To obtain a quantum mechanical expression for the quadrupole coupling, we simply replace the classical ρ by its quantum mechanical operator $\rho^{(\mathrm{op})}$, given by

$$\rho^{(\mathrm{op})}(\boldsymbol{r}) = \sum_k q_k \underline{\rho}(\boldsymbol{r} - \boldsymbol{r}_k), \tag{9.13}$$

where the sum runs over the nuclear particles $1, 2, \ldots k \ldots N$, of charge q_k. Since the neutrons have zero charge, and the protons a charge e, we can simply sum over the protons:

$$\rho^{(\mathrm{op})}(\boldsymbol{r}) = e \sum_{\mathrm{protons}} \delta(\boldsymbol{r} - \boldsymbol{r}_k). \tag{9.14}$$

By substituting (9.14) into the classical expression for $Q_{\alpha\beta}$, we obtain the quadrupole operator $Q_{\alpha\beta}^{(\mathrm{op})}$:

$$\begin{aligned} Q_{\alpha\beta}^{(\mathrm{op})} &= \int (3x_\alpha x_\beta - \delta_{\alpha\beta} r^2)\, \rho^{(\mathrm{op})}(\boldsymbol{r})\, d\tau \\ &= e \sum_{\mathrm{protons}} \int (3x_\alpha x_\beta - \delta_{\alpha\beta} r^2)\, \delta(\boldsymbol{r} - \boldsymbol{r}_k)\, d\tau \\ &= e \sum_{\mathrm{protons}} (3x_{\alpha k} x_{\beta k} - \delta_{\alpha\beta} r_k^2). \end{aligned} \tag{9.15}$$

We have, then, a quadrupole term for the Hamiltonian $\mathscr{H}_Q$, given by

$$\mathscr{H}_Q = \tfrac{1}{6} \sum_{\alpha,\beta} V_{\alpha\beta} Q_{\alpha\beta}^{(\mathrm{op})}. \tag{9.16}$$

The expressions of (9.15) and (9.16) look exceedingly messy to handle because they involve all the nuclear particles. They appear to require us to treat the nucleus as a many-particle system, a complication we have avoided in discussing the magnetic couplings. Actually a similar problem is involved in both magnetic dipole and electric quadrupole cases, but we have simply avoided discussion in the magnetic case.

The quadrupole interaction represented by (9.15) enables us to treat problems of much greater complexity than those we encounter in a discussion of resonance phenomena. When performing resonances, we are in general concerned only with the ground state of a nucleus, or perhaps with an excited state when the excited state is sufficiently long-lived. The eigenstates of the nucleus are characterized by the total angular momentum I of each state, $2I + 1$ values of a component of angular momentum, and a set of other quantum numbers η, which we shall not bother to specify. Since we shall be concerned only with the spatial reorientation of the nucleus for a given nuclear energy state, we shall be concerned only with matrix elements diagonal in both I and η. Thus we shall need only matrix elements of the quadrupole operator, such as

---

$$\Delta E = \tfrac{1}{2} \sum_\alpha V_{\alpha\alpha} \int r^2 \rho\, d\tau = -\frac{4\pi e}{6} |\psi(0)|^2 \int r^2 \rho\, d\tau.$$

This ΔE will be different for two nuclei of the same charge but different charge distributions (isotopes), or for two nuclei of the same mass and charge but different nuclear states (isomers). In an electronic transition between an s and a p-state, ΔE will make a contribution that will in general be different for different isotopes or isomers. Effects also show up in nuclear transitions [9.2].

$$(Im\eta | Q_{\alpha\beta}^{(\mathrm{op})} | Im'\eta).$$

These can be shown to obey the equation

$$(Im\eta | Q_{\alpha\beta}^{(\mathrm{op})} | Im'\eta) = C(Im | \tfrac{3}{2}(I_\alpha I_\beta + I_\beta I_\alpha) - \delta_{\alpha\beta} I^2 | Im') \tag{9.17}$$

where C is a constant, different for each set of the quantum numbers I and η. In order to justify (9.17), we need to digress to discuss the Clebsch-Gordan coefficients, the so-called irreducible tensor operators T_{LM}, and the Wigner-Eckart theorem.

