/2)-1/2}\right)^{\ell_3-\mu_3}\right\}^{(2\ell_3)} \bullet^{2\ell_3} (\sqcup)^{\alpha}(\sqcup)^{\beta} \end{aligned} \tag{10.105}$$

The $\sqcup$'s are here written as vertical lines because of space limitations, but the left-right notion of a $\sqcup$ must be retained. Here this if indicated as an arrowhead.

To carry out the contractions, it is noted that the individual contractions of the spinor basis elements are nonzero only between $\mathfrak{e}^{(1/2)1/2}$ and $\mathfrak{e}^{(1/2)-1/2}$. Thus, for a given possible way in which the contractions have a non-zero contribution, the numbers γ_- of $\mathfrak{e}^{(1/2)-1/2}$ and γ_+ of $\mathfrak{e}^{(1/2)1/2}$ on the lefthand side of the set of γ contractions must respectively equal the numbers of $\mathfrak{e}^{(1/2)1/2}$ and $\mathfrak{e}^{(1/2)-1/2}$ on the righthand side. Likewise for the α and β sets of contractions. Refer to the definition of the 3-j spinor tensor and the associated discussion for the specific meaning of α, β and γ. Note that the labeling here of which is γ_- and which is γ_+ is according to the basis element on the lefthand side (upper row) of the possible contraction! In this way, a set of contractions having a non-zero value must satisfy the counting constraints

$$\begin{aligned} \alpha = \alpha_+ + \alpha_- \qquad & \beta = \beta_+ + \beta_- \qquad \gamma = \gamma_+ + \gamma_- \\ \ell_1 + \mu_1 = \beta_+ + \gamma_+ \qquad & \ell_1 - \mu_1 = \beta_- + \gamma_- \\ \ell_2 + \mu_2 = \alpha_+ + \gamma_- \qquad & \ell_2 - \mu_2 = \alpha_- + \gamma_+ \\ \ell_3 + \mu_3 = \alpha_- + \beta_- \qquad & \ell_3 - \mu_3 = \alpha_+ + \beta_+. \end{aligned} \tag{10.106}$$

Examination of these relations show that there is one independent parameter, which is chosen to be γ_-. This choice of pararmeterization is made because the result leads to a formula for the 3-j's that coincides exactly with that of Edmonds [1].

For the purpose of carrying out the contractions, each symmetric set of basis spinors must be partitioned into two symmetric sets, consistent with the above constraints. In particular, the first set of $2\ell_1$ basis spinors is partitioned according into the β and γ sets. The numbers of ways that the β set contains β_- $\boldsymbol{\mathfrak{e}}^{(1/2)-1/2}$'s and β_+ $\boldsymbol{\mathfrak{e}}^{(1/2)1/2}$'s is the combinatorial factor

$$\binom{\beta}{\beta_-}$$

with an analogous quantity for the γ set. The sum of all the possible ways of carrying out this partitioning is

$$\sum_{\gamma_-}\binom{\gamma}{\gamma_-}\binom{\beta}{\beta_-}=\sum_{\gamma_-}\binom{\gamma}{\gamma_-}\binom{\beta}{\ell_1-\mu_1-\gamma_-}=\binom{\beta+\gamma}{\ell_1-\mu_1}, \tag{10.107}$$

which is the number of terms in the symmetric set of order $2\ell_1$. This summation equation is just an example of the binomial addition theorem listed in Appendix 1 of Edmonds [1]. It implies that the fraction of ways in which the $2\ell_1$ basis spinors are partitioned consistent with the labeling of β_- and γ_- is

$$W(\beta_-,\gamma_-)=\binom{\gamma}{\gamma_-}\binom{\beta}{\beta_-}\binom{2\ell_1}{\ell_1+\mu_1}^{-1}. \tag{10.108}$$

Analogous quatities for the other two symmetric sets are $W(\alpha_-,\gamma_-)$ and $W(\alpha_-,\beta_-)$.

A typical contraction is that of the β indices. This is calculated as

$$\begin{aligned}
&\left\{\left(\boldsymbol{\mathfrak{e}}^{(1/2)1/2}\right)^{\beta_+}\left(\boldsymbol{\mathfrak{e}}^{(1/2)-1/2}\right)^{\beta_-}\right\}^{(\beta)}\bullet^{\beta}\left(\sqcup\right)^{\beta}\\
&\left\{\left(\boldsymbol{\mathfrak{e}}^{(1/2)1/2}\right)^{\beta_-}\left(\boldsymbol{\mathfrak{e}}^{(1/2)-1/2}\right)^{\beta_+}\right\}^{(\beta)}\bullet^{\beta}\left(\sqcup\right)^{\beta}\\
=\;&\left(\boldsymbol{\mathfrak{e}}^{(1/2)1/2}\right)^{\beta_-}\left(\boldsymbol{\mathfrak{e}}^{(1/2)-1/2}\right)^{\beta_+}\bullet^{\beta}\left\{\left(\boldsymbol{\mathfrak{e}}^{(1/2)1/2}\right)^{\beta_+}\left(\boldsymbol{\mathfrak{e}}^{(1/2)-1/2}\right)^{\beta_-}\right\}^{(\beta)}\\
=\;&(-1)^{\beta_+}/\tbinom{\beta}{\beta_-}.
\end{aligned} \tag{10.109}$$

Note the transposition of factors that arises from the fact that the $\sqcup$'s are contracted into both $\boldsymbol{\mathfrak{e}}$ factors from the right. The symmetrization only needs to be applied once, and then only one term from the symmetrized set contributes, hence the fraction. Since the contraction is made from the righthand side of both spinors, this results in the transposition of the order of spinors when forming a direct contraction. Then since $\boldsymbol{\mathfrak{e}}^{(1/2)-1/2}\bullet\,\boldsymbol{\mathfrak{e}}^{(1/2)1/2}=-1$ while $\boldsymbol{\mathfrak{e}}^{(1/2)1/2}\bullet\,\boldsymbol{\mathfrak{e}}^{(1/2)-1/2}=1$, the sign is determined by the number of $\boldsymbol{\mathfrak{e}}^{(1/2)1/2}$'s on the "original" lefthand side (uppermost) spinor tensor, namely β_+.

Combining the various terms together, the contraction of the symmetrized sets is the sum

$$\begin{aligned}
&\sum_{\gamma_-}\frac{(-1)^{\alpha_++\beta_++\gamma_+}}{\binom{\alpha}{\alpha_+}\binom{\beta}{\beta_+}\binom{\gamma}{\gamma_+}}W(\beta_-,\gamma_-)W(\alpha_-,\beta_-)W(\alpha_-,\gamma_-)\\
=&\sum_{\gamma_-}(-1)^{\alpha_++\beta_++\gamma_+}\binom{\alpha}{\alpha_+}\binom{\beta}{\beta_+}\binom{\gamma}{\gamma_+}\left[\binom{2\ell_1}{\ell_1+\mu_1}\binom{2\ell_2}{\ell_2+\mu_2}\binom{2\ell_3}{\ell_3+\mu_3}\right]^{-1}.
\end{aligned} \tag{10.110}$$

On inserting this result into the equation for the 3-j symbol and simplifying the result, it is found that

$$\begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ \mu_1 & \mu_2 & \mu_3 \end{pmatrix} = \delta_{\mu_1+\mu_2+\mu_3,0}(-1)^{\ell_1-\ell_2-\mu_3}\sqrt{\frac{\alpha!\beta!\gamma!}{(L+1)!}}$$
$$\times\left[(\ell_1-\mu_1)!(\ell_1+\mu_1)!(\ell_2-\mu_2)!(\ell_2+\mu_2)!(\ell_3-\mu_3)!(\ell_3+\mu_3)!\right]^{1/2}$$
$$\times\sum_{\gamma_-}\frac{(-1)^{\gamma_-}}{\gamma_-!(\ell_1+\ell_2-\ell_3-\gamma_-)!(\ell_2+\mu_2-\gamma_-)!(\ell_3-\ell_1-\mu_2+\gamma_-)!(\ell_3-\ell_2+\mu_1+\gamma_-)!(\ell_1-\mu_1-\gamma_-)!}. \quad (10.111)$$

This is identical to Edmonds Eq. (3.6.11) after relabelling and transforming Edmonds' Clebsch Gordan result into a 3-j. The parameter γ_- is the same as z in Edmonds' formula.

10.8 Spinor - Cartesian Transformation

A Cartesian vector belongs to a weight 1 irreducible representation of the rotation group. Thus only the spinor tensors of integer weight, and combinations of even order, can be associated with Cartesian tensors. Only the Cartesian vector-symmetric second order spinor relations are discussed here, the higher ordered tensor relations follow from these.

A general weight 1 spinor tensor $\mathbf{\Psi}$ has three independent components, usually expressed as

$$\mathbf{\Psi} = \mathfrak{e}^{(1)1}\Psi_1 + \mathfrak{e}^{(1)0}\Psi_0 + \mathfrak{e}^{(1)-1}\Psi_{-1}, \quad (10.112)$$

while a Cartesian vector $\mathbf{A}$ has the three independent components usually expressed in the form

$$\mathbf{A} = \hat{x}A_x + \hat{y}A_y + \hat{z}A_z. \quad (10.113)$$

Since these are both weight 1 irreducible representations of the rotation group, there must be a way to write the spinor tensor in Cartesian form, and vice versa, the Cartesian vector as a symmetric second order spinor tensor. An obvious comment about such a correspondence is that, if the Cartesian vector is written in spherical tensor form, then the components must be proportional. Moreover, the magnitudes of the components in the different representations must be the same since the normalizations correspond, but there is still a question of the phase. Two possible choices are the $\mathbf{e}^{(1)\mu}$, Eqs. (5.11-5.12), and the $\mathfrak{e}^{(1)\mu}$, Eq. (5.28), bases of Cartesian vectors. Clearly with the notation chosen in this book, it is the latter that is consistent with the spinor basis that has been presented (an argument for this will be presented shortly). Thus the association is based on writing $\mathbf{A}$ in the form [$\mathfrak{e}$ the Cartesian basis]

$$\mathbf{A} = \mathfrak{e}^{(1)1}A_1 + \mathfrak{e}^{(1)0}A_0 + \mathfrak{e}^{(1)-1}A_{-1}, \quad (10.114)$$

with components

$$A_1 = i\frac{A_x - iA_y}{\sqrt{2}}, \qquad A_0 = -iA_z, \qquad A_{-1} = -i\frac{A_x + iA_y}{\sqrt{2}}. \quad (10.115)$$

Then the symmetric second order spinor $\mathfrak{A}$ (here to be considered as a unique way of writing the capital Greek letter alpha) equivalent to the vector $\mathbf{A}$ is [now the $\mathfrak{e}$ is the spinor tensor basis]

$$\mathfrak{A} = \mathfrak{e}^{(1)1}A_1 + \mathfrak{e}^{(1)0}A_0 + \mathfrak{e}^{(1)-1}A_{-1}. \quad (10.116)$$

This dual usage of the basis elements $\mathfrak{e}^{(1)\mu}$ may be confusing, and if much computation is done using both spinor and Cartesian tensors, then a notational difference would be necessary. But here, only the elementary correspondences are being discussed, so an enhanced notation has not been introduced.

That the $\mathfrak{e}$ Cartesian basis is appropriate is argued as follows. The standard Cartesian vector, for example, the position vector $\mathbf{r}$, is real, with real components x, y and z. Applying this constraint to the vector $\mathbf{A}$, its $\mathfrak{e}^{(1)\mu}$ components, see Eqs. (10.115), satisfy

$$A_1^* = A_{-1} \qquad A_0^* = -A_0. \tag{10.117}$$

Inherently spinors involve the complex field, so reality of a spinor tensor $\boldsymbol{\Psi}$ can be interpreted as that it is equal to its adjoint,

$$\boldsymbol{\Psi}^\dagger = \boldsymbol{\Psi}. \tag{10.118}$$

It was argued in Sec. 10.1, Eq. (10.6), that the adjoint exchanges covariant and contravariant basis sets. This is automatically extended to the spinor tensor basis sets, so in particular

$$\mathfrak{e}^{(1)\mu\dagger} = \mathfrak{e}^{(1)}_\mu = (-1)^{1-\mu}\mathfrak{e}^{(1)-\mu}. \tag{10.119}$$

It is noted that this is also satisfied by the Cartesian form of this basis set. From this it follows that, if $\boldsymbol{\Psi}^\dagger = \boldsymbol{\Psi}$, then

$$\begin{aligned} \boldsymbol{\Psi}^\dagger &= \mathfrak{e}^{(1)-1}\Psi_1^* - \mathfrak{e}^{(1)0}\Psi_0^* + \mathfrak{e}^{(1)1}\Psi_{-1}^* \\ = \boldsymbol{\Psi} &= \mathfrak{e}^{(1)1}\Psi_1 + \mathfrak{e}^{(1)0}\Psi_0 + \mathfrak{e}^{(1)-1}\Psi_{-1}, \end{aligned} \tag{10.120}$$

and the components satisfy the relations

$$\Psi_1^* = \Psi_{-1}, \qquad \Psi_0^* = -\Psi_0. \tag{10.121}$$

These are exactly the reality relations for the components of a Cartesian vector expressed in the $\mathfrak{e}$ basis, Eq. (10.117). Thus, in order to interpret the self-adjointness of an even ordered spinor tensor as equivalent to the reality of the corresponding Cartesian tensor, the connection between even ordered spinors and Cartesian tensors is to be made via the $\mathfrak{e}$ basis sets.

On expressing the weight 1 spinor tensor basis set explicitly in terms of second order spinor tensors, so that a weight 1 spinor is written as

$$\mathfrak{A} = \sum_{\mu\nu} \mathfrak{e}^{(1/2)\mu}\mathfrak{e}^{(1/2)\nu}\mathfrak{A}_{\mu\nu}, \tag{10.122}$$

the relation between the components of a symmetric second order spinor tensor $\mathfrak{A}_{\mu\nu}$ and a Cartesian vector $\mathbf{A}_m$ can be expressed in matrix form according to

$$\begin{pmatrix} \mathfrak{A}_{1/2,1/2} \\ \mathfrak{A}_{1/2,-1/2} \\ \mathfrak{A}_{-1/2,1/2} \\ \mathfrak{A}_{-1/2,-1/2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 & 0 \\ 0 & 0 & -i \\ 0 & 0 & -i \\ -i & 1 & 0 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}. \tag{10.123}$$

The inverse relation is

$$\begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i & 0 & 0 & +i \\ 1 & 0 & 0 & 1 \\ 0 & i & i & 0 \end{pmatrix} \begin{pmatrix} \mathfrak{A}_{1/2,1/2} \\ \mathfrak{A}_{1/2,-1/2} \\ \mathfrak{A}_{-1/2,1/2} \\ \mathfrak{A}_{-1/2,-1/2} \end{pmatrix}. \tag{10.124}$$

The corresponding relation in terms of the contravariant spinor tensor components $\mathfrak{A}^{\mu\nu}$ follow from

$$\mathfrak{A}^{\mu\nu} = (-1)^{1+\mu+\nu}\mathfrak{A}_{-\mu,-\nu}. \tag{10.125}$$

It is noted that these relations are opposite to those given in Ref. [16] because of a difference in the role of covariant and contravariant basis sets.

10.8.1 Cayley-Klein representation of a vector

The Cayley-Klein representation of the vector $\mathbf{A}$ is obtained by first writing the second order spinor of Eq. (10.123) representing the vector $\mathbf{A}$ in a mixed covariant-contravariant component form,

$$\mathfrak{A}_\mu^{\ \nu} = \sum_{\nu'} \mathfrak{g}^{\nu\nu'}\mathfrak{A}_{\mu\nu'}, \tag{10.126}$$

and then expressing this in matrix form (the matrix order is taken as μ before ν and 1/2 before -1/2). In terms of the vector components of $\mathbf{A}$, this matrix is

$$(\mathfrak{A}_\mu^{\ \nu}) = \frac{-i}{\sqrt{2}}\begin{pmatrix} A_z & A_x - iA_y \\ A_x + iA_y & -A_z \end{pmatrix} = \frac{-i}{\sqrt{2}}\mathbf{A}\cdot\boldsymbol{\sigma}. \tag{10.127}$$

The matrix (neglecting the prefactor of $-i/\sqrt{2}$) is the Cayley-Klein representation of the Cartesian vector $\mathbf{A}$, and is conveniently related to $\mathbf{A}$ via the vector of Pauli spin matrices $\boldsymbol{\sigma}$.

This form of writing a vector is often useful for carrying out rotations of the vector. In particular, a rotation of $\mathbf{A}$ is equivalent to a similarity transformation of the Cayley-Klein matrix. To arrive at such a connection, a rotation of the covariant form of a second order spinor is first considered, and this is then rewritten to conform with a similarity transformation of the Cayley-Klein matrix.

The rotation of the covariant form of a second order spinor by an angle θ about the $\hat{n}$ axis is expressed as

$$\mathfrak{A}'_{\mu\nu} \equiv \sum_{\mu'\nu'} \mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)_\mu^{\mu'}\mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)_\nu^{\nu'}\mathfrak{A}_{\mu'\nu'}. \tag{10.128}$$

On transforming this into a mixed covariant-contravariant component form, the rotated spinor tensor is

$$\begin{aligned}\mathfrak{A}'^{\ \nu}_{\mu} &\equiv \sum_{\mu'\nu'\nu_1\nu_2} \mathfrak{g}^{\nu\nu_1}\mathfrak{g}_{\nu_2\nu'}\mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)_\mu^{\mu'}\mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)_{\nu_1}^{\nu_2}\mathfrak{A}_{\mu'}^{\ \nu'} \\ &= \sum_{\mu'\nu'} \mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)_\mu^{\mu'}\mathfrak{A}_{\mu'}^{\ \nu'}X_{\nu'}^{\ \nu}. \end{aligned} \tag{10.129}$$

The quantity

$$\begin{aligned} X_{\nu'}^{\ \nu} &= \sum_{\nu_1\nu_2} \mathfrak{g}^{\nu\nu_1}\mathfrak{g}_{\nu_2\nu'}\mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)_{\nu_1}^{\nu_2} \\ &= (-1)^{\nu-\nu'}\mathfrak{R}_{\hat{n}}^{(1/2)}(\theta)_{-\nu}^{-\nu'} = \mathfrak{R}_{\hat{n}}^{(1/2)}(-\theta)_{\nu'}^{\nu} \end{aligned} \tag{10.130}$$

is found to be exactly the rotation matrix for $-\theta$, the inverse rotation, so the action of a rotation of a vector is equivalent to a similarity transformation of the corresponding Cayley-Klein matrix. It is also seen by comparison of its elements, that this matrix is the adjoint of the original rotation matrix, consistent with the standard requirement for an inverse operator in a vector space over the complex field.

10.9 Discussion of Spinors

As mentioned earlier in this chapter, all treatments of spinors in the literature appear to deal only with spinors as a set of components. In contrast, the emphasis here has been on the notion of a vector space of spinors in which there is a "dot" product. To relate to spinor components needs a basis set. A natural basis set is the set of eigenvectors of the rotation generator about a particular axis, standardly the $\hat{z}$ axis, so the generator used is $G_{\hat{z}}$. There is no requirement that these eigenvectors be orthogonal with respect to the "dot" product, in particular, a dot product is inherently a rotational invariant so the dot product of an eigenvector of $G_{\hat{z}}$ (having a nonzero eigenvalue) with itself can only be zero. In such a situation, this basis set is one of a pair of biorthogonal basis sets.

In this presentation it has been chosen to write the eigenvectors of $G_{\hat{z}}$ as contravariant vectors, with superscript indices. The biorthogonal basis set are then covariant vectors, written with subscripts. The other major choice in assigning the properties of the basis vectors, and the associated expansion components of any spinor, is the idempotency of $\boldsymbol{\epsilon}$. These two choices imply the particular relations (10.46) between the covariant and contravariant basis elements. A change in either or both of these choices change the detailed formulae for the spinor properties and the consequent relations to Cartesian vectors.

The antisymmetry of the metrics $\mathfrak{g}^{\mu\nu}$ and $\mathfrak{g}_{\mu\nu}$ are well known in the literature, but their relation to the dot products of the corresponding contravariant and covariant basis sets does not seem to be emphasized. Likewise the relation between the identity $\boldsymbol{\sqcup}$ and the invariant $\boldsymbol{\epsilon}$, namely as different combinations of contravariant and covariant versions of the same quantity, also appears new. At least, the author is not aware of these relations being expressed in the literature.

It is possible to proceed further, in particular to get equations for the 6-j symbols and their higher homologs. The rotation matrices for higher ℓ values is another topic. But this chapter was aimed at showing how the methods of irreducible Cartesian tensors could be applied to another problem rather than to give a detailed treatment of spinors. It is felt that this has been done.

Chapter 11

Applications to Quantum Mechanics

The 3-dimensional rotation group describes the properties of successive rotations of any object. In particular, this book has emphasized the properties of rotating Cartesian vectors and tensors and the decomposition of tensors into a sum of tensors irreducible under the rotation group. But standardly the first introduction to rotations that a person comes into contact with, is the rotation of some physical object, and the dynamics of such physical motion involves the angular momentum, whether using classical mechanics or quantum mechanics. In quantum mechanics, the commutation relations of position and momentum immediately imply certain commutation relations for the components of the angular momentum. Neglecting a factor of $\hbar$ (Planck's constant divided by 2π) these are the same as the commutation relations of the rotation generators, and in fact the angular momentum is the generator for a rotation of a physical body. This connection may be misinterpreted as an identity, with the result that anything dealing with a rotation is synonymous with it being involved with angular momentum, rather than only with the rotation of physical objects. This book has carefully tried to distinguish the general properties of rotations, such as the rotational properties of a tensor, from the physical rotation of a physical object. But clearly there is an interplay between these mathematical and physical concepts. In particular, a rotation can be applied to any object described in 3-dimensional space, such as a tensor, whereas angular momentum is part of mechanics and is a property of a physical system. A situation where this distinction is especially important, is when the rotation of angular momentum tensors is described. Then clearly the mathematical rotation of the tensor must be distinguished from the physical vector quantity, namely the angular momentum.

