Physics 544 Problems

1. Prove that the commutation relations among the components of $\vec{J}$, as well as the action of these operators on $|JM\rangle$, remain valid in a representation defined by the following replacements:

$$J_+ \longrightarrow -\nu\frac{\partial}{\partial\mu}, \quad J_- \longrightarrow -\mu\frac{\partial}{\partial\nu}, \quad J_z \longrightarrow -\frac{1}{2}\left(\mu\frac{\partial}{\partial\mu} - \nu\frac{\partial}{\partial\nu}\right)$$

$$|JM\rangle \longrightarrow (-1)^{J-M}\left[(J-M)!(J+M)!\right]^{-1/2}\mu^{J-M}\nu^{J+M}$$

Make the substitutions $\mu = \rho\sin\varphi$, $\nu = \rho\cos\varphi$, and find J_y in terms of ρ and φ. Prove

$$\exp\left(\frac{1}{2}\beta\frac{\partial}{\partial\varphi}\right)\left(\sin^a\varphi\cos^b\varphi\right) = \sin^a\left(\varphi + \tfrac{1}{2}\beta\right)\cos^b\left(\varphi + \tfrac{1}{2}\beta\right),$$

Expand the quantities on the right-hand side of this equation and thereby derive

$$d^J_{MN}(\beta) = \sum_t \frac{(-1)^t\left[(J+M)!(J-M)!(J+N)!(J-N)!\right]^{1/2}}{(J+M-t)!(J-N-t)!\,t!\,(t+N-M)!}$$

$$\times\left(\cos\frac{\beta}{2}\right)^{2J+M-N-2t}\left(\sin\frac{\beta}{2}\right)^{2t+N-M}$$

3. Using Rodrigues' Formula

$$P_l^m(\mu) = \frac{(1-\mu^2)^{m/2}}{2^l\, l!} \frac{d^{l+m}}{d\mu^{l+m}} (\mu^2 - 1)^l$$

together with $\dfrac{d^{l+m}}{d\mu^{l+m}} (\mu^2-1)^l = \dfrac{d^{l+m}}{d\mu^{l+m}} \left\{ (\mu-1)^l (\mu+1)^l \right\}$

prove that

$$P_l^m(\mu) = \frac{1}{2^l} \sum_t (-1)^{t-m} \frac{l!\,(l+m)!}{(l-t)!\,(t-m)!\,t!\,(l+m-t)!}$$

$$\times (1+\mu)^{l-t+m/2} (1-\mu)^{t-m/2}$$

and therefore

$$C_m^l(\beta,\alpha) = \mathcal{D}_{m0}^l(\alpha,\beta,\gamma)^* = (-1)^m \mathcal{D}_{0m}^l(-\gamma,\beta,-\alpha).$$

Give a physical interpretation of this result in terms of symmetric top eigenfunctions.

Judd "Angular Momentum Theory For Diatomic Molecules"

1.3 ROTATIONS

One of the most remarkable features of angular momentum vectors is their usefulness in constructing rotation operators. Consider, for example,

$$\exp(-i\alpha l_z)\ (x \pm iy)\ \exp(i\alpha l_z).$$

To evaluate this quantity [4], we take as our starting point

$$l_z(x \pm iy) = (x \pm iy)(l_z \pm 1).$$

Thus

$$l_z^2(x \pm iy) = l_z(x \pm iy)(l_z \pm 1) = (x \pm iy)(l_z \pm 1)^2,$$

and, in general,

$$l_z^n(x \pm iy) = (x \pm iy)(l_z \pm 1)^n.$$

On expanding the exponential, we at once see that

$$\exp(-i\alpha l_z)\ (x \pm iy) = (x \pm iy)\ \exp(-i\alpha(l_z \pm 1)),$$

and so

$$\exp(-i\alpha l_z)\ (x \pm iy)\ \exp(i\alpha l_z) = (x \pm iy)\ \exp(\mp i\alpha). \qquad (1.7)$$

Since l_z commutes with z, we can immediately write down

$$\exp(-i\alpha l_z)\ z\ \exp(i\alpha l_z) = z. \qquad (1.8)$$

In many cases, the algebra of the transformation may be sufficient for our purposes. However, if we wish to put a geometrical interpretation on the equations, two options are open to us. We can imagine either that the operator $\exp(-i\alpha l_z)$ rotates the vector **r** through an angle $-\alpha$ about the z axis, or else that it rotates the coordinate frame by an angle $+\alpha$ about the axis. To make sure that all spins and momenta are similarly transformed, we have merely to use $\exp(-i\alpha J_z)$, where **J** is the total angular momentum of the system.