9.3 Clebsch-Gordan Coefficients, Irreducible Tensor Operators, and the Wigner-Eckart Theorem

The Wigner-Eckart theorem is one of the most useful theorems in quantum mechanics. In order to state it, we must introduce the Clebsch-Gordan coefficients $C(LJ'J; MM_{J'}M_J)$, and the irreducible tensor operators T_{LM}. We shall first state the Wigner-Eckart theorem and then define the Clebsch-Gordan coefficients. Next we shall discuss irreducible tensor operators, and lastly we shall indicate the derivation of the Wigner-Eckart theorem.

We consider a set of wave functions characterized by quantum numbers J J' for the total angular momentum, M_J or $M_{J'}$ for the z-component of angular momentum, and as many other quantum numbers η or η' as are needed to specify the state. We are then concerned with calculating the matrix elements of the operators T_{LM}, using these functions as the basis functions. The Wigner-Eckart theorem states that all such matrix elements are related to the appropriate Clebsch-Gordan coefficients through a set of quantities $(J\eta \| T_L \| J'\eta')$ that depend on J, J', η, η' and L but which are independent of M_J, $M_{J'}$, and M. Stated mathematically, the Wigner-Eckart theorem is

$$(JM_J\eta | T_{LM} | J'M_{J'}\eta') = C(J'LJ; M_{J'}MM_J)(J\eta \| T_L \| J'\eta'). \tag{9.18}$$

Let us now define the Clebsch-Gordan coefficients. They are encountered when one discusses the addition of two angular momenta to form a resultant. We therefore consider a system made up of two parts. Let us describe one part of the system by the quantum numbers L and M, to describe the total angular momentum of that part and its z-component. Let us use the quantum numbers J' and $M_{J'}$ correspondingly for the second part of the system. For the system as a whole we introduce quantum numbers J and M_J. We have, then, wave functions ψ_{LM} and $\phi_{J'M_{J'}}$, to describe the two parts, and Ψ_{JM_J} for the whole system. The function Ψ_{JM_J} can be expressed as a linear combination of product functions of the two parts, since such products form a complete set:

$$\Psi_{JM_J} = \sum_{\substack{J'M_{J'} \\ LM}} C(J'LJ;M_{J'}MM_J)\,\phi_{J'M_{J'}}\psi_{LM}\,. \tag{9.19}$$

The coefficients $C\,(J'LJ;\ M_{J'}MM_J)$ are called the *Clebsch-Gordan coefficients.* Certain of their properties are very well known. For example, $C(J'LJ;\ M_{J'}MM_J)$ vanishes unless $M_J = M + M_{J'}$. A second property, often called the *triangle rule*, is that $C(J'LJ;\ M_J'\ MM_J)$ vanishes unless J equals one of the values $J' + L, J' + L - 1, \ldots |J' - L|$, a fact widely used in atomic physics.

Let us now define the irreducible tensor operators T_{LM}. Suppose we have a system whose angular momentum operators have components J_x, J_y, and J_z. We define the raising and lowering operators J^+ and J^- as usual by the relations

$$\begin{aligned} J^+ &\equiv J_x + iJ_y \\ J^- &\equiv J_x - iJ_y\,. \end{aligned} \tag{9.20}$$

One can construct functions G of the operators of the system and examine the commutators such as (J^+, G), (J^-, G), and (J_z,G). It is often possible to define a family of $2L + 1$ operators (L is an integer) labeled by an integer $M(M = L, L - 1, \ldots - L)$ which we shall term *irreducible tensor operators* T_{LM}, which obey the commutation rules

$$\begin{aligned} (J^\pm, T_{LM}) &= \sqrt{L(L+1) - M(M\pm1)}\,T_{LM\pm1} \\ (J_z, T_{LM}) &= MT_{LM}\,. \end{aligned} \tag{9.21}$$

An example of such a set for $L = 1$ is

$$\begin{aligned} T_{11} &= \frac{-1}{\sqrt{2}}\,J^+ \\ T_{10} &= J_z \\ T_{1-1} &= \frac{1}{\sqrt{2}}\,J^-\,. \end{aligned} \tag{9.22}$$

