promoted to a vacancy in the $g\frac{9}{2}$ state. Once again the large difference in angular momentum explains the isomeric decay.

Thus in a very satisfactory way the position of the islands of isomerism on the nuclear chart find an explanation within the framework of the shell model. It should be noted that all excited states do not have such simple configurations as we have been picturing above. Those states which are as simple as this are referred to as *single-particle states*. However, it is clear that as well as single-particle states it must also be expected that there will exist excited states involving the promotion of two or even more particles.

6.12 Summary

The shell model, originating in an attempt to meet the challenge of explaining magic numbers and based on the arbitrary assumption of spin-orbit coupling, produces a level scheme which enables quantum numbers to be assigned to nucleons in complex nuclei. With the additional assumption that nucleons pair so as to cancel angular momentum, a scheme of ground-state spins in excellent agreement with measured ground-state spin values for odd-A nuclei can be constructed. In some cases the spins of excited states of nuclei can be explained on the basis of one particle being promoted from the lowest energy configuration and in particular the existence of islands of isomerism has a simple interpretation within the shell model. We shall see in the following chapters that the shell model has also a role to play in the interpretation of the measured electric and magnetic moments of nuclei.

Chapter 7
Nuclear Moments 1

7.1 Single-particle magnetic dipole moment

We saw in section 6.9 that cancellation of angular momentum takes place as long as there is an even number of nucleons in the nucleus; when there is an odd number of nucleons the total spin of the nucleus can be identified with the angular momentum of the one unpaired nucleon. Now it is found that (even, even) nuclei, which, as seen above, invariably have zero spin, also have zero magnetic dipole moment. It would therefore seem instructive to consider whether the observed finite magnetic dipole moments of odd-A stable nuclei can be explained as arising from the motion of the single unpaired nucleon. We now proceed to consider the magnetic moment to be expected to arise from the single nucleon in a given quantum state.

First however we have recourse to classical physics to define the basic terms used in atomic and nuclear magnetic studies. A particle with electric charge e, measured in electrostatic units, and mass M, moving in a circular orbit of radius r with constant angular velocity ω, is equivalent to a current $e\omega/2\pi c$ flowing so as to enclose an area πr^2. The equivalent magnetic dipole moment from classical electromagnetism is $e\omega r^2/2c$. We note that the angular momentum of the particle about an axis normal to the orbit and through its centre is $Mr^2\omega$. Thus the ratio of magnetic moment to angular momentum, the *gyromagnetic ratio*, is $e/2Mc$. Denoting the magnetic dipole moment by μ and the angular momentum by I we thus have

$$\frac{\mu}{I} = \text{constant} = \gamma, \qquad 7.1$$

say, where γ is independent of ω and r. This simple result for a circular orbit is true in the general case, where the orbit may be elliptic. In the quantum-mechanical case, the maximum value of angular momentum along a specified direction for a particle in an l-state is $l\hbar$ and the measured associated dipole moment would therefore be expected to be $le\hbar/2Mc$. If we define the constant quantity $e\hbar/2Mc$ to be the standard unit of magnetic moment, then the magnetic moment in terms of this standard unit is numerically equal to l. In the case of the electron, $e\hbar/2Mc$ is termed the *Bohr magneton*. When we apply the same ideas to the nucleon, the analogous quantity is termed the *nuclear magneton*. The larger value of the nucleon mass means that the nuclear magneton is 1/1836 times the Bohr magneton. Thus on the whole, since the angular momenta in both cases is of the order of $\hbar$, nuclear magnetic moments are expected to be smaller by this factor than atomic magnetic moments. When the accepted values of the constants are inserted in the expression $e\hbar/2Mc$, the nuclear magneton is found to be $5{\cdot}050 \times 10^{-31}$ J G^{-1}.

We now consider the magnetic moment which classical physics attributes to a rotating charged body. Assume that the charge is distributed through the volume to give a charge density ρ_e, which may vary from point to point. Let the mass be distributed in such a way as to give a mass density ρ, which also may vary from point to point. Take an element of the body of volume dV at a distance $\bar{r}$ from the axis of rotation. This element is equivalent to an orbiting particle having a charge $\rho_e\, dV$ and a mass $\rho\, dV$. It will therefore contribute to the magnetic moment an amount

$$d\mu = (\rho\, dV)\bar{r}^2\omega\left[\frac{\rho_e\, dV}{2\rho\; dV c}\right],$$

where ω is the angular velocity. If ρ_e and ρ are constants, or have the same dependence on the space coordinates, then we can write

$$\rho_e = K\rho,$$

where K is a constant. The total charge

$$e = \int \rho_e\, dV = K\int \rho\, dV = KM,$$

where M is the total mass. In this special case therefore

$$\frac{\rho_e}{\rho} = K = \frac{e}{M}.$$

Integrating over the whole body we then have

$$\mu = \frac{e\omega}{2Mc}\int \rho\bar{r}^2\, dV = \frac{e}{2Mc} \times \text{angular momentum.}$$

