# Chapter 8

# Irreducible Representations of SO(2) and SO(3)

*The shortest path between two truths in the real domain passes through the complex domain.*
    —Jacques Hadamard[1]

Some of the most useful aspects of group theory for applications to physical problems stem from the orthogonality relations of characters of irreducible representations. The widespread impact of these relations stems from their role in constructing and resolving new representations from direct products of irreducible representations. Direct products are especially important in applications involving continuous groups, with the construction of higher dimensional irreducible representations, the derivation of angular momentum coupling rules, and the characterization of families of elementary particles all relying on the formation and decomposition of direct products.

Although the notion of an irreducible representation can be carried over directly from our development of discrete groups through Schur's first lemma, a transcription of Schur's second lemma and the Great Orthogonality Theorem to the language of continuous groups requires a separate discussion. This is because proving the latter two theorems

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[1]Quoted in *The Mathematical Intelligencer* **13**(1), 1991.

necessitates performing summations over group elements and invoking the Rearrangement Theorem (Theorem 2.1). This theorem guarantees the following equality

$$\sum_g f(g) = \sum_g f(g'g) \,, \tag{8.1}$$

where the summation is over elements $g$ in a group $G$, $g'$ is any other element in $G$, and $f$ is some function of the group elements. The crucial point is that the same quantities appear on both sides of the equation; the only difference is the order of their appearance. To proceed with the proofs of these theorems for continuous groups requires an equality analogous to (8.1):

$$\int f(R) \, \mathrm{d}R = \int f(R'R) \, \mathrm{d}R \,, \tag{8.2}$$

where $R$ and $R'$ are the elements of a continuous group and $f$ is some function of these elements. To appreciate the issues involved, we write the integral on the left-hand side of (8.2) as an integral over the parameters

$$\int f(R) \, \mathrm{d}R = \int f(R)g(R) \, \mathrm{d}a \,, \tag{8.3}$$

where $g(R)$ is the density of group elements in parameter space in the neighborhood of $R$. The equality in (8.2) will hold provided that the density of group elements is arranged so that the density of the points $R'R$ is the same as that of the points $R$. Our task is to find the form of $g(R)$ which ensures this. A related concept that will arise is the notion of the "order" of the continuous group as the volume of its elements in the space defined by the parameters of the group.

This chapter is devoted to the characters and irreducible representations of SO(2) and SO(3). For SO(2), we will show that the density of group elements is uniform across parameter space, so the density function reduces to a constant. But, for SO(3), we will need to carry out the determination of the density function in (8.3) explicitly. This will illustrate the general procedure which is applicable to any group. For both SO(2) and SO(3), we will derive the basis functions for their irreducible representations which will be used to obtain the corresponding characters and to demonstrate their orthogonality

# 8.1 Orthogonality of Characters for SO(2)

The structure of SO(2) is simple enough that many of the results obtained for discrete groups can be taken over directly with little or no modification. The basis of this claim is that the Rearrangement Theorem for this group is, apart from the replacement of the sum by an integral, a direct transcription of that for discrete groups which, together with this group being Abelian, renders the calculation of characters a straightforward exercise.

## 8.1.1 The Rearrangement Theorem

We first show that the rearrangement theorem for this group is

$$\int_0^{2\pi} R(\varphi')R(\varphi)\,\mathrm{d}\varphi = \int_0^{2\pi} R(\varphi)\,\mathrm{d}\varphi\,.$$

This implies that the weight function appearing in (8.3) is unity, i.e., the density of group elements is uniform in the space of the parameter $\varphi$. Using the fact that $R(\varphi')R(\varphi) = R(\varphi' + \varphi)$, we have

$$\int_0^{2\pi} R(\varphi')R(\varphi)\,\mathrm{d}\varphi = \int_0^{2\pi} R(\varphi' + \varphi)\,\mathrm{d}\varphi\,.$$

We now introduce a new integration variable $\theta = \varphi' + \varphi$. Since $\varphi'$ is fixed, we have that $\mathrm{d}\varphi = \mathrm{d}\theta$. Then, making the appropriate changes in the upper and lower limits of integration, and using the fact that $R(\varphi + 2\pi) = R(\varphi)$, yields

$$\int_0^{2\pi} R(\varphi' + \varphi)\,\mathrm{d}\varphi = \int_{\varphi'}^{\varphi'+2\pi} R(\theta)\,\mathrm{d}\theta$$

$$= \int_{\varphi'}^{2\pi} R(\theta)\,\mathrm{d}\theta + \int_{2\pi}^{\varphi'+2\pi} R(\theta)\,\mathrm{d}\theta$$

$$= \int_{\varphi'}^{2\pi} R(\theta)\,\mathrm{d}\theta + \int_0^{\varphi'} R(\theta)\,\mathrm{d}\theta$$

$$= \int_0^{2\pi} R(\theta)\,\mathrm{d}\theta\,,$$

which verifies our assertion.