Another example of a T_{1M} can be constructed for an atom with spin and orbital angular momentum operators $\boldsymbol{s}$ and $\boldsymbol{l}$, respectively, and total angular momentum $\boldsymbol{J}$. Then we define the operators

$$\begin{aligned} l^+ &= l_x + il_y \\ l^- &= l_x - il_y\,. \end{aligned} \tag{9.23}$$

One can then verify that the operators T_{1M}, defined by

$$\begin{aligned} T_{11} &= -\frac{l^+}{\sqrt{2}} \\ T_{10} &= l_z \\ T_{1-1} &= \frac{l^-}{\sqrt{2}} \end{aligned} \tag{9.24}$$

obey (9.21). (Actually the operators of (9.24) form components of an irreducible tensor T_{1M} with respect to the operators l^+, l^-, and l_z as well as J^+, J^-, and J_z). We may write the T_{1M}'s of (9.22) as $T_{1M}(\boldsymbol{J})$, to signify that they are functions of the components J_x, J_y, and J_z of $\boldsymbol{J}$. The T_{1M}'s of (9.24) are in a similar manner signified as $T_{1M}(\boldsymbol{l})$.

It is helpful to have a more physical feeling for the definition of the operators T_{LM} by the commutation rules of (9.21). We realize that angular momentum operators can be used to generate rotations, as discussed in Chapter 2. It is not surprising, therefore, that (9.21) can be shown to guarantee that T_{LM} transforms under rotations of the coordinate axes into linear combinations $T_{LM'}$, in exactly the same way that the spherical harmonics Y_{LM} transform into linear combinations of $Y_{LM'}$'s. This theorem is shown in Chapter 5 of *Rose*'s excellent book [9.3].

We shall wish to compute matrix elements of the T_{LM}'s. We are familiar with the fact that it is possible to derive expressions for the matrix elements of angular momentum from the commutation rules among the components. It is possible to compute the matrix elements of the T_{LM}'s by means of (9.21) in a similar manner. Let us illustrate.

We have in mind a set of commuting operators J^2, J_z, plus others, with eigenvalues J, M_J, and η. We use η to stand for all other quantum numbers needed. We wish to compute matrix elements such as

$$(JM_J\eta|T_{LM}|J'M_{J'}\eta')\,. \tag{9.25}$$

By means of the commutation rule

$$[J_z, T_{LM}] = MT_{LM} \tag{9.26}$$

we have

$$(JM_J\eta|[J_z, T_{LM}]|J'M_{J'}\eta') = M(JM_J\eta|T_{LM}|J'M_{J'}\eta')\,. \tag{9.27a}$$

But

$$\begin{aligned} (JM_J\eta|[J_z, T_{LM}]|J'M_{J'}\eta') &= \underbrace{(JM_J\eta|J_zT_{LM}|J'M_{J'}\eta)}_{1} - \underbrace{(JM_J\eta|T_{LM}J_z|J'M_{J'}\eta')}_{2} \\ &= (M_J - M_{J'})\,(JM_J\eta|T_{\mathrm{LM}}|J'M_{J'}\eta') \end{aligned}$$

where the last step follows from allowing the Hermitian operator J_z to operate on the function to its left in term 1 and to its right in term 2.

Therefore

$$(M_J - M_{J'})(JM_J\eta|T_{LM}|J'M_{J'}\eta) = M(JM_J\eta|T_{LM}|J'M_{J'}\eta)\,. \tag{9.27b}$$

Eq.(9.27b) shows that

$$(JM_J\eta|T_{LM}|J'M_{J'}\eta') = 0 \quad \text{unless} \quad M_J - M_{J'} = M\,. \tag{9.28}$$

In a similar way we may find conditions on the matrix elements of the other terms of (9.21). Thus

$$(JM_J\eta|[J^\pm, T_{LM}]|J'M_{J'}\eta') = \sqrt{L(L+1) - M(M\pm 1)}(JM_J\eta|T_{LM\pm1}|J'M_{J'}\eta'). \tag{9.29}$$