If on the other hand ρ_e and ρ do not have the same dependence on the space coordinates (i.e. the mass and charge distributions are dissimilar) then

$$\mu = \frac{\omega}{2c}\int \bar{r}^2\rho_e\, dV = \text{angular momentum} \times \frac{1}{2c}\,\frac{\int \bar{r}^2\rho_e\, dV}{\text{moment of inertia}}.$$

As an example, consider a sphere, radius R, of constant density, with the charge located entirely in a surface layer of thickness t, where $t \ll R$. Taking a ring element,

$$dV = 2\pi\bar{r}tR\, d\theta,$$

where θ is the usual spherical polar coordinate, and

$$\int \bar{r}^2\rho_e\, dV = \int_0^{\pi} 2\pi R^4 t\rho_e \sin^3\theta\, d\theta = \tfrac{2}{3}eR^2,$$

since e, the total charge, equals $4\pi R^2 t\rho_e$.

$$\text{Thus}\quad \mu = \text{angular momentum} \times \frac{1}{2c} \times \frac{\frac{2}{3}eR^2}{\frac{2}{5}MR^2} = \text{angular momentum} \times \frac{5}{6}\,\frac{e}{Mc}.$$

$$\text{Therefore}\quad \frac{\mu}{I} = \frac{e}{2Mc}\,\frac{5}{3}.$$

We thus see that in the general case a numerical coefficient is involved which is dependent on the charge and mass distributions. We therefore modify equation 7.1 by introducing the so called g-factor, writing

$$\frac{\mu}{I} = g\gamma. \tag{7.2}$$

In the case of the electron, Dirac's theory leads to a predicted value for g of 2, and this is in good agreement with the electron's measured magnetic dipole moment. In the case of the nucleon, there is no similar theoretical guidance and we use the measured values of μ together with equation 7.2 to arrive at the value of g. For the proton, $\mu_p = 2{\cdot}7934$ nuclear magnetons, and therefore the g-factor, which for rotational or spin angular momentum we shall denote by g_{sp}, will be $\mu_p/\frac{1}{2} = 5{\cdot}5868$. It is found experimentally that the neutron, despite its having zero net electric charge, has a finite magnetic dipole moment. This indicates that the neutron has internal electrical structure with different positive and negative charge distributions, the total charge being zero. The measured magnetic moment in the case of the neutron is $-1{\cdot}9135$ nuclear magnetons, the negative sign indicating that the direction of the dipole is related to the spin direction as it would be for a negatively charged body. The corresponding g-factor, $g_{sn} = \mu_n/\frac{1}{2} = -3{\cdot}8270$. It is convenient to modify equation 7.1 when applied to orbital motion by introducing in this case too a g-factor. For the proton, which behaves in this respect as a classical point charge, the value of this g-factor g_{lp} will be unity. The neutron, again as would be expected on the classical view, makes no contribution to the magnetic moment by virtue of its orbital motion and therefore $g_{ln} = 0$.

7.2 Relationship of magnetic moment to nuclear spin

Let the nucleon be in an l-state. Then the angular-momentum vector diagram when spin-orbit coupling is assumed is drawn in Figure 29. The orbital angular momentum of absolute magnitude $\sqrt{[l(l+1)]}\,\hbar$ we denote by $\mathbf{l}$, the spin angular momentum by $\mathbf{s}$ and their resultant by $\mathbf{j}$, where, as in section 6.7, $\mathbf{j} = \mathbf{l} + \mathbf{s}$. The vectors $\mathbf{l}$ and $\mathbf{s}$ precess about $\mathbf{j}$, which in turn precesses about the direction of an applied magnetic field. $\mathbf{j}$ has a component $j\hbar$ along the field direction. If the g_l and g_s factors were equal then the same diagram, suitably scaled, would represent the magnetic dipole-moment vectors. However we have seen that the g_l and g_s factors are not equal for either type of nucleon. The magnetic moment associated with $\mathbf{l}$ will have a component along the direction of $\mathbf{j}$ and also a component perpendicular to it. The perpendicular component will time-average