This chapter starts with a review of the properties of angular momentum (in quantum mechanics). The eigenvectors of rigid rotors and the Wigner-Eckart theorem are related to previously defined quantities and properties of the rotation group. The chapter finishes with a discussion of tensors of the angular momentum, their traces and angular momentum superoperators. Most of this presentation involves the relation between quantum states and Cartesian tensors and this is limited here to quantum states with integer angular momentum. This has been done in order to use the basis set $\mathbf{e}^{(\ell)m}$ that naturally lead to the phase relations appearing in most of the scientific literature. For the treatment of 1/2-integral angular momenta, it is the spinor tensors that need to be used and these have inherently a different phase convension associated with the $\mathfrak{e}^{(\ell)m}$ basis set. Rather than present both systems, or use the latter system for all states, the choice of restricting the presentation has been made.

11.1 Eigenvectors of the Angular Momentum

A major aspect of quantum mechanics is the commutation relation between the position $\mathbf{r}_{\rm op}$ and momentum $\mathbf{p}_{\rm op}$ operators, $\mathbf{r}_{\rm op}\mathbf{p}_{\rm op} - \mathbf{p}_{\rm op}\mathbf{r}_{\rm op} = i\hbar\mathbf{U}$. This implies that the components of the (rotational) angular momentum $\mathbf{J} = \mathbf{r}_{\rm op}\times\mathbf{p}_{\rm op}$ satisfy the commutation relations

$$J_j J_k - J_k J_j = i\hbar J_\ell, \tag{11.1}$$

where j, k and ℓ label the components according to a righthand orthogonal coordinate system. There are three obvious ways of studying the properties of the quantum theory of rotational angular momentum. First is based on the wavefunction method of satisfying the position-momentum commutation relation by identifying the momentum operator $\mathbf{p}_{\rm op}$ with the differential operator $-i\hbar\partial/\partial\mathbf{r}$. Then any quantum state describing the position of a physical system is described by a wavefunction $\psi(\mathbf{r}) = \langle\mathbf{r}|\psi\rangle$. This is known as the position representation of the abstract (Dirac) quantum state $|\psi\rangle$. Note the distinction between the position and momentum operators $\mathbf{r}_{\rm op}$, $\mathbf{p}_{\rm op}$ and the position and momentum parameters $\mathbf{r}$ and $\mathbf{p}$. Second is an alternate wavefunction method of satisfying the position-momentum commutation relation, namely by identifying the position operator $\mathbf{r}_{\rm op}$ as the differential operator $i\hbar\partial/\partial\mathbf{p}$ with the momentum wavefunction $\psi(\mathbf{p}) = \langle\mathbf{p}|\psi\rangle$ being the momentum representation of the quantum state $|\psi\rangle$. Third and last is to deal with quantum states and the angular momentum operators in an abstract manner. This is the most elegant method and also the most general, in that this approach can be generalized to include states of the spin angular momentum as well as those of the rotational angular momentum. All three approaches have their utility and arise in the following discussion, but most of the development is done using the abstract operator approach. As well, in most of the following discussion, the presence of degrees of freedom other than rotation is ignored, while in real applications such other degrees of freedom usually play an important, if not crucial, role. But here, since the emphasis is only on those aspects of the physical system that are associated with its angular momentum, this restriction is appropriate.

It should be remarked that position $|\mathbf{r}\rangle$ and momentum $|\mathbf{p}\rangle$ ket states, and their associated bra states, $\langle\mathbf{r}|$ and $\langle\mathbf{p}|$, are not elements of Hilbert space [in terms of which quantum mechanics is correctly formulated] but are considered as idealized quantum states having Dirac delta normalization, as originally formulated by Dirac [33]. They are in common use because they greatly simplify the connection between the abstract and the position and momentum representations of quantum states.

Consistent with this book's theme on Cartesian tensors, the quantum commutation relations are usually expressed in tensor form, thus the tensor form of Eq. (11.1) is

$$[\mathbf{J},\mathbf{J}]_- = i\hbar\boldsymbol{\mathcal{E}}\cdot\mathbf{J}. \tag{11.2}$$

But in writing this equation it is only the quantum operator aspect of this relation that is interchanged by the commutator whereas the tensorial aspect is not. To emphasize this distinction, it is useful to expand this tensor equation as

$$[\mathbf{J},\mathbf{J}]_- = \mathbf{J}\mathbf{J} - (\mathbf{J}\mathbf{J})^t = i\hbar\boldsymbol{\mathcal{E}}\cdot\mathbf{J}, \tag{11.3}$$

where $(\ )^t$ denotes the tensor transpose. This may be clearer if the two operators are not the same, for example

$$[\mathbf{A}, \mathbf{B}]_- \equiv \mathbf{AB} - (\mathbf{BA})^t. \tag{11.4}$$

For the angular momentum case with both operators the same, the commutator vanishes if the transpose was not present, whereas with different operators the combination of operators without the transpose could be non-zero.

11.1.1 Abstract Properties

Since the components of the angular momentum don't commute, it follows that any eigenvector of one component cannot, except under exceptional circumstances, also be an eigenvector of another component of the angular momentum. But it also follows from the commutation relations that $\mathbf{J}\cdot\mathbf{J}$ commutes with all components of the angular momentum, so that angular momentum eigenvectors can be classified according to an eigenvalue of one angular momentum component and according to the eigenvalue of the magnitude of the angular momentum. It is standard to use the $\hat{z}$ component of the angular momentum $m\hbar$ to classify the eigenvectors of the angular momentum and this is used here, thus

$$J_{\hat{z}}|jm\rangle = m\hbar|jm\rangle, \tag{11.5}$$

with j parameterizing the magnitude of the angular momentum. A connection between these eigenvectors can be obtained using the raising and lowering operators $J_\pm \equiv J_{\hat{x}} \pm iJ_{\hat{y}}$, which satify the commutation relations

$$J_{\hat{z}}J_\pm = J_\pm(J_{\hat{z}} \pm \hbar). \tag{11.6}$$

It follows that

$$J_{\hat{z}}J_\pm|jm\rangle = (m \pm 1)\hbar J_\pm|jm\rangle, \tag{11.7}$$

which implies that $J_\pm|m\rangle$ is a $J_{\hat{z}}$ eigenstate with eigenvalue $(m \pm 1)\hbar$. Using the fact that $\mathbf{J}\cdot\mathbf{J}$ can be written in the form

$$\mathbf{J}\cdot\mathbf{J} = J_\mp J_\pm + J_{\hat{z}}(J_{\hat{z}} \pm \hbar), \tag{11.8}$$

it follows that

$$\langle jm|J_\mp J_\pm|jm\rangle = [C_j - m(m \pm 1)]\hbar^2\langle jm|jm\rangle, \tag{11.9}$$

where C_j is the eigenvalue of $\mathbf{J}\cdot\mathbf{J}$ that is associated with the parameter j. Thus, if all the $|jm\rangle$ are to be normalized, then

$$J_\pm|jm\rangle = \sqrt{C_j - m(m \pm 1)}\hbar|j(m \pm 1)\rangle \tag{11.10}$$

gives a definite relation (including the phase) between those normalized eigenvectors of $J_{\hat{z}}$ which are also parameterized by a given j. This assignment of a phase relation between different eigenvectors is due to Condon and Shortley [21] and a now standard convention. The set of such eigenvectors is finite only if the raising and lowering operations both stop at some upper m_u and lower m_d values, namely that these m values satisfy

$$C_j = m_u(m_u + 1) = m_d(m_d - 1). \tag{11.11}$$

Clearly this is satisfied only if $m_d = -m_u$ and, since $m_u - m_d$ must be an integer [since each raising and/or lowering changes the $J_{\hat{z}}$ eigenvalue by $\hbar$], it follows that C_j can be set equal to $j(j + 1)$ for some positive integer or half-integer, and for a given value of j, there are $2j+1$ eigenvalues of $J_{\hat{z}}$, having eigenvalues $-j\hbar, (-j+1)\hbar, \cdots, (j-1)\hbar, j\hbar$. An immediate consequence of this is that $J_{\hat{z}}$ satisfies the polynomial equation

$$\prod_{n=0}^{2j}[J_{\hat{z}} - (j-n)\hbar] = 0, \tag{11.12}$$

restricted to the manifold of states classified by $\mathbf{J}\cdot\mathbf{J} = j(j+1)\hbar^2$. This is an example of the Cayley-Hamilton theorem, see for example Greub [34].

Except for the factors of $\hbar$, this discussion about the eigenvalues of $J_{\hat{z}}$ parallels the discussion in Chapter 5 for the eigenvalues of a generator of the 3-dimensional rotation group. The parallelism can be continued by considering

$$|\psi(\chi)\rangle \equiv e^{-iJ_{\hat{n}}\chi/\hbar}|\psi\rangle \tag{11.13}$$

to be the rotation of the state $|\psi\rangle$ by an angle χ about the $\hat{n}$ axis. In this way the set of angular momentum components, divided by $\hbar$ are exactly the generators of rotations of quantum states. Starting from a given state $\psi\rangle$, the action of all possible rotations generates a representation of the rotation group. This is in general reducible and can be reduced into its irreducible components. Since $\mathbf{J}\cdot\mathbf{J}$ commutes with all components of the angular momentum and since an eigenvector of $J_{\hat{z}}$ can be transformed into $2j+1$ eigenvectors of $J_{\hat{z}}$ by products of the raising and/or lowering operators $J_\pm$, such a set of states $\{|jm\rangle\}$ forms the basis for a $2j+1$-dimensional irreducible representation of the rotation group, which is parameterized by the magnitude of angular momentum quantum number j. By the completeness of the eigenvectors of the angular momentum, any state $|\psi\rangle$ can be expanded in terms of the $|jm\rangle$, namely

$$|\psi\rangle = \sum_{jm}|jm\rangle\langle jm|\psi\rangle, \tag{11.14}$$

with expansion coefficients $\langle jm|\psi\rangle$. It is assumed throughout that the basis elements $|jm\rangle$ are normalized and that there are no degrees of freedom other than the angular momentum.

11.1.2 Position Representation

Since the commutator of the rotational angular momentum operator $\mathbf{J}$ and $\mathbf{r}_{\text{op}}$ is

$$[\mathbf{J}, \mathbf{r}_{\text{op}}]_- = [\mathbf{r}_{\text{op}}\times\mathbf{p}_{\text{op}}, \mathbf{r}_{\text{op}}]_- = -i\hbar\mathbf{r}_{\text{op}}\times\mathsf{U} = i\hbar\boldsymbol{\mathcal{E}}\cdot\mathbf{r}_{\text{op}}, \tag{11.15}$$

it follows from the properties of the exponential of a commutator, see appendix A.16, that the operator transformation

$$\begin{aligned}\mathbf{r}_{\text{op}}(\hat{n},\chi) &\equiv e^{i\chi J_{\hat{n}}/\hbar}\mathbf{r}_{\text{op}}e^{-i\chi J_{\hat{n}}/\hbar} = e^{-\chi\hat{n}\cdot\boldsymbol{\mathcal{E}}\cdot}\mathbf{r}_{\text{op}} \\ &= [\hat{n}\hat{n} + \cos\chi(\mathsf{U} - \hat{n}\hat{n}) - \sin\chi\hat{n}\cdot\boldsymbol{\mathcal{E}}]\cdot\mathbf{r}_{\text{op}} = \mathsf{R}_{\hat{n}}(\chi)\cdot\mathbf{r}_{\text{op}},\end{aligned} \tag{11.16}$$

is identical to the rotation of the vector $\mathbf{r}_{\text{op}}$, compare with Eqs. (2.90-2.92). A special case of this is

$$\mathbf{r}_{\text{op}}(\hat{z},\chi) = (1-\cos\chi)\hat{z}z_{\text{op}} + \cos\chi\mathbf{r}_{\text{op}} + \sin\chi\hat{z}\times\mathbf{r}_{\text{op}} = \mathsf{R}_{\hat{z}}(\chi)\cdot\mathbf{r}_{\text{op}}. \tag{11.17}$$

Equation (11.16) relates a quantum transformation of the vector position operator to a vector transformation of this same vector operator. It is noted that, while $e^{-i\chi J_{\hat{n}}/\hbar}$ is the operator for a rotation of a quantum state by $+\chi$ about the $\hat{n}$ axis, the corresponding rotation of an operator has the adjoint of the transformation on the left of the operator on which it acts. This is essentially the difference between the Heisenberg versus Schrödinger pictures for operator versus state transformations, and it is seen that this is equivalent to the rotation of the vector $\mathbf{r}_{\rm op}$, as a vector, by this same angle $+\chi$. It is emphasized that these are the transformations of a "vector" operator. In contrast, a typical component of Eq. (11.16) [specializing $\hat{n}$ to $\hat{z}$ for simplicity of presentation] is

$$\begin{aligned} e^{i\chi J_{\hat{z}}/\hbar} x_{\rm op} e^{-i\chi J_{\hat{z}}/\hbar} &= \hat{x}\cdot e^{i\chi J_{\hat{z}}/\hbar}\mathbf{r}_{\rm op} e^{-i\chi J_{\hat{z}}/\hbar} \\ &= \hat{x}\cdot\mathsf{R}_{\hat{z}}(\chi)\cdot\mathbf{r}_{\rm op} = x_{\rm op}\cos\chi - y_{\rm op}\sin\chi. \end{aligned} \tag{11.18}$$

In carrying out the calculation for the component transformation, the basis vectors are taken as constant, both quantum mechanically and for the vector rotation, thus this represents an active rotation (by $-\chi$) in terms of both quantum and vector transformations, corresponding to the inverse of the (Schrödinger) transformation of the state and equivalent to the $+\chi$ rotation of an operator in the Heisenberg picture.

As an application of Eq. (11.16), if $|\mathbf{r}\rangle$ is an eigenvector of $\mathbf{r}_{\rm op}$, then

$$e^{i\chi J_{\hat{n}}/\hbar}\mathbf{r}_{\rm op} e^{-i\chi J_{\hat{n}}/\hbar}|\mathbf{r}\rangle = \mathsf{R}_{\hat{n}}(\chi)\cdot\mathbf{r}|\mathbf{r}\rangle, \tag{11.19}$$

or equivalently

$$\mathbf{r}_{\rm op} e^{-i\chi J_{\hat{n}}/\hbar}|\mathbf{r}\rangle = \mathsf{R}_{\hat{n}}(\chi)\cdot\mathbf{r} e^{-i\chi J_{\hat{n}}/\hbar}|\mathbf{r}\rangle. \tag{11.20}$$

Expressed in other terms, $e^{-i\chi J_{\hat{n}}/\hbar}|\mathbf{r}\rangle$ is an eigenvector of $\mathbf{r}_{\rm op}$ with eigenvalue $\mathsf{R}_{\hat{n}}(\chi)\cdot\mathbf{r}$, equivalently,

$$e^{-i\chi J_{\hat{n}}/\hbar}|\mathbf{r}\rangle = |\mathsf{R}_{\hat{n}}(\chi)\cdot\mathbf{r}\rangle. \tag{11.21}$$

This identification allows a connection to be made between the operator rotation of the state $|\mathbf{r}\rangle$ and the rotation of the parameter $\mathbf{r}$ that characterizes the state, specifically

$$e^{-i\chi J_{\hat{n}}/\hbar}|\mathbf{r}\rangle = |\mathsf{R}_{\hat{n}}(\chi)\cdot\mathbf{r}\rangle = |e^{\chi\hat{n}\cdot(\mathbf{r}\times\partial/\partial\mathbf{r}}\mathbf{r}\rangle. \tag{11.22}$$

A more useful way of employing this result is to examine the rotational properties of the position representation of a state, thus

$$\begin{aligned} \langle\mathbf{r}|e^{-i\chi J_{\hat{n}}/\hbar}|\psi\rangle &= \langle e^{i\chi J_{\hat{n}}/\hbar}\mathbf{r}|\psi\rangle = \langle\mathsf{R}_{\hat{n}}(-\chi)\cdot\mathbf{r}|\psi\rangle \\ &= \psi(\mathsf{R}_{\hat{n}}(-\chi)\cdot\mathbf{r}) = e^{-\chi\hat{n}\cdot(\mathbf{r}\times\partial/\partial\mathbf{r})}\psi(\mathbf{r}). \end{aligned} \tag{11.23}$$

In the second equation on the first line, $\mathbf{r}$ is interpreted as labelling the quantum state on which the rotation operator acts, whereas in the second line it is the rotated $\mathbf{r}$ that labels the position wavefunction. As a function, the rotation of the parameter on which it depends is equivalent to the exponential differential operator acting on the function. The difference between how the state label in Eq. (11.22) is changed versus how the position representation in Eq. (11.23) is changed should be noticed. Finally, for Eq. (11.23), the differential operator can be identified as the position representation of the angular momentum

$$\mathbf{J}_{\rm pos} \equiv \frac{\hbar}{i}\mathbf{r}\times\frac{\partial}{\partial\mathbf{r}}, \tag{11.24}$$

then the connection

$$\langle \mathbf{r}| e^{-i\chi J_{\hat{n}}/\hbar} |\psi\rangle = e^{-i\chi \hat{n}\cdot\mathbf{J}_{\text{pos}}} \psi(\mathbf{r}) \tag{11.25}$$

between the abstract and position representations of the angular momentum operator can be made. It is also instructive to notice how a positive rotation of a ket (ψ) is equivalent to the negative rotation of the bra ($\mathbf{r}$) so that the relative properties of the ket and bra are retained.

It is an easy exercise to show that, as differential operators,

$$[\mathbf{J}_{\text{pos}}, \mathbf{J}_{\text{pos}}]_- = i\hbar \boldsymbol{\mathcal{E}} \cdot \mathbf{J}_{\text{pos}}, \tag{11.26}$$

which is equivalent to the commutation relations of the components of the abstract angular momentum operator, Eq. (11.1). If the unit position vector $\hat{r}$ is given in polar coordinates by $\theta,\ \phi$, based on the standard righthand coordinate system $\hat{x},\ \hat{y},\ \hat{z}$, then a straightforward calculation shows that

$$\begin{aligned} \hat{z}\cdot\mathbf{J}_{\text{pos}} &= \frac{\hbar}{i}\frac{\partial}{\partial\phi}, \\ \hat{x}\cdot\mathbf{J}_{\text{pos}} &= \frac{\hbar}{i}\left[-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right], \\ \hat{y}\cdot\mathbf{J}_{\text{pos}} &= \frac{\hbar}{i}\left[\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right]. \end{aligned} \tag{11.27}$$

Particularly important combinations of these differential operators are

$$\mathbf{J}_{\text{pos}}\cdot\mathbf{J}_{\text{pos}} = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{11.28}$$

and

$$J_{\text{pos},+} \equiv (\hat{x} + i\hat{y})\cdot\mathbf{J}_{\text{pos}} = \hbar\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]. \tag{11.29}$$

The well behaved solutions of these differential equations are the spherical harmonics, as is shown in an indirect manner after some comments are made introducing the ket for the unit vector $\hat{r}$.

Once the position representation of the angular momentum operators are expressed in terms of the two angle variables, there is no need to keep the magnitude of the position vector $\mathbf{r} = r\hat{r}$. [When evaluating these operators according to Eq. (11.24) it was necessary to treat all three Cartesian components of $\mathbf{r}$ as independent in carrying out the differentiations.] In particular, the position ket can be expressed as the product

$$|\mathbf{r}\rangle = |r\rangle|\hat{r}\rangle, \tag{11.30}$$

and only the orientation ket $|\hat{r}\rangle$, which can also be written as $|\theta,\phi\rangle$ using the polar angles of $\hat{r}$, is affected by the angular momentum. The Dirac delta normalization of these two pieces of $|\mathbf{r}\rangle$ are to be

$$\begin{aligned} \langle \hat{r}'|\hat{r}\rangle &= \delta(\hat{r}' - \hat{r}) = \frac{\delta(\theta' - \theta)}{\sin\theta}\delta(\phi' - \phi), \\ \langle r'|r\rangle &= \frac{\delta(r' - r)}{r^2} \end{aligned} \tag{11.31}$$

so that the contractions

$$\int d\hat{r}\langle \hat{r}'|\hat{r}\rangle f(\hat{r}) = \int \sin\theta d\theta \int d\phi \frac{\delta(\theta' - \theta)}{\sin\theta}\delta(\phi' - \phi) f(\theta,\phi) = f(\hat{r}') \tag{11.32}$$

and

$$\int r^2 dr \langle r'|r\rangle f(r) = f(r') \tag{11.33}$$

are valid. The orientation kets (and bras) are useful when only rotational motion is involved, equivalently when there is no relevance for the magnitude of a position vector.