Suppose that two rectangular coordinate frames F and F' share the same origin but are arbitrarily oriented, one with respect to the other. To bring F into coincidence with F', a single rotation will, of course, suffice; but if the allowed axes of rotation are specified in advance, then three successive rotations are, in general, necessary. If we rotate F first by γ about its z axis, then by β about the y axis of F (i.e., about the original y axis, not the new one), and finally by α about the z axis of F (i.e., about the same axis as the first rotation), the rotation operator is

$$D(\omega) = \exp(-i\alpha J_z)\ \exp(-i\beta J_y)\ \exp(-i\gamma J_z), \qquad (1.9)$$

where ω is an abbreviation for the three Euler angles α, β, and γ. Let (xyz) be the coordinates of a point in F and $(\xi\eta\zeta)$ its coordinates in F'. Then

$$\xi = D(\omega) x D(\omega)^{-1},$$

with similar equations for η and ζ. For future reference, the results are written out in full:

$$\begin{aligned}
\xi &= x(\cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma) \\
&\quad + y(\sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma) - z\sin\beta\cos\gamma, \\
\eta &= x(-\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma) \\
&\quad + y(-\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma) + z\sin\beta\sin\gamma, \\
\zeta &= x\cos\alpha\sin\beta + y\sin\alpha\sin\beta + z\cos\beta. \qquad (1.10)
\end{aligned}$$

The inverses can be written down by making the replacements

$$x \to \xi, \quad y \to \eta, \quad z \to \zeta, \quad \alpha \to -\gamma, \quad \beta \to -\beta, \quad \gamma \to -\alpha.$$

All these equations can be obtained by repeated use of Eqs. (1.7)–(1.8) and cyclic permutations of them. In carrying through the calculations, we must avoid using equations such as

$$e^a e^b = e^{a+b} = e^{b+a} = e^b e^a,$$

which only hold if a and b commute. (The correct form of equations of this type has been discussed by Messiah [5].)

There exists an alternative way of making the transformation above. First, F is rotated by α about its z axis, then this second frame (say F'') is rotated by β about the new y axis. Finally, this third frame is rotated by γ about its z axis. A detailed analysis reveals that the frame so obtained coincides with F' (see Problem 1.1).

1.4 ROTATION MATRICES

Corresponding to the coordinate transformations (1.10), any operator T becomes T', where

$$T' = D(\omega) T D(\omega)^{-1}.$$

The effect of $D(\omega)$ on a ket $|J, M'\rangle$ can only be to produce a linear combination of kets with the same J, since $D(\omega)$ is a function of the components of **J**, for which Eqs. (1.3) are valid. Let us therefore write

$$D(\omega)\ |JM'\rangle = \sum_{M''} \mathfrak{D}_{M''M'}{}^{J}(\omega)\ |JM''\rangle$$

and determine the numerical coefficients $\mathfrak{D}_{M''M'}{}^{J}(\omega)$. (For simplicity, the amas have been omitted from the kets.) Setting the bra $\langle JM|$ to the of both sides of this equation, and writing $M' = N$, we get

$$M\,|\,D(\omega)\,|\,JN\rangle = \mathfrak{D}_{MN}{}^{J}(\omega)$$
$$= \langle JM\,|\exp(-i\alpha J_z)\exp(-i\beta J_y)\exp(-i\gamma J_z)\,|\,JN\rangle$$
$$= \exp(-i(\alpha M + \gamma N))\,d_{MN}{}^{J}(\beta),$$

ere

$$d_{MN}{}^{J}(\beta) = \langle JM\,|\exp(-i\beta J_y)\,|\,JN\rangle.$$

e derivation of the explicit form of $d_{MN}{}^{J}(\beta)$ is outlined in Problem (1.2); final answer is

$$d_{MN}{}^{J}(\beta) = \sum_t (-1)^t \frac{[(J+M)!(J-M)!(J+N)!(J-N)!]^{1/2}}{(J+M-t)!(J-N-t)!t!(t+N-M)!} \times (\cos\beta/2)^{2J+M-N-2t}(\sin\beta/2)^{2t+N-M}. \qquad (1.11)$$

This expression for $d_{MN}{}^{J}(\beta)$ enables many symmetry properties of the ation matrices to be rapidly written down. For example,

$$d_{MN}{}^{J}(\beta) = d_{-N-M}{}^{J}(\beta), \qquad (1.12)$$
$$d_{NM}{}^{J}(\beta) = d_{MN}{}^{J}(-\beta) = (-1)^{M-N}d_{MN}{}^{J}(\beta), \qquad (1.13)$$

m which we can deduce

$$\mathfrak{D}_{MN}{}^{J}(\omega)^* = (-1)^{M-N}\mathfrak{D}_{-M-N}{}^{J}(\omega). \qquad (1.14)$$

expression such as $d_{MN}{}^{J}(\pi-\beta)$ is slightly more difficult to handle. wever, we have only to write $t = J - t' - N$, and the sum over t' can expressed in terms of $d_{-MN}{}^{J}(\beta)$. The result is

$$d_{MN}{}^{J}(\pi-\beta) = (-1)^{J-N}d_{-MN}{}^{J}(\beta) = (-1)^{J+M}d_{M-N}{}^{J}(\beta). \qquad (1.15)$$