But

$$\begin{aligned}(JM_J\eta|J^\pm\, T_{LM}|J'M_{J'}\eta')\\ &= (JM_J\eta|J^\pm|JM_J\mp 1\eta)(JM_J\mp 1\eta|T_{LM}|J'M_{J'}\eta')\\ &= \sqrt{J(J+1)-(M_J\mp 1)M_J}\,(JM_J\mp 1\eta|T_{LM}|J'M_{J'}\eta')\,.\end{aligned} \tag{9.30}$$

By combining (9.29) and (9.30), we obtain the other recursion relations:

$$\begin{aligned}&\sqrt{J(J+1)-(M_J\mp 1)M_J}\,(JM_J\mp 1\eta|T_{LM}|J'M_{J'}\eta')\\ &-(JM_J\eta|T_{LM}|J'M_{J'}\pm 1\eta')\sqrt{J'(J'+1)-M_{J'}(M_{J'}\pm 1)}\\ &\qquad = \sqrt{L(L+1)-M(M\pm 1)}\,(JM_J\eta|T_{LM\pm1}|J'M_{J'}\eta')\,.\end{aligned} \tag{9.31}$$

We note that the only nonvanishing terms must satisfy (9.27b) However if any one term in (9.31) satisfies this relation, all do. Eq. (9.27b) and (9.31) constitute a set of recursion relations relating matrix elements for T_{LM} to one another and to those of $T_{LM'}$. These equations turn out to be sufficient to enable one to solve for all T_{LM} matrix elements for given J,J',η,η' in terms of any one matrix element.

A further insight into the significance of the recursion relations is shown by returning to the Clebsch-Gordan coefficients. In so doing, we shall sketch the proof of the Wigner-Eckart theorem.

As is shown by *Rose*, the C's obey recursion relations identical to those of the T_{LM}'s. We shall derive one-the selection rule on M, M_J, and $M_{J'}$. Consider the operator

$$J_z \equiv L_z + J_z'\,. \tag{9.32}$$

where

$$\begin{aligned}J_z\Psi_{JM_J} &= M_J\Psi_{JM_J}\\ L_z\psi_{LM} &= M\psi_{LM}\\ J_z'\phi_{J'M_{J'}} &= M_{J'}\phi_{J'M_{J'}}\,.\end{aligned} \tag{9.33}$$

Then consider the following matrix element of the operator J_z:

$$\begin{aligned}(\psi_{LM}\phi_{J'M_{J'}}, J_z\Psi_{JM_J}) &= M_J(\psi_{LM}\phi_{J'M_{J'}}, \Psi_{JM_J})\\ &= M_J C(J'LJ;M_{J'}MM_J)\end{aligned} \tag{9.34}$$

where we have let J_z operate to the right. But, writing J_z as $L_z + J_z'$ and operating on the functions to the left, we get

$$(\psi_{LM}\phi_{J'M_{J'}}, J_z\psi_{JM_J}) = (M + M_{J'})C(J'LJ;M_{J'}MM_J)\,. \tag{9.35}$$

By equating (9.34) and (9.35), we find

$$(M + M_{J'} - M_J)C(J'LJ;M_{J'}MM_J) = 0. \tag{9.36}$$

This equation is quite analogous to (9.27b), provided we replace

$$(JM_J\eta|T_{LM}|J'M_{J'}\eta')$$

by

$$C(J'LJ;M_{J'}MM_J)\,.$$

One can proceed in a similar manner to compute matrix elements of the raising and lowering operators, to get equations similar to (9.31). In fact the $C(J'LJ;M_{J'}MM_J)$'s obey the recursion relations identical to those of the $(JM_J\eta|T_{LM}|J'M_{J'}\eta')$'s. As a result, one can say that the C's and the matrix elements of T_{LM}'s are related. The relationship is called the *Wigner-Eckart theorem*:

$$(JM_J\eta|T_{LM}|J'M_{J'}\eta') = C(J'LJ;M_{J'}MM_J)(J\eta\|T_L\|J'\eta') \tag{9.37}$$

where the notation $(J\eta\|T_L\|J'\eta')$ stands for a quantity that is a constant for a given J,L,J',η,η' independent of M_J, $M_{J'}$, and M.