From the above relations, it follows that the position representation $\langle \hat{r}|jm\rangle$ of the angular momentum eigenvector satifies the differential equations

$$\begin{aligned}\langle \hat{r}|J_{\hat{z}}|jm\rangle &= m\hbar\langle \hat{r}|jm\rangle = \hat{x}\cdot\mathbf{J}_{\text{pos}}\langle \hat{r}|jm\rangle = \frac{\hbar}{i}\frac{\partial}{\partial\phi}\langle \hat{r}|jm\rangle, \\ \langle \hat{r}|\mathbf{J}\cdot\mathbf{J}|jm\rangle &= j(j+1)\hbar^2\langle \hat{r}|jm\rangle = \mathbf{J}_{\text{pos}}\cdot\mathbf{J}_{\text{pos}}\langle \hat{r}|jm\rangle. \end{aligned} \tag{11.34}$$

The first equation can be immediately integrated to obtain the ϕ dependence of $\langle \hat{r}|jm\rangle$ as

$$\langle \hat{r}|jm\rangle = A_{jm}(\theta)e^{im\phi} \tag{11.35}$$

for some function $A_{jm}(\theta)$ of θ. On the basis that the wavefunction is single valued and that $\phi = 0$ and $\phi = 2\pi$ give the same value of $\hat{r}$, it follows that m must be an integer. That also means that j must also be an integer, so that only integer order irreducible representations of the rotation group have a position representation. Rather than solving the second equation to get the θ dependence of $A_{jm}(\theta)$, a procedure analogous to that used by Edmonds [1] is used, specifically using the raising and lowering operators. It is first noticed that

$$\begin{aligned}\langle \hat{r}|J_+|jj\rangle = 0 &= J_{\text{pos},+}\langle \hat{r}|jj\rangle = \hbar\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]\langle \hat{r}|jj\rangle \\ &= \hbar\left[\frac{\partial}{\partial\theta} - j\cot\theta\right]\langle \hat{r}|jj\rangle. \end{aligned} \tag{11.36}$$

It follows that the position representation of this angular momentum eigenvector has the detailed angle dependence

$$\langle \hat{r}|jj\rangle = A_j \sin^j\theta e^{ij\phi}. \tag{11.37}$$

Normalization according to $\langle jj|jj\rangle = 1$ evaluates the magnitude of the constant, and with a proper choice of phase

$$\langle \hat{r}|jj\rangle = \frac{(-1)^j}{2^j j!}\sqrt{\frac{(2j+1)!}{4\pi}}\sin^j\theta e^{ij\phi} \tag{11.38}$$

is recognized as the spherical harmonic $Y_{jj}(\theta,\phi)$, Eq. (5.86). Since both the angular momentum kets and the spherical harmonics satisfy the lowering and raising operators with Condon Shortley phases, it follows that for all m,

$$\langle \hat{r}|jm\rangle = Y_{jm}(\hat{r}). \tag{11.39}$$

11.1.3 Tensorial Representaion

An association with tensors can be made via Eq. (11.39), namely from Eq. (5.75) it is seen that

$$\langle \hat{r}|jm\rangle = \left(\frac{(2j+1)!}{4\pi 2^j (j!)^2}\right)^{1/2} (\hat{r})^j \odot^j \mathbf{e}^{(j)m}. \tag{11.40}$$

This associates the basis tensor with the angular momentum state $|jm\rangle$, while a sufficient power of $\hat{r}$ is dotted into the basis tensor to make a scalar and thus be interpreted as a quantum mechanical bracket. Such an association implies that $\mathbf{e}^{(j)m}$ is associated with an eigenvector of the quantum mechanical angular momentum operator $J_{\hat{z}}$ with eigenvalue $m\hbar$. But since the basis tensors are sums of products of the vector basis elements, which were taken as constants (i.e. angular momentum invariants) when arriving at the component rotation properties, Eq. (11.18), a direct application of $\mathbf{J}$ or $\mathbf{J}_{\rm pos}$ gives a value of zero. And if one tries to replace $\mathbf{r}_{\rm op}$ in Eq. (11.16) by $\hat{x}+i\hat{y}$, etc., the wrong sign is obtained. Thus, if the association of $\mathbf{e}^{(j)m}$ with $|jm\rangle$, together with its proper eigenvalue is to be made, then there must be a representation of the angular momentum operator. Clearly, when acting on a tensor of order p, this is accomplished by taking the angular momentum operator as ($\hbar$ times) the tensor rotation generator $\mathbf{G}^{(p)}$ of Eq. (3.3), that is,

$$\mathbf{J}_{\rm p-order\ tensors} = \hbar\mathbf{G}^{(p)}. \tag{11.41}$$

This gives another way of representing rotational states in quantum mechanics, in particular the eigenvector equation

$$\hat{z}\cdot\mathbf{J}_{\rm j-order\ tensors}\mathbf{e}^{(j)m} = m\hbar\mathbf{e}^{(j)m}. \tag{11.42}$$

is obtained.

11.1.4 Momentum Representation

The above treatment can be repeated for the momentum representation. This is started with

$$[\mathbf{J},\mathbf{p}_{\rm op}]_- = [\mathbf{r}_{\rm op}\times\mathbf{p}_{\rm op},\mathbf{p}_{\rm op}]_- = -[\mathbf{p}_{\rm op}\times\mathbf{r}_{\rm op},\mathbf{p}_{\rm op}]_- = -i\hbar\mathbf{p}_{\rm op}\times\mathbf{U} = i\hbar\boldsymbol{\varepsilon}\cdot\mathbf{p}_{\rm op} \tag{11.43}$$

as a relation between $\mathbf{J}$ as an angular momentum operator and the vectorial rotation generator $\boldsymbol{\varepsilon}\cdot$ when acting on the vector momentum operator $\mathbf{p}_{\rm op}$. Since this is exactly the same relation as for the position operator it follows that the momentum representation of an angular momentum ket is, up to a phase η_j (the relative phases for m are fixed by the Condon Shortley convention), the corresponding spherical harmonic of the unit momentum direction $\hat{p}$ having polar angles $\zeta,\ \xi$, that is,

$$\langle\hat{p}|jm\rangle = \eta_j Y_{jm}(\hat{p}) = \eta_j Y_{jm}(\zeta,\xi). \tag{11.44}$$

If only the momentum representation is to be used in a scientific development, then the phases η_j can be set to 1, but if both position and momentum representations are to be used, they must be chosen so that the two representations are consistent. The consistency constraint is due to the fact that the position $\mathbf{r}$ is even (invariant) to time reversal while the momentum $\mathbf{p}$ is odd. These symmetry properties have to be attached to the directions $\hat{r},\ \hat{p}$ since the magnitudes are always positive [35]. Denoting by $\theta_{\rm op}$ the time reversal operator, it is known that this is antiunitary [3]

$$\langle\Psi|\Phi\rangle = \langle\theta_{\rm op}\Phi|\theta_{\rm op}\Psi\rangle = \langle\theta_{\rm op}\Psi|\theta_{\rm op}\Phi\rangle^* \tag{11.45}$$

where * designates the complex conjugate. When acting on spin-free states $\theta_{\rm op}$ is the operation of taking the complex conjugate and satisfies $\theta_{\rm op}^2 = 1_{\rm op}$, the identity operator. It is assumed that the position and momentum directional kets satisfy the physical symmetry conditions

$$\theta_{\rm op}|\hat{r}\rangle = |\hat{r}\rangle \qquad\qquad \theta_{\rm op}|\hat{p}\rangle = |-\hat{p}\rangle. \tag{11.46}$$

From the antiunitary property of $\theta_{\rm op}$, the position representation of an angular momentum state satisfies

$$\langle\theta_{\rm op}\hat{r}|\theta_{\rm op}jm\rangle = \langle\hat{r}|jm\rangle^* = Y_{jm}(\hat{r})^* = (-1)^m Y_{j,-m}(\hat{r}). \quad (11.47)$$

Then, since $\langle\hat{r}|$ is unchanged by time reversal, it follows that

$$\theta_{\rm op}|jm\rangle = (-1)^m|j,-m\rangle. \quad (11.48)$$

With this result, the application of time reversal to the momentum representation of an angular momentum state is

$$\langle\theta_{\rm op}\hat{p}|\theta_{\rm op}jm\rangle = \langle\hat{p}|jm\rangle^* = \eta_j^* Y_{jm}(\hat{p})^* = \eta_j^*(-1)^m Y_{j,-m}(\hat{p}). \quad (11.49)$$

The calculation of this quantity using the direct action of $\theta_{\rm op}$ on the abstract states gives the alternate evaluation

$$\langle\theta_{\rm op}\hat{p}|\theta_{\rm op}jm\rangle = (-1)^m\langle-\hat{p}|j,-m\rangle = (-1)^{j+m}\eta_j Y_{j,-m}(\hat{p}). \quad (11.50)$$

Since these two evaluations must be identical, it follows that η_j can have two possible values, $\eta_j = (\pm i)^j$. This assignment of η_j depends on the constraints of time reversal symmetry and the association given by Eq. (11.39) between $\langle\hat{r}|jm\rangle$ and the spherical harmonic.

A different choice for the phase for the relation between $\langle\hat{r}|jm\rangle$ and the spherical harmonic would imply a different phase relation between $\langle\hat{p}|jm\rangle$ and the corresponding spherical harmonic for $\hat{p}$, but any set of phases is always constrained by the condition

$$\langle\hat{r}|\hat{p}\rangle = \sum_{jm}\langle\hat{r}|jm\rangle\langle jm|\hat{p}\rangle = \sum_{jm} Y_{jm}(\hat{r})(\pm i)^j Y_{jm}(\hat{p})^*. \quad (11.51)$$

This follows [36] from the requirement of the time reversal symmetry,

$$\langle\hat{r}|\hat{p}\rangle = \langle\theta_{\rm op}\hat{r}|\hat{p}\rangle = \langle\hat{r}|\theta_{\rm op}\hat{p}\rangle^* = \langle\hat{r}|-\hat{p}\rangle^*, \quad (11.52)$$

and the expansion of the inner product in terms of spherical harmonics. Thus it is seen that it is inconsistent to assign both $\langle\hat{r}|jm\rangle$ and $\langle\hat{p}|jm\rangle$ as being the corresponding spherical harmonics without added phase factors that satisfy Eq. (11.51).

Another way of proving Eq. (11.51) is by examining the asymptotic behaviour of the standard relation

$$\langle\mathbf{r}|\mathbf{p}\rangle = \frac{1}{h^{3/2}}e^{i\mathbf{r}\cdot\mathbf{p}/\hbar} = \frac{4\pi}{h^{3/2}}\sum_{jm}(i)^j j_j(rp/\hbar)Y_{jm}(\hat{r})Y_{jm}(\hat{p})^* \quad (11.53)$$

for large $rp/\hbar \to \infty$. This depends on the asymptotic expansion of the spherical Bessel function $j_j(x)$ together with ignoring the $j\pi/2$ in the resulting sine function as an averaging effect over the large values of $rp/\hbar$

$$j_j(x) \sim \frac{\sin(x - j\pi/2)}{x} \underset{\rm ave}{\sim} \frac{\sin x}{x}. \quad (11.54)$$

Then the inner product factors into a magnitude factor and an angle dependent factor, namely

$$\langle\mathbf{r}|\mathbf{p}\rangle \sim \frac{2\sin(rp/\hbar)}{rp(h)^{1/2}}\sum_{jm}(i)^j Y_{jm}(\hat{r})Y^*_{jm}(\hat{p}). \quad (11.55)$$

The sum is the same as $\langle\hat{r}|\hat{p}\rangle$ with the positive choice of $(i)^j$ and an argument can be made [35] for the prefactor to be the scalar product between states for the magnitudes of **r** and **p**.

11.2 Symmetric Top Eigenvectors

Here the symmetric top is assumed to be rigid, so only rotational motion is considered. In terms of position space, the orientation of a symmetric top is specified by the direction of its symmetry axis, which is also unique if the symmetric top has no reflection symmetry along the symmetry axis (no σ_h symmetry). Since the top can rotate, have angular momentum and rotational energy, about any axis, it is important to fix a coordinate system within the top, called the body-fixed coordinate system. It is common to label the body-fixed coordinate system as $\hat{\mathbf{X}}$, $\hat{\mathbf{Y}}$ and $\hat{\mathbf{Z}}$ with $\hat{\mathbf{Z}}$ being the symmetry axis. A unique prescription for specifying the orientation of the top is to consider it initially in an orientation so that the body-fixed coordinate system $\hat{\mathbf{X}}$, $\hat{\mathbf{Y}}$, $\hat{\mathbf{Z}}$ and laboratory-fixed coordinate system $\hat{x}$, $\hat{y}$, $\hat{z}$ coincide. Then a rotation R is made to put the body-fixed frame into the desired orientation. Any such rotation can be considered as first rotating the symmetry axis from $\hat{z}$ to $\hat{\mathbf{Z}} = \mathbf{R}\cdot\hat{z}$, and then a rotation made about the symmetry axis in the body-fixed coordinate system, compare the description of a rotation in terms of Euler angles, Sec. 2.5.2.

Any function of the orientation of a symmetric top can be decomposed into irreducible representations of the 3-dimensional rotation group. Since it is standardly of interest to specify the states that are eigenvectors of the angular momentum, this involves introducing spherical bases for both the body-fixed and laboratory frames. The latter is the standard set, Eq. (5.48), which depends on the vector basis set of Eqs. (5.11-5.12). Since these are classified according to their behaviour under a rotation about the $\hat{z}$ axis, the action of the component of the angular momentum operator $\mathbf{J}_{\text{j−order tensors}}$ is given by Eq. (11.42). The body fixed spherical basis set is built from the vector basis set

$$\mathbf{E}^{(1)1} \equiv -\frac{\hat{\mathbf{X}} + i\hat{\mathbf{Y}}}{\sqrt{2}} = \mathbf{R}\cdot\mathbf{e}^{(1)1}; \quad \mathbf{E}^{(1)0} \equiv \hat{\mathbf{Z}} = \mathbf{R}\cdot\mathbf{e}^{(1)0}; \quad \mathbf{E}^{(1)-1} \equiv \frac{\hat{\mathbf{X}} - i\hat{\mathbf{Y}}}{\sqrt{2}} = \mathbf{R}\cdot\mathbf{e}^{(1)-1}, \tag{11.56}$$

each of these being related to the corresponding $\mathbf{e}^{(1)\mu}$ by the rotation from laboratory frame to body frame. For $k > 0$, a set of spherical basis tensors for describing the jth irreducible representation of the rotation group in the body-fixed frame is then

$$\mathbf{E}^{(j)k} = N_{jk}\left[\left(\mathbf{E}^{(1)1}\right)^k \left(\mathbf{E}^{(1)0}\right)^{j-k}\right]^{(j)} = \mathbf{R}^{(j)}\odot^j \mathbf{e}^{(j)k}, \tag{11.57}$$

while for $k < 0$, the kth power of $\mathbf{E}^{(1)1}$ is replaced by the $|k|$th power of $\mathbf{E}^{(1)-1}$. The normalization factor is given by Eq. (5.55). A covariant body-fixed basis set is defined in an analogous way.

For a symmetric top having magnitude j and $\hat{z}$ component m of the angular momentum in the laboratory frame, it's state $|jm\rangle$ is taken as being represented by the tensor $\mathbf{e}^{(j)m}$. The selection of a state having a particular orientation (rotation R) with internal (body fixed) angular momentum $\hat{\mathbf{Z}}$ component $k\hbar$, whose meaning is the bra $\langle R, jk|$, is represented by the covariant tensor $\mathbf{E}_k^{(j)}$. Then the corresponding wavefunction is

$$\begin{aligned}\Psi_{jkm}(R) &= N_{jkm}\mathbf{E}_k^{(j)}\odot^j \mathbf{e}^{(j)m} \\ &= N_{jkm}\mathbf{e}_k^{(j)}\odot^j \left(\mathbf{R}^{-1}\right)^{(j)}\odot^j \mathbf{e}^{(j)m} = N_{jkm} D_{km}^{(j)}(R^{-1}).\end{aligned} \tag{11.58}$$

The normalization factor N_{jkm}, chosen so that an integration over all rotations R gives

$$\int \Psi_{j'k'm'}(R)^*\Psi_{jkm}(R)dR = \delta_{j'j}\delta_{k'k}\delta_{m'm}, \tag{11.59}$$

is

$$N_{jkm} = \sqrt{\frac{2j+1}{8\pi^2}}, \tag{11.60}$$

provided R is parameterized by the Euler angles, compare Eq. (9.52). With the connection between covariant and contravariant basis tensors, Eq. (9.41) shows how the wavefunction can be expressed as

$$\Psi_{jkm}(R) = (-1)^{m+k} N_{jkm} D^{(j)}_{-m,-k}(R). \tag{11.61}$$

This is somewhat like the wavefunction given by Rose [2] (page 55), but Rose's k and m appear to be interchanged and without the phase factor. A more explicit form for the wavefunction can be given when the rotation R is expressed in terms of the Euler angles α, β and γ, specifically from Eq. (11.58),

$$\begin{aligned}
\Psi_{jkm}(\alpha\beta\gamma) &= \sqrt{\frac{2j+1}{8\pi^2}} e^{ik\gamma} D^{(j)}_{km}(R_{\hat{y}}(-\beta)) e^{im\alpha} \\
&= (-1)^{m+k} \sqrt{\frac{2j+1}{8\pi^2}} e^{im\alpha} D^{(j)}_{mk}(R_{\hat{y}}(-\beta)) e^{ik\gamma} \\
&= (-1)^{m+k} \sqrt{\frac{2j+1}{8\pi^2}} \mathcal{D}^{(j)}_{mk}(\alpha,\beta,\gamma).
\end{aligned} \tag{11.62}$$

The second form is obtained by using a symmetry of the rotation matrices, Eq. (9.20), and a reordering of the factors, which is in turn recognized as being the wavefunction given by Wigner [3] and Edmonds [1], except for a factor of $(-1)^{m+k}$, compare Eq. (9.21).

As written in Eq. (11.58), each of the two jth order tensors carries an angular momentum quantum number so its direct association with a bracket such as $\langle R|jkm\rangle$ does not appear to be quite right. On the other hand, if the tensorial contraction is written

$$\langle R|jkm\rangle = \Psi_{jkm}(R) = N_{jkm} \mathbf{R}^{(j)} \odot^{2j} \mathbf{e}^{(j)}_k \mathbf{e}^{(j)m}, \tag{11.63}$$

then the contraction separates what can be regarded as the orientation bra from the angular momentum ket, which now appears as the direct product of a covariant and a contravariant basis set. This is what is used here to make a connection with the calculation of eigenvalues for the various angular momenta.

First is the square of the angular momentum, which can be calculated by applying the abstract operator to the abstract ket, or the corresponding tensorial operator *to one of* the basis tensors, thus

$$\mathbf{J}\cdot\mathbf{J}|jkm\rangle = j(j+1)\hbar^2|jkm\rangle \iff \hbar^2 \mathbf{G}^{(j)} \odot^j \mathbf{G}^{(j)} \odot^j \mathbf{e}^{(j)m} = j(j+1)\hbar^2 \mathbf{e}^{(j)m}, \tag{11.64}$$

with $\mathbf{e}^{(j)}_k$ unaffected, and the calculation is of the laboratory fixed total angular momentum. It is interpreted that the angular momentum is to be determined by a laboratory fixed observer. Second is as an eigenvector of $J_{\hat{z}}$, which for a symmetric top wavefunction can be calculated in the differing ways,

$$\begin{aligned}
\langle R|J_{\hat{z}}|jkm\rangle &= m\hbar\langle R|jkm\rangle, \\
&= N_{jkm} \mathbf{R}^{(j)} \odot^{2j} \mathbf{e}^{(j)}_k \left[\hbar \mathbf{G}^{(j)}_{\hat{z}} \mathbf{e}^{(j)m}\right], \\
&= \frac{\hbar}{i}\frac{\partial}{\partial\alpha} \Psi_{jkm}(R),
\end{aligned} \tag{11.65}$$

with the last form coming from the expression of the wavefunction as a function of Euler angles. In carrying out the tensorial representation of the angular momentum operator, this has been applied to the contravariant tensor basis element. Lastly, this state is also an eigenvector of $J_{\hat{\mathbf{Z}}}$, again applied to the basis vector for the laboratory fixed part of the state,

$$\begin{aligned} \langle R|J_{\hat{\mathbf{Z}}}|jkm\rangle &= k\hbar\langle R|jkm\rangle \\ &= N_{jkm}\mathbf{R}^{(j)}\odot^{2j}\mathbf{e}_k^{(j)}\left[\hbar\mathbf{G}_{\hat{\mathbf{Z}}}^{(j)}\odot^j\mathbf{e}^{(j)m}\right]. \end{aligned} \tag{11.66}$$

To carry out the effect of the rotation generator, it is recognized that the generator for rotating about the body-fixed $\hat{\mathbf{Z}}$ axis can be written

$$\mathbf{G}_{\hat{\mathbf{Z}}}^{(j)} = \mathbf{G}_{\mathbf{R}\cdot\hat{z}}^{(j)} = \mathbf{R}^{(j)}\odot^j\mathbf{G}_{\hat{z}}^{(j)}\odot^j(\mathbf{R}^{(j)})^{-1}, \tag{11.67}$$

making use of the rotational invariance of $\boldsymbol{\mathcal{E}}$. The calculation of the tensor contractions in the tensorial representation of the matrix element is then

$$\begin{aligned} \mathbf{R}^{(j)}\odot^{2j}\mathbf{e}_k^{(j)}\left[\hbar\mathbf{G}_{\hat{\mathbf{Z}}}^{(j)}\odot^j\mathbf{e}^{(j)m}\right] &= \mathbf{R}^{(j)}\odot^{2j}\mathbf{e}_k^{(j)}\left[\hbar\mathbf{R}^{(j)}\odot^j\mathbf{G}_{\hat{z}}^{(j)}\odot^j(\mathbf{R}^{(j)})^{-1}\odot^j\mathbf{e}^{(j)m}\right] \\ &= \mathbf{e}_k^{(j)}\odot^j\hbar\mathbf{G}_{\hat{z}}^{(j)}\odot^j(\mathbf{R}^{(j)})^{-1}\odot^j\mathbf{e}^{(j)m} \\ &= k\hbar\mathbf{e}_k^{(j)}\odot^j(\mathbf{R}^{(j)})^{-1}\odot^j\mathbf{e}^{(j)m} = k\hbar D_{km}^{(j)}(R^{-1}) \\ &= \frac{\hbar}{i}\frac{\partial}{\partial\gamma}D_{km}^{(j)}(-\gamma,-\beta,-\alpha). \end{aligned} \tag{11.68}$$

The hamiltonian for a rigid rotor is

$$H = \frac{J_{\hat{\mathbf{X}}}^2}{2I_X} + \frac{J_{\hat{\mathbf{Y}}}^2}{2I_Y} + \frac{J_{\hat{\mathbf{Z}}}^2}{2I_Z}, \tag{11.69}$$

with moments of inertia I_X, I_Y and I_Z about the body-fixed axes. If the rotor is symmetric, $I_X = I_Y$, the hamiltonian simplifies to

$$H = \frac{\mathbf{J}\cdot\mathbf{J}}{2I_X} + \left(\frac{1}{2I_Z} - \frac{1}{2I_X}\right)J_{\hat{\mathbf{Z}}}^2. \tag{11.70}$$

Clearly the wavefunctions Ψ_{jkm} are the eigenvectors of this hamiltonian with eigenvalues

$$E_{jkm} = \frac{j(j+1)\hbar^2}{2I_X} + \left(\frac{1}{2I_Z} - \frac{1}{2I_X}\right)k^2\hbar^2, \tag{11.71}$$

independent of m. This simplifies further if the rotor is spherical, $I_X = I_Y = I_Z$.