## 8.1.2 Characters of Irreducible Representations

We can now use Schur's first lemma for SO(2). Since SO(2) is an Abelian group, this first lemma requires all of the irreducible representations to be one-dimensional (cf. Problem 4, Problem Set 5). Thus, every element is in a class by itself and the characters must satisfy the same multiplication rules as the elements of the group:

$$\chi(\varphi)\chi(\varphi') = \chi(\varphi + \varphi') \,. \tag{8.4}$$

The character corresponding to the unit element, $\chi(0)$, which must map onto the identity for ordinary multiplication, is clearly unity for all irreducible representations:

$$\chi(0) = 1 \,. \tag{8.5}$$

Finally, we require the irreducible representations to be single-valued, i.e., an increase in the rotation angle by $2\pi$ does not change the effect of the rotation. Thus,

$$\chi(\varphi + 2\pi) = \chi(\varphi) \,. \tag{8.6}$$

The three conditions in (8.4), (8.5), and (8.6) are sufficient to determine the characters of all of the irreducible representations of SO(2).

We will proceed by writing Eq. (8.4) as a differential equation and using (8.5) as an "initial condition" and (8.6) as a "boundary condition." In (8.4), we set $\varphi' = \mathrm{d}\varphi$,

$$\chi(\varphi)\chi(\mathrm{d}\varphi) = \chi(\varphi + \mathrm{d}\varphi) \,,$$

and expand both sides of this equation to first order in $\mathrm{d}\varphi$:

$$\chi(\varphi)\left[\chi(0) + \frac{\mathrm{d}\chi}{\mathrm{d}\varphi}\bigg|_{\varphi=0}\mathrm{d}\varphi\right] = \chi(\varphi) + \frac{\mathrm{d}\chi}{\mathrm{d}\varphi}\mathrm{d}\varphi \,.$$

Then, using (8.5) and cancelling common terms, this equation reduces to a first-order ordinary differential equation for $\chi(\varphi)$:

$$\frac{\mathrm{d}\chi}{\mathrm{d}\varphi} = \chi_0'\chi(\varphi) \,,$$

where $\chi_0' = \chi'(0)$ is to be determined. The general solution to this equation is

$$\chi(\varphi) = A\,e^{\chi_0'\varphi}\,,$$

where $A$ is a constant of integration which is also to be determined. In fact, by setting $\varphi = 0$ and invoking (8.5), we see that $A = 1$. The requirement (8.6) of single-valuedness, when applied to this solution, yields the condition that

$$e^{\chi_0'(\varphi+2\pi)} = e^{\chi_0'\varphi}\,,$$

or,

$$e^{2\pi\chi_0'} = 1\,.$$

The most general solution of this equation is $\chi_0' = im$, where $i^2 = -1$ and $m$ is any integer. This produces an infinite sequence of characters of the irreducible representations of SO(2):

$$\chi^{(m)}(\varphi) = e^{im\varphi}, \qquad m = \ldots, -2, -1, 0, 1, 2, \ldots \tag{8.7}$$

The identical representation corresponds to $m = 0$. In contrast to the case of finite groups, we see that SO(2) has an infinite set of irreducible representations, albeit one that is countably infinite.

## 8.1.3  Orthogonality Relations

Having determined the characters for SO(2), we can now examine the validity of the orthogonality theorems for characters which were discussed for discrete groups in Theorem 5.1. We proceed heuristically and begin by observing that the exponential functions in (8.7) are orthogonal over the interval $0 \le \varphi < 2\pi$:

$$\int_0^{2\pi} e^{i(m'-m)\varphi}\,\mathrm{d}\varphi = 2\pi\delta_{m,m'}\,.$$

By writing this relation as

$$\int_0^{2\pi} \chi^{(m)*}(\varphi)\chi^{(m')}(\varphi)\,\mathrm{d}\varphi = 2\pi\delta_{m,m'}\,, \tag{8.8}$$

we obtain an orthogonality relation of the form in Eq. (5.4), once we identify the "order" of SO(2) as the quantity

$$\int_0^{2\pi} \mathrm{d}\varphi = 2\pi \,.$$

This is the "volume" of the group in the space of the parameter $\varphi$, which lies in the range $0 \leq \varphi < 2\pi$, given that the density function is unity, according to the discussion in thew preceding section. Note that the integration over $\varphi$ is effectively a sum over classes.

**Example 8.1.** Consider the representation of SO(2) derived in Section 7.2:

$$R(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \,. \tag{8.9}$$

Since SO(2) is an Abelian group, this representation must be reducible. We can decompose this representation into its irreducible components by using either the analogue of the Decomposition Theorem (Section 5.3) for continuous groups or, more directly, by using identities between complex exponential and trigonometric functions:

$$\chi(\varphi) \equiv \mathrm{tr}[R(\varphi)]$$

$$= 2\cos\varphi$$

$$= \mathrm{e}^{i\varphi} + \mathrm{e}^{-i\varphi} \,.$$

A comparison with (8.7) yields

$$\chi(\varphi) = \chi^{(1)}(\varphi) + \chi^{(-1)}(\varphi) \,,$$

so the representation in (8.9) is a direct sum of the irreducible representations corresponding to $m = 1$ and $m = -1$.[2] ∎

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[2]This example illustrates the importance of the field used in the entries of the matrices for SO(2). If we are restricted to *real* entries, then the representation in (8.9) is *irreducible*. But, if the entries are *complex*, then this example shows that this representation is *reducible*.