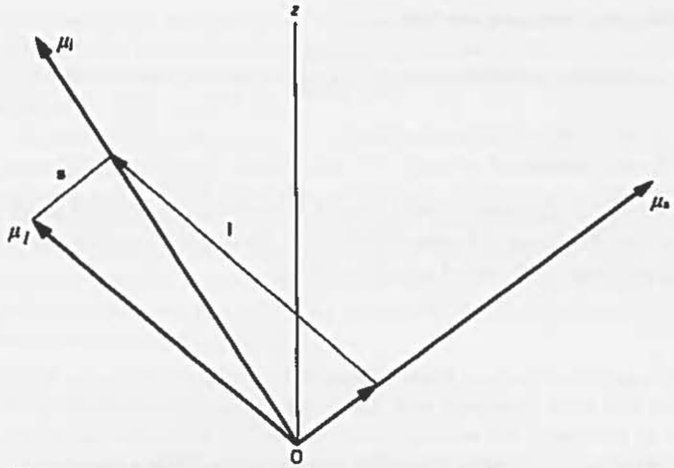

Figure 29 Contributions to nuclear magnetic dipole moment, arising from nucleon orbital and spin angular momenta, plotted on an angular-momentum vector diagram. Note that μ_j is only one component of the resultant of μ_l and μ_s

to zero. Similarly for the components associated with s. If we then take the sum of the components along j and resolve this sum along and perpendicular to the field direction, again the perpendicular component can be discounted and the measured dipole moment is the component of the sum along the field direction, when the angle between j and the field is the smallest of the discrete number of permitted angles. Carrying out this programme we have, for the sum of the components of the moments along j, the expression

$$\frac{1}{\hbar}[g_l|\mathbf{l}|\cos(\mathbf{l},\mathbf{j}) + g_s|\mathbf{s}|\cos(\mathbf{s},\mathbf{j})].$$

Resolving this along the field direction, the observed moment is found to be given by μ, where

$$\mu = \frac{1}{\hbar}[g_l|\mathbf{l}|\cos(\mathbf{l},\mathbf{j}) + g_s|\mathbf{s}|\cos(\mathbf{s},\mathbf{j})]\cos(\mathbf{j}, Oz)$$

$$= \frac{g_l[l(l+1)+j(j+1)-s(s+1)] + g_s[s(s+1)+j(j+1)-l(l+1)]}{2(j+1)},$$

using the elementary trigonometrical formula for the cosine of the angle in a triangle.

Take now the case $j = l + s$. We substitute $\frac{1}{2}$ for s and $j - \frac{1}{2}$ for l, and find

$$\mu_{l+\frac{1}{2}} = g_l(j-\tfrac{1}{2}) + \tfrac{1}{2}g_s = lg_l + \tfrac{1}{2}g_s.$$

For $j = l - s$, we have $s = \frac{1}{2}$ and $l = j + \frac{1}{2}$, and therefore

$$\mu_{l-\frac{1}{2}} = \frac{j}{j+1}[g_l(j+\tfrac{3}{2}) - \tfrac{1}{2}g_s] = \frac{j}{j+1}[(l+1)g_l - \tfrac{1}{2}g_s].$$

We must treat the cases of the proton and neutron separately, as their g-factors are different. If the particle concerned is a proton ($g_{lp} = 1$, $g_{sp} = 5{\cdot}5863$) and we take the case $j = l + \frac{1}{2}$, then $\mu_p = j + 2{\cdot}29$.

For a proton and $j = l - \frac{1}{2}$,

$$\mu_p = \frac{j}{j+1}(j - 1{\cdot}29)$$

$$= j - 2{\cdot}29\frac{j}{j+1}.$$

For a neutron ($g_{ln} = 0$, $g_{sn} = -3{\cdot}8270$) and $j = l + \frac{1}{2}$,

$$\mu_n = -1{\cdot}91.$$

For a neutron and $j = l - \frac{1}{2}$,

$$\mu_n = 1{\cdot}91\frac{j}{j+1}.$$

7.3 Schmidt lines

If we now use these results in conjunction with the shell-model hypothesis (namely the assumption that the spin and magnetic moment in odd-A nuclei

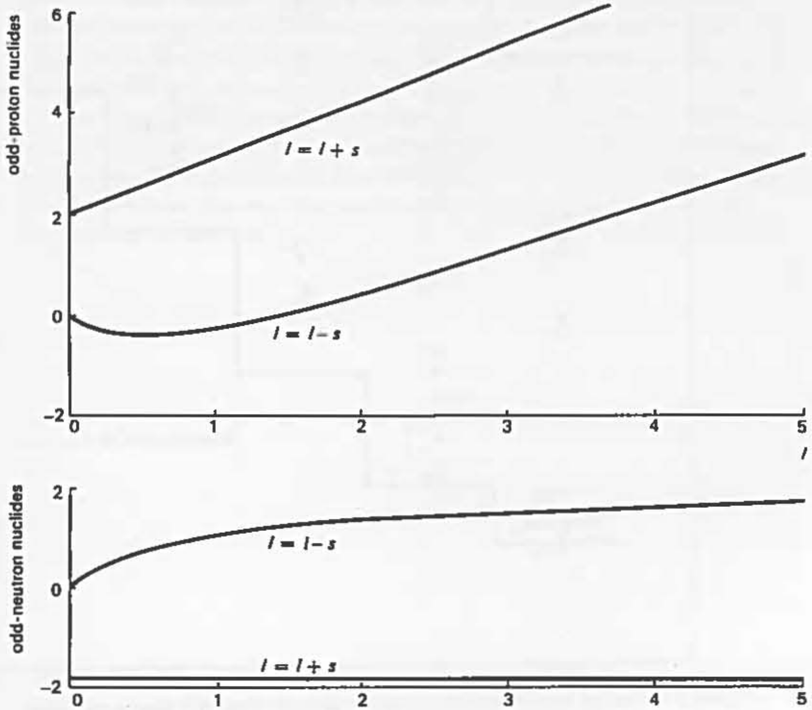

Figure 30 The theoretical Schmidt lines of magnetic dipole moment plotted against nuclear spin quantum number