As we can see specifically from (9.22) and (9.24), for a given L and M there may be a variety of functions, all of which are T_{LM}'s. The Clebsch-Gordan coefficient is the same for all functions T_{LM} that have the same L and M, but the constant $(J\eta\|T_L\|J'\eta')$ will depend on what variable is used to construct the T_{LM}'s.

To illustrate this point further, let us consider a particle with spin $\boldsymbol{s}$ and orbital angular momentum $\boldsymbol{l}$ and position $\boldsymbol{r}$. The total angular momentum $\boldsymbol{J}$ is given by

$$\boldsymbol{J} = \boldsymbol{s} + \boldsymbol{l} \tag{9.38}$$

where

$$l_x = \frac{1}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$l_y = \frac{1}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \tag{9.39}$$
$$l_z = \frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right).$$

We shall now list two T_{2M}'s: one a function of the angular momentum $\boldsymbol{J}$; the other, of the coordinate $\boldsymbol{r}$. One can verify that the functions of Table 9.1, which we shall call $T_{2M}(\boldsymbol{J})$ and $T_{2M}(\boldsymbol{r})$. indeed obey the commutation rules of (9.21) with respect to J^+, J^-, and J_z.

Table 9.1

	$T_{2M}(\boldsymbol{J})$	$T_{2M}(\boldsymbol{r})$
T_{22}	J^{+2}	$(x+iy)^2$
T_{21}	$-(J_zJ^+ + J^+J_z)$	$-2z(x+iy)$
T_{20}	$\sqrt{\frac{2}{3}}(3J_z{}^2 - J^2)$	$\sqrt{\frac{2}{3}}(3z^2 - r^2)$
T_{2-1}	$J_zJ^- + J^-J_z$	$2z(x-iy)$
T_{2-2}	J^{-2}	$(x-iy)^2$

We have used the notation $T_{2M}(\boldsymbol{r})$ as shorthand for a T_{2M} constructed from the components x,y, and z of $\boldsymbol{r}$. There is an obvious similarity between $T_{2M}(\boldsymbol{J})$ and $T_{2M}(\boldsymbol{r})$: Replacement of J^+ by $(x+iy)$, J^- by $(x-iy)$, J_z by z will convert $T_{2M}(\boldsymbol{J})$ into $T_{2M}(\boldsymbol{r})$. This similarity is a direct consequence of the similarity of the commutation relations of components of $\boldsymbol{J}$ and $\boldsymbol{r}$ with J_x, J_y, and J_z:

$$[J_x, y] = iz \tag{9.40a}$$
$$[J_x, J_y] = iJ_z, \text{ etc.} \tag{9.40b}$$

where (9.40a) can be verified by means of (9.38) and (9.39) It is clear that any function $G(x, y, z)$ of x, y, z, constructed from a function $G(J_x, J_y, J_z)$ of J_x, J_y, J_z by direct substitution of x for J_x, and so on, will obey the same commutation rules with respect to J_x, J_y, and J_z. Thus, if a function of J_x, J_y, J_z is known to be a T_{LM}, the same will be true of the function formed by replacing J_x, J_y, J_z by x, y, z, respectively. The only caution we note in procedures such as this is that we must remember that the components of some operators do not commute among themselves; so that for example in $T_{21}(\boldsymbol{J})$ we have the symmetrized product $J^+J_z + J_zJ^+$, not $2J^+J_z$. The method of direct replacement will work for other variables as long as they obey commutation relations such as those of (9.40) For an excellent review article including tables of T_{LM}'s of various L and M, see [9.4].