If we recall that the adjoint of an operator product AB is given by $B)^\dagger = B^\dagger A^\dagger$, it is at once seen that $D(\omega)^\dagger = D(\omega)^{-1}$, since the Carte- n components of **J** are Hermitian [6]. It follows that $D(\omega)$ is a unitary erator, and that the matrices $\mathfrak{D}_{MN}{}^{J}(\omega)$, where M and N label the rows d columns respectively, are unitary matrices. Thus

$$\sum_{M'} \mathfrak{D}_{M'N}{}^{J}(\omega)^*\mathfrak{D}_{M'M}{}^{J}(\omega) = \delta(M,N),$$
$$\sum_{M'} \mathfrak{D}_{MM'}{}^{J}(\omega)\mathfrak{D}_{NM'}{}^{J}(\omega)^* = \delta(M,N). \qquad (1.16)$$

If a ket can be represented by a wavefunction $\psi(\mathbf{r})$, then the effect of (ω) is to rotate the contours of $\psi(\mathbf{r})$. However, the sense of the rotation

is opposite to that for **r** itself. To see this, take $\psi(\mathbf{r})$ in the hypothetical form of the Dirac delta function $\delta(\mathbf{r}-\mathbf{R})$. Suppose that **r** becomes $\mathbf{r}+\mathbf{a}$ under the action of $D(\omega)$. Then the wavefunction becomes $\delta(\mathbf{r}+\mathbf{a}-\mathbf{R})$, and the singularity moves from **R** to $\mathbf{R}-\mathbf{a}$.

1.5 SPHERICAL TENSORS

Operators that transform under rotations in the same manner as the kets $|JM\rangle$ are of great importance. If the $2k+1$ operators $T_q^{(k)}$, where $-k \le q \le k$, satisfy

$$D(\omega)T_q^{(k)}D(\omega)^{-1} = \sum_{q'} \mathfrak{D}_{q'q}{}^{k}(\omega)T_{q'}^{(k)}, \qquad (1.17)$$

then they are said to form the components of a spherical tensor $\mathbf{T}^{(k)}$ of rank k. It is clear that the commutation relations that the $T_q^{(k)}$ obey with respect to **J** are of crucial importance in determining the form of the right-hand side of Eq. (1.17). In fact, we can follow Racah [7] and use these commutation relations as an equivalent way of defining a tensor operator. They run

$$[J_z, T_q^{(k)}] = qT_q^{(k)},$$
$$[J_\pm, T_q^{(k)}] = [k(k+1) - q(q\pm 1)]^{1/2}T_{q\pm 1}^{(k)}. \qquad (1.18)$$

The similarity between these conditions and Eqs. (1.3) illustrates the correspondence between tensor operators and kets.

The vector **J** is itself a tensor operator. To satisfy Eqs. (1.18), we must define the components as follows:

$$J_1^{(1)} = -\sqrt{\tfrac{1}{2}}\,J_+, \qquad J_0^{(1)} = J_z, \qquad J_{-1}^{(1)} = \sqrt{\tfrac{1}{2}}\,J_-.$$

No adjustment needs to be made for the spherical harmonics Y_{lm}; they are tensors for which $k = l$ and $q = m$. It is often more convenient to use the tensors $\mathbf{C}^{(k)}$, for which

$$C_q^{(k)}(\theta\phi) = \sqrt{\frac{4\pi}{2k+1}}\,Y_{kq}(\theta,\phi).$$

It is found, for example, that

$$C_{\pm 1}^{(1)} = \mp\sqrt{\frac{1}{2}}\,\frac{x \pm iy}{r}, \qquad C_0^{(1)} = \frac{z}{r}. \qquad (1.19)$$

Here and elsewhere, the radical sign applies only to the fraction immediately following it.

1.6 DOUBLE TENSORS

In the previous sections we have specified $D(\omega)$ in terms of the components of the total angular momentum **J**, and it is through the commutation relations with this operator that tensor operators have been defined. It is often useful, however, to consider the properties of operators with respect to other angular momenta before examining their features overall. Commuting angular momenta turn out to be particularly valuable for separating and characterizing the properties of operators in the different spaces spanned by the angular momenta. The orbital and spin spaces, to which correspond the total orbital and total spin angular momentum respectively, constitute perhaps the most familiar example. If we have two commuting angular momenta **J** and **J**′, then a double tensor $\mathbf{T}^{(kk')}$ can be defined by specifying that the $(2k+1)$ components $T_{qq'}^{(kk')}$ for which $-k \le q \le k$ behave as a tensor with respect to **J** for any choice of q'; and, reciprocally, the $(2k'+1)$ components $T_{qq'}^{(kk')}$ for which $-k' \le q' \le k'$ behave as a tensor with respect to **J**′ for any choice of q. The double tensor $\mathbf{T}^{(kk')}$ possesses $(2k+1)(2k'+1)$ components in all.