## 8.2 Basis Functions for Irreducible Representations

We were able to determine the characters for all of the irreducible representations of SO(2) without any knowledge of the representations themselves. But this is not the typical case for continuous groups. We will see, for example, when determining the characters for SO(3) that we will be required to construct explicit representations of rotations corresponding to different classes. The action of these rotations on the basis functions will determine the representation of that class and the character will be calculated directly from this representation. As an introduction to that discussion, in this section we will determine the basis functions of the irreducible representations of SO(2).

We begin by calculating the eigenvalues of the matrix in (8.9) from $\det(R - \lambda I) = 0$:

$$\begin{vmatrix} \cos\varphi - \lambda & -\sin\varphi \\ \sin\varphi & \cos\varphi - \lambda \end{vmatrix} = (\cos\varphi - \lambda)^2 + \sin^2\varphi$$

$$= \lambda^2 - 2\lambda\cos\varphi + 1 = 0 \,.$$

Solving for $\lambda$ yields

$$\lambda = \cos\varphi \pm i\sin\varphi = \mathrm{e}^{\pm i\varphi} \,. \tag{8.10}$$

The corresponding eigenvectors are proportional to $x \pm iy$. Thus, operating on these eigenvectors with $R(\varphi)$ (see below) generates the irreducible representations corresponding to $m = 1$ and $m = -1$ in (8.7), i.e., the characters $\chi^{(1)}(\varphi)$ and $\chi^{(-1)}(\varphi)$.

Obtaining the basis functions for the other irreducible representations of SO(2) is now a matter of taking appropriate direct products, since

$$\chi^{(m)}(\varphi)\chi^{(m')}(\varphi) = \chi^{(m+m')}(\varphi) \,.$$

In particular, the $m$-fold products $(x \pm iy)^m$ generate irreducible representations for the $m$-fold direct product, as discussed in Sec. 6.5. This

can be verified directly from the transformation (8.9) applied to $x$ and $y$:

$$x' = x \cos \varphi - y \sin \varphi \,,$$

$$y' = x \sin \varphi + y \cos \varphi \,.$$

Then,

$$
\begin{aligned}
(x' \pm iy')^m &= \left[ x \cos \varphi - y \sin \varphi \pm i(x \sin \varphi + y \cos \varphi) \right]^m \\
&= \left[ x(\cos \varphi \pm i \sin \varphi) \pm iy(\cos \varphi \pm i \sin \varphi) \right]^m \\
&= \left[ (x \pm iy) \, \mathrm{e}^{\pm i\varphi} \right]^m \\
&= (x \pm iy)^m \, \mathrm{e}^{\pm im\varphi} \,.
\end{aligned}
$$

Therefore, we can now complete the character table for SO(2), including the basis functions which generate the irreducible representations:

| SO(2) | $E$ | $R(\varphi)$ |
|:---:|:---:|:---:|
| $\Gamma^{\pm m}\colon\ (x \pm iy)^m$ | $1$ | $\mathrm{e}^{\pm im\varphi}$ |

We note for future reference that the basis functions $(x \pm iy)^m$ could have been derived in a completely different manner. Consider Laplace's equation in two dimensions:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \,.$$

This equation is invariant under all the elements of SO(2), as can be easily verified. The general solution to this equation is

$$u(x, y) = F(x + iy) + G(x - iy) \,,$$

where $F$ and $G$ are arbitrary functions. Thus, if we are interested in solutions which are homogeneous polynomials of degree $m$, we can

choose in turn solutions with $F(s) = s^m$ and $G(s) = 0$ and then with $F(s) = 0$ and $G(s) = s^m$. We thereby obtain the expressions

$$u(x, y) = (x \pm iy)^m \tag{8.11}$$

as solutions of Laplace's equations which are also the basis functions of the irreducible representations of SO(2). These functions are the analogues in two dimensions of spherical harmonics, which are the solutions of Laplace's equations in three dimensions. These will be discussed later in this chapter.

# 8.3 Axis–Angle Representation of Proper Rotations in Three Dimensions

The three most common parametrizations of proper rotations were discussed in Section 7.4. For the purposes of obtaining the orthogonality relations for the characters of SO(3), the representation in terms of a fixed axis about which a rotation is carried out—the axis–angle representation—is the most convenient. We begin this section by showing how this representation emerges naturally from the basic properties of orthogonal matrices.

## 8.3.1 Eigenvalues of Orthogonal Matrices

Let $A$ be any proper rotation matrix in three dimensions. Denoting the eigenvalues of $A$ by $\lambda_1$, $\lambda_2$, and $\lambda_3$, and the corresponding eigenvalues by $\boldsymbol{u}_1$, $\boldsymbol{u}_2$, and $\boldsymbol{u}_3$, we then have

$$A\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$$

for $i = 1, 2, 3$. We can also form the adjoint of each equation:

$$\boldsymbol{u}_i^\dagger A^{\mathrm{t}} = \lambda^* \boldsymbol{u}_i^\dagger \,.$$