Returning now to (9.37), let us consider two T_{LM}'s, one a function of variables q and the other a function of variables p. Then (9.37) tells us that

$$(JM_J\eta|T_{LM}(q)|J'M_{J'}\eta') = (JM_J\eta|T_{LM}(p)|J'M_{J'}\eta')\frac{(J\eta||T_L(q)||J'\eta')}{(J\eta||T_L(p)||J'\eta')}. \tag{9.41}$$

Since the factor $(J\eta||T_L(q)||J'\eta')/(J\eta||T_L(p)||J'\eta')$ is a constant (that is, independent of M, M_J, and $M_{J'}$), we see that we can compute all the matrix elements of $T_{LM}(q)$ of fixed J, J', η, and η' from knowledge of the constant and of the matrix elements $(JM_J\eta|T_{LM}(p)|J'M_{J'}\eta')$.

One word of caution is necessary. It may be that (9.41) is not meaningful, since for some operators p, the matrix element $(JM_J\eta|T_{LM}(p)|J'M_{J'}\eta')$ vanishes even though the matrix element $(JM_J\eta|T_{LM}(q)|J'M_{J'}\eta')$ does not. An example of such a case is when $T_{LM}(p)$ is made up of components of $\boldsymbol{J}$. Then all matrix elements in which $J' \neq J$ vanish. Of course $(J||T_2(\boldsymbol{J})||J')$ vanishes too, so that (9.41) becomes indeterminant.

9.4 Quadrupole Hamiltonian—Part 2

We now apply the Wigner-Eckart theorem to evaluate the matrix elements of $Q_{\alpha\beta}^{(\mathrm{op})}$. Now

$$Q_{\alpha\beta}^{(\mathrm{op})} = e\sum_k^{\text{protons}}(3x_{\alpha k}x_{\beta k} - \delta_{\alpha\beta}r_k^2). \tag{9.42}$$

By recalling that I_x, I_y, and I_z are the operators of the total angular momentum of the nucleus

$$I_x = \sum_k l_{xk} + s_{xk}, \quad \text{etc., for } I_y \text{ and } I_z, \tag{9.43}$$

where l_{xk} and s_{xk} are the x-components of the orbital and spin angular momentum of the kth nucleon; and by recalling that

$$[l_{xk}, y_k] = iz_k \quad [s_{xk}, y_k] = 0, \text{ etc.}, \tag{9.44}$$

we see that

$$[I_x, y_k] = iz_k, \text{ etc.} \tag{9.45}$$

The terms $3x_{\alpha k}x_{\beta k} - \delta_{\alpha\beta}r_k^2$ are linear combinations of $T_{2M}(\boldsymbol{r}_k)$'s such as found in the right-hand column of Table 9.1.

Equation (9.41) applies in a somewhat more general form not only to T_{LM}'s but also to functions that are linear combinations of T_{LM}'s, all of the *same* L. Thus consider such a function $F(p)$, which is a function of the operators p:

$$F(p) = \sum_M a_M T_{LM}(p)\,. \tag{9.46}$$

Let us define a function $G(q)$ of the operators q, using the same coefficients a_M:

$$G(q) \equiv \sum_M a_M T_{LM}(q)\,. \tag{9.47}$$

Then one can easily verify, using (9.41, 46, 47), that

$$(JM_J\eta\,|\,G(q)\,|\,J'M_{J'}\eta') = (JM_J\eta\,|\,F(p)\,|\,J'M_{J'}\eta')\frac{(J\eta\|T_L(q)\|J'\eta')}{(J\eta\|T_L(p)\|J'\eta')}\,. \tag{9.48}$$

We may apply this theorem to show that

$$(Im\eta\,|\,e\sum_k^{\text{protons}}(3x_{\alpha k}x_{\beta k} - \delta_{\alpha\beta}r_k^2)\,|\,Im'\eta) = \left(Im\eta\left|\,3\frac{(I_\alpha I_\beta + I_\beta I_\alpha)}{2} - \delta_{\alpha\beta}I^2\right|Im'\eta\right)C \tag{9.49}$$

where C is a constant,[3] the same for all m, m', α, and β. We can express C in terms of the matrix element for which $m = m' = I$, $\alpha = \beta = z$ as follows:

$$\begin{aligned}(II\eta\,|\,e\sum_k^{\text{protons}}(3z_k^2 - r_k^2)\,|\,II\eta) &= C(II\eta\,|\,3I_z^2 - I^2\,|\,II\eta)\\ &= CI(2I-1)\,.\end{aligned} \tag{9.50}$$