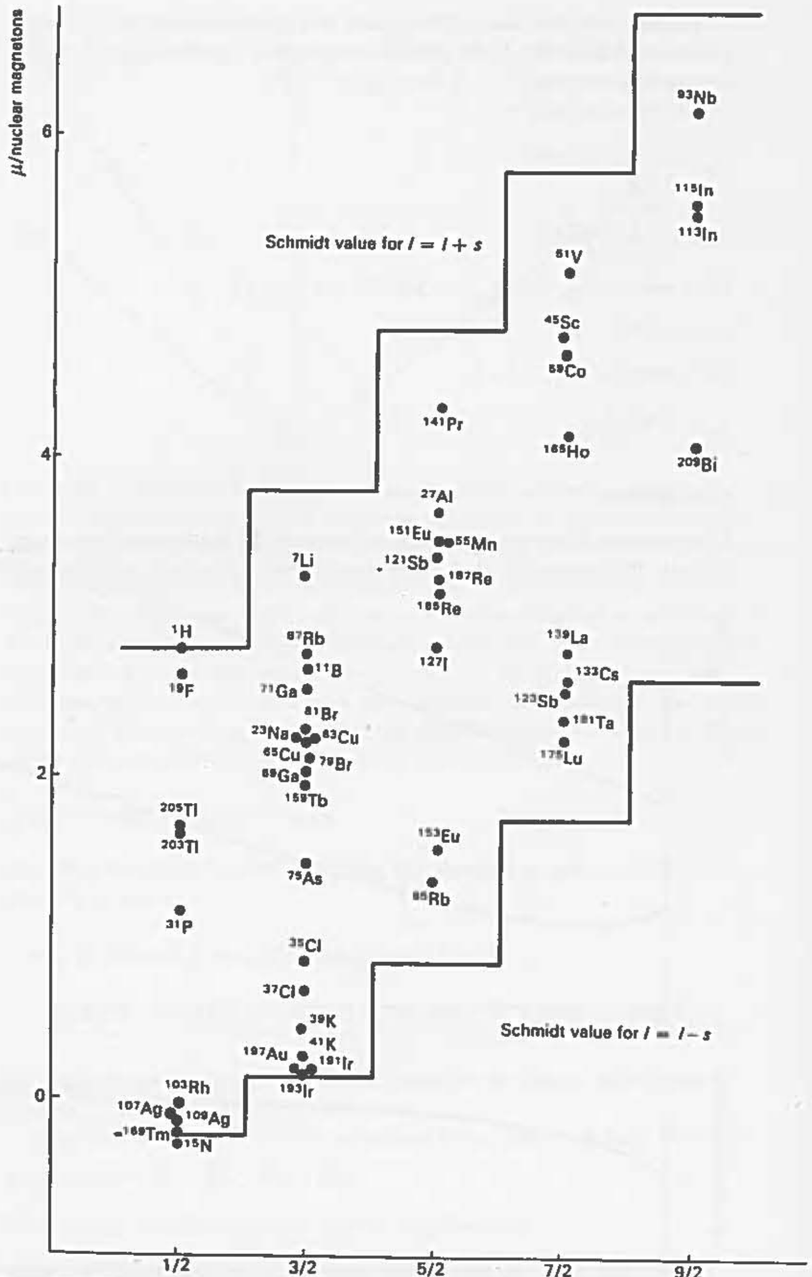

Figure 31 Plot of experimental values of nuclear magnetic dipole moment against nuclear spin quantum number of odd-A nuclei containing an odd number of protons

arise solely from the motion of the unpaired nucleon), then I, the nuclear spin, can be equated with j. The predicted magnetic dipole moments for odd-A nuclei will then be as in Table 4. I has, of course, only discrete values. However, if we