These eigenvalue equations imply

$$\boldsymbol{u}_i^\dagger \boldsymbol{u}_i = \boldsymbol{u}_i^\dagger A^{\mathrm{t}} A \boldsymbol{u}_i = |\lambda_i^2| \boldsymbol{u}_i^\dagger \boldsymbol{u}_i \,,$$

which shows that $|\lambda_i^2| = 1$, i.e., that the modulus of every eigenvalue of an orthogonal matrix is unity [cf. (8.10)]. The most general form of such a quantity is a complex number of the form $e^{i\varphi}$ for some angle $\varphi$. But these eigenvalues are also the roots of the characteristic equation $\det(A - \lambda I) = 0$ so, according to the Fundamental Theorem of Algebra,[3] if they are complex, they must occur in complex conjugate pairs (because the coefficients of this polynomial, which are obtained from the entries of $A$, are real). Hence, the most general form of the eigenvalues of an orthogonal matrix in three dimensions is

$$\lambda_1 = 1, \qquad \lambda_2 = e^{i\varphi}, \qquad \lambda_3 = e^{-i\varphi}. \tag{8.12}$$

The eigenvector corresponding to $\lambda_1 = 1$, which is unaffected by the action of $A$, thereby defines the axis about which the rotation is taken. The quantity $\varphi$ appearing in $\lambda_2$ and $\lambda_3$ defines the angle of rotation about this axis.

## 8.3.2   The Axis and Angle of an Orthogonal Matrix

In this section, we show how the axis and angle of an orthogonal matrix can be determined from its matrix elements. We take the axis of the rotation to be a unit vector $\boldsymbol{n}$, which is the eigenvector corresponding to the eigenvalue of unity:

$$A\boldsymbol{n} = \boldsymbol{n}. \tag{8.13}$$

This equation and the orthogonality of $A$ $(AA^{\mathrm{t}} = A^{\mathrm{t}}A = 1)$ enables us to write

$$A^{\mathrm{t}}\boldsymbol{n} = A^{\mathrm{t}}A\boldsymbol{n} = \boldsymbol{n}. \tag{8.14}$$

Subtracting (8.14) from (8.13) yields

$$(A - A^{\mathrm{t}})\boldsymbol{n} = 0.$$

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[3]K. Hoffman and R. Kunze, *Linear Algebra* 2nd edn (Prentice–Hall, Englewood Cliffs, NJ, 1971), p. 138.

In terms of the matrix elements $a_{ij}$ of $A$ and the components $n_i$ of $\boldsymbol{n}$, we then have

$$(a_{12} - a_{21})n_2 + (a_{13} - a_{31})n_3 = 0\,,$$

$$(a_{21} - a_{12})n_1 + (a_{23} - a_{32})n_3 = 0\,,$$

$$(a_{31} - a_{13})n_1 + (a_{32} - a_{23})n_2 = 0\,.$$

Notice that these equations involve only the *off-diagonal* elements of $A$. The solution of these equations yield the relations

$$\frac{n_2}{n_1} = \frac{a_{31} - a_{13}}{a_{23} - a_{32}}, \qquad \frac{n_3}{n_1} = \frac{a_{12} - a_{21}}{a_{23} - a_{32}}, \qquad (8.15)$$

which, when combined with the normalization condition

$$\boldsymbol{n}{\cdot}\boldsymbol{n} = n_1^2 + n_2^2 + n_3^2 = 1$$

determines $\boldsymbol{n}$ uniquely.

The angle of the rotation can be determined from the invariance of the trace of $A$ under similarity transformations. Noting that the trace is the sum of the eigenvalues, and using (8.12), we have

$$a_{11} + a_{22} + a_{33} = 1 + e^{i\varphi} + e^{-i\varphi} = 1 + 2\cos\varphi\,, \qquad (8.16)$$

so $\varphi$ is determined only by the *diagonal* elements of $A$.

### 8.3.3   Normal Form of an Orthogonal Matrix

We conclude this section by deriving the form of a rotation matrix in an orthogonal coordinate system which naturally manifests the axis and angle. The diagonal form of a rotation matrix is clearly given by

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\varphi} & 0 \\ 0 & 0 & e^{i\varphi} \end{pmatrix}.$$

The eigenvector $\boldsymbol{n}$ corresponding to $\lambda_1 = 1$ is the axis of the rotation and can always be chosen to be real. However, the eigenvectors of $\lambda_2 =$

$e^{i\varphi}$ and $\lambda_3 = e^{-i\varphi}$ are inherently complex quantities. An orthonormal set can be chosen as

$$\boldsymbol{n}_2 = \tfrac{1}{2}\sqrt{2}(0, 1, i), \qquad \boldsymbol{n}_2 = \tfrac{1}{2}\sqrt{2}(0, 1, -i),$$

respectively. Since we are interested in transformations of real coordinates, we must perform a unitary transformation from this complex basis to a real orthogonal basis, in which case our rotation matrix $\Lambda$ will no longer be diagonal. The required unitary matrix which accomplishes this is

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \tfrac{1}{2}\sqrt{2} & \tfrac{1}{2}i\sqrt{2} \\ 0 & \tfrac{1}{2}\sqrt{2} & -\tfrac{1}{2}i\sqrt{2} \end{pmatrix}.$$

Thus,

$$R = U^{-1}\Lambda U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix}. \qquad (8.17)$$

When expressed in this basis, the rotation matrix clearly displays the axis of rotation through the entry $R_{11} = 1$, and the angle of rotation through a 2×2 rotational submatrix in a plane perpendicular to this axis.