An important example of **J** and **J**′ can be constructed from the coordinates (xyz) and $(\xi\eta\zeta)$. Since the nine quantities $(xyz,\ \xi\eta\zeta,\ \alpha\beta\gamma)$ are connected by just three equations—namely, Eqs. (1.10)—any six of them can be taken as independent variables. If $(xyz,\ \xi\eta\zeta)$ are chosen for this role, we can define two angular momentum vectors $\boldsymbol{l}$ and $\boldsymbol{\lambda}$ by means of the equations

$$l_x = \frac{1}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \tag{1.20}$$

$$\lambda_\xi = \frac{1}{i}\left(\eta\frac{\partial}{\partial \zeta} - \zeta\frac{\partial}{\partial \eta}\right), \tag{1.21}$$

together with their cyclic permutations over the respective triads (xyz) and $(\xi\eta\zeta)$. Having taken $(xyz,\ \xi\eta\zeta)$ as independent variables, we know that

$$[\boldsymbol{l}, \boldsymbol{\lambda}] = 0,$$

so we can make the identifications $\boldsymbol{l} = \mathbf{J}$, $\boldsymbol{\lambda} = \mathbf{J}'$.

A physical interpretation can be given to $\boldsymbol{l}$ and $\boldsymbol{\lambda}$. The vector $\boldsymbol{l}$ is evidently the orbital angular momentum of a particle measured with respect to a frame F; but since the partial derivatives $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$ that occur in $\boldsymbol{l}$ imply differentiation in which ξ, η, and ζ are held constant, the particle is stationary in F'. In other words, the frame F' turns relative to F in such a way that the motion of the particle is precisely followed. We may evidently express $\boldsymbol{l}$ in terms of the Euler angles through which the relative position of F and F' is defined. When this is done, we get

$$l_x \pm il_y = ie^{\pm i\alpha}\left(\cot\beta\frac{\partial}{\partial\alpha} \mp i\frac{\partial}{\partial\beta} - \frac{1}{\sin\beta}\frac{\partial}{\partial\gamma}\right),$$

$$l_z = -i\frac{\partial}{\partial\alpha}. \tag{1.22}$$

In a similar way, $\boldsymbol{\lambda}$ represents the orbital angular momentum of a particle which is stationary in F. For this case,

$$\lambda_\xi \pm i\lambda_\eta = ie^{\mp i\gamma}\left(\cot\beta\frac{\partial}{\partial\gamma} \pm i\frac{\partial}{\partial\beta} - \frac{1}{\sin\beta}\frac{\partial}{\partial\alpha}\right),$$

$$\lambda_\zeta = i\frac{\partial}{\partial\gamma}. \tag{1.23}$$

The partial derivatives $\partial/\partial\alpha$, $\partial/\partial\beta$, and $\partial/\partial\gamma$ in Eqs. (1.22) are not the same as those in Eqs. (1.23): the former correspond to a scheme in which $(\xi\eta\zeta)$ are held constant, the latter to one in which (xyz) are held constant. If we wish to use $\boldsymbol{l}$ and $\boldsymbol{\lambda}$ to investigate the tensorial properties of functions solely of the Euler angles, this distinction is irrelevant. Without further ado, we can take the right-hand sides of Eqs. (1.22) and (1.23) for two commuting operators $\boldsymbol{l}$ and $\boldsymbol{\lambda}$.

Consider, for example, $\mathfrak{D}_{MN}^{J}(\omega)^*$. We see at once that

$$[l_z, \mathfrak{D}_{MN}^{J}(\omega)^*] = M\mathfrak{D}_{MN}^{J}(\omega)^*, \tag{1.24}$$

since the dependence of the $\mathfrak{D}^*$ function on α is simply $e^{iM\alpha}$. The commutation with respect to $l_\pm$ is more difficult to work out, though quite straightforward if $\cot\beta$ and $\csc\beta$ are converted to functions of half angles through the expressions

$$\cot\beta = \frac{\cos^2\beta/2 - \sin^2\beta/2}{2\sin\beta/2\cos\beta/2}, \qquad \csc\beta = \frac{\cos^2\beta/2 + \sin^2\beta/2}{2\sin\beta/2\cos\beta/2}$$

before combination with the expression for $d_{MN}^{J}(\beta)$ given in Eq. (1.11). The result is

$$[l_x \pm il_y, \mathfrak{D}_{MN}^{J}(\omega)^*] = [J(J+1) - M(M\pm 1)]^{1/2}\mathfrak{D}_{M\pm1,N}^{J}(\omega)^*. \tag{1.25}$$

So, for a given N (and ω), the functions $\mathfrak{D}_{MN}^{J}(\omega)^*$ behave as tensor components $T_M^{(J)}$ with respect to $\boldsymbol{l}$.

When we turn to λ, a slight complication arises. The commutation relations turn out to be

$$[\lambda_\xi, \mathfrak{D}_{MN}{}^J(\omega)^*] = -N\mathfrak{D}_{MN}{}^J(\omega)^*,$$

$$[\lambda_\xi \pm i\lambda_\eta, \mathfrak{D}_{MN}{}^J(\omega)^*] = -[J(J+1) - N(N \mp 1)]^{1/2}\mathfrak{D}_{M,N\mp 1}{}^J(\omega)^*. \qquad (1.26)$$

To get a minus sign in the first equation, we need to assign a tensor component q of $-N$ to $\mathfrak{D}_{MN}{}^J(\omega)^*$. The minus sign in the second equation requires an alternation of sign with N for the tensor components. This is most conveniently achieved by means of a phase factor $(-1)^{J-N}$. The presence of J in the phase serves to eliminate complex quantities when N is half-integral.