Since the quantum number η is assumed to be associated with a variable that commutes with I^2 and I_z, we can omit it in evaluating the right-hand equality of (9.50). We shall also define a symbol eQ:

$$eQ = (II\eta\,|\,e\sum_k^{\text{protons}}(3z_k^2 - r_k^2)\,|\,II\eta)\,. \tag{9.51}$$

Q is called the *quadrupole moment* of the nucleus. We have, by combining (9.50) and (9.51),

$$C = \frac{eQ}{I(2I-1)}\,. \tag{9.52}$$

The fact that we are concerned with matrix elements internal to one set of quantum numbers I, η enables us to use (9.49) and (9.52) to replace $Q_{\alpha\beta}^{(\text{op})}$ in the Hamiltonian. All matrix elements diagonal in I and η are just what we should calculate by adding an effective quadrupolar contribution $\mathscr{H}_Q$ to the Hamiltonian:

$$\mathscr{H}_Q = \frac{eQ}{6I(2I-1)}\sum_{\alpha,\beta} V_{\alpha\beta}[\tfrac{3}{2}(I_\alpha I_\beta + I_\beta I_\alpha) - \delta_{\alpha\beta}I^2]\,. \tag{9.53}$$

[3] Do not confuse C with the symbol for the Clebsch-Gordan coefficients.

It is interesting to note that of the nine components of $Q_{\alpha\beta}^{(\text{op})}$, only one nuclear constant, eQ, is needed. The reason is as follows: The fact that the nucleus is in a state of definite angular momentum is equivalent to the classical statement that the charge has cylindrical symmetry. Taking z as the symmetry axis, the energy change on reorientation depends, then, only on the *difference* between the charge distribution parallel and transverse to z.

$$\int z^2\rho\,d\tau \quad\text{and}\quad \int x^2\rho\,d\tau\,.$$

This gives us the critical quantity

$$\begin{aligned}\int(z^2 - x^2)\rho\,d\tau &= \tfrac{1}{2}\int(2z^2 - x^2 - y^2)\rho\,d\tau\\ &= \tfrac{1}{2}\int(3z^2 - r^2)\rho\,d\tau\,.\end{aligned} \tag{9.54}$$

The last integral, we see, is the classical equivalent of our eQ.

The effective quadrupole interaction of (9.53) applies for an arbitrary orientation of the rectangular coordinates $\alpha = x,y,z$. The tensor coupling to the symmetric (in x, y, z) tensor $V_{\alpha\beta}$ can be simplified by choice of a set of principal axes relative to which $V_{\alpha\beta} = 0$ for $\alpha \neq \beta$. In terms of these axes, we have

$$\mathscr{H}_Q = \frac{eQ}{6I(2I-1)}[V_{xx}(3I_x^2 - I^2) + V_{yy}(3I_y^2 - I^2) + V_{zz}(3I_z^2 - I^2)]\,. \tag{9.55}$$

This expression can be rewritten, using LaPlace's equation $\sum_\alpha V_{\alpha\alpha} = 0$, to give

$$\mathscr{H}_Q = \frac{eQ}{4I(2I-1)}[V_{zz}(3I_z^2 - I^2) + (V_{xx} - V_{yy})(I_x^2 - I_y^2)]\,. \tag{9.56}$$

Eq. (9.56) shows that only two parameters are needed to characterize the derivatives of the potential: V_{zz} and $V_{xx} - V_{yy}$. It is customary to define two symbols, η and q, called the *asymmetry parameter* and the *field gradient*, by the equations

$$\begin{aligned} eq &= V_{zz}\\ \eta &= \frac{V_{xx} - V_{yy}}{V_{zz}}\,.\end{aligned} \tag{9.57}$$

The case of axial symmetry, often a good approximation, is handled by taking the axis to be the z-direction, giving $\eta = 0$.

Since we have seen that the raising and lowering operators often provide particularly convenient selection rules, it is useful to write (9.53) in terms of I^+, I^-, and I_z for an arbitrary (that is, nonprincipal) set of axes. By defining