Table 4

	Proton (*odd Z : even N*)	*Neutron* (*even Z : odd N*)
$j = l + s$	$I + 2{\cdot}29$	$-1{\cdot}91$
$j = l - s$	$I - 2{\cdot}29\,\dfrac{I}{I+1}$	$1{\cdot}91\,\dfrac{I}{I+1}$

treat it as a continuous variable for diagrammatic purposes, then the predictions for the μ-values lie on the lines shown in Figure 30. These are known as the *Schmidt lines.* In Figures 31 and 32 histograms are drawn to correspond to the discrete values of I. On the diagrams are plotted the measured dipole moments for a series of nuclei. It can be seen that the agreement is by no means perfect. However, the lines clearly set limits to the measured values. In most cases the measured value falls much closer to one line than to the other and in these cases an assignment of the nucleus to one group or the other can be made with some confidence. This is important as it provides a means of discovering, once the j-value has been determined from a measurement of I, which of the two possible l-values has to be assigned to the unpaired nucleon. This in turn permits us to establish the parity of the nucleus, positive parity arising from zero and even values of l, negative parity from odd l-values. We return in a later chapter to the discrepancy between the measured and the 'single-particle' value of magnetic dipole moment.

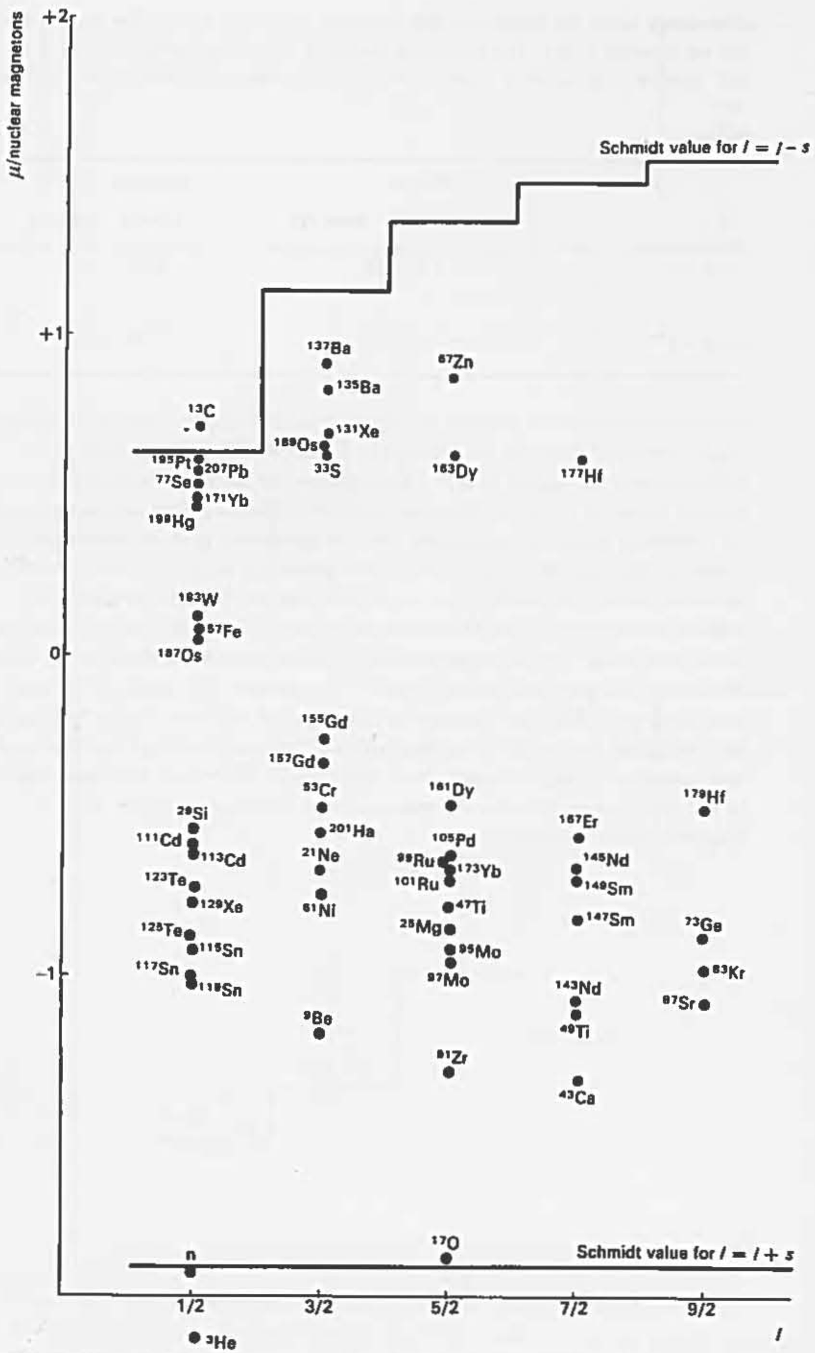

Figure 32 Plot of experimental values of nuclear magnetic dipole moment against nuclear spin quantum number for odd-A nuclei with an odd number of neutrons

7.4 Nuclear electric moments

The shell model claims to provide wave functions for the individual nucleons and hence should enable a prediction to be made of the spatial distribution of nucleons within the nuclear volume. As far as the protons are concerned, the prediction can be tested experimentally by investigating the static electric moments associated with the distribution. The measurement of these electric moments is related to the energy of the charge distribution as a function of its orientation when it is placed in an electric field. We therefore begin by discussing on the basis of classic electrostatics the energy relation between an external electric field and the internal distribution of nuclear charge.