We can now define a double tensor $\mathbf{D}^{(JJ)}$ through the equation

$$D_{M,-N}{}^{(JJ)} = (-1)^{J-N}(2J+1)^{1/2}\mathfrak{D}_{MN}{}^J(\omega)^*. \qquad (1.27)$$

The factor $(2J+1)^{1/2}$ simplifies various calculations, as we shall see later on. It is understood that $\mathbf{D}^{(JJ)}$ refers to a specific value of the Euler triad ω.

1.7 COUPLING

The coupling of two angular momenta **A** and **B** to form a third, **C**, is familiar to all spectroscopists. It is supposed that **A** and **B** refer to different physical systems, or else to independent parts of the same system. This guarantees that **A** and **B** commute, thereby ensuring that **C**, which is defined by $\mathbf{C} = \mathbf{A} + \mathbf{B}$, satisfies the commutation relations (1.2). To simplify the notation as much as possible, let us write the eigenvalues of $\mathbf{A}^2$ and A_z as $A(A+1)$ and a respectively. Two types of ket are now available for describing the combined scheme. We can choose either the uncoupled form $|Aa, Bb\rangle$, or the coupled form $|Cc\rangle$. For a given A and B, there are $(2A+1)(2B+1)$ kets of the first kind; and if we use the fact that C can run with integral steps from $A+B$ down to $|A-B|$, it can be easily checked that there are an equal number of coupled kets. The unitary transformation that connects the two descriptions can be written

$$|Cc\rangle = \sum_{a,b} (Aa, Bb \mid Cc) \mid Aa, Bb\rangle. \qquad (1.28)$$

The coefficients $(Aa, Bb \mid Cc)$ are the celebrated Clebsch–Gordan (CG) coefficients. Phases can be chosen so that they are all real. By operating on both sides of Eq. (1.28) with C_z $(= A_z + B_z)$, we at once see that $a + b = c$, so the sum effectively runs over a single index. Owing to the unitarity of Eq. (1.28), we have

$$\sum_{a,b} (Cc \mid Aa, Bb)(Aa, Bb \mid C'c') = \delta(c, c')\delta(C, C'), \qquad (1.29)$$

$$\sum_{C,c} (Aa, Bb \mid Cc)(Cc \mid Aa', Bb') = \delta(a, a')\delta(b, b'). \qquad (1.30)$$

It would be out of place in this introduction to go deeply into the properties of the CG coefficients. Nowadays they are often replaced by the 3-j symbol [8], which is defined by

$$\begin{pmatrix} A & B & C \\ a & b & c \end{pmatrix} = (-1)^{A-B-c}(2C+1)^{-1/2}(Aa, Bb \mid C\,-c). \qquad (1.31)$$

The 3-j symbol exhibits the symmetries of the CG coefficient in a particularly transparent form. Even permutations of the columns leave the numerical value of the symbol unchanged, while odd permutations of the columns or a reversal in sign of the entries of the lower row produce a phase factor $(-1)^{A+B+C}$. Over the years, many tabulations of the CG coefficients and 3-j symbols have been made. The numerical tables of Rotenberg *et al.* [9] are some of the most extensive. Edmonds [1] gives the algebraic forms of a number of the more simple 3-j symbols. Several of these are assembled in Appendix I. A method for finding an explicit expression for the general CG coefficient is outlined in Problem 1.3.

To indicate that A and B are coupled to C, the ket $|Cc\rangle$ is often more completely written as $|(AB)Cc\rangle$. The arrangement of symbols is of some significance, since the explicit form for the CG coefficient appearing in Eq. (1.28) permits the interchange $Aa \leftrightarrow Bb$ only when the phase $(-1)^{A+B-C}$ is included. So

$$|(AB)Cc\rangle = (-1)^{A+B-C} \mid (BA)Cc\rangle. \qquad (1.32)$$

Tensor operators, like kets, can be coupled. Thus we may write

$$(\mathbf{T}^{(A)}\mathbf{U}^{(B)})_c{}^{(C)} = \sum_{a,b} (Aa, Bb \mid Cc) T_a{}^{(A)} U_b{}^{(B)}. \qquad (1.33)$$

It is traditional [7] to define a scalar product by the equation

$$(\mathbf{T}^{(A)} \cdot \mathbf{U}^{(A)}) = \sum_a (-1)^a T_a{}^{(A)} U_{-a}{}^{(A)}.$$

From Edmonds' text, we at once find that

$$(Aa, A\,-a \mid 00) = (-1)^{-A+a}(2A+1)^{-1/2}, \qquad (1.34)$$

so that

$$(\mathbf{T}^{(A)} \cdot \mathbf{U}^{(A)}) = (-1)^A(2A+1)^{1/2}(\mathbf{T}^{(A)}\mathbf{U}^{(A)})^{(0)}. \qquad (1.35)$$