## 8.3.4 Parameter Space for SO(3)

The axis-angle representation of three-dimensional rotations provides a convenient parametrization of all elements of SO(3). We have seen that every element of SO(3) can be represented by a unit vector corresponding to the rotation axis and a scalar corresponding to the rotation angle. Thus, consider the space defined by the three quantities

$$(n_1\varphi, n_2\varphi, n_3\varphi), \qquad (8.18)$$

where $n_1^2 + n_2^2 + n_3^2 = 1$. Every direction is represented by a point on the unit sphere. Thus, defining an azimuthal angle $\phi$ and a polar angle
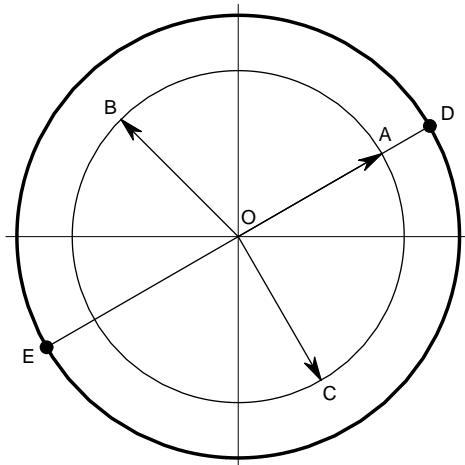
Figure 8.1: Two-dimensional representation of the parameter space of SO(3) as the interior of a sphere of radius $\pi$. The point $A$ represents a rotation whose axis is along the direction $OA$ and whose angle is the length of $OA$. The points at $A$, $B$ and $C$ correspond to rotations with the same angle but about axis along different directions. This defines the classes of SO(3). The diametrically opposite points at $D$ and $E$ correspond to the same operation.

$\theta$ according to the usual conventions in spherical polar coordinates, the parameter space of SO(3) can be represented as

$$(\varphi \cos \phi \sin \theta, \varphi \sin \phi \sin \theta, \varphi \cos \theta) , \tag{8.19}$$

where

$$0 \le \varphi \le \pi, \qquad 0 \le \phi \le 2\pi, \qquad 0 \le \theta \le \pi .$$

We can now see directly that this parameter space corresponds to the interior of a sphere of radius $\pi$ (Fig. 8.1). For every point *within* the sphere, there is a unique assignment to an element of SO(3): the *direction* from the radius to the point corresponds to the direction of the rotation axis and the *distance* from the point to the origin represents the rotation angle. Two diametrically opposed points on the surface of the sphere ($\varphi = \pi$) correspond to the same rotation, since a rotation by $\pi$ about $\boldsymbol{n}$ is the same as a rotation by $-\pi$ about this axis which, in turn, is the same as a rotation by $\pi$ about $-\boldsymbol{n}$ (whatever the sense of rotation).

Another useful feature of the axis-angle parametrization is the representation of classes of SO(3). Consider two elements of SO(3) which have the same angle of rotation $\varphi$ but about different axes $\boldsymbol{n}$ and $\boldsymbol{n}'$. We denote these operations by $R(\boldsymbol{n}, \varphi)$ and $R(\boldsymbol{n}', \varphi)$. Let $U(\boldsymbol{n}, \boldsymbol{n}')$ denote the rotation of $\boldsymbol{n}$ into $\boldsymbol{n}'$. The inverse of this operation then rotates $\boldsymbol{n}'$ into $\boldsymbol{n}$. The relationship between $R(\boldsymbol{n}, \varphi)$, $R(\boldsymbol{n}', \varphi)$, and $U(\boldsymbol{n}, \boldsymbol{n}')$ is, therefore,

$$R(\boldsymbol{n}, \varphi) = \left[ U(\boldsymbol{n}, \boldsymbol{n}') \right]^{-1} R(\boldsymbol{n}', \varphi) U(\boldsymbol{n}, \boldsymbol{n}') \,,$$

i.e., $R(\boldsymbol{n}, \varphi)$ and $R(\boldsymbol{n}', \varphi)$ are related by a similarity transformation and, therefore, belong to the *same equivalence class.* Referring to Fig. 8.1, equivalence classes of SO(3) correspond to operations which lie on the same radius. Thus, *a summation over the classes of SO(3) is equivalent to a sum over spherical shells.*

# 8.4   Orthogonality Relations for SO(3)

The axis-angle representation of rotations provides, in addition to a conceptual simplicity of elements of SO(3) in parameter space, a natural framework within which to discuss the integration over the elements of SO(3) and thereby to obtain the Rearrangement Theorem for this group. In this section, we derive the density function $g$ in (8.3) for this group and then use this to identify the appropriate form of the orthogonality relations for characters

## 8.4.1   The Density Function

As discussed in the introduction, one of the basic quantities of interest for continuous groups is the density of group elements as a function of position in parameter space. To determine this function for SO(3), we first consider the elements in the neighborhood of the identity and then examine the behavior of these points under an arbitrary element of SO(3). Referring to the discussion in Section 7.4.2, these elements correspond to rotations by infinitesimal angles $\varphi_1$, $\varphi_2$, and $\varphi_3$ about each of the three coordinate axes. The rotation matrix associated with

this transformation is

$$\delta R = \begin{pmatrix} 1 & -\varphi_3 & \varphi_2 \\ \varphi_3 & 1 & -\varphi_1 \\ -\varphi_2 & \varphi_1 & 1 \end{pmatrix}.$$

The identity of SO(3) corresponds to the origin in the three-dimensional parameter space, $\varphi_1 = \varphi_2 = \varphi_3 = 0$, and is indicated by the point O in Fig. 8.1. For infinitesimal rotation angles, the parameter space spanned by $\delta R$ is associated with an infinitesimal volume element in the neighborhood of the origin.