We assume that the nucleus has a spin I and that by virtue of the rotation the averaged nuclear charge, which is the quantity measured experimentally, will be symmetric about the axis of I. We therefore limit our treatment to distributions having axial symmetry.

7.5 Multipole expansion of the electric potential

Consider $V(R, \theta)$, the electric potential at a point P with coordinates (R, θ), outside the volume of the charge distribution. As V must satisfy Laplace's equation, we can write

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0. \qquad 7.3$$

This can be transformed into the usual spherical coordinates. As we are assuming symmetry of the charge about the z-axis, the differential coefficient with respect to ϕ will be zero. Thus the transformed equation (see equation 6.2) is

$$\left[\frac{\partial^2}{\partial R^2} + \frac{2}{R}\frac{\partial}{\partial R} + \frac{1}{R^2}\frac{\partial^2}{\partial \theta^2} + \frac{\cot\theta}{R^2}\frac{\partial}{\partial \theta}\right] V = 0. \qquad 7.4$$

If a solution with the variables separated, of the form $V(R, \theta) = F(R)G(\theta)$, be assumed, then

$$\frac{R^2}{F(R)}\frac{d^2F(R)}{dR^2} + \frac{2R}{F(R)}\frac{dF(R)}{dR} = -\frac{1}{G(\theta)}\frac{d^2G(\theta)}{d\theta^2} - \frac{\cot\theta}{G(\theta)}\frac{dG(\theta)}{d\theta} \qquad 7.5$$

and each side of this equation must then be independent of R and θ. Let this constant be $l(l+1)$. The right-hand side of the equation then, with $\mu = \cos\theta$, reduces to

$$(1-\mu^2)\frac{d^2G}{d\mu^2} - 2\mu\frac{dG}{d\mu} + l(l+1)G = 0.$$

As noted in section 6.3, if we limit the choice of l to zero or positive integral values, this equation has as a solution $G = P_l(\cos\theta)$, where $P_l(\cos\theta)$ is a Legendre polynomial.

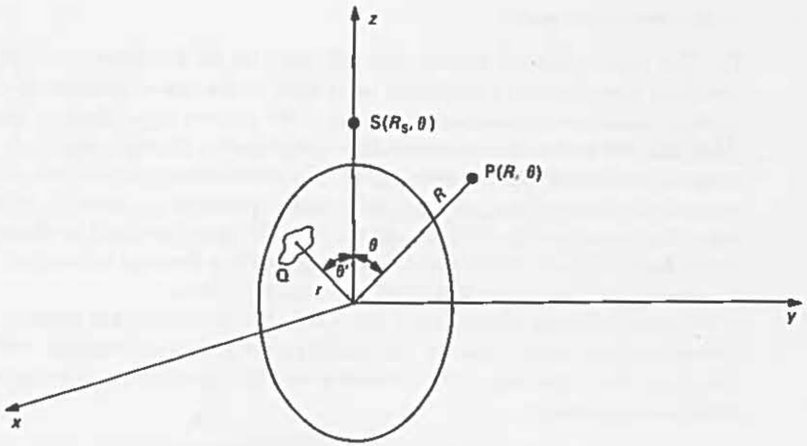

Figure 33 Charge distribution symmetrical about z-axis

Taking now the left-hand side of the equation we have

$$R^2 \frac{d^2F(R)}{dR^2} + 2R\frac{dF(R)}{dR} = l(l+1)F(R). \qquad 7.6$$

Assuming a solution of the form $F(R) = a_n/R^n$, where n is a positive integer (thus ensuring that $F(R)$ has the physically necessary property of tending to zero as R tends to infinity), and substituting in equation 7.6, we find that

$$n(n+1)\frac{a_n}{R^n} - 2n\frac{a_n}{R^n} = l(l+1)\frac{a_n}{R^n}.$$

If $F(R)$ is to be a solution, then we must have $n = l+1$. For the solution of equation 7.4 we therefore finally have

$$V(R,\theta) = \frac{1}{R}\sum_{l=0}^{\infty}\frac{a_l}{R^l}P_l(\cos\theta). \qquad 7.7$$