(3) $$\frac{d}{d\chi}\left[\sin^l \chi \left(\frac{d}{d\cos\chi}\right)^l C_{n-1}(\cos\chi)\right]$$

$$= \cot\chi\left[l\sin^l\chi\left(\frac{d}{d\cos\chi}\right)^l C_{n-1}(\cos\chi)\right]$$

$$- \sin^{l+1}\chi\left(\frac{d}{d\cos\chi}\right)^{l+1} C_{n-1}(\cos\chi),$$

(4) $$(1-\mu^2)\frac{d^{l+1}}{d\mu^{l+1}}C_{n-1}(\mu) - (2l+1)\mu\frac{d^l}{d\mu^l}C_{n-1}(\mu)$$

$$= -(n^2-l^2)\frac{d^{l-1}}{d\mu^{l-1}}C_{n-1}(\mu).$$

Assemble these results to prove Eq. (2.25).

2.4 By multiplying both sides of the equation

$$C_t(\mu)C_{t'}(\mu) = \sum_s \Delta(tt's)C_s(\mu) \qquad (\mu \equiv \cos\chi)$$

by $C_{t''}(\cos\chi)\sin^2\chi\, d\chi$ and integrating over χ, prove that the coefficient of $h^t g^{t'} f^s$ in

$$\int_{-1}^{1}(1-\mu^2)^{1/2}(1-2\mu h+h^2)^{-1}(1-2\mu g+g^2)^{-1}(1-2\mu f+f^2)^{-1}\,d\mu$$

is $\frac{1}{2}\pi\Delta(tt's)$. Show that this is equal to the coefficient of $h^t g^{t'} f^s$ in

$$\tfrac{1}{2}\pi\{(1-gh)(1-hf)(1-fg)\}^{-1}$$

and deduce that $\Delta(tt's) = 1$ if t, t', and s satisfy the triangular condition and if, in addition, $t+t'+s$ is even: otherwise $\Delta(tt's) = 0$.

2.5 Derive Eq. (2.40) from the requirement that $C_{n-1}(\cos\chi)$, being a function of an angle between two radii vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ of the hypersphere, is a scalar under rotations generated by $(J_{ab})_1 + (J_{ab})_2$.

3

R(4) in Physical Systems

3.1 THE RIGID ROTATOR

The notion of a rigid rotator is an abstraction. Its significance for us lies in the fact that, when treating the motion of a physical object in quantum mechanics, we usually separate out the coordinates ω that refer specifically to the orientation of the object from those that represent internal motion. The resulting differential equation satisfied by the Euler angles ω is identical to that occurring in the quantum treatment of a classical rigid rotator. For this reason, the properties of this rather artificial object are relevant to us. Casimir [20] and van Winter [31] have given more complete treatments than the sketch presented here.

The rigid rotator is visualized as an object possessing three principal moments of inertia, I_1, I_2, and I_3. It is convenient to fix a frame F' in the rotator so that the ξ, η, and ζ axes coincide with the principal axes. A point $(\xi\eta\zeta)$ embedded in the rotator can be assigned coordinates (xyz) in a laboratory-fixed frame F. The connection with the Euler angles ω $(= \alpha\beta\gamma)$ is specified by Eqs. (1.10). The classical kinetic energy T of the rotator is given by

$$T = \tfrac{1}{2}(I_1\omega_1^2 + I_2\omega_2^2 + I_3\omega_3^2), \tag{3.1}$$

where ω_i is the angular velocity of the object about principal axis i. To relate this to $\dot\alpha$, $\dot\beta$, and $\dot\gamma$, we consider an infinitesimal displacement of the rotator. Since the frame F' is carried with the rotator, we are easily able to find dx, dy, and dz in terms of $d\alpha$, $d\beta$, and $d\gamma$ by taking ξ, η, and ζ to be constant and differentiating the inverses of Eqs. (1.10). If, however, the frame F' had not moved with the rotator, the point $(\xi\eta\zeta)$ fixed in the rotator would have been assigned coordinates $(\xi + d\xi,\ \eta + d\eta,\ \zeta + d\zeta)$, and the increments $d\xi$, $d\eta$, and $d\zeta$ can be immediately found by substituting dx for x, etc., in Eqs. (1.10). We get

$$\omega_1 = \left(\frac{\eta\dot\zeta - \zeta\dot\eta}{\eta^2 + \zeta^2}\right)_{\xi=0} = \dot\beta \sin\gamma - \dot\alpha \sin\beta\cos\gamma,$$

$$\omega_2 = \left(\frac{\zeta\dot\xi - \xi\dot\zeta}{\zeta^2 + \xi^2}\right)_{\eta=0} = \dot\beta \cos\gamma + \dot\alpha \sin\beta\sin\gamma,$$

$$\omega_3 = \left(\frac{\xi\dot\eta - \eta\dot\xi}{\xi^2 + \eta^2}\right)_{\zeta=0} = \dot\alpha\cos\beta + \dot\gamma.$$