A special case of the symmetric top case is when the molecule is linear, so that $I_Z = 0$. Then only the $k = 0$ eigenvalue is allowed (has finite energy). In this case, the eigenvectors simplify to

$$\Psi_{j0m}(R) = N_{j0m}\mathbf{E}_0^{(j)}\odot^j\mathbf{e}^{(j)m} = \sqrt{\frac{(2j+1)!}{8\pi^2 2^j(j!)^2}}[\hat{r}]^{(j)}\odot^j\mathbf{e}^{(j)m} = \sqrt{\frac{1}{2\pi}}Y_{jm}(\hat{r}), \tag{11.72}$$

on the basis that $\mathsf{R}\cdot\hat{z} = \hat{r}$ and from Eq. (5.48),

$$\mathbf{E}_0^{(j)} = \mathsf{R}^{(j)}\odot^j \mathbf{e}_0^{(j)} = \sqrt{\frac{(2j)!}{2^j(j!)^2}}[\hat{r}]^{(j)}. \tag{11.73}$$

The extra factor of $\sqrt{1/2\pi}$ in front of the spherical harmonic is associated with the normalization for the γ integration. Since there is now no dependence on γ, all reference to that quantity can be eliminated and the result simplified. These calculations show how the tensorial method can be consistently used for studying the properties of molecular rotational states.

11.2.1 Anomalous commutation relations

The components of the angular momentum operator satisfy the commutation relations of Eq. (11.1). It is inherently assumed in that statement that the components are with respect to a space-fixed (laboratory-fixed) coordinate system. On the other hand, in the body-fixed coordinate system, the commutation relations have the opposite sign. This arises because the coordinate axes rotate with the angular momentum according to Eq. (11.15), for example, $\hat{\mathbf{X}}$ is a position vector so that

$$[\mathbf{J}, \hat{\mathbf{X}}]_- = i\hbar\boldsymbol{\mathcal{E}}\cdot\hat{\mathbf{X}}. \tag{11.74}$$

The typical body-fixed angular momentum commutation relation then becomes

$$\begin{aligned}
[J_{\hat{\mathbf{X}}}, J_{\hat{\mathbf{Y}}}]_- &= \hat{\mathbf{X}}\cdot\mathbf{J}\hat{\mathbf{Y}}\cdot\mathbf{J} - \hat{\mathbf{Y}}\cdot\mathbf{J}\hat{\mathbf{X}}\cdot\mathbf{J} \\
&= \hat{\mathbf{X}}\cdot[\mathbf{J}, \hat{\mathbf{Y}}]_-\cdot\mathbf{J} + \hat{\mathbf{Y}}\hat{\mathbf{X}}{:}\mathbf{J}\mathbf{J} - \hat{\mathbf{Y}}\cdot[\mathbf{J}, \hat{\mathbf{X}}]_-\cdot\mathbf{J} - \hat{\mathbf{X}}\hat{\mathbf{Y}}{:}\mathbf{J}\mathbf{J} \\
&= i\hbar\hat{\mathbf{X}}\cdot\boldsymbol{\mathcal{E}}{:}\hat{\mathbf{Y}}\mathbf{J} + i\hbar\hat{\mathbf{Y}}\hat{\mathbf{X}}{:}\boldsymbol{\mathcal{E}}\cdot\mathbf{J} - i\hbar\hat{\mathbf{Y}}\cdot\boldsymbol{\mathcal{E}}{:}\hat{\mathbf{X}}\mathbf{J} \\
&= -i\hbar J_{\hat{\mathbf{Z}}} + i\hbar J_{\hat{\mathbf{Z}}} - i\hbar J_{\hat{\mathbf{Z}}} = -i\hbar J_{\hat{\mathbf{Z}}}.
\end{aligned} \tag{11.75}$$

A related commutation is the fact that the commonents of the angular momentum in the body-fixed frame commute with those in the laboratory-fixed frame, for example, $\mathbf{J}_{\hat{\mathbf{X}}}$ commutes with $\mathbf{J}$, namely

$$[\mathbf{J}, \mathbf{J}_{\hat{\mathbf{X}}}]_- = \mathbf{0}. \tag{11.76}$$

This is what allows a symmetric top eigenvector to have both body-fixed and laboratory-fixed angular momentum component eigenvalues. According to van Vleck [37], these anomalous commutation rules were first discovered by O. Klein [38].

11.3 Wigner-Eckart Theorem

A common problem arising in quantum mechanics is that of evaluating the matrix element of an operator between two quantum states, each of the three quantities belonging to irreducible representations of the rotation group and each an eigenvector of the corresponding rotation generator $G_{\hat{z}}$. The value of the matrix element can then be separated into the product of a 3-j symbol associated with the directional properties of the three quantities and a reduced matrix element independent of directional properties but determining the quantum mechanical properties of the matrix element. This is usually referred to as the Wigner-Eckart theorem [39–41]. Here this result is examined using Cartesian tensor methods.

Let $A^{(\ell)\mu}$ be a quantum operator belonging to the weight ℓ irreducible representation of the rotation group, and being an eigenvector of a rotation about the $\hat{z}$ axis with eigenvalue μ. A matrix element of this operator between quantum states $|ajm\rangle$ and $|a'j'm'\rangle$ is (jm and $j'm'$ are the angular momentum eigenvalues of the states while $a,\ a'$ label other degrees of freedom)

$$\langle a'j'm'|A^{(\ell)\mu}|ajm\rangle. \tag{11.77}$$

For integer j there is a tensor valued ket $|\boldsymbol{\psi}_a^{(j)}\rangle$ whose spherical components correspond to the kets $|ajm\rangle$. This could be found, for example, by

$$|\boldsymbol{\psi}_a^{(j)}\rangle = \sum_m |ajm\rangle \mathbf{e}_m^{(j)}. \tag{11.78}$$

Similarly, the connections for the bra state [the complex conjugate in the definition of a bra state is equivalent to a change from contravariant to covariant basis elements, Eq. (5.60)] and for the operator are

$$\begin{aligned} \langle\boldsymbol{\psi}_{a'}^{(j')}| &= \sum_{m'} \mathbf{e}^{(j')m'}\langle a'j'm'| \\ \mathbf{A}^{(\ell)} &= \sum_\mu A^{(\ell)\mu}\mathbf{e}_\mu^{(\ell)}. \end{aligned} \tag{11.79}$$

With these associations, the original matrix element can be expressed in the form

$$\langle a'j'm'|A^{(\ell)\mu}|ajm\rangle = \mathbf{e}_{m'}^{(j')}\odot^{j'}\langle\boldsymbol{\psi}_{a'}^{(j')}|\mathbf{A}^{(\ell)}|\boldsymbol{\psi}_a^{(j)}\rangle\odot^{j+\ell}\mathbf{e}^{(j)m}\mathbf{e}^{(\ell)\mu}. \tag{11.80}$$

Since the matrix element of the tensor valued states and operator is a rotational invariant, it must be a multiple of a 3-j tensor, thus

$$\langle\boldsymbol{\psi}_{a'}^{(j')}|\mathbf{A}^{(\ell)}|\boldsymbol{\psi}_a^{(j)}\rangle = (i)^{j+\ell-j'}\mathbf{V}(j',\ell,j)\langle\psi_{a'}^{(j')}||A^{(\ell)}||\psi_a^{(j)}\rangle, \tag{11.81}$$

with reduced matrix element $\langle\psi_{a'}^{(j')}||A^{(\ell)}||\psi_a^{(j)}\rangle$. The phase factor has been inserted in order to obtain the same reduced matrix elements as those standardly used. That such a phase factor is needed is due to the fact that the 3-j symbols are naturally associated with the $\mathfrak{e}^{(j)\mu}$ basis tensors whereas the standard formalism of quantum mechanics uses the $\mathbf{e}^{(j)\mu}$ basis tensors. As a consequence, the contractions of Eq. (11.80) give a 3-j symbol,

$$\langle a'j'm'|A^{(\ell)\mu}|ajm\rangle = (-1)^{j'-m'}\begin{pmatrix} j' & \ell & j \\ -m' & \mu & m \end{pmatrix}\langle\psi^{(j')}||A^{(\ell)}||\psi^{(j)}\rangle. \tag{11.82}$$

This is the standard manner in which the Wigner-Eckart theorem is written, with the reduced matrix element given by

$$\begin{aligned} \langle\psi^{(j')}||A^{(\ell)}||\psi^{(j)}\rangle. &= (i)^{j+\ell-j'}\mathbf{V}(j,\ell,j')\odot^{j'+\ell+j}\langle\boldsymbol{\psi}_{a'}^{(j')}|\mathbf{A}^{(\ell)}|\boldsymbol{\psi}_a^{(j)}\rangle \\ &= \sum_{m'\mu m}(-1)^{j'-m'}\begin{pmatrix} j' & \ell & j \\ -m' & \mu & m \end{pmatrix}\langle a'j'm'|A^{(\ell)\mu}|ajm\rangle. \end{aligned} \tag{11.83}$$

Here the connection to irreducible Cartesian tensors has been presented for states with integer j. For half-integer j, the analogous calculation could be done using spinor tensors, whose phase conventions are the same as the $\mathfrak{e}^{(j)\mu}$, whether written in terms of spinor or Cartesian tensors, but with the change in basis, the reduction of the tensorial matrix element, Eq. (11.81), is replaced by

$$\langle \mathbf{\Psi}_{a'}^{(j')}|\mathfrak{A}^{(\ell)}|\mathbf{\Psi}_{a}^{(j)}\rangle = \boldsymbol{\mathcal{W}}(j',\ell,j)\langle \psi_{a'}^{(j')}||A^{(\ell)}||\psi_{a}^{(j)}\rangle, \tag{11.84}$$

involving spinor tensors, in order to get the phases to agree with Eq. (11.82).

A first example illustrating these quantities is the evaluation of the matrix elements of the multipole moments for a rigid diatomic molecule. Standardly the wavefunctions used are $Y_{jm}(\hat{r})$ and the multipole moments are multiples of the spherical harmonics in position, $Y_{\ell\mu}(\hat{r})$. Direct integration, see Eq. (7.39) but with complex conjugation for the bra state, gives

$$\langle j'm'|Y_{\ell\mu}(\hat{r})|jm\rangle = (-1)^{m'}\left[\frac{(2j'+1)(2\ell+1)(2j+1)}{4\pi}\right]^{1/2}\begin{pmatrix} j' & \ell & j \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} j' & \ell & j \\ -m' & \mu & m \end{pmatrix}. \tag{11.85}$$

Thus by direct calculation, the reduced matrix element is

$$\langle j'||\mathbf{Y}^{(\ell)}(\hat{r})||j\rangle = (-1)^{j'}\left[\frac{(2j'+1)(2\ell+1)(2j+1)}{4\pi}\right]^{1/2}\begin{pmatrix} j' & \ell & j \\ 0 & 0 & 0 \end{pmatrix}. \tag{11.86}$$

The corresponding tensor operator is

$$\mathbf{Y}^{(\ell)}(\hat{r}) = \sum_{\mu}\mathbf{e}_{\mu}^{(\ell)}Y_{\ell\mu}(\hat{r}) = \boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})/\sqrt{4\pi}. \tag{11.87}$$

with analogous expressions for the tensor valued ket and bra. Then the reduced matrix element as calculated by tensor methods, using Eq. (7.21), is

$$\begin{aligned}\langle j'||\mathbf{Y}^{(\ell)}(\hat{r})||j\rangle &= (-i)^{j+\ell-j'}\mathbf{V}(j,\ell,j')\odot^{j+\ell+j'}\frac{1}{(4\pi)^{3/2}}\int \boldsymbol{\mathcal{Y}}^{(j')}(\hat{r})\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})\boldsymbol{\mathcal{Y}}^{(j)}(\hat{r})d\hat{r} \\ &= (-1)^{j'}\left[\frac{(2j'+1)(2\ell+1)(2j+1)}{4\pi}\right]^{1/2}\begin{pmatrix} j' & \ell & j \\ 0 & 0 & 0 \end{pmatrix},\end{aligned} \tag{11.88}$$

in agreement with the direct calculation of the matrix element in spherical tensor representation.

A second example is the reduced matrix element for the angular momentum operator, defined according to the above as

$$\langle j'm'|\mathbf{J}\cdot\mathbf{e}^{(1)\mu}|jm\rangle = (-1)^{j'-m'}\begin{pmatrix} j' & 1 & j \\ -m' & \mu & m \end{pmatrix}\langle j'||\mathbf{J}||j\rangle. \tag{11.89}$$

It is immediately clear that $j' = j$ since the angular momentum operator does not change the magnitude of the angular momentum. For the special case that $\mu = 0$, $m' = m$ and $\mathbf{J}\cdot\mathbf{e}^{(1)0} = J_{\hat{z}}$, so the evaluation of the matrix element is easy,

$$\begin{aligned} m\hbar &= (-1)^{j-m}\begin{pmatrix} j & 1 & j \\ -m & 0 & m \end{pmatrix}\langle j||\mathbf{J}||j\rangle \\ &= \frac{m}{\sqrt{j(j+1)(2j+1)}}\langle j||\mathbf{J}||j\rangle,\end{aligned} \tag{11.90}$$

so the reduced matrix element is

$$\langle j'||\mathbf{J}||j\rangle = \delta_{j'j}\hbar\sqrt{j(j+1)(2j+1)}. \tag{11.91}$$

The calculation of reduced matrix elements of higher ordered tensors of the angular momentum operator is included in the next section.

11.4 Tensors of Angular Momentum

The tensor product of the angular momentum operator with itself gives a second order tensor operator. This dual nature of being both a tensor and an operator is an extension of the dual nature of $\mathbf{J}$ itself. A well known relation of this type is the set of commutation relations for the angular momentum components, which can be combined together into the single tensorial equality

$$[\mathbf{J}, \mathbf{J}]_{-} = i\hbar\boldsymbol{\varepsilon}\cdot\mathbf{J}. \tag{11.92}$$

This inherently involves the tensor $\mathbf{JJ}$, but also exemplifies a situation in which a vector does not commute with itself. An alternate way of writing this vector commutation relation is

$$\mathbf{J}\times\mathbf{J} = -\mathbf{JJ}:\boldsymbol{\varepsilon} = i\hbar\mathbf{J}. \tag{11.93}$$

These two equations illustrate the interplay of operator and tensor properties. Specifically, the commutator form interchanges the order in which the operators act quantum mechanically but leave the tensorial order fixed, compare the discussion of Eq. (11.3). In contrast, the second equation changes the tensorial order of the operators but leaves the quantum order of action fixed. Since both results are the same, the effect of the two procedures have the same effect.

Generally one can take the tensor product an arbitrary number of times, in particular p times to get an pth order tensor of the angular momentum. Such a tensor can be reduced into parts that are irreducible under the rotation group acting on the tensorial directions. It must be understood that such an action is a tensorial operation and has nothing to do with the action of the angular momentum as a quantum operator. The tensorial and quantum operator properties are separate but there can be consequences of the dual properties as well as relations between these properties, as exemplified in the previous paragraph. But the tensorial reduction has no knowledge of whether a vector is an operator or not, so the irreducible tensors are just the same as those of Chap. 3, specifically an irreducible Cartesian tensor $[\mathbf{J}]^{(\ell)}$ of weight ℓ is symmetric and traceless in all pairs of indices.

The simplest irreducible tensor of angular momentum (besides the vector $\mathbf{J}$) is

$$[\mathbf{J}]^{(2)} = \frac{1}{2}\left[\mathbf{JJ} + (\mathbf{JJ})^t\right] - \frac{1}{3}\mathbf{J}\cdot\mathbf{J}\mathbf{U}. \tag{11.94}$$

Here $(\ )^t$ denotes the tensor transpose and is explicitly needed since $\mathbf{J}$ does not commute with itself. This can also be recognized as

$$[\mathbf{J}]^{(2)} = \mathbf{E}^{(2)}\odot^2\mathbf{JJ}. \tag{11.95}$$

With the aid of the vector commutation relation, Eq. (11.92), the reduction of the tensor product of two $\mathbf{J}$'s can be written as

$$\mathbf{JJ} = [\mathbf{J}]^{(2)} + \frac{1}{2}i\hbar\boldsymbol{\varepsilon}\cdot\mathbf{J} + \frac{1}{3}\mathbf{J}\cdot\mathbf{J}\mathbf{U}, \tag{11.96}$$

namely into its weight 2, 1 and 0 parts. For an ordinary vector (one that commutes with itself) the weight 1 part of this vanishes, which is also indicated by the presence of $\hbar$ in that term. While the angular momentum operator is hermitian, the above shows that the product $\mathbf{JJ}$ is not hermitian because of the presence of i in the weight 1 part of its reduction. On the other hand, $[\mathbf{J}]^{(2)}$ is hermitian. Such properties can be extended to the reduction of the pth tensor product of $\mathbf{J}$.

The generalization to form a highest weight ℓ tensor of the angular momentum can be found using the $\mathsf{E}^{(\ell)}$ projector, namely

$$[\mathbf{J}]^{(\ell)} = \mathsf{E}^{(\ell)} \odot^{\ell} \mathbf{JJ} \cdots \mathbf{J}, \tag{11.97}$$

with ℓ $\mathbf{J}$'s. A complete contraction $[\mathbf{J}]^{(\ell)} \odot^{\ell} [\mathbf{J}]^{(\ell)}$ of this tensor with itself is a polynomial of order ℓ in $\mathbf{J \cdot J}$ that provides a means of normalizing the tensor. But this contraction differs in nature from the position analog, Eq. (4.6),

$$[\mathbf{r}]^{(\ell)} \odot^{\ell} [\mathbf{r}]^{(\ell)} = \frac{2^{\ell}(\ell!)^2}{(2\ell)!} r^{2\ell} = r^{2\ell} \overline{P}_{\ell}(1), \tag{11.98}$$

because of the angular momentum commutation relations. The effect of the commutation relations is equivalent to the discreteness of the angular momentum in quantum mechanics and its effect is found by use of this discreteness. Thus for a magnitude quantum number j of the angular momentum, there are only $2j+1$ independent quantum states and, for example, $J_{\hat{z}}^{2j+1}$ is not an independent operator, but determined by the Cayley-Hamilton theorem, Eq. (11.12). As a consequence, $[\mathbf{J}]^{(2j+1)} = \mathbf{0}$ because there is an insufficient number of independent operators (in particular its $\hat{z}\hat{z} \cdots \hat{z}$ component) for this to exist. Such a constraint can be expressed by stating that

$$[\mathbf{J}]^{(\ell)} \odot^{\ell} [\mathbf{J}]^{(\ell)} = A_{\ell} \left[\mathbf{J \cdot J} - \frac{\ell - 1}{2} \left(\frac{\ell - 1}{2} + 1 \right) \hbar^2 \right] [\mathbf{J}]^{(\ell-1)} \odot^{\ell-1} [\mathbf{J}]^{\ell-1)} \tag{11.99}$$

for some constant A_{ℓ}, on the basis that the contractions are polynomials in $\mathbf{J \cdot J}$ for which the lefthand side must vanish if $j = (\ell - 1)/2$, whereas the remaining contraction on the right does not. Iteration of this gives

$$[\mathbf{J}]^{(\ell)} \odot^{\ell} [\mathbf{J}]^{(\ell)} = \overline{P}_{\ell}(1) \prod_{n=0}^{\ell-1} \left[\mathbf{J \cdot J} - \frac{n}{2} \left(\frac{n}{2} + 1 \right) \hbar^2 \right], \tag{11.100}$$

with the constant determined by the fact that for $\mathbf{J}$ replaced by $\mathbf{r}$ and $\hbar \to 0$, this must reduce to being equivalent to the classical expression, Eq. (11.98). This result was derived by Schwinger [42] and the method of derivation given here is a variant of that presented in [43]. Zemach's recursion relation [44]

$$\mathbf{J} \cdot [\mathbf{J}]^{(\ell)} = \frac{\ell}{2\ell - 1} \left[\mathbf{J \cdot J} - \frac{1}{4}(\ell^2 - 1)\hbar^2 \right] [\mathbf{J}]^{(\ell-1)} \tag{11.101}$$

is obtained by contracting both sides with $\ell - 1$ $\mathbf{J}$'s and using the ratio of normalization constants.

The analog of the $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$ are the operators

$$\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J}) \equiv \left(\frac{2\ell + 1}{[\mathbf{J}]^{(\ell)} \odot^{\ell} [\mathbf{J}]^{(\ell)}} \right)^{1/2} [\mathbf{J}]^{(\ell)}. \tag{11.102}$$

These are normalized so that

$$(2j+1)^{-1} \mathrm{Tr} \mathcal{P}_j \boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J}) \boldsymbol{\mathcal{Y}}^{(\ell')}(\mathbf{J}) = \delta_{\ell\ell'} \mathsf{E}^{(\ell)}, \tag{11.103}$$

corresponding to the quantum trace over the $2j+1$ states of the magnitude j angular momentum quantum number,

$$\mathcal{P}_j \equiv \sum_m |jm\rangle\langle jm| = |\boldsymbol{\psi}^{(j)}\rangle \odot^j \langle \boldsymbol{\psi}^{(j)}| \tag{11.104}$$

being the projector onto this set of states. This restriction is analogous to the restriction that it is only the unit vector $\hat{r}$ that appears in the normalization of the $\boldsymbol{\mathcal{Y}}^{(\ell)}(\hat{r})$. As defined here, the emphasis is on taking the average over the independent variable, whether $\hat{r}$ or quantum state, hence the factors of $1/(4\pi)$ or $1/(2j+1)$. It is noted that the projector is a rotational invariant (it is easy to show that it commutes with all rotation generators $J_{\hat{x}}$, $J_{\hat{y}}$ and $J_{\hat{z}}$) and has been written both as a sum over angular momemtum component states and as the tensor contraction of the ket and bra tensor states, Eqs. (11.78) and (11.79), associated with angular momentum magnitude $j\hbar$.