The values of the constants a_l will depend on the distribution of charge within the central volume. We can find the form of this dependence by considering the potential at the point S whose coordinates are $(R_S, 0)$. Since $P_l(1) = 1$ for all values of l, the potential at S, from equation 7.7, is given by

$$V(R_S,0) = \frac{1}{R_S}\sum_{l=0}^{\infty}\frac{a_l}{R_S^l}. \qquad 7.8$$

The potential at S can also be expressed directly in terms of the charge distribution. If $\rho_e(r,\theta')$ is the charge density at Q, the point (r,θ') within the nucleus, and $d\tau$ is an element of volume containing the point Q, then

$$V(R_S,0) = \int\frac{\rho_e(r,\theta')}{SQ}d\tau$$
$$= \int\frac{\rho_e(r,\theta')\,d\tau}{\sqrt{(R_S^2 + r^2 - 2rR_S\cos\theta')}}$$
$$= \frac{1}{R_S}\int\frac{\rho_e(r,\theta')\,d\tau}{\sqrt{\{1 - 2(r/R_S)\cos\theta' + r^2/R_S^2\}}} \qquad 7.9$$

Now, as can be shown by expanding by the binomial theorem,

$$\frac{1}{\sqrt{(1-2x\cos\theta + x^2)}} = \sum_{n=0}^{\infty}x^n P_n(\cos\theta).$$

Hence we can express equation 7.9 as

$$V(R_S,0) = \frac{1}{R_S}\sum_{n=0}^{\infty}\int\frac{\rho_e(r,\theta')r^n}{R_S^n}P_n(\cos\theta')\,d\tau. \qquad 7.10$$

If now we compare the coefficients of $1/R_S^{l+1}$ in equations 7.8 and 7.10, we see that

$$a_l = \int\rho_e(r,\theta')r^l P_l(\cos\theta')\,d\tau$$

is the relationship between the coefficients and the charge distribution.

7.6 Definition of the static electric moments

We proceed to consider the physical meaning to be attributed to the coefficients a_l in the above multipole expansion.

Since $P_0(\cos\theta) = 1$, for all values of θ, it follows that

$$a_0 = \int\rho_e(r,\theta')\,d\tau = Ze.$$

The first coefficient is thus seen to equal the total charge within the nuclear volume.

Thus, if in equation 7.7 R is assumed to be so large that we need only consider the first term in the series, the potential for the given distribution is the same as that for a point charge.

Proceeding to the next term we find that, since $P_1(\cos\theta) = \cos\theta$, we have

$$a_1 = \int\rho_e(r,\theta')r\cos\theta'\,d\tau = \int\rho_e(r,\theta')z\,d\tau. \qquad 7.11$$

This expression is the component of the first moment of the charge taken parallel to the z-axis. Note that the components of the first moment parallel to the other axes are zero because of the symmetry. The simplest distribution giving rise to a finite moment of this order and having net zero charge is the dipole formed by the displacement of equal and opposite charges e equal and opposite distances d from the origin. For this distribution $a_1 = 2ed$. At great distances from the dipole the potential as a function of θ is, to the order R^{-2}, given by

$$V = \frac{2ae}{R^2}\cos\theta,$$

in line with the angular-dependent factor in the second term of equation 7.7.

Thus, if we wish to include the second term in equation 7.7, we can regard the general charge distribution as equivalent to a point charge at the centre plus a dipole also at the centre, the dipole moment being calculated from equation 7.11. When the charges in the distribution are all of the same sign, a dipole moment can arise if the charges are not symmetrically distributed about the point with respect to which the potential is calculated. This point will normally be the centre of mass of the system. We shall see later that, in fact, nuclei do not have finite electric dipole moments.

The third term in equation 7.7 involves $P_2(\cos\theta)$, which is equal to $\frac{1}{2}(3\cos^2\theta - 1)$. Hence we have

$$a_2 = \tfrac{1}{2}\int \rho_e(r,\theta')r^2(3\cos^2\theta - 1)\,d\tau = \tfrac{1}{2}\int \rho_e(r,\theta')(3z^2 - r^2)\,d\tau. \qquad 7.12$$

We now introduce

$$Q = \frac{1}{e}\int \rho_e(r,\theta')(3z^2 - r^2)\,d\tau$$

and can therefore write $a_2 = \frac{1}{2}eQ$. We call Q the *quadrupole moment* and on this definition, which is that now commonly used in nuclear physics, it has the dimensions of area.

The simple distribution shown in Figure 34, which is the symmetrical displacement of equal and opposite dipoles from the origin, is seen to have zero net charge and zero dipole moment. The quadrupole moment as defined above is given by $Q = 4b^2$, since $z = r$ for this linear quadrupole. The potential at P is thus

$$V_P = \frac{eb^2}{R^3}(3\cos^2\theta - 1),$$

to lowest order in R^{-1}.

This process of developing multipoles which are equivalent to the terms in equation 7.7 can be continued in an obvious way to higher orders. However, while electric quadrupole moments are of important current interest in nuclear physics, information about possible moments of higher order is not yet accessible to the experimentalist.