Readers with a well-developed geometrical perception could no doubt write down these expressions for ω_i without any preliminaries, as do Landau and Lifshitz [32]. The generalized momenta are defined by

$$p_\alpha = \partial T/\partial\dot\alpha = -I_1\omega_1 \sin\beta\cos\gamma + I_2\omega_2\sin\beta\sin\gamma + I_3\omega_3\cos\beta,$$

$$p_\beta = \partial T/\partial\dot\beta = I_1\omega_1\sin\gamma + I_2\omega_2\cos\gamma,$$

$$p_\gamma = \partial T/\partial\dot\gamma = I_3\omega_3.$$

We now make the replacements $p_\alpha = -i\hbar\partial/\partial\alpha$, etc., and, after having done this, express $I_i\omega_i$ as sums of these derivatives. The result is

$$I_1\omega_1 = -\hbar\lambda_\xi, \qquad I_2\omega_2 = -\hbar\lambda_\eta, \qquad I_3\omega_3 = -\hbar\lambda_\zeta, \tag{3.2}$$

where λ is given by Eqs. (1.23). The quantum-mechanical Hamiltonian for the rigid rotator is thus

$$T = \frac{1}{2}\hbar^2\left(\frac{\lambda_\xi^2}{I_1} + \frac{\lambda_\eta^2}{I_2} + \frac{\lambda_\zeta^2}{I_3}\right). \tag{3.3}$$

Of course, we could have appealed to classical mechanics for Eq. (3.3) instead of Eq. (3.1). However, the intervening analysis is important for establishing the negative signs in Eqs. (3.2).

To assign quantum numbers to the eigenfunctions of T, we seek operators that commute with it. Now, we have already determined that l, defined in Eqs. (1.22), commutes with every component of λ. Hence the eigenvalues $J(J+1)$ and M of the two mutually commuting operators l^2 and l_z can be used to label the eigenfunctions. Of course, $l^2 = \lambda^2$, and the two quantum numbers J and M correspond to the total angular momentum of the rigid rotator and its z projection in the laboratory frame. The eigenfunction ψ can only depend on the Euler angles ω, since these are the only dynamical variables appearing in the Hamiltonian. As $\mathfrak{D}_{MN}^J(\omega)^*$ is an eigenfunction of l^2 and l_z, it is highly convenient to expand $\psi(\omega)$ in terms of the $\mathfrak{D}$ functions. This is possible because the $\mathfrak{D}$ functions (like the spherical harmonics Y_{nlm}) form a complete set. Thus the eigenfunction corresponding to a specified J and M takes the form

$$\psi(\omega) = \sum_N a_N \mathfrak{D}_{MN}^J(\omega)^* \tag{3.4}$$

for the rigid rotator.

The coefficients a_N in Eq. (3.4) depend on the moments of inertia, I_i. If two of these (say I_1 and I_2) are equal, the rigid rotator is called a *symmetric top*. For this special case, we can write

$$T = \frac{1}{2}\hbar^2\left[\frac{1}{I_1}\lambda^2 + \left(\frac{1}{I_3} - \frac{1}{I_1}\right)\lambda_\zeta^2\right],$$

and this expression for T commutes with λ_ζ as well as with l^2 and l_z. From Section 1.6, we know $\mathfrak{D}_{MN}^J(\omega)^*$ is an eigenfunction of λ_ζ with eigenvalue $-N$, so a single $\mathfrak{D}$ function is an eigenfunction of the symmetric top. We impose a normalization condition and write

$$\psi(\omega) = \{(2J+1)/8\pi^2\}^{1/2}\mathfrak{D}_{MN}^J(\omega)^* \tag{3.5}$$

Since $I_3\omega_3 = -\hbar\lambda_\zeta$, the angular momentum of the symmetric top about the symmetry axis ζ is $\hbar N$ for the eigenfunction of Eq. (3.5). The eigenvalues of T are

$$\frac{1}{2}\hbar^2\left[\frac{J(J+1)}{I_1} + \left(\frac{1}{I_3} - \frac{1}{I_1}\right)N^2\right], \tag{3.6}$$

and we must necessarily have $J \geq |N|$. Unless $I_1 = I_3\ (= I_2)$, in which case the symmetric top reduces to a *spherical rotator*, each energy level for which $|N| > 0$ possesses a degeneracy of $2(2J+1)$. The levels of a spherical rotator exhibit a degeneracy of $(2J+1)^2$. Needless to say, any linear combination of the solutions (3.5) that correspond to the same energy is itself a solution.

Although the eigenfunctions $\psi(\omega)$ of Eq. (3.5) form basis functions for an irreducible representation of $R(4)$ if we let M and N run between their limits of $-J$ and J, they correspond to a single energy level only for the spherical rotator. This is because the operators λ_ξ and λ_η do not commute with the Hamiltonian of the symmetric top. The group $R(4)$ is said to be a *noninvariance* group for this system.