We now follow the infinitesimal transformation $\delta R$ by a *finite* transformation $R(\boldsymbol{n}, \varphi)$, i.e., we form the product $R\,\delta R$. This generates a volume element in the neighborhood of $R$ and the product $R\,\delta R$ can be viewed as transformation of the volume near the origin to that near $R$. The Jacobian of this transformation is the relative change of volume near the origin to that near $R$ or, equivalently, is the relative change of the *density* of operations near the origin to that near $R$. According to the discussion in the introduction, this is the information required from the density function for SO(3).

We have already seen that equivalence classes of SO(3) are comprised of all rotations with the same rotation angle, regardless of the direction of the rotation axis. Thus, the density function is expected to depend only on $\varphi$. Referring to Fig. 8.1, this means that the density of elements depends only on the "radial" distance from the origin, not on the direction, so we can choose $R$ in accordance with this at our convenience. Therefore, in constructing the matrix $R\,\delta R$, we will use for $R$ a matrix of the form in (8.17). Thus,

$$R\,\delta R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} 1 & -\varphi_3 & \varphi_2 \\ \varphi_3 & 1 & -\varphi_1 \\ -\varphi_2 & \varphi_1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & -\varphi_3 & \varphi_2 \\ \varphi_3\cos\varphi + \varphi_2\sin\varphi & \cos\varphi - \varphi_1\sin\varphi & -\varphi_1\cos\varphi - \sin\varphi \\ \varphi_3\sin\varphi - \varphi_2\cos\varphi & \sin\varphi - \varphi_1\cos\varphi & -\varphi_1\sin\varphi + \cos\varphi \end{pmatrix}.$$

We can now use (8.15) and (8.16) to determine the axis $\boldsymbol{n}'$ and angle $\varphi'$ of this product. The angle is determined from

$$1 + 2\cos\varphi' = 1 + 2\cos\varphi - 2\varphi_1 \sin\varphi\,,$$

which, upon cancelling common factors, becomes

$$\cos\varphi' = \cos\varphi - \varphi_1 \sin\varphi\,.$$

Using the standard trigonometric formula for the cosine of a sum, we find, to first order in $\varphi_1$, that

$$\varphi' = \varphi + \varphi_1\,.$$

The *unnormalized* components of $\boldsymbol{n}'$ are determined from (8.15) to be

$$n_1' = -2\varphi_1 \cos\varphi - 2\sin\varphi\,,$$

$$n_2' = \varphi_3 \sin\varphi - \varphi_2(1 + \cos\varphi)\,,$$

$$n_3' = -\varphi_2 \sin\varphi - \varphi_3(1 + \cos\varphi)\,.$$

To normalize the axis, we first determine the length based on these components. To first order in the $\varphi_i$, we find

$$|\boldsymbol{n}'| = 2\varphi_1 \cos\varphi + 2\sin\varphi\,.$$

Thus, the components of the normalized rotation axis of $R\,\delta R$ are

$$n_1' = 1\,,$$

$$n_2' = -\tfrac{1}{2}\varphi_3 + \tfrac{1}{2}\varphi_2 \frac{1 + \cos\varphi}{\sin\varphi}\,,$$

$$n_3' = \tfrac{1}{2}\varphi_2 + \tfrac{1}{2}\varphi_3 \frac{1 + \cos\varphi}{\sin\varphi}\,.$$

Expressed in terms of the parametrization in (8.18), $R\,\delta R$ is given by

$$(n_1'\varphi', n_2'\varphi', n_3'\varphi') =$$

$$\left\{ \varphi + \varphi_1, \tfrac{1}{2}\varphi\left( -\varphi_3 + \varphi_2 \frac{1 + \cos\varphi}{\sin\varphi} \right), \tfrac{1}{2}\varphi\left( \varphi_2 + \varphi_3 \frac{1 + \cos\varphi}{\sin\varphi} \right) \right\}\,.$$

This defines the transformation from the neighborhood of the origin to the neighborhood near $R\,\delta R$. The Jacobian $J$ of this transformation, obtained from

$$J = \det\left|\frac{\partial(n_i'\varphi')}{\partial\varphi_j}\right|,\tag{8.20}$$

determines how the density of elements of SO(3) near the origin is transformed to the density of points near $R$. By taking the derivatives in (8.20) to obtain the entries $(i,j)$ in the Jacobian matrix, we obtain

$$J = \begin{vmatrix} 1 & 0 & 0 \\ 0 & \varphi\dfrac{1+\cos\varphi}{2\sin\varphi} & -\tfrac{1}{2}\varphi \\ 0 & \tfrac{1}{2}\varphi & \varphi\dfrac{1+\cos\varphi}{2\sin\varphi} \end{vmatrix} = \frac{\varphi^2}{2(1-\cos\varphi)}\,.$$