The matrix elements of the operator $\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})$ are given in terms of 3-j symbols and reduced matrix elements

$$\langle j'm'|\mathcal{Y}^{(\ell)\mu}(\mathbf{J})|jm\rangle = (-1)^{j'-m'} \begin{pmatrix} j' & \ell & j \\ -m' & \mu & m \end{pmatrix} \langle j'||\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})||j\rangle. \tag{11.105}$$

This also conforms to the components of the tensorial form (11.81) of the Wigner Eckart theorem (the detailed equations in the following are restricted to integer j, but there is an analogous treatment using spinor tensors for 1/2-integer angular momentum)

$$\langle \boldsymbol{\psi}^{(j')}|\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})|\boldsymbol{\psi}^{(j)}\rangle = (i)^{j+\ell-j'} \mathbf{V}(j',\ell,j)\langle j'||\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})||j\rangle. \tag{11.106}$$

For $\ell = 1$ the reduced matrix element can be calculated by direct evaluation of a typical matrix element and is a variant of Eq. (11.91),

$$\langle j'||\boldsymbol{\mathcal{Y}}^{(1)}(\mathbf{J})||j\rangle = \delta_{j'j}\sqrt{3(2j+1)}. \tag{11.107}$$

It is noticed that this is dimensionless (no $\hbar$). This and the other reduced matrix elements can be calculated, up to a possible sign, from the tensorial contraction of Eq. (11.103) and using the tensorial form of Eq. (11.104) for the projector

$$\begin{aligned} \mathrm{Tr}\mathcal{P}_j\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})\odot^\ell\mathcal{P}_j\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J}) &= (2j+1)(2\ell+1) \\ = \quad & (-1)^\ell\mathbf{V}(j,\ell,j)\odot^{2j+\ell}\mathbf{V}(j,\ell,j)\langle j||\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})||j\rangle^2 \\ = \quad & \langle j||\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})||j\rangle^2. \end{aligned} \tag{11.108}$$

As a consequence, the reduced matrix element of the tensor of the angular momentum is

$$\langle j'||\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})||j\rangle = \delta_{j'j}\sqrt{(2\ell+1)(2j+1)}, \tag{11.109}$$

with the Kronecker delta function added. The choice of sign can be checked by examining the relative phases of the trace over three $\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})$'s, see the following paragraph.

The trace over three angular momentum tensors necessarily has the form

$$\mathrm{Tr}\mathcal{P}_j\boldsymbol{\mathcal{Y}}^{(\ell_1)}(\mathbf{J})\boldsymbol{\mathcal{Y}}^{(\ell_2)}(\mathbf{J})\boldsymbol{\mathcal{Y}}^{(\ell_3)}(\mathbf{J}) = C(\ell_1,\ell_2,\ell_3|j)\mathbf{V}(\ell_1,\ell_2,\ell_3) \tag{11.110}$$

for some, to be determined, coefficient $C(\ell_1,\ell_2,\ell_3|j)$. Now the trace can be calculated using a $|jm\rangle$ basis set and a sum over the resulting 3-j symbols, or using the tensorial states. It is the latter that is followed here. Inserting the tensorial form for the projector $\mathcal{P}_j$ between each pair of $\boldsymbol{\mathcal{Y}}^{(\ell)}$'s, the combination of 3-j tensors that results is

$$\begin{aligned}&(\underbrace{\mathsf{I})^j \odot^j \mathbf{V}(j,\ell_1,j)\odot^j \mathbf{V}(j,\ell_2,j)\odot^j \mathbf{V}(j,\ell_3,j)\odot^j (\mathsf{I}}) ^j \\ &= (-1)^{\ell_1+\ell_2+\ell_3}\mathbf{V}(\ell_1,\ell_2,\ell_3)\left\{\begin{matrix}\ell_1 & \ell_2 & \ell_3\\ j & j & j\end{matrix}\right\}\end{aligned} \tag{11.111}$$

and the coefficient for the evaluation of the trace of three $\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})$'s is

$$\begin{aligned}C(\ell_1,\ell_2,\ell_3|j) &= (-i)^{\ell_1+\ell_2+\ell_3}(2j+1)^{3/2}\\ &\quad\times\sqrt{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}\left\{\begin{matrix}\ell_1 & \ell_2 & \ell_3\\ j & j & j\end{matrix}\right\}.\end{aligned} \tag{11.112}$$

One of the simplest cases of this is

$$C(1,1,1|j) = \frac{3i(2j+1)}{\sqrt{2j(j+1)}}, \tag{11.113}$$

which can easily be checked by direct calculation of the trace. An immediate consequence of the general formula is that the scalar product of three $\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})$'s is

$$\begin{aligned}&\boldsymbol{\mathcal{Y}}^{(\ell_1)}(\mathbf{J})\boldsymbol{\mathcal{Y}}^{(\ell_2)}(\mathbf{J})\mathcal{P}_j\boldsymbol{\mathcal{Y}}^{(\ell_3)}(\mathbf{J})\odot^{\ell_1+\ell_2+\ell_3}\mathbf{V}(\ell_3,\ell_2,\ell_1) = (i)^{\ell_1+\ell_2+\ell_3}(2j+1)^{1/2}\\ &\quad\times\sqrt{(2\ell_1+1)(2\ell_2+1)(2\ell_3+1)}\left\{\begin{matrix}\ell_1 & \ell_2 & \ell_3\\ j & j & j\end{matrix}\right\}\\ &= (i)^{\ell_1+\ell_2+\ell_3}(2j+1)^{-1}\langle j||\boldsymbol{\mathcal{Y}}^{(\ell_1)}(\mathbf{J})||j\rangle\langle j||\boldsymbol{\mathcal{Y}}^{(\ell_2)}(\mathbf{J})||j\rangle\\ &\quad\times\langle j||\boldsymbol{\mathcal{Y}}^{(\ell_3)}(\mathbf{J})||j\rangle\left\{\begin{matrix}\ell_1 & \ell_2 & \ell_3\\ j & j & j\end{matrix}\right\},\end{aligned} \tag{11.114}$$

with the last form expressed in terms of reduced matrix elements. The projector $\mathcal{P}_j$ is included in order to determine which magnitude of the angular momentum quantum number j is to be used in evaluating the various terms. A special case is for $\ell_1,\ \ell_2,\ \ell_3 = \ell,\ \ell+1,\ 1$

$$\begin{aligned}&\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})\boldsymbol{\mathcal{Y}}^{(\ell+1)}(\mathbf{J})\mathcal{P}_j\boldsymbol{\mathcal{Y}}^{(1)}(\mathbf{J})\odot^{2\ell+2}\mathbf{V}(1,\ell+1,\ell) = (i)^{2\ell+2}(2j+1)^{-1}\\ &\quad\times\langle j||\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})||j\rangle\langle j||\boldsymbol{\mathcal{Y}}^{(\ell+1)}(\mathbf{J})||j\rangle\langle j||\boldsymbol{\mathcal{Y}}^{(1)}(\mathbf{J})||j\rangle\left\{\begin{matrix}\ell & \ell+1 & 1\\ j & j & j\end{matrix}\right\}.\end{aligned} \tag{11.115}$$

Since the reduced matrix element $\langle j||\boldsymbol{\mathcal{Y}}^{(1)}(\mathbf{J})||j\rangle$ has been calculated directly, Eq. (11.107), and the lefthand side is, except for a numerical factor, determined by $[\mathbf{J}]^{(\ell+1)}\odot^{\ell+1}[\mathbf{J}]^{(\ell+1)}$, this equation determines the product of reduced matrix elements

$$\langle j||\boldsymbol{\mathcal{Y}}^{(\ell)}(\mathbf{J})||j\rangle\langle j||\boldsymbol{\mathcal{Y}}^{(\ell+1)}(\mathbf{J})||j\rangle = (2j+1)\sqrt{(2\ell+1)(2\ell+3)}. \tag{11.116}$$

This provides a recursive means of determining that Eq. (11.109) has the correct phase for the general reduced matrix element, since the first element is already determined by Eq. (11.107).

11.5 Traces of Products of J

This is the extension of Sec. 4.2 to a particular vector operator whose components do not commute. Besides the obvious difference between having a trace rather than an integral, the magnitude of the quantum vector operator cannot be separated from its directional properties, so there needs to be some contraint on the magnitude of the quantum operator, here the insertion of the projector $\mathcal{P}_j$ for the angular momentum. Thus the study here are the traces

$$\mathrm{Tr}\mathcal{P}_j(\mathbf{J})^n = \mathrm{Tr}\mathcal{P}_j\mathbf{J}\mathbf{J}\cdots\mathbf{J}.$$

For the unit position vector $\hat{r}$ discussed in Sec. 4.2, a complete and general classification of the integrals was easily carried out. The angular momentum case is significantly harder and no general result is known by the author. Thus the discussion is limited to general considerations and to listing the traces for n up to 6. The cases of n up to 4 have been given previously in Ref. [13].

Since the trace is a rotational invariant, this nth order tensor is a linear combination of products of $\boldsymbol{\mathsf{U}}$ and $\boldsymbol{\mathcal{E}}$. Moreover, because the product of two $\boldsymbol{\mathcal{E}}$'s is a linear combination of 3 $\boldsymbol{\mathsf{U}}$'s, see Eq. (2.84), at most one $\boldsymbol{\mathcal{E}}$ is needed for forming the nth invariant tensor. Thus, if n is even, the integral is expressible as a linear combination of terms each having $n/2$ $\boldsymbol{\mathsf{U}}$'s, while for odd n there is one $\boldsymbol{\mathcal{E}}$ and $(n-3)/2$ $\boldsymbol{\mathsf{U}}$'s in each term. The only other symmetry that appears available is due to the cyclic invariance of the trace, so the resulting tensor must also be invariant to a cyclic permutation of the n directions of the tensor.

The cases of n=0,1,2,3 are straightforward. In particular, for n=0,1 and 2

$$\mathrm{Tr}\mathcal{P}_j = 2j+1; \qquad \mathrm{Tr}\mathcal{P}_j\mathbf{J} = \mathbf{0}; \qquad \mathrm{Tr}\mathcal{P}_j\mathbf{J}\mathbf{J} = \frac{2j+1}{3}j(j+1)\hbar^2\boldsymbol{\mathsf{U}}. \tag{11.117}$$

For n=3, the trace is proportional to $\boldsymbol{\mathcal{E}}$, namely

$$\mathrm{Tr}\mathcal{P}_j\mathbf{J}\mathbf{J}\mathbf{J} = a_3\boldsymbol{\mathcal{E}}, \tag{11.118}$$

with the coefficient a_3 calculated by contracting with $\boldsymbol{\mathcal{E}}$

$$\boldsymbol{\mathcal{E}} \odot^3 \mathrm{Tr}\mathcal{P}_j\mathbf{J}\mathbf{J}\mathbf{J} = -\mathrm{Tr}\mathcal{P}_j\mathbf{J}\times\mathbf{J}\cdot\mathbf{J} = -i(2j+1)j(j+1)\hbar^3 = -6a_3. \tag{11.119}$$

Consequently the trace is given by

$$\mathrm{Tr}\mathcal{P}_j\mathbf{J}\mathbf{J}\mathbf{J} = \frac{i(2j+1)j(j+1)\hbar^3}{6}\boldsymbol{\mathcal{E}}. \tag{11.120}$$

This is equivalent to the evalustion of the trace of the product of three $\boldsymbol{\mathcal{Y}}^{(1)}(\mathbf{J})$'s, as calculated in the previous section.

The n=4 case is the first one involving more than one $\boldsymbol{\mathsf{U}}$. There are three ways of forming a 4th order tensor from two $\boldsymbol{\mathsf{U}}$'s, so the trace of 4 $\mathbf{J}$'s can be written

$$\mathrm{Tr}\mathcal{P}_j\mathbf{J}\mathbf{J}\mathbf{J}\mathbf{J} = a_4\boldsymbol{\mathsf{U}}\boldsymbol{\mathsf{U}} + b_4\boldsymbol{\mathsf{U}\!\!\mathsf{U}} + c_4\boldsymbol{\Cup}, \tag{11.121}$$

with coefficients a_4, b_4 and c_4 to be determined. The invariance to a cyclic permutation of the directions of the tensor implies that $c_4 = a_4$, so only two quantities need to be determined. First, if $\boldsymbol{\mathsf{U}}$ is double dotted into this equation from the left

$$j(j+1)\hbar^2\mathrm{Tr}\mathcal{P}_j\mathbf{J}\mathbf{J} = \frac{(2j+1)j^2(j+1)^2\hbar^4}{3}\boldsymbol{\mathsf{U}} = (3a_4+b_4+c_4)\boldsymbol{\mathsf{U}}. \tag{11.122}$$

Second, if the antisymmetric combination of the first two directions of the tensors on each side is taken, then

$$\begin{aligned}\mathrm{Tr}\mathcal{P}_j\left[\mathbf{JJ}-(\mathbf{JJ})^t\right]\mathbf{JJ} &= i\hbar\boldsymbol{\mathcal{E}}\cdot\mathrm{Tr}\mathcal{P}_j\mathbf{JJJ}=\frac{-(2j+1)j(j+1)\hbar^4}{6}\boldsymbol{\mathcal{E}}\cdot\boldsymbol{\mathcal{E}} \\ &= (b_4-c_4)\left[\mathbf{\cup\!\!\cup}-\mathbf{\cup\!\!\cup}\right]. \end{aligned} \tag{11.123}$$

Since the remaining tensors in this equation are negatives of each other, this gives two equations for $a_4 = c_4$ and b_4, which when solved, gives

$$\mathrm{Tr}\mathcal{P}_j(\mathbf{J})^4=\frac{(2j+1)j(j+1)\hbar^4}{30}\left[(2j^2+2j+1)\left(\mathbf{UU}+\mathbf{\cup\!\!\cup}\right)+(2j^2+2j-4)\mathbf{\cup\!\!\cup}\right]. \tag{11.124}$$

Asymptotically as $j\to\infty$, this reduces to a factor of $(2j+1)(j\hbar)^4/15$ times the sum of all three permutations of $\mathbf{UU}$, in analogy to Eq. (4.25), with the replacement of the degeneracy factor $2j+1$ by the surface area 4π and including the magnitude of the angular momentum $(j\hbar)^4$. For reference, the classical limit is in fact: take $j\hbar$ constant while $\hbar\to 0$ and $j\to\infty$. It is also noted that projecting the first two indices of Eq. (11.124) with $\mathbf{E}^{(2)}$ gives

$$\mathrm{Tr}\mathcal{P}_j[\mathbf{J}]^{(2)}\mathbf{JJ}=\frac{(2j+1)j(j+1)(2j-1)(2j+3)\hbar^4}{30}\mathbf{E}^{(2)}, \tag{11.125}$$

in agreement with Eq. (11.103) taking into account the normalization of the $\boldsymbol{\mathcal{Y}}^{(2)}(\mathbf{J})$.

For n=5, the trace is expressed as a linear combination of tensors with one $\mathbf{U}$ and one $\boldsymbol{\mathcal{E}}$. While such tensors are not all independent, see the typical relation (2.87), here the cyclic symmetry of the trace is stressed. Thus the trace is a combination of two sets of tensors, each set being a sum of the cyclic permutations of a member of that set,

$$\begin{aligned}\mathrm{Tr}\mathcal{P}_j(\mathbf{J})^5 &= a_5\left[\mathbf{U}\boldsymbol{\mathcal{E}}+\boldsymbol{\mathcal{E}}\!\!\mathbf{U}+\boldsymbol{\mathcal{E}}\mathbf{U}+\boldsymbol{\mathcal{E}}\mathbf{U}+\mathbf{U}\!\boldsymbol{\mathcal{E}}\!\mathbf{U}\right] \\ &\quad +b_5\left[\mathbf{U}\!\!\boldsymbol{\mathcal{E}}+\boldsymbol{\mathcal{E}}\!\!\mathbf{U}+\boldsymbol{\mathcal{E}}\mathbf{U}+\mathbf{U}\!\boldsymbol{\mathcal{E}}+\boldsymbol{\mathcal{E}}\!\mathbf{U}\right]. \end{aligned} \tag{11.126}$$

The doubledot contraction of $\boldsymbol{\mathcal{E}}$ with this gives

$$\begin{aligned}\boldsymbol{\mathcal{E}}:\mathrm{Tr}\mathcal{P}_j(\mathbf{J})^5 &= -i\hbar\mathrm{Tr}\mathcal{P}_j(\mathbf{J})^4 \\ &= a_5\left[-3\mathbf{UU}-3\mathbf{\cup\!\!\cup}+2\mathbf{\cup\!\!\cup}\right]+b_5\left[\mathbf{UU}+\mathbf{\cup\!\!\cup}-4\mathbf{\cup\!\!\cup}\right]. \end{aligned} \tag{11.127}$$

On making use of the expression of $\mathrm{Tr}\mathcal{P}_j(\mathbf{J})^4$, a solution for the coefficients a_5 and b_5 can be obtained,

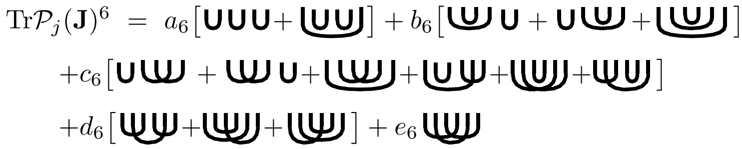
$$a_5=\frac{i\hbar^5(2j+1)j^2(j+1)^2}{30};\qquad b_5=\frac{i\hbar^5(2j+1)j(j+1)[j(j+1)-1]}{30}. \tag{11.128}$$

A check on these results is that the doubledot contraction of Eq. (11.126) with $\mathbf{U}$ agrees with Eq. (11.120). For use in the calculation of the trace of 6 **J**'s, the relation of Eq. (2.87) and its cyclic permutations can be used to rewrite Eq. (11.126) in the form

$$\begin{aligned}\mathrm{Tr}\mathcal{P}_j(\mathbf{J})^5 &= \frac{i(2j+1)\hbar^5 j(j+1)}{30}\Big\{[3j(j+1)-1]\left(\boldsymbol{\mathcal{E}}\!\!\mathbf{U}+\boldsymbol{\mathcal{E}}\!\mathbf{U}+\boldsymbol{\mathcal{E}}\mathbf{U}\right) \\ &\quad +[j(j+1)-2]\left(\boldsymbol{\mathcal{E}}\mathbf{U}-\boldsymbol{\mathcal{E}}\mathbf{U}+\boldsymbol{\mathcal{E}}\!\!\mathbf{U}\right)\Big\}. \end{aligned} \tag{11.129}$$

This also illustrates that there are only 6 linearly independent rotationally invariant fifth order tensors, as according to the parentage scheme of Sec. 3.5.

The trace of 6 **J**'s can be calculated in a similar way, but the details are much more complicated than the previous cases. Essentially there are 15 rotationally invariant tensors on which the trace depends and these are all linearly independent as can be seen by parentage arguments. A classification by cyclic symmetry allows the trace to be written in the form



(11.130)

Doubledot contractions with $\mathbf{U}$ and $\boldsymbol{\varepsilon}$ relate this trace with Eq. (11.124) to give three equations for the 5 coefficients, and provided the contraction is done on the left, with Eq. (11.129), to give 4 more equations. These 7 equations for the 5 coefficients can be shown to be consistent, and solved to give

$$\begin{aligned} a_6 = d_6 &= \frac{(2j+1)j(j+1)\hbar^6}{210}[2j^2(j+1)^2 - 9j(j+1) + 10] \\ b_6 &= \frac{(2j+1)j(j+1)\hbar^6}{210}[2j^2(j+1)^2 + 19j(j+1) - 11] \\ c_6 &= \frac{(2j+1)j(j+1)\hbar^6}{210}[2j^2(j+1)^2 - 2j(j+1) - 4] \\ e_6 &= \frac{(2j+1)j(j+1)\hbar^6}{210}[2j^2(j+1)^2 - 30j(j+1) + 17]. \end{aligned} \quad (11.131)$$

Such calculations can be extended to higher n, but the general structure of the result is not readily apparent.

It is noted that in all the above cases, the coefficient of each tensorial term in $\mathrm{tr}(\mathbf{J})^n$ is $2j+1$ times a polynomial of degree $[n/2]$ in $j(j+1)$. Moreover, for n even, the leading term is

$$(2j+1)\hbar^n(2)^{n/2}(n/2)!/(n+1)!.$$

This agrees with the normalization of $\int(\hat{r})^n d\hat{r}$, Sec. 4.2, except for the replacement of 4π by $2j+1$ (the respective volume of the space) and the multiplication by $[j(j+1)\hbar^2]^{n/2}$. That this asociation should occur is because, in the classical mechanical limit, $\hbar \to 0$, $j \to \infty$, with $j\hbar$ constant, the trace is equivalent to the integral over all angular momentum directions, and thus similar in structure to the $\hat{r}$ integral. Some of this structure has been noted by Dalton [45], who discusses one method of calculating the trace of a product of angular momentum operator components. Tables of such traces are given for $n \leq 10$ by Ambler, et al [46] for both Cartesian and spherical tensor components, calculated via computer using the commutation relations.

Another possible way of calculating the trace of an arbitrary number of angular momentum components is to use the Wigner-Eckart theorem, Eq. (11.89), for a single **J** component with magnitude j and then calculate the trace of $(\mathbf{J})^n$ by repeated matrix multiplication of the 3-j symbols. For a spherical component of **J** in particular, the matrix of the corresponding 3-j symbol has only one entry in each row and column, so this should be an efficient way of calculating such a trace. The author is not aware of any implementation of this method. Of course, what the author considers more efficient, is that in any problem that involves a tensor product of **J**'s, this product should be decomposed into its irreducible parts and then the trace of the tensor is just the invariant part.

11.6 Angular Momentum Superoperators

The word superoperator was introduced by Crawford [47] to designate an operator acting on an operator, equivalently a transformation of an operator. The action of taking the commutator of a given operator with whatever operator is to be transformed is such a superoperator. Specifically the act of taking the commutator of $J_{\hat{n}}$ with another operator is denoted here by

$$\mathcal{J}_{\hat{n}} A \equiv [J_{\hat{n}}, A]_- . \tag{11.132}$$

This can be specialized to the components of the angular momentum in some coordinate system, for example to those associated with the $\hat{x}$, $\hat{y}$ and $\hat{z}$ unit vectors. It can also be generalized to the vector angular momentum, namely the angular momentum superoperator is defined as

$$\boldsymbol{\mathcal{J}} A \equiv [\mathbf{J}, A]_- . \tag{11.133}$$

The action of the square of such a superoperator, for example $\mathcal{J}_{\hat{n}}$, gives

$$\mathcal{J}_{\hat{n}}^2 A = J_{\hat{n}}^2 A - 2 J_{\hat{n}} A J_{\hat{n}} + A J_{\hat{n}}^2 , \tag{11.134}$$

while the qth power gives

$$\mathcal{J}_{\hat{n}}^q A = \sum_k \binom{q}{k} (-1)^{q-k} J_{\hat{n}}^k A J_{\hat{n}}^{q-k} . \tag{11.135}$$

This can easily be proven by induction. It follows that

$$e^{-i\mathcal{J}_{\hat{n}}\chi/\hbar} A = e^{-iJ_{\hat{n}}\chi/\hbar} A e^{iJ_{\hat{n}}\chi/\hbar} . \tag{11.136}$$

This is another simple calculation, based on expanding the exponential of the superoperator, apply Eq. (11.135), and recognize that the two sums can be calculated independently, with each giving an exponential. There is nothing unique about $\mathcal{J}_{\hat{n}}$ in this derivation so that the same result is valid for any commutator superoperator. $e^{-i\mathcal{J}_{\hat{n}}\chi/\hbar}$ is also a superoperator in that it is a transformation of operators, but this transformation is not equivalent to being the commutator of some operator with A.

Since $e^{-iJ_{\hat{n}}\chi/\hbar}$ rotates a quantum state, Eq. (11.13), it follows that Eq. (11.136) describes a rotation of the operator A. According to this association, if $A = J_{\hat{x}}$ and $\hat{n}$ chosen, for example, to equal $\hat{z}$, the transformation of $J_{\hat{x}}$ is the rotation

$$e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar} J_{\hat{x}} = J_{\hat{x}} \cos\chi + J_{\hat{y}} \sin\chi . \tag{11.137}$$

This can be verified by examining the repeated action of the commutator, in particular these just cycle between $J_{\hat{x}}$ and $J_{\hat{y}}$ because

$$\mathcal{J}_{\hat{z}} J_{\hat{x}} = i\hbar J_{\hat{y}}, \qquad \mathcal{J}_{\hat{z}} J_{\hat{y}} = -i\hbar J_{\hat{x}} . \tag{11.138}$$

Thus, on expanding the exponential and separating the even and odd powers of $\mathcal{J}_{\hat{z}}$, Eq. (11.137) is obtained. An alternate method is to notice the derivatives

$$\begin{aligned}\frac{\partial}{\partial\chi}e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{x}} &= e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}\frac{-i\mathcal{J}_{\hat{z}}}{\hbar}J_{\hat{x}} = e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{y}} \\ \frac{\partial^2}{\partial\chi^2}e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{x}} &= e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}\frac{-\mathcal{J}_{\hat{z}}^2}{\hbar^2}J_{\hat{x}} = -e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{x}}. \end{aligned} \tag{11.139}$$

Integration of the second order differential equation implies that

$$e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{x}} = B\cos\chi + C\sin\chi \tag{11.140}$$

with operators B and C evaluated to agree with the initial ($\chi = 0$) values of the (rotated) operator and its derivative. This again gives Eq. (11.137). Products and powers of the angular momentum components can be similarly rotated, each component being rotated independently since

$$e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}AB = \left(e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}A\right)\left(e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}B\right), \tag{11.141}$$

namely the rotation of a product of operators is the product of the rotated operators.

This quantum rotation, when applied to the angular momentum vector $\mathbf{J}$, is found by rotating each component [note that this transformation is a quantum transformation and the basis vectors are constants to this transformation], so that

$$\begin{aligned} e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}\mathbf{J} &= \hat{x}e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{x}} + \hat{y}e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{y}} + \hat{z}e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}J_{\hat{z}} \\ &= \hat{x}(J_{\hat{x}}\cos\chi + J_{\hat{y}}\sin\chi) + \hat{y}(J_{\hat{y}}\cos\chi - J_{\hat{x}}\sin\chi) + \hat{z}J_{\hat{z}} \\ &= [\hat{z}\hat{z} + (\mathsf{U} - \hat{z}\hat{z})\cos\chi + \sin\chi\,\hat{z}\cdot\boldsymbol{\mathcal{E}}\,]\cdot\mathbf{J}. \end{aligned} \tag{11.142}$$

This must be contrasted with the vector rotation of $\mathbf{J}$ as a vector, as described by Eq. (2.90). It is seen that the angles are opposite, namely

$$e^{-i\mathcal{J}_{\hat{z}}\chi/\hbar}\mathbf{J} = \mathsf{R}_{\hat{z}}(-\chi)\cdot\mathbf{J}. \tag{11.143}$$

This is due to the fact that the quantum rotation transforms one angular momentum component into another, whereas the vector rotation merely realignes the component of the vector along a new direction. Compare the discussion here with that of the action of the commutator of $J_{\hat{n}}$ on the position operator $\mathbf{r}_{\rm op}$, Eq. (11.16). There the emphasis was on rotating a quantum state, whereas here the emphasis is on the rotation of an operator. As stated there, this relation is similar to the difference between the Schrödinger and Heisenberg pictures, in that a forward rotation of one is the reverse rotation of the other.

The commutator of two angular momentum superoperators is proportional to another angular momentum superoperator. This is exemplified by

$$[\mathcal{J}_{\hat{x}}, \mathcal{J}_{\hat{y}}]_- = i\mathcal{J}_{\hat{z}}, \tag{11.144}$$

which can be proved by applying both sides to an arbitrary operator. This is exactly the same commutation relations as those for the angular momentum. Clearly the other components of the angular momentum superoperators satify the analogous commutation relations. This shows that the angular momentum superoperators are the generators of the rotation group when acting on operators. As well, the commutation of one superoperator with another superoperator, say $\mathcal{A}$, can be considered as a transformation $\mathfrak{J}_{\hat{z}}$ of the superoperator $\mathcal{A}$ according to

$$\mathfrak{J}_{\hat{z}}\mathcal{A} \equiv [\mathcal{J}_{\hat{z}}, \mathcal{A}]_{-}. \tag{11.145}$$

This defines what might be called a supersuperoperator. Such a procedure can be repeated indefinitely, with each new level giving another representation of the rotation group. It is not known if there are any applications for such a hierarchy of transformations, but it is noted that such a scheme can be defined.

Appendix A

Some Formalities of Linear Algebra

The object of this appendix is to provide the reader with a cursory introduction to some of the basic notions of linear algebra that are used in this book. In writing this appendix I found the books by Greub [34], Boerner [5], Geroch [48] and Choquet-Bruhat, et al [49] particularly useful, but everyone will find their own preferred treatments of this vast subject.

The objects of importance in this book are groups and their representations, vector spaces and tensors. These are discussed in turn but the dependence of the topics is not simply ordered, in particular, representation theory and the theory of Lie groups depend on vector space concepts but vector spaces are defined in terms of groups.

A.1 Group Theory

Fundamentals

The most primitive structure that is of importance in this work is a group, and it also forms the basis of more complicated structures. Its formal definition is:

A **group** $\mathcal{G}$ is a set of elements $\{g_j\}$ with a composition $*$ such that:

1. for every pair of elements $g_j,\ g_k,\ g_j * g_k$ is an element of the group and this composition is associative, namely $(g_j * g_k) * g_\ell = g_j * (g_k * g_\ell)$ for all $g_j,\ g_k,\ g_\ell$.
2. there is an identity element g_0 satisfying $g_0 * g_j = g_j * g_0 = g_j$.
3. for every element g_j there is an inverse g_j^{-1} satisfying $g_j^{-1} * g_j = g_j * g_j^{-1} = g_0$.

The number of elements can be finite or infinite, while the composition $*$ is usually designated as being either addition $+$, with identity $g_0 = 0$, or multiplication, used here without any composition indicator, as for example $g_j g_k$, and identity $g_0 = 1$.

In certain groups, the composition of group elements is commutative, that is $g_j * g_k = g_k * g_j$ for all group elements, in which case the group is classified as being **commutative** or **Abelian**. Otherwise the group is classified as **non-commutative** or **non-Abelian**.

Many different types of sets of elements may constitute a group. Two groups may have the same number of elements (the **order** of the group) and the same composition rules for their elements, constituting what might be called the **composition table**. Clearly in such a case, the two groups can be mapped 1-1 onto each other and are referred to as being **isomorphic**. More commonly the relation is many-to-1, that is, several group elements of the first group $\mathcal{G}$ can be mapped to the same group element of the second group $\mathcal{H}$, in which case the mapping is referred to as a **homomorphism**, provided the composition tables of the two groups are compatible. That is, if $g_1 * g_2 = g_3$ in the group $\mathcal{G}$, the mapped elements $(g_j \rightarrow h_j)$ must satisfy $h_1 * h_2 = h_3$ according to the composition rules of $\mathcal{H}$. A trivial example is when all elements of a multiplicative group are mapped onto the identity 1. Clearly the composition table of the group is preserved under such a mapping, no matter what the composition table is for the multiplicative group.

Essentials of Representation Theory

A particularly useful type of group, is a group of operators on a vector space, namely a set of operators that multiply together in such a way that they form a group. The usefulness of such a set of objects is that the underlying vector space allows the group to be studied numerically, whereas in general, an (abstract) group has only abstractly stated elements and rules of composition. A **representation** of an abstract group $\mathcal{G}$ is a homomorphism to a group of operators $\mathcal{H}$ on a vector space. Commonly this set of operators is written in matrix form without any mention of the underlying vector space. But, while this can always be done as long as the vector space is of finite dimension or equivalently, the order of $\mathcal{H}$ is finite, any matrix representation is associated with a basis for the underlying vector space. In this book, the emphasis is on those representation spaces that are tensor product spaces based on a real 3-dimensional vector space, see Chap. 3, or in Chap. 10, are spinor tensor spaces based on a complex 2-dimensional vector space.

Under the group action, vectors of the representation space are (generally) changed into other vectors and the subspace spanned by a set of vectors is changed into a (generally) different subspace. But it can happen that an object, or more generally a subspace, remains **invariant** (i.e. the same object or subspace) under the action of all elements of the group. In the case of a subspace, individual vectors may change under the action of a group element, but the resultant vector is again a vector in the subspace. As long as the subspace is neither the whole space or the zero element, the vector space can be decomposed into two or more subspaces, each of which is invariant. Such a process reduces the size of the representation. If no reduction of the representation is possible, the representation is **irreducible**. It is an important property of a group, as to what irreducible representations are possible.

Some Notations

All groups discussed in this book are of infinite order. This book also uses a variety of elementary permutation symmetry properties which could be discussed using group theory language, but are not, since their group theoretical properties are not emphasized, nor even commented upon, in this book.

Classically, the infinite groups arose as groups of matrices and the notation for classifying these groups is based on the properties of the corresponding sets of matrices. But of more fundamental importance is the parameterization of the group by a set of continuous variables. The basic consequences of having such a parameterization is discussed in the following subsection. Here the notations for the most common matrix groups are summarized.

The most general $n \times n$ matrix group consist of all those matrices that are non-singular. This can be restricted to real matrices, the general linear group $GL(n,\mathbb{R})$, or to allow complex matrices, $GL(n,\mathbb{C})$ [$\mathbb{R}$ is the field of real numbers while $\mathbb{C}$ is the field of complex numbers. If the determinant of the matrices is restricted to being 1, the groups are given the designation of being "special", thus there are the special linear groups, $SL(n,\mathbb{R})$ and $SL(n,\mathbb{C})$, these are also referred to as being unimodular groups. The next restriction is to the orthogonal groups $O(n)$ of real orthogonal matrices, (real matrices whose transposes are their inverses), and the complex analog, the unitary groups $U(n)$ of unitary matrices (matrices whose adjoints [complex conjugate transposes] are their inverses). Again the restriction of the determinant to be 1 leads to the special orthogonal groups $SO(n)$ and special unitary groups $SU(n)$. There are other types of matrix groups but they are not discussed here.

Lie Groups

Rotation groups are examples of **Lie groups**. Here the order of the group is not only infinite, but continuously and differentiably infinite. Thus, for rotations in a plane, the angle of rotation θ parameterizes the rotation and is a continuous variable. Technically, a Lie group is a **differential manifold** as well as a group with the group action and manifold structure in some sense compatible with each other. Being a manifold essentially means that the group is locally a vector space in which any open set about an arbitrary element g is locally isomorphic to an n-dimensional Euclidean space, for some n. This serves to provide n parameters (at least locally) for the group. Neglecting the technical features, the essence of the manifold structure is that it provides a way of parameterizing the group elements. Being differentiable means that this local isomorphism is smooth enough that it makes sense to differentiate with respect to the n parameters and to give group actions of infinitesimal size. These can be chosen in any direction associated with a direction in the isomorphic n-dimensional Euclidean space, which is referred to as the **tangent space** of the manifold, at the element g. There are thus n linearly independent derivatives and these determine n linearly independent **group generators** G_j of $\mathcal{G}$. It is a property of a Lie group that the group generators can be exponentiated to generate the whole group, for example the set of group elements

$$g_j(\theta) = e^{-i\theta G_j}, \tag{A.1}$$

for an arbitrary real number θ, is a 1-parameter subgroup of $\mathcal{G}$. A general element of $\mathcal{G}$ can be obtained by an appropriate product of one or more such exponentials. In this book, the $-i$ factor is inserted for convenience and has the effect that the generators then act as hermitian operators in any representation of the group. For example, for a matrix Lie group, it should be noted that all of the above description is based on thinking of a group element in terms of both being a matrix and as a point in the manifold parameterizing the matrix. This duality of descriptions allows a more global picture of what the group is about through its manifold structure while the details of the exact actions are obtained from the details of the matrices. Consistent with the matrix group case, a generator is thought of both as a vector in the tangent space of the identity and as a (hermitian) matrix, hence its operator properties.

As well as their vector space properties, the generators can be multiplied together, not only to generate 1-parameter subgroups, but to relate the actions of different generators, assuming of course that the Lie group has more that one generator. Fundamental to this are the properties of the combination

$$g_{jk}(\theta_j,\theta_k) \equiv e^{-i\theta_j G_j} e^{-i\theta_k G_k} e^{i\theta_j G_j} e^{i\theta_k G_k} \tag{A.2}$$

of group elements based on the actions of two generators of the group [note that the group composition is here multiplication and no special character is inserted to indicate that this multiplication is to be carried out]. It is noticed that $g_{jk}(\theta_j, \theta_k)$ is the identity if either θ_j or θ_k vanishes. Thus for small θ_j and θ_k, the variation of $g_{jk}(\theta_j, \theta_k)$ from the identity is proportional to the product of the parameters $\theta_j\theta_k$ and a generator G_{jk} associated with $g_{jk}(\theta_j, \theta_k)$ can be found by examining the behaviour of $g_{jk}(\theta_j, \theta_k)$ for small θ_j and θ_k. It should be remarked that an exponentiation of such a generator does NOT give the set of group elements of Eq. (A.2) since the latter is a two parameter set of group elements and generally not even a subgroup of $\mathcal{G}$, but it does determine the behaviour of $g_{jk}(\theta_j, \theta_k)$ for small values of these parameters. Expanding in powers of the parameters, Eq. (A.2) gives, to all quadratic terms

$$g_{jk}(\theta_j, \theta_k) = 1 - \theta_j\theta_k[G_jG_k - G_kG_j] + \cdots. \tag{A.3}$$

Thus the generator that arises naturally from this combination of group elements is the commutator

$$G_{jk} = -i[G_j, G_k]_- = \sum_\ell c^\ell_{jk} G_\ell. \tag{A.4}$$

Since the generators span the n dimensional tangent space, the generator G_{jk} must be a linear combination of the G_j's with **structure constants** c^ℓ_{jk}, this expansion being given above. With commutation as the rule for multiplication, the vector space of generators becomes the **Lie algebra** of the Lie group. It is the Lie algebra that describes the commutation properties of the Lie group and distinguishes one Lie group from another. An immediate property of commutators is the **Jacobi identity**,

$$[G_i, [G_j, G_k]_-]_- = [[G_i, G_j]_-, G_k]_- + [G_j, [G_i, G_k]_-]_-. \tag{A.5}$$

This is usually written in a form so that all terms are on the same side of the equality sign. The above shows how the action of commutation of G_i with a commutator is equivalent to the successive commutation of G_i with each of the terms in the commutator, very similar to the action of differentiation of a product.

The groups of importance in this book are the 1-parameter group of rotations in a plane discussed in Sec. 2.3 having the unit circle as its manifold and the 3-dimensional rotation group discussed in Sec. 2.5 having the projective sphere P_3 of radius π as its differential manifold. Since a rotation leaves orthogonal vectors orthogonal, the rotation groups are orthogonal groups, the above being the groups $SO(2)$ and $SO(3)$. They are "special" since any rotation can be thought of as a continuous transformation from the identity, so the determinant cannot change from its value for the identity, namely 1. The properties of the generators of $SO(3)$ are discussed in Sec. 5.1. The Lie algebra associated with this group naturally generates the Lie group $SU(2)$, of which $SO(3)$ is a restriction. The group $SU(2)$ is naturally associated with spinors, the space of 2-dimensional complex vectors. This is discussed in Chap. 10.

Since the generators (Lie algebra) determine the group, they also determine the possible irreducible representations of the group. The action of a generator in a particular irreducible representation is as a (hermitian) operator acting on the vector space. Such an operator has eigenvectors and eigenvalues, the latter being called the **weights** of the irreducible representation. Moreover, at least for the rotation groups, an irreducible representation is classified by the **maximum weight** (eigenvalue) of any one of the generators. The possible maximum weights of the 3-dimensional rotation group are either integer or 1/2-integer. Irreducible Cartesian Tensors, see Chap. 3, are irreducible representations having integer maximum weights. As it turns out, there is an odd number of weights in such an irreducible representation, which means that the dimension of the representation is of odd dimension. It is also of note that the space of any Cartesian tensor is of odd dimension and this emphasis on odd dimensionality is presumably connected to the fact that rotations in the building block of Cartesian tensors, namely the 3-dimensional vector space, form an irreducible representation of integer weight. The irreducible representations of the 3-dimensional rotation group having 1/2-integer maximum weights are double-valued, requiring a rotation of 4π to get back to the starting point. Technically it might be argued that such a representation is not a representation of $SO(3)$ at all, but of the **covering group** $SU(2)$, whose generators are the same but whose manifold is a two-sheeted Riemann surface.

An especially important, but obvious, set of 0-dimensional irreducible representations is the set of group invariants, that is, those objects that are unchanged by the action of any group element. Since the group is generated by the generators, it is only necessary to examine the action of the generators on an object to distinguish if it is an invariant. One useful set of objects is the set of generators themselves, or more generally functions of them. An invariant function of the generators is variously referred to as a **Casimir operator, Casimir element or Casimir invariant**. Clearly, as a group element, such a function commutes with all group generators. Thus if, as a group element, a Casimir invariant C is an operator that acts on the vectors of an irreducible representation, then **Schur's Lemma** states that the effect of C is to merely multiply each vector in the irreducible representation by the same constant. [This can be be seen as follows — since C has at least one eigenvector and eigenvalue, then the whole irreducible representation can be generated from this eigenvector by the actions of the various group elements, meanwhile the eigenvalue of C stays unchanged and is a common constant.] Such constants can be used to classify the irreducible representations. For the set of generators common to $SO(3)$ and $SU(2)$, there is only one Casimir invariant, namely $G_{\hat{x}}^2 + G_{\hat{y}}^2 + G_{\hat{z}}^2$. The $p\underline{\text{th}}$ order tensorial form for this is given by Eq. (3.15).

A.2 Vector Spaces

Fundamentals

Mathematical objects are standardly built up of objects with simpler structures and combinations of rules of action. An important step in this direction is first the notion of a field and then of a vector space. Specifically, a field has two types of action and a vector space three.

A **field** is defined as a commutative group under addition "+" and, excluding the additive identity which is standardly designated as "0", is a commutative group under multiplication, sometimes denoted by "·", but usually without any explicit designation, and multiplicative identity "1". As well, these operations satisfy the distributive law $a(b+c) = ab + ac$ for all field elements $a,\ b,\ c$. Of prime importance are the well known fields of real $\mathbb{R}$ and complex numbers $\mathbb{C}$.

A **vector space** V (whose elements are called **vectors**, and generally in this book, are written in boldface), is defined as a commutative group under addition "+" with identity "**0**" together with a field such that multiplication of vectors by field elements satifies the associative and distributive laws together with the specification of the action of the multiplicative identity of the field, namely:

1. $a(b\mathbf{v}) = (ab)\mathbf{v}$ for all $a,\ b$ field elements and any vector $\mathbf{v}$.

2. $(a+b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}$ and $a(\mathbf{v}_j + \mathbf{v}_k) = a\mathbf{v}_j + a\mathbf{v}_k$, for all $a,\ b$ field elements and all vectors $\mathbf{v},\ \mathbf{v}_j,\ \mathbf{v}_k$.

3. $1\mathbf{v} = \mathbf{v}$.

The field elements are standardly referred to as **scalars**. A **subspace** of V is a subset of V which satisfies the conditions of being a vector space in its own right.

Of importance is the notion of linear dependence, namely if there are non-zero field elements a_j and vectors $\mathbf{v}_j$ such that

$$\sum_j a_j \mathbf{v}_j = \mathbf{0}, \tag{A.6}$$

then the set of vectors $\{\mathbf{v}_j\}$ are linearly dependent. That is, it is possible to solve for (at least) one of the vectors in terms of the others. If no such set of a_j exist, then the set of vectors is said to be **linearly independent**. The maximum number of linearly independent vectors in V is the **dimension** $\dim(V)$ of V. This can be finite or infinite. A set of $\dim(V)$ linearly independent vectors $\mathbf{v}_j$ is a **basis** of V and any element $\mathbf{u}$ of V can be expressed as a linear combination

$$\mathbf{u} = \sum_j u_j \mathbf{v}_j \tag{A.7}$$

of the basis elements with **expansion coefficients** u_j. If the dimension is infinite, there is the question of whether the infinite sum converges, but such questions are not discussed here.

Inner Product

Given a basis $\{\mathbf{v}_j\}$, then for any pair of vectors $\mathbf{u}$, $\mathbf{w}$, their expansion coefficients u_j and w_j relative to this basis, the **scalar product** or **inner product**

$$\langle \mathbf{u} | \mathbf{w} \rangle \equiv \sum_j u_j^* w_j \tag{A.8}$$

can be defined [Complex conjugation of the u_j is standardly taken if the field is the complex numbers]. An inner product defines whether two vectors are to be considered as orthogonal

$$\langle \mathbf{u} | \mathbf{w} \rangle = 0 \tag{A.9}$$

and what **norm** (a measure of the magnitude of a vector)

$$\|\mathbf{u}\| \equiv \sqrt{\langle \mathbf{u} | \mathbf{u} \rangle} \geq 0 \tag{A.10}$$

a vector space element has. Other definitions of a norm are also important for certain purposes but only the above definition is used inthis book. It is noted that Eq. (A.8) implies that the basis elements are **orthonormal**,

$$\langle \mathbf{v}_j | \mathbf{v}_k \rangle = \delta_{jk}, \tag{A.11}$$

that is, satisfying both Eqs. (A.9) and (A.10) with unit norm. By the above definition, the inner product is linear in the second vector and antilinear in the first, so that complex conjugation is equivalent to an interchange of the two vectors in the inner product, namely

$$\begin{aligned} &\langle a_j \mathbf{u}_j + a_k \mathbf{u}_k | b_\ell \mathbf{w}_\ell + b_m \mathbf{w}_m \rangle \\ = \;& a_j^* b_\ell \langle \mathbf{u}_j | \mathbf{w}_\ell \rangle + a_j^* b_m \langle \mathbf{u}_j | \mathbf{w}_m \rangle + a_k^* b_\ell \langle \mathbf{u}_k | \mathbf{w}_\ell \rangle + a_k^* b_m \langle \mathbf{u}_k | \mathbf{w}_m \rangle \\ &\langle \mathbf{u} | \mathbf{w} \rangle^* = \langle \mathbf{w} | \mathbf{u} \rangle. \end{aligned} \tag{A.12}$$

In the above discussion, the inner product is defined in terms of whatever basis set is chosen. This can always be done, but it must be recognized that all the properties of the inner product, particularly orthogonality, depends on the chosen basis set. More standardly, an inner product that satisfies the **sesquilinear** condition of Eq. (A.12) together with the positivity condition $\langle \mathbf{u}|\mathbf{u}\rangle > 0$ for all $\mathbf{u} \neq \mathbf{0}$ suggests itself from the context of the problem being addressed. The other properties, including Eq. (A.8), then follow after choosing a basis that is orthonormal with respect to this inner product. As long as the choices of inner product and basis are such that the basis elements are orthonormal, there are a number of simplifying features to working with the expansion coefficients. In particular, the expansion coefficients of $\mathbf{u}$ in terms of the basis $\{\mathbf{v}_j\}$ are given by the inner products $u_j = \langle \mathbf{v}_j|\mathbf{u}\rangle$. An important aspect of having a norm is that $d(\mathbf{u}, \mathbf{w}) \equiv \|\mathbf{u} - \mathbf{w}\|$ is a measure of the distance between the two vectors $\mathbf{u}$ and $\mathbf{w}$. This **metric** clearly distinguishes between whether the two vectors are, or are not, equal.

It should also be noted that the manner of writing an inner product differs between the physical-chemical formalism and the mathematical. The above is the way physics and chemistry write an inner product, especially in quantum mechanics, and is due to Dirac [33], whereas mathematicians standardly use

$$(\mathbf{w}, \mathbf{u}) = \langle \mathbf{u}|\mathbf{w}\rangle. \tag{A.13}$$

Thus the role of the two vectors are interchanged in the two ways of writing the inner product, namely that in mathematical formalism the inner product is antilinear in the second vector rather than the first, in contrast to the way it is written here.

This book deals almost exclusively with finite dimensional vector spaces, which are generally referred to as Euclidean spaces. An infinite dimensional space with inner product and appropriate rules for interpreting limits and infinite sums is known as a Hilbert space. This is the vector space standardly used for expressing the quantum mechanics of particles with position and momentum.

Algebras

An **algebra** A is a vector space with the extra property that elements of A can be multiplied together. This multiplication is usually not indicated by any special symbol. But the multiplication of elements has to be consistent with the vector space multiplication by scalars in the sense that

$$a(xy) = (ax)y = x(ay) \tag{A.14}$$

for all $x, y \in A$ and all scalars a. Two types of algebras are of importance in this book. The first type is a **Lie algebra** in which the multiplication is anticommutative, $xy = -yx$ and satisfies the Jacobi identity $x(yz) + y(zx) + z(xy) = 0$. This is exemplified by the multiplication being commutation and indicated by $[x, y]_-$, see Eqs. (A.4) and (A.5) and the associated discussion for their relation to a Lie group. The second type is an **associative algebra**, in which the multiplication is associative

$$u(vw) = (uv)w. \tag{A.15}$$

It should be noted that a Lie algebra is not associative.

The set of linear transformations of a vector space into itself is an associative algebra, see the subsubsection following the next one. The next subsubsection is devoted to the derivation of an important formula of an associative algebra.

The Exponential of a Commutator

Let A and B be elements of a associative algebra with $\mathcal{A}$ denoting "the commutation of A with", for example, $\mathcal{A}B \equiv [A,B]_- = AB - BA$. Then it follows that the exponential of $\mathcal{A}$ acting on B is given by

$$e^{\mathcal{A}}B = e^{A}Be^{-A}. \tag{A.16}$$

This can be proven as the solution of the differential equation

$$\frac{d}{dt}e^{\mathcal{A}t}B = \mathcal{A}e^{\mathcal{A}t}B, \tag{A.17}$$

with $t = 1$. Namely the second form of Eq. (A.16) also satisfies this differential equation.

A more direct proof is by expansion of the exponentials. To do this, it is necessary to introduce some notation to distinguish whether A is to multiply B on the left, namely AB or on the right BA. Define $A_L B \equiv AB$ for left multiplication and $A_R B \equiv BA$ for right multiplication. Thus the action of commutation is

$$\mathcal{A}B = (A_L - A_R)B = AB - BA. \tag{A.18}$$

It is noted that A_L and A_R commute, for example

$$(A_L)^n(A_R)^m B = (A_R)^m(A_L)^n B = A^n B A^m. \tag{A.19}$$

Then the exponential of the $\mathcal{A}$ acting on B can be expanded and rewritten in the sequence of forms

$$\begin{aligned} e^{\mathcal{A}}B &= \sum_n \frac{\mathcal{A}^n}{n!}B = \sum_n \frac{(A_L - A_R)^n}{n!}B \\ &= \sum_{n,m} \frac{1}{n!}\binom{n}{m}(A_L)^m(-A_R)^{n-m}B \\ &= \sum_{m,p} \frac{A^m}{m!}B\frac{(-A)^p}{p!} = e^{A}Be^{-A}. \end{aligned} \tag{A.20}$$

Here the index $n - m$ has been replaced by p and the double summation re-ordered so that the m and p summations independently go from 0 to infinity. This completes the proof of the identity, Eq. (A.16).

Linear Operators

These are also referred to as **linear transformations** or **linear mappings**, and describe a mapping from one vector space to another, or to the scalars, the latter being called **linear functionals** or **linear forms**. The linearity of a linear operator $\mathbf{T}$ means that, acting on the linear combination of vectors in a vector space, the result is the linear combination of $\mathbf{T}$ acting on the individual vectors, namely

$$\mathbf{T}(a\mathbf{v} + b\mathbf{u}) = a\mathbf{T}\mathbf{v} + b\mathbf{T}\mathbf{u}. \tag{A.21}$$

Depending on the subject specialization, these different terms are, or are not distinguished, at least that is the author's understanding. Linear operators and linear functionals seem more in vogue in the physics and chemistry literature, so these are the terms generally used in this book. It is easily seen that the linear functionals of a vector space V constitutes a vector space, the **dual vector space** V^* whose dimension is the same as that of V. In particular, for a fixed vector $\mathbf{u}$, the inner product $\langle \mathbf{u}|\mathbf{w}\rangle$ defines a linear functional from the vector space V to the scalars. The Reisz representation theorem states that, given any linear functional, there is a $\mathbf{u}$ so that the linear functional can be written as an inner product involving $\mathbf{u}$. Thus, for a vector space in which an inner product is defined, there is a 1-1 correspondence between the elements of the vector space and the linear functionals. In such a case the vector space V can also be identified as the space of linear functionals on V^*, that is, $V = V^{**}$. For finite dimensional spaces and Hilbert spaces, this is always the case, but in general infinite dimensional spaces do not have this reciprocity. In quantum mechanics it is convenient to write the linear functional associated with $\mathbf{u}$ as $\langle \mathbf{u}|$, known as a "bra" state after Dirac's separation of a "bracket" $\langle \mathbf{u}|\mathbf{w}\rangle$ into its "bra" and "ket" parts. The author finds this type of notation extremely useful so it will be found in various parts of this book.

More generally, linear mappings or linear transformations can be defined from one vector space to another, the most important being the linear transformations from V into V, and is more specially referred to as an **endomorphism** while the physics and chemistry literature usually calls such a linear transformation an **operator**, especially in quantum mechanics. If T is such a linear transformation (usually designated in this book as a capital sans serif letter), its action on $\mathbf{u}$ is often written as just the product $\mathbf{w} = \mathsf{T}\mathbf{u}$ to give the vector $\mathbf{w}$. Several special designations for such an action are used in this book. For 3-dimensional vectors, a "dot product" $\mathbf{w} = \mathsf{T}\cdot\mathbf{u}$ is used, while for spinors, a "bullet" $\mathbf{w} = \mathsf{T}\bullet\mathbf{u}$ is used, and the vectors are written as boldface Greek letters. But in the quantum mechanical applications of Chap. 11, no symbol is used to indicate the action of an operator, which is the usual quantum mechanics practice. Given an orthonormal basis $\{\mathbf{v}_j\}$, the vectors can be represented as column vectors of their expansion coefficients and the operator by a matrix with elements $T_{jk} = \langle \mathbf{v}_j|\mathsf{T}\mathbf{v}_k\rangle$. The vector space equation $\mathbf{w} = \mathsf{T}\mathbf{u}$ is then equivalent to the matrix equation $w_j = \sum_k T_{jk}u_k$. It is noted that, if the basis is not orthonormal, then there are some extra factors arising from the non-orthogonality of the different basis elements that must be included and complicate the mathematical detail. Since the vector resulting from the action of an operator can again be operated upon, the set of operators have both addition and multiplication composition rules, as well as multiplication by scalars, so is an algebra, specifically an associative algebra.

A vector $\mathbf{u}$ satisfying $\mathsf{T}\mathbf{u} = \lambda\mathbf{u}$ is called an **eigenvector** of T with **eigenvalue** λ. The standard method of calculating the eigenvalues of T is to use an orthonormal basis to get its matrix representation and then find the eigenvalues as the roots of the **characteristic polynomial** $P(\lambda) \equiv \det(\lambda\delta_{jk} - T_{jk})$, [the determinant of the indicated combination of matrices]. Then the corresponding eigenvectors are obtained by solving $\mathsf{T}\mathbf{u} = \lambda\mathbf{u}$ for each of the eigenvalues. There are some possible complications which are standardly not stressed in carrying out this program. While n roots of the characteristic polynomial always exist if the vector space is n-dimensional and the scalars are the complex numbers, in general their corresponding eigenvectors do not exist. For example, the characteristic polynomial $P(\lambda) = (\lambda - 1)^2$ of the 2×2 matrix

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \tag{A.22}$$

has 1 as a double root, but only the single eigenvector

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{A.23}$$

with eigenvalue 1. This is an example of a matrix in Jordan normal form. Such a complication can only occur when the characteristic polynomial has several equal roots. If a root is different from all the other roots, then there is an egenvector corresponding to that root, specifically there is at least one eigenvector for each root that is different.

A useful approach for understanding what an operator $\mathbf{T}$ does, is to look for subspaces that are invariant under the action of $\mathbf{T}$. Clearly an eigenvector of $\mathbf{T}$ determines a one dimensional subspace that is unchanged (invariant) under the action of $\mathbf{T}$. [Multiplication by a scalar does not count, it is the subspace itself that is invariant, not the individual vectors.] In general, starting with an arbitrary vector $\mathbf{w}$, then either $\mathbf{Tw}$ is proportional to $\mathbf{w}$ and $\mathbf{w}$ is an eigenvector of $\mathbf{T}$, or $\mathbf{w}$ and $\mathbf{Tw}$ are linearly independent. In the later case the process can be repeated to produce $\mathbf{T}^2\mathbf{w} \equiv \mathbf{TTw}$. If this is linearly dependent on $\mathbf{w}$ and $\mathbf{Tw}$, then the 2-dimensional vector subspace determined by the basis $\mathbf{w}$ and $\mathbf{Tw}$ is invariant to $\mathbf{T}$, that is, $\mathbf{T}$ acting on any vector in this subspace is a vector in this subspace. On the other hand, if $\mathbf{w}$, $\mathbf{Tw}$ and $\mathbf{T}^2\mathbf{w}$ are linearly independent, then consider whether the three vectors are the basis for a 3-dimensional invariant subspace by examining whether $\mathbf{T}^3\mathbf{w}$ is in this subspace. This process can be repeated until an invariant subspace is found. For an n-dimensional vector space this procedure must end since there are at most n linearly independent vectors and the whole space is invariant under the action of $\mathbf{T}$. In particular, $\mathbf{T}^n\mathbf{w}$ must be linearly dependent on the set $S \equiv \{\mathbf{T}^m\mathbf{w} | m = 0 \cdots n-1\}$.

A particularly simple case to understand is if $\mathbf{T}$ and $\mathbf{w}$ are such that all the elements of this set S are all linearly independent, in which case this set of vectors forms a basis for the vector space. Then the dependence of $\mathbf{T}^n\mathbf{w}$ on this set determines a polynomial

$$P(\mathbf{T}) = \sum_{m=0}^{n} p_m \mathbf{T}^m \tag{A.24}$$

such that $P(\mathbf{T})\mathbf{w} = \mathbf{0}$. It also follows that $P(\mathbf{T})\mathbf{T}^m\mathbf{w} = \mathbf{0}$ for all m, namely for all elements of the set S, and $P(\mathbf{T})\mathbf{u} = \mathbf{0}$ for every vector $\mathbf{u}$ in V since S is a basis for V. Thus $P(\mathbf{T}) = 0$ is an operator identity. This polynomial, evaluated as a function of λ, namely $P(\lambda) = \sum_{m=0}^{n} p_m \lambda^m$, is the characteristic polynomial for $\mathbf{T}$. This connection, which is known as the **Cayley-Hamilton-theorem**, is clear for $P(\mathbf{T})$ acting on any eigenvector of $\mathbf{T}$. The argument is more elaborate when $\mathbf{T}$ has less than n eigenvectors. Similarly, if not all the elements of S are linearly independent, then it is necessary to repeat the procedure starting with a different vector, say $\mathbf{w}'$, that is linearly independent of the set S. No attempt is made here to treat all the various special cases, but after sufficient effort, the Cayley-Hamiltonian-theorem can again be obtained.

An important aspect of having a characteristic polynomial is that, for every distinct root of the polynomial, there is at least one eigenvector. In the case in which several roots are the same, it may occur that there are not as many eigenvectors as there are equal roots, the matrix of Eq. (A.22) illustrating what might then happen. An argument that any operator $\mathbf{T}$ has at least one eigenvector, whose corresponding eigenvalue is a root of its characteristic polynomial, is presented here. Elaborations along the same lines could be used to prove the more general statement that each distinct root has at least one eigenvector. As a polynomial, $P(\mathbf{T})$ can be factored

$$P(\mathbf{T}) = A \prod_{j=1}^{n} (\mathbf{T} - \lambda_j) \tag{A.25}$$

with possibly some scale factor A. Now for any vector $\mathbf{w}$, $P(\mathbf{T})\mathbf{w} = \mathbf{0}$ so if $\prod_{j=2}^{n}(\mathbf{T} - \lambda_j)\mathbf{w}$ is a nonzero vector, then $\prod_{j=2}^{n}(\mathbf{T} - \lambda_j)\mathbf{w}$ is an eigenvector of $\mathbf{T}$ with eigenvalue λ_1. Otherwise

$\prod_{j=2}^{n}(\mathsf{T} - \lambda_j)\mathbf{w} = \mathbf{0}$. In the latter case, repeat the argument leaving off the factors containing λ_1 and λ_2. If that does not lead to an eigenvector, repeat the operation until a nonzero vector is obtained, which vanishes when acted upon by the next factor, say $(\mathsf{T} - \lambda_k)$. Then $\prod_{j=k+1}^{n}(\mathsf{T} - \lambda_j)\mathbf{w}$ is an eigenvector of T corresponding to λ_k. Since the procedure started with a nonzero vector $\mathbf{w}$, this must occur at some stage. This proves that T has at least one eigenvector for some root λ_k of its characteristic polynomial. As stated earlier, the procedure could be elaborated upon to yield an eigenvector for each distinct root of the characteristic polynomial.

If an inner product has been defined for the vector space, then it follows that for any operator T, there is an **adjoint** operator $\mathsf{T}^\dagger$ defined so that

$$\langle \mathsf{T}^\dagger \mathbf{u} | \mathbf{w} \rangle = \langle \mathbf{u} | \mathsf{T}\mathbf{w} \rangle \tag{A.26}$$

for all $\mathbf{u}$ and $\mathbf{w}$. [With an orthonormal basis, the matrix for $\mathsf{T}^\dagger$ is just the complex conjugate transpose of the matrix corresponding to T.] Particular classes of operators are the **hermitian** operators, defined as those satisfying $\mathsf{T}^\dagger = \mathsf{T}$, and the **unitary** operators, defined as those that satify $\mathsf{T}^\dagger\mathsf{T} = \mathbf{1}$. They are particular cases of **normal** operators, defined as those that satisy the commutation relation $\mathsf{T}^\dagger\mathsf{T} = \mathsf{T}\mathsf{T}^\dagger$. A normal operator has n eigenvectors, whose corresponding eigenvalues are real if the operator is hermitian and complex of unit magnitude if the operator is unitary. In each of these cases, the operator can be written in terms of its n eigenvalues λ_j and corresponding *normalized* eigenvectors $\mathbf{v}_j$ as

$$\mathsf{T} = \sum_j |\mathbf{v}_j\rangle \lambda_j \langle \mathbf{v}_j|, \tag{A.27}$$

with the right-hand side designating the linear functional that selects out that component of the vector on which T acts which lies in the $\mathbf{v}_j$ direction. This expansion is known as the **spectral representation** of the operator T.

The proof that a normal operator has n orthogonal eigenvalues takes two steps. Firstly it is shown that, if $\mathbf{v}$ is an eigenvector of T with eigenvalue λ, then it is also an eigenvector of $\mathsf{T}^\dagger$, but with eigenvalue λ^*. This follows from the set of identities

$$\begin{aligned} \|(\mathsf{T}^\dagger - \lambda^*\mathbf{1})\mathbf{v}\|^2 &= \langle (\mathsf{T}^\dagger - \lambda^*\mathbf{1})\mathbf{v} | (\mathsf{T}^\dagger - \lambda^*\mathbf{1})\mathbf{v}\rangle = \langle \mathbf{v} | (\mathsf{T} - \lambda\mathbf{1})(\mathsf{T}^\dagger - \lambda^*\mathbf{1})\mathbf{v}\rangle \\ &= \langle \mathbf{v} | (\mathsf{T}^\dagger - \lambda^*\mathbf{1})(\mathsf{T} - \lambda\mathbf{1})\mathbf{v}\rangle = \langle (\mathsf{T} - \lambda\mathbf{1})\mathbf{v} | (\mathsf{T} - \lambda\mathbf{1})\mathbf{v}\rangle \\ &= \|(\mathsf{T} - \lambda\mathbf{1})\mathbf{v}\|^2 = 0. \end{aligned} \tag{A.28}$$

The second step involves showing that a normal operator T maps any vector $\mathbf{w}$ orthogonal to an eigenvector $\mathbf{v}$ into a vector again orthogonal to this $\mathbf{v}$. This easily follows from

$$\langle \mathsf{T}\mathbf{w} | \mathbf{v} \rangle = \langle \mathbf{w} | \mathsf{T}^\dagger \mathbf{v} \rangle = \lambda^* \langle \mathbf{w} | \mathbf{v} \rangle = 0. \tag{A.29}$$

Thus, everytime an eigenvector is found, the subspace orthogonal to that eigenvector is such that T is a normal operator restricted to that subspace and thus has an eigenvector in that subspace. This can be repeated until all of V is used up, proving that T has n orthogonal eigenvectors.

The individual elements of the sum in the spectral representation involve the projections

$$\mathsf{P}_j \equiv |\mathbf{v}_j\rangle\langle \mathbf{v}_j| \tag{A.30}$$

onto the corresponding eigenvectors. In general, a **projection operator P** is defined as an **idempotent** [$\mathsf{P}\mathsf{P} = \mathsf{P}$] operator which is also hermitian. It has the important property of dividing up the vector space V into a subspace $\mathsf{P}V$ and its **orthogonal complement** $(\mathbf{1} - \mathsf{P})V$. That is, for $\mathbf{u} \in \mathsf{P}V$ and $\mathbf{w} \in (\mathbf{1} - \mathsf{P})V$, these vectors are orthogonal, namely $\langle \mathbf{u} | \mathbf{w} \rangle = 0$.

A.3 Cartesian Tensors and Polyadics

The word tensor has different connotations for different people. In a lot of the physics and engineering literature, tensors arise when dealing with curvilinear coordinate systems. Then various derivatives and relations between derivatives describe tangents and curvatures of the coordinate system. Such topics are now described as part of the theory of differential manifolds where the objects are referred to as **tensor fields**. This is NOT the object of study in this book. Rather the topic is **Cartesian tensors** and the coordinate system is flat, or as far as used in this book, there is no sense of any dependence of the coordinate system on its place in space and/or time.

The operations involving vectors have so far either produced new vectors or elements of the field used in defining the vector space. What is discussed now is the product of two or more vector spaces to form a new vector space. It is standard to recognize two different ways in which this can be done, namely the **Cartesian product** and the **tensor product**. The presentation of these constructions given here aims at clearly distinguishing between the two different types of product and commenting on three ways that are in use to define the tensor product. Certain names have been adopted by the author to distinguish these three ways of defining tensors, but these are only the authors attempt at clarification and are not of use in the literature. Of the three methods, it is the first that is closest to the way that this book uses tensors and which is elaborated the most in the following.