3.2 REVERSED ANGULAR MOMENTUM

To convert $\psi(\omega)$ of Eq. (3.5) to the form of a ket, we write

$$\psi(\omega) = [(2J+1)/8\pi^2]^{1/2}\mathfrak{D}_{MN}{}^{J}(\omega)^* = (-1)^{J-N}\,|J, M, -N\rangle. \quad (3.7)$$

The reason for the phase factor $(-1)^{J-N}$ and the minus sign preceding N in the ket is precisely the same as the reason for their appearance in Eq. (1.27). Both quantum numbers M and $-N$ are on a similar footing with respect to l and λ. Thus M and $-N$ specify the eigenvalues of l_z and λ_ζ, and the properties of the shift operators $l_x \pm il_y$ and $\lambda_\xi \pm i\lambda_\eta$ are also matched.

The presence of $-N$ rather than N in the ket may seem distasteful. As has just been pointed out in the previous section, the angular momentum of the symmetric top about the symmetry axis is $\hbar N$, and not $-\hbar N$. It might therefore seem more natural to write $|J, MN\rangle$ for $\psi(\omega)$ and to introduce the vector $\lambda' = -\lambda$, so that N now appears as the eigenvalue of λ_ζ'. Unfortunately, these modest adjustments entail another change. Unlike λ, the vector λ' is not an angular momentum vector, since it satisfies the commutation relations

$$[\lambda_\xi', \lambda_\eta'] = -i\lambda_\zeta', \quad (3.8)$$

etc., in which $-i$ appears on the right-hand side instead of i. However, this is not entirely satisfactory, since λ' represents, in one sense, an angular momentum: it is, in fact, the total angular momentum l of the rigid rotator projected onto axes coinciding instantaneously with those of the frame F' fixed in the rotator. To see this, we write $l = l^{(10)}$ in the double-tensor notation of Section 1.7. To project $l^{(10)}$ onto the axes of F', we have merely to construct $(\mathbf{D}^{(11)}l^{(10)})^{(01)}$. Using Eqs. (1.22)–(1.23), we find

$$\lambda' = (\mathbf{D}^{(11)}l^{(10)})^{(01)}. \quad (3.9)$$

(An alternative method to the direct approach for obtaining this result is outlined in Problem 3.2.) Van Vleck [33] realized that matters could be arranged to make it permissible to take Eq. (3.8) as the standard form for the commutation relations for the components of an angular momentum vector. The sign of i can have no significance in quantum mechanics: one merely has to be consistent. However, if we accept Eq. (3.8) and its cyclic permutations as defining an angular momentum vector, a normal angular momentum vector $\mathbf{P}$ satisfies anomalous commutation relations. To correct this, Van Vleck defined, for such a vector, the reversed angular momentum $\tilde{\mathbf{P}}$ by the equation

$$\tilde{\mathbf{P}} = -\mathbf{P}, \quad (3.10)$$

and now the components of $\tilde{\mathbf{P}}$ satisfy commutation relations of the type (3.8). The kets $|\tilde{P}, \tilde{M}_P\rangle$ are to be used, in which $\tilde{M}_P$ is the eigenvalue of $\tilde{P}_\zeta$.

The change of sign of an angular momentum vector corresponds to time reversal. This can be seen to be associated with the replacement $i \to -i$ by substituting $-\mathbf{p}$ for $\mathbf{p}$ in the fundamental commutation relations (1.1). Freed [34] has described in detail the procedures to follow when the method of reversed angular momentum is adopted.

It is not necessary to take Van Vleck's extreme position. Carrington *et al.* [35] have pointed out that the commutation relations (3.8) can be corrected by setting

$$\lambda_\xi' = \lambda_\xi'', \qquad \lambda_\eta' = -\lambda_\eta'', \qquad \lambda_\zeta' = \lambda_\zeta'',$$

for then λ'' satisfies the commutation relations of an ordinary angular momentum vector.

Alternatively, all these adjustments can be avoided by accepting Eq. (3.7), and this is the course we shall follow here. The price we pay is a certain asymmetry between the frames F and F' to which our double tensors are referred (see Problem 3.2).

3.3 REDUCED MATRIX ELEMENTS

An important matrix element for eigenstates of the rigid rotator is

$$\langle JMN\,|\,D_{pq}{}^{(kk)}\,|\,J'M'N'\rangle. \quad (3.11)$$

The notation of Eq. (3.7) is followed in bra and ket. (Thus N is the eigenvalue of λ_ζ.) From this equation and from Eq. (1.27), the matrix element (3.11) is equal to

$$(-1)^{J+N+J'+N'+k+q}[J, k, J']^{1/2}\frac{1}{8\pi^2}\int \mathfrak{D}_{M-N}{}^{J}(\omega)\mathfrak{D}_{p-q}{}^{k}(\omega)^*\mathfrak{D}_{M'-N'}{}^{J'}(\omega)^*\,d\omega.$$

The integral can be readily evaluated from Eqs. (1.14) and (1.45).

On the other hand, the WE theorem can be applied to the matrix element (3.11). Since we are dealing with a double tensor, two 3-j symbols appear,