Notice that

$$\lim_{\varphi\to 0} J = 1\,,$$

so that the normalization of the volume in parameter space is such that the volume near the unit element is unity. Hence, the *density* of elements in parameter space is the *reciprocal* of $J$, so the density function $g$ in (8.3) is

$$g(\varphi) = \frac{2}{\varphi^2}(1-\cos\varphi)\,.\tag{8.21}$$

## 8.4.2 Integrals in Parameter Space

The density function in (8.21) now permits us to carry out integral over the group. Thus, for a function $F(\varphi,\Omega)$, where $\Omega$ denotes the angular variables in the parametrization in (8.19), we have

$$\iint g(\varphi)F(\varphi,\Omega)\varphi^2\,\mathrm{d}\varphi\,\mathrm{d}\Omega\,,$$

where we have used the usual volume element for spherical polar coordinates. Using the density function in (8.21), this integral becomes

$$\iint 2(1-\cos\varphi)F(\varphi,\Omega)\mathrm{d}\varphi\,\mathrm{d}\Omega\,.$$

We can now establish the orthogonality relation for characters. If we denote the characters for two irreducible representations of SO(3) by $\chi^\mu(\varphi)$ and $\chi^\nu(\varphi)$, then we have

$$\iint 2(1 - \cos\varphi)\chi^\mu(\varphi)\chi^\nu(\varphi)\mathrm{d}\varphi\,\mathrm{d}\Omega = \delta_{\mu,\nu}\iint 2(1 - \cos\varphi)\mathrm{d}\varphi\,\mathrm{d}\Omega\,.$$

The integral on the right-hand side of this equation, which has the value $8\pi^2$, corresponds to the volume of SO(3) in parameter space. The integral over the angular variables on the left-hand side yields $2 \times 4\pi$, so cancelling common factors, we obtain

$$\int_0^\pi (1 - \cos\varphi)\chi^\mu(\varphi)\chi^\nu(\varphi)\,\mathrm{d}\varphi = \pi\delta_{\mu,\nu}\,. \tag{8.22}$$

This is the orthogonality relation for characters of SO(3).

## 8.5 Irreducible Representations and Characters for SO(3)

For SO(2), we were able to determine the characters of the irreducible representations directly, i.e., without having to determine the basis functions of these representations. The structure of SO(3), however, does not allow for such a simple procedure, so we must determine the basis functions from the outset.

### 8.5.1 Spherical Harmonics

We proceed as in Section 8.2 by determining the homogeneous polynomial solutions of Laplace's equation, now in three dimensions:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0\,.$$

We seek solutions of the form

$$u(x, y, z) = \sum_{a,b} c_{ab}(x + iy)^a (x - iy)^b z^{\ell - a - b}\,,$$

which are homogeneous polynomials of degree $\ell$. In spherical polar coordinates,

$$x = r\cos\phi\sin\theta, \qquad y = r\sin\phi\sin\theta, \qquad z = r\cos\theta\,,$$

where $0 \le \phi < 2\pi$ and $0 \le \theta \le \pi$, these polynomial solutions transform to

$$u(r,\theta,\phi) = \sum_{a,b} c_{ab} r^\ell \sin^{a+b}\theta \cos^{\ell-a-b}\theta\, \mathrm{e}^{i(a-b)\phi}\,. \qquad (8.23)$$

Alternatively, Laplace's equation in spherical polar coordinates is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2} = 0\,.$$

When the method of separation of variables is used to find solutions of this equation of the form $u(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$, the stipulation that the solution be single-valued with respect changes in $\phi$ by $2\pi$,

$$u(r,\theta,\phi+2\pi) = u(r,\theta,\phi)\,,$$

requires that

$$\Phi(\phi) \propto \mathrm{e}^{im\phi}\,,$$

where $m$ is an integer. Comparing this expression with the corresponding factor in (8.23), we see that $a - b = m$. Since the ranges of both $a$ and $b$ are between 0 and $\ell$, we see that there are $2\ell + 1$ values of $m$ consistent with homogeneous polynomial solutions of degree $\ell$. The corresponding values of $m$ are $-\ell \le m \le \ell$. The $2\ell + 1$ independent homogeneous polynomials of degree $\ell$ are called the **spherical harmonics** and denoted by $Y_{\ell m}(\theta,\phi)$. Their functional form is

$$Y_{\ell m}(\theta,\phi) \propto P_m^\ell(\theta)\,\mathrm{e}^{im\phi}\,, \qquad (8.24)$$

where $P_m^\ell(\theta)$ is a **Legendre function**. In the following discussion, we will utilize only the exponential factor in the spherical harmonics.

## 8.5.2 Characters of Irreducible Representations

The $Y_{\ell m}(\theta, \phi)$ form a $(2\ell + 1)$-dimensional representation of SO(3). Thus, for a general rotation $R$, we have

$$R Y_{\ell m}(\theta, \phi) = \sum_{m'=-\ell}^{\ell} Y_{\ell m'}(\theta, \phi) . \Gamma^{\ell}_{m'm}(R)$$

To determine the character of this representation, it is convenient to again invoke the fact that the classes of SO(3) are determined only by the rotation angle, not by the direction of the rotation axis. Thus, we can choose a rotation axis at our convenience and we therefore focus on rotations through an angle $\varphi$ about the $z$-axis. In this case, the form of (8.24) allows us to write

$$R_z(\varphi) Y_{\ell m}(\theta, \phi) = Y_{\ell m}(\theta, \phi - \varphi) = \mathrm{e}^{-im\varphi} Y_{\ell m}(\theta, \phi) .$$