Cartesian product

The Cartesian product $V \times W$ of the two vector spaces V and W simply treats elements of the two vector spaces as pairs of vectors. In order for the result to be a vector space, the two vector spaces must necessarily be over the same field and the two operation of vector addition and scalar multiplication need to be defined. A common notation is, given $\mathbf{v} \in V$ and $\mathbf{w} \in W$, then $(\mathbf{v}, \mathbf{w}) \in V \times W$. Note that this is NOT the inner product of the two vectors as in Eq. (A.13), though it shares the same notation in many mathematical treatments. The addition of two vectors in the Cartesian product is calculated by summing the separate vector space elements,

$$(\mathbf{v}_1, \mathbf{w}_1) + (\mathbf{v}_2, \mathbf{w}_2) = (\mathbf{v}_1 + \mathbf{v}_2, \mathbf{w}_1 + \mathbf{w}_2), \tag{A.31}$$

so the sum is again an “ordered” pair of vectors, the first vector in V and the second in W. Multiplication by scalars involves multiplying both elements of a pair $(\mathbf{v}, \mathbf{w})$ by the same field element, thus

$$a(\mathbf{v}, \mathbf{w}) = (a\mathbf{v}, a\mathbf{w}). \tag{A.32}$$

The construction of a Cartesian product is actually a very familiar thing and it may only be this author who gets confused by the word “product”. It is more like an “extension” of the vector space V by the vector space W to get more components. Presumably the word “product” comes from the requirement that an element of $V \times W$ assigns a vector in each of V and W, even if one of these is $\mathbf{0}$. The most common example of a Cartesian product is the standard 3-dimensional vector space in which we live, which can be viewed as the Cartesian product of three 1-dimensional vector spaces.

As implied by the last sentence, the construction of Cartesian products can be repeated to get, for example, the vector space $V \times W \times X$ as long as X is another vector space over the same field as V and W, and of course a vector space can be producted any number of times with itself. The dimension of the Cartesian product $\times_j V_j$ of a set of vector spaces $\{V_j\}$ is the sum $\sum_j \dim(V_j)$ of the dimensions of those vector spaces.

Tensors as Polyadics

The tensor product of two vectors was described in Chap. 2 in what could be viewed as a physical picture. More accurately, this is the picture emphasized by Gibbs [14], who referred to this combination, for 3-dimensional vectors, as a **dyad**. That is, if $\mathbf{r}_1$ and $\mathbf{r}_2$ are two 3-dimensional vectors, the dyad $\mathbf{r}_1\mathbf{r}_2$ is a quantity with two directions, or with the use of a coordinate system, a quantity with two indices, see Eq. (2.9) and the associated discussion. The standard mathematical notation for this product is $\mathbf{r}_1 \otimes \mathbf{r}_2$. This approach can be applied to form the tensor product of vectors in different vector spaces. Thus for arbitrary vector spaces V and W, the tensor product of $\mathbf{v} \in V$ and $\mathbf{w} \in W$ is denoted by the quantity $\mathbf{v} \otimes \mathbf{w}$, being simultaneously a vector in V and a vector in W. These quantities are to be considered as (some of the) elements of a vector space $V \otimes W$. For that to be the case, both V and W must be defined over the same field and the two vector space operations of addition and multiplication in $V \otimes W$ must be defined. Firstly, addition implies that linear combinations of tensor products of two vectors need to be included, for example, for $\mathbf{v}_1,\ \mathbf{v}_2 \in V$ and $\mathbf{w}_1,\ \mathbf{w}_2 \in W$, then

$$\mathbf{v}_1 \otimes \mathbf{w}_1 + \mathbf{v}_2 \otimes \mathbf{w}_2 \in V \otimes W. \tag{A.33}$$

For 3-dimensional vector spaces, Gibbs called such a combination a **dyadic**. Secondly, multiplication of a tensor product of two vectors by a field element can assign the scalar to either the first or the second vector in the product, namely

$$a(\mathbf{v} \otimes \mathbf{w}) = (a\mathbf{v}) \otimes \mathbf{w} = \mathbf{v} \otimes (a\mathbf{w}), \tag{A.34}$$

but not simultaneously to both. It is useful to note how these two properties distinguish the tensor product space $V \otimes W$ from the Cartesian product space $V \times W$. Addition in the latter is done in such a way that the sum is again a pair of vectors, one in each of V and W, whereas the tensor product has sums of pairs as elements of its space. Multiplication by a scalar is also different, according to whether both vectors are multiplied by the field element in the Cartesian product, or only one vector is multiplied by the field element in the tensor product.

But there is a further requirement in defining the tensor product (or dyadic for the 3-dimensional case), namely if in the addition of two or more tensor products, there is a linear dependence among either the V or W vectors arising in the sum of tensor products, then this set of tensor products are not to be taken as linearly independent. Specifically, equalities of the type

$$a\mathbf{v}_1 \otimes \mathbf{w}_1 + b\mathbf{v}_2 \otimes \mathbf{w}_1 = (a\mathbf{v}_1 + b\mathbf{v}_2) \otimes \mathbf{w}_1 \tag{A.35}$$

and

$$\mathbf{v}_1 \otimes (a\mathbf{w}_1) + \mathbf{v}_1 \otimes (b\mathbf{w}_2) = \mathbf{v}_1 \otimes (a\mathbf{w}_1 + b\mathbf{w}_2) \tag{A.36}$$

are to be imposed. This cuts the dimensionality of $V \otimes W$ to the simple product of the dimensions of V and W, whereas without such a constraint, the dimensionality is infinite, and the **free vector space** consisting of the linear combination of all possible tensor products $\mathbf{v} \otimes \mathbf{w}$ is formed. Possibly a simpler way of understanding this constraint, is to consider a basis $\{\mathbf{v}_j\}$ of V and a basis $\{\mathbf{w}_k\}$ for W, and consider the tensor product space $V \otimes W$ as the vector space with basis $\{\mathbf{v}_j \otimes \mathbf{w}_k\}$. Thus, if $\dim(V) = n$ and $\dim(W) = m$, then as stated above, the tensor product has dimension $\dim(V \otimes W) = nm$. In contrast, the Cartesian product has dimension $\dim(V \times W) = n + m$.

Drew [15] extended Gibb's dyads and dyadics to the definition of **polyads** and **polyadics**. Thus, given a set $\{\mathbf{r}_j\}$ of 3-dimensional vectors, $\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3$ is a triad, $\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4$ a tetrad and $\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4\mathbf{r}_5$ a pentad while a sum of triads is in general a triadic, a sum of tetrads a tetradic, etc. Clearly this can be generalized to any **order** to give n-ads and n-adics. The generalizations of the constraints (A.35) and (A.36) are to be applied to the definition of the space of n-adics, or equivalently this is a vector space having the 3^n basis elements $\hat{r}_1 \cdots \hat{r}_n$, where each $\hat{r}_j$ is one of the three basis elements of the space of 3-dimensional vectors. Drew considers polyadic analysis to be "tensor analysis restricted to Cartesian tensors". In this way, the title of this book might better be called "Irreducible Polyadics", but the word polyadics appears very little in the literature whereas tensor analysis is well used.

The application of these notions to a set of vector spaces $\{V_j\}$, some or all of which may be the same, is obvious. This gives rise to an algebra of tensors in which multiplication is the tensor product. This algebra is associative and distributive, but in general only commutative if all the V_j are the same.

Tensors as Multilinear Functionals

A **bilinear functional F**, also called a **bilinear form**, is a mapping from the Cartesian product $V \times W$ of two vector spaces to the scalars that is linear in each of the vector spaces V and W. That is, given $(\mathbf{v}, \mathbf{w}) \in V \times W$ and scalar a, the bilinear form satisfies

$$\mathsf{F}(a\mathbf{v}, \mathbf{w}) = a\mathsf{F}(\mathbf{v}, \mathbf{w}) = \mathsf{F}(\mathbf{v}, a\mathbf{w}) \tag{A.37}$$

and the addition rules

$$\mathsf{F}(a_1\mathbf{v}_1 + a_2\mathbf{v}_2, \mathbf{w}) = a_1\mathsf{F}(\mathbf{v}_1, \mathbf{w}) + a_2\mathsf{F}(\mathbf{v}_2, \mathbf{w}) \tag{A.38}$$

and

$$\mathsf{F}(\mathbf{v}, a_1\mathbf{w}_1 + a_2\mathbf{w}_2) = a_1\mathsf{F}(\mathbf{v}, \mathbf{w}_1) + a_2\mathsf{F}(\mathbf{v}, \mathbf{w}_2). \tag{A.39}$$

This can immediately be generalized to an arbitrary number of vector spaces to give **multilinear functionals**, equivalently called **multilinear forms** whose **order** is the number of vector spaces that are involved.

Specializing this to the vector space V and its dual V^*, a multilinear functional T on p replicas of V^* and q replicas of V is defined as a tensor of order $p+q$, or in more detail of **type** (p, q). Provided the order of the vectors in the Cartesian product $(\mathbf{w}_1, \cdots, \mathbf{w}_p, \mathbf{v}_1, \cdots, \mathbf{v}_q)$ is such that all the vectors $\{\mathbf{w}_j\}$ of V^* appear before the vectors $\{\mathbf{v}_k\}$ of V, then the space of such tensors is defined as the tensor product space

$$\overbrace{V \otimes V \otimes \cdots V}^{p} \otimes \overbrace{V^* \otimes V^* \otimes \cdots V^*}^{q}$$

of p replicas of V and q replicas of V^*. Note that V is equivalent to the linear functionals on V^* and V^* equivalent to the linear functionals on V, so the roles of p and q in the tensor product space and in the Cartesian product appear to be interchanged. If V, and thus V^* is of dimension n, then this tensor space is a vector space of dimension n^{p+q}. Clearly other orders for the Cartesian product may occur and the tensor product space is then similarly ordered. The name of product anticipates a multiplicative property both of the tensors and of the space of tensors. Thus given a tensor T_1 of type (p_1, q_1) and a tensor $\mathbf{T}_2$ of type (p_2, q_2), then the tensor product $\mathbf{T} = \mathbf{T}_1 \otimes \mathbf{T}_2$ is defined as the element of a tensor space of type $(p_1 + p_2, q_1 + q_2)$ such that

$$\begin{aligned} &\mathbf{T}(\mathbf{w}_1, \cdots, \mathbf{w}_{p_1}, \mathbf{v}_1, \cdots, \mathbf{v}_{q_1}, \mathbf{w}_{p_1+1}, \cdots, \mathbf{w}_{p_1+p_2}, \mathbf{v}_{q_1+1}, \cdots, \mathbf{v}_{q_1+q_2}) \\ &= \mathbf{T}_1(\mathbf{w}_1, \cdots, \mathbf{w}_{p_1}, \mathbf{v}_1, \cdots, \mathbf{v}_{q_1}) \mathbf{T}_2(\mathbf{w}_{p_1+1}, \cdots, \mathbf{w}_{p_1+p_2}, \mathbf{v}_{q_1+1}, \cdots, \mathbf{v}_{q_1+q_2}), \end{aligned} \tag{A.40}$$

where the $\{\mathbf{w}_j\}$ are elements of V^* and $\{\mathbf{v}_k\}$ are elements of V. Together with the obvious addition of two tensors of the same type, this multiplication defines a tensor algebra which is not commutative.

For the Cartesian tensors that are the subject of interest in this book, $V^* = V$ and the inner product of the two vectors is the dot product $\cdot$. Thus all tensors can be classified as of type $(p, 0)$, or by their order p. This is different for the case of spinors where contravariant and covariant vectors are distinguished. The essential difference is that now the vector space is defined over the complex field and the inner product is not linear in the bra state. Thus a distinction needs to be made but it is shown in Chap. 10 how an association, Eq. (10.46) between the contravariant and covariant basis elements can be obtained. But even in that chapter only tensors of order p were considered as the generalization of Cartesian tensors, so the antilinear nature of the transformation from contravariant to covariant temsors did not need to appear.

The Tensor Product and the Composition of Maps

The third way of defining tensors, actually the tensor product space, involves specifying various maps from one vector space to another and their compositions and relations one to another. This method of definition is foreign to this author so the definition is presented with little comment.

A tensor product of V and W is defined as a vector space $V \otimes W$ together with a bilinear mapping μ from $V \times W$ to $V \otimes W$ (linear in each vector space in the Cartesian product), with the condition that, given any other vector space X and any bilinear mapping ν from $V \times W$ to X, there is a unique mapping ϕ from $V \otimes W$ to X such that $\nu = \phi\mu$ (the product indicating successive mappings). This condition can be proven to provide the same effect as the pair of constraints listed in what has been referred to here as the polyadic approach.

The order of contraction of 3-dimensional tensors

The order of carrying out one or more contractions between tensors of order greater than 1 can be carried out in a variety of ways. In this book, the system has been to contract nearest directions first and to work outwards till all indicated contractions have been carried out. Comments are made here about the alternate system used by Gibbs [14] and Drew [15]. This is done using polyads to illustrate their approach since the question of which vectors are contracted together can be clearly indicated.

The double-dot contraction of the dyad **ab** with the dyad **cd** is the scalar

$$\mathbf{ab}{:}\mathbf{cd} = (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) \tag{A.41}$$

in Gibbs' and Drew's system [Gibb's Chap. V, Eq. (56); Drew, Sec. 2.8-1], whereas it is

$$\mathbf{ab}{:}\mathbf{cd} = (\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c}) \tag{A.42}$$

in the system used here. However, if only a single dot is involved, namely only a partial contraction of this pair of dyads, then Gibbs and Drew [Gibbs Chap. V, Eq. (23); Drew, Eq. (2.6-7)] use

$$\mathbf{ab}\cdot\mathbf{cd} = \mathbf{ad}(\mathbf{b}\cdot\mathbf{c}), \tag{A.43}$$

namely a contraction of the nearest neighboring vectors, the same as used in this book. This author finds their system confusing.

Polydot contractions are elaborated upon by Drew, in his Sec. 2.8-1. Consider his Eq. (2.8-4) as illustrative of his system, which is the 3-fold contraction of a pentad with a tetrad

$$\begin{aligned} \mathbf{abcde} \odot^3 \mathbf{hjks} &= \mathbf{ab}(\mathbf{cde} \odot^3 \mathbf{hjk})\mathbf{s} \\ &= \mathbf{abs}(\mathbf{c}\cdot\mathbf{h})(\mathbf{d}\cdot\mathbf{j})(\mathbf{e}\cdot\mathbf{k}). \end{aligned} \tag{A.44}$$

Here the 3-fold contraction has been written with $\odot^3$ rather than using three vertical dots, which is what Drew writes there, and the second line does does appear in Drew's equation, but is implied by his Eq. (2.8-1). What is important to note, is that it is now not the first three vectors of the pentad that is contracted, but the last three, yet in the subsequent contraction, the order of contraction is to be in the order in which the vectors appear in the triads. Again this seems confusing to this author. Carrying out the contractions, starting from the nearest directions in the convention adopted in this book, of the above, gives

$$\begin{aligned} \mathbf{abcde} \odot^3 \mathbf{hjks} &= \mathbf{ab}(\mathbf{cde} \odot^3 \mathbf{hjk})\mathbf{s} \\ &= \mathbf{abs}(\mathbf{c}\cdot\mathbf{k})(\mathbf{d}\cdot\mathbf{j})(\mathbf{e}\cdot\mathbf{h}), \end{aligned} \tag{A.45}$$

and seems to be an approach that can be consistently applied to all situations.

Appendix B

Calculation of $D^{(\ell)}_{mn}(0,\beta,0)$

The calculation given here is based entirely on Irreducible Cartesian Tensor methods. The matrix elements are defined by Eq. (9.18) in terms of the spherical tensor basis elements, which are in turn given explicitly in terms of vector quantities by Eq. (5.49). A rotation of a tensor involves the rotation of each of its directions, so according to the expansion of $\mathbf{e}^{(\ell)n}$ the rotation of this tensor is

$$R^{(\ell)}_{\hat{y}}(\beta)\mathbf{e}^{(\ell)n} = N_{\ell n}\sum_t a_t^{\ell|n|}\left\{[\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{e}^{(1)\nu}]^{|n|}[\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{e}^{(1)0}]^{\ell-|n|-2t}[\mathbf{U}]^t\right\}^{(\ell)}, \tag{B.1}$$

where $\nu \equiv n/|n|$ is used as an abbreviation for ± 1, corresponding to whether n is ≥ 0 or < 0. $\mu \equiv m/|m|$ plays the analogous role for m, to be used presently. It is noticed that this tensor is traceless as well as symmetric, so when calculating the scalar product of $\mathbf{e}^{(\ell)}_m$ with this rotated tensor using the analog of the expansion (5.49), only the component of $\mathbf{e}^{(\ell)}_m$ with no $\mathbf{U}$'s is needed, thus

$$\begin{aligned} D^{(\ell)}_{mn}(0,\beta,0) &= \mathbf{e}^{(\ell)}_m \odot^\ell \mathbf{R}^{(\ell)}_{\hat{y}}(\beta)\odot^\ell \mathbf{e}^{(\ell)n} = N_{\ell m}N_{\ell n}\sum_t a_t^{\ell|n|} \\ &\times \left\{[\mathbf{e}^{(1)}_\mu]^{|m|}[\mathbf{e}^{(1)}_0]^{\ell-|m|}\right\}^{(\ell)}\odot^\ell[\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{e}^{(1)\nu}]^{|n|}[\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{e}^{(1)0}]^{\ell-|n|-2t}[\mathbf{U}]^t. \end{aligned} \tag{B.2}$$

The symmetrization is needed on only one of the expansions of the basis elements. It follows that either $\mathbf{e}^{(1)}_\mu$ or $\mathbf{e}^{(1)}_0$ is dotted into each direction of the rotated tensor and the symmetrization is accounted for by considering all possible ways of carrying out these contractions. Since each direction of the rotated tensor can be dotted into two possible vectors, it is a set of combinatorial factors that determines the number of possible ways in which the contraction can be carried. The number of ways in which p $\mathbf{e}^{(1)}_\mu$'s can be dotted into $|n|$ $\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{e}^{(1)\nu}$'s, q $\mathbf{e}^{(1)}_\mu$'s dotted into $\ell-|n|-2t$ $\mathbf{R}_{\hat{y}}(\beta)\cdot\mathbf{e}^{(1)0}$'s and r $\mathbf{e}^{(1)}_\mu$'s dotted into the $2t$ directions of the $\mathbf{U}$'s is

$$N^{\ell|n|t}_{|m|;pqr} = \binom{|n|}{p}\binom{\ell-|n|-2t}{q}\binom{2t}{r}\delta_{p+q+r,|m|}. \tag{B.3}$$

According to the function

$$f(u) \equiv \sum_{|m|pqr} u^{|m|}N^{\ell|n|t}_{|m|;pqr} = (1+u)^\ell \tag{B.4}$$

the sum of $N^{\ell|n|t}_{|m|;pqr}$ over p, q and r is the coefficient of $u^{|m|}$ in the power series expansion of $f(u)$,

$$\sum_{pqr} N^{\ell|n|t}_{|m|;pqr} = \binom{\ell}{|m|}. \tag{B.5}$$

It is moreover noticed that $\mathbf{e}^{(1)}_\mu \cdot \mathbf{e}^{(1)}_\mu = 0$, so that only the $r = 0$ terms contribute to the calculation of the rotational matrix elements, thus

$$\begin{aligned} D^{(\ell)}_{mn}(0,\beta,0) &= \frac{N_{\ell m} N_{\ell n}}{\binom{\ell}{|m|}} \sum_{tp} a^{\ell|n|}_t N^{\ell|n|t}_{|m|;p,|m|-p,0} \left[D^{(1)}_{\mu\nu}(0,\beta,0)\right]^p \\ \times \left[D^{(1)}_{0\nu}(0,\beta,0)\right]^{|n|-p} &\left[D^{(1)}_{\mu 0}(0,\beta,0)\right]^{|m|-p} \left[D^{(1)}_{00}(0,\beta,0)\right]^{\ell-|m|-|n|-2t+p}. \end{aligned} \tag{B.6}$$

For the special case in which $m, n > 0$, a substitution of the values for the $D^{(1)}(0,\beta,0)$ matrix elements from Eq. (9.23) with subsequent simplification gives

$$\begin{aligned} D^{(\ell)}_{mn}(0,\beta,0) &= \frac{(-1)^m m! n!}{2^\ell} \left[\frac{(\ell-m)!(\ell-n)!}{(\ell+m)!(\ell+n)!}\right]^{1/2} (\sin\beta)^{m+n} \\ &\times \sum_{tp} \frac{(-1)^{t+p}(2\ell-2t)!(\cos\beta)^{\ell+p-m-n-2t}}{t!p!(\ell-t)!(m-p)!(n-p)!(\ell+p-m-n-2t)!(1-\cos\beta)^p}. \end{aligned} \tag{B.7}$$

To get closer to the standard formula arrived at by using spinors [1–3], the half angle formulas of the trigonometric functions are used, specifically $\cos\beta = \cos^2\frac{\beta}{2} - \sin^2\frac{\beta}{2}$. Then expand the power of the cos, and as well, introduce the expansion of $1 = (\cos^2\frac{\beta}{2} + \sin^2\frac{\beta}{2})^{2t}$. This gives an equation that is homogeneous of degree 2ℓ in the trigonometric functions of $\beta/2$, which can be written in the form

$$\begin{aligned} D^{(\ell)}_{mn}(0,\beta,0) &= (-1)^{\ell-n} m! n! 2^{m+n-\ell} \left[\frac{(\ell-m)!(\ell-n)!}{(\ell+m)!(\ell+n)!}\right]^{1/2} \\ &\times \sum_\sigma (\cos\frac{\beta}{2})^{m+n+2\sigma} (\sin\frac{\beta}{2})^{2\ell-m-n-2\sigma} \sum_{tp} \frac{(-1)^t (2t)!(2\ell-2t)!}{2^p t! p! (\ell-t)!(m-p)!(n-p)!} \\ &\times \sum_a \frac{(-1)^a}{(2t+a-\sigma)!(\ell+p-m-n-2t-a)!a!(\sigma-a)!}. \end{aligned} \tag{B.8}$$

This has a structure similar to the standard formula, Eq. (9.19). It is not clear how the triple sum over p, t and a can be accomplished to yield the standard formula, but computationally, it is easy to show that the expressions are numerically equal.

Symbol Index

As a general rule, scalar quantities are written in lightface, vectors in boldface, tensors in sans serif and spinors as Greek boldface. Spherical tensors with what might be referred to as the spinor phase are written in Euler style. In general irreducible representations of the rotation group are denoted by their **weight** ℓ while the **order** (number of directions) of a tensor is denoted by p. These are not always rigorously followed, in particular in the first four chapters where the basic formalism is being developed. As a further consequence, this also leads to some redundancy in the listing of symbols.

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