The odd electric moments – dipole, octupole, etc. – are zero for a nuclear system which has a definite parity, whether that parity be positive or negative. This is so because the amplitude of the wave function being unaltered when

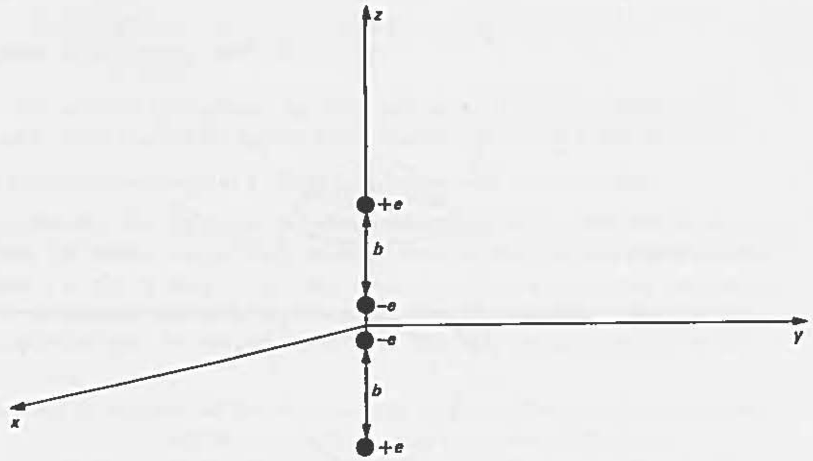

Figure 34 System of four point charges having zero net charge, zero net dipole moment and finite quadrupole moment with symmetry about the z-axis. Note that in a constant electric field the dipoles experience equal and opposite couples; the system experiences no resultant couple. However, in a field with a constant gradient parallel to the z-axis the couples on the dipoles are no longer equal, so that the system experiences a resultant couple. The net force on each dipole is equal and opposite if the field gradient is constant so that there is no resultant force on the system

$(-x, -y, -z)$ is substituted for (x, y, z) means that $\rho_e(r,\theta')$, which is proportional to ψ^2, is unaltered on this transformation. For odd values of l however $P_l(\cos\theta)$, the other factor in the integral defining the moment of the multipole, is an odd function in $\cos\theta$. The above parity transformation, which changes the sign of $\cos\theta$, thus changes the sign of $P_l(\cos\theta)$. Consequently when the integration is performed over the whole volume for odd values of l the result is zero. Similar arguments applied to the magnetic moments show that if the nuclear system has a definite parity, then the *even* magnetic moments – i.e. quadrupole etc. – are zero. The fact that these predictions seem to be borne out when nuclear electric and magnetic moments are measured indicates that nuclei do have a definite parity. We note that this means that their shapes must be symmetrical about the xy plane. Thus spheres and ellipsoids of revolution are permitted but a pear shape would violate the parity requirement.

7.7 Quadrupole moment of deformed sphere

In the interpretation of quadrupole moments we shall have occasion to picture nuclei as slightly deformed spheres. We now proceed to calculate the quadrupole moment of a uniformly charged sphere, slightly deformed to become an ellipsoid of revolution, having a semi-axis length c along the z-axis and semi-axes each length b along the x- and y-axes.

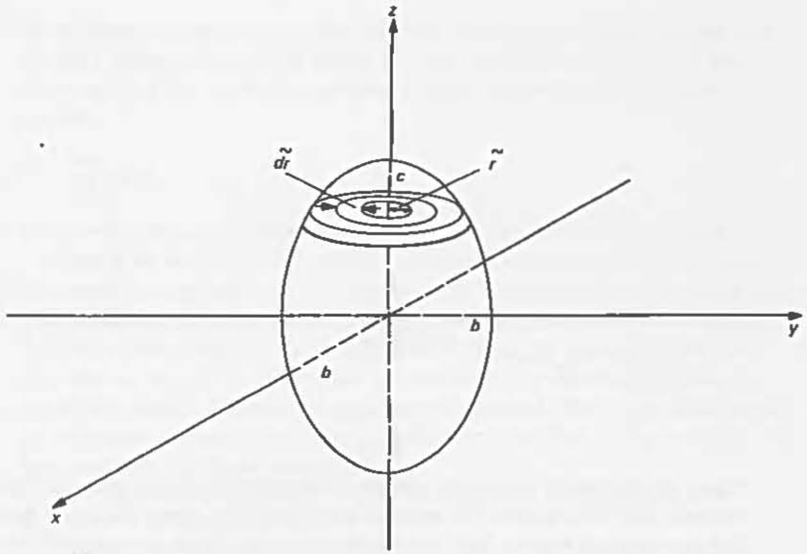

Figure 35 Division of spheroid into ring elements for the calculation of its quadrupole moment

The quadrupole moment Q will then be given by

$$eQ = \int \rho_e (3z^2 - r^2)\, d\tau$$

$$= \int \rho_e (3z^2 - z^2 - \tilde{r}'^2) 2\pi \tilde{r}'\, d\tilde{r}'\, dz,$$

where the volume element $d\tau$ has