Thus, the corresponding transformation matrix is given by

$$\Gamma^{\ell}[R_z(\varphi)] = \begin{pmatrix} \mathrm{e}^{-i\ell\varphi} & 0 & \cdots & 0 \\ 0 & \mathrm{e}^{-i(\ell-1)\varphi} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathrm{e}^{i\ell\varphi} \end{pmatrix} . \tag{8.25}$$

The character $\chi^{(\ell)}(\varphi)$ of this class is obtained by taking the trace of this matrix:

$$\chi^{(\ell)}(\varphi) = \mathrm{e}^{-i\ell\varphi} + \mathrm{e}^{-i(\ell-1)\varphi} + \cdots + \mathrm{e}^{i\ell\varphi}$$

$$= \mathrm{e}^{-i\ell\varphi}\left( 1 + \mathrm{e}^{i\varphi} + \mathrm{e}^{2i\varphi} + \cdots + \mathrm{e}^{2\ell i\varphi} \right)$$

$$= \mathrm{e}^{-i\ell\varphi} \frac{1 - \mathrm{e}^{-(2\ell+1)i\varphi}}{1 - \mathrm{e}^{i\varphi}}$$

$$= \frac{\mathrm{e}^{(\ell+1/2)i\varphi} - \mathrm{e}^{-(\ell+1/2)i\varphi}}{\mathrm{e}^{i\varphi/2} - \mathrm{e}^{-i\varphi/2}}$$

$$= \frac{\sin\left[(\ell + \tfrac{1}{2})\varphi\right]}{\sin\left(\tfrac{1}{2}\varphi\right)} .$$

The orthogonality integral for these characters takes the form

$$\int_0^\pi (1 - \cos\varphi) \frac{\sin\left[(\ell + \frac{1}{2})\varphi\right] \sin\left[(\ell' + \frac{1}{2})\varphi\right]}{\sin^2\left(\frac{1}{2}\varphi\right)} \, \mathrm{d}\varphi \, .$$

Using the trigonometric identity

$$2\sin^2\left(\tfrac{1}{2}\varphi\right) = 1 - \cos\varphi$$

enables us to write the orthogonality integral as

$$\int_0^\pi \sin\left[(\ell + \tfrac{1}{2})\varphi\right] \sin\left[(\ell' + \tfrac{1}{2})\varphi\right] \mathrm{d}\varphi = \tfrac{1}{2}\pi\delta_{\ell,\ell'} \, ,$$

where the right-hand side of this equation follows either from (8.22) or from the orthogonality of the sine functions over $(0, \pi)$.

It is possible to show directly, using Schur's first lemma, that the spherical harmonics form a basis for $(2\ell + 1)$-dimensional *irreducible* representations of SO(3). However, this requires invoking properties of the Legendre functions in (8.24). If we confine ourselves to the matrices in (8.25) then we can show that a matrix that commutes with all such rotation matrices must reduce to a diagonal matrix. If we then consider rotations about any other direction, which requires some knowledge of the Legendre functions, we can then show that this constant matrix must, in fact, be a constant multiple of the unit matrix. Hence, according to Schur's first lemma, these representations are irreducible. We can now construct the character table for SO(3) with the basis functions which generate the irreducible representations:

| SO(3) | $E$ | $R(\varphi)$ |
|---|---|---|
| $\Gamma^\ell$: $Y_{\ell m}(\theta, \phi)$ | 1 | $\dfrac{\sin\left[(\ell + \frac{1}{2})\varphi\right]}{\sin\left(\frac{1}{2}\varphi\right)}$ |

## 8.6   Summary

In this chapter, we have shown how the orthogonality relations developed for finite groups must be adapted for continuous groups, using

SO(2) and SO(3) as examples. For SO(2), which is a one-parameter Abelian group, this proved to be a straightforward matter. However, the corresponding calculations for SO(3) required us to determine explicitly the density function to produce the appropriate form of the orthogonality relations. We found that the there are an infinite sequence of irreducible representations of dimensionality $2\ell + 1$, where $\ell \geq 0$. Because of the connection between SO(3) and angular momentum, the structure of these irreducible representations has several physical consequences:

- For systems that possess spherical symmetry, the energy eigenstates have degeneracies of $2\ell + 1$. The fact that there is a greater degeneracy for the hydrogen atom is due to a "hidden" SO(4) symmetry.[4]

- The formation and decomposition of direct products of the irreducible representations of SO(3) forms the basis of angular momentum coupling rules (Problem 6, Problem Sets 10) and the classification of atomic spectra.[5]

- When atoms are placed within crystals, the original spherical symmetry is lowered to the symmetry of the crystal. This causes levels which were degenerate in the spherically-symmetric environment to split. Such "crystal-field" effects are important for many aspects for electrons in crystalline solids.[6]

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[4]H.F. Jones, *Groups, Representations and Physics* (Institute of Physics, Bristol, 1998), pp. 124–127.

[5]E.P. Wigner, *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (Academic, New York, 1959), pp. 177–194.

[6]M. Tinkham, *Group Theory and Quantum Mechanics* (McGraw–Hill, New York, 1964), pp. 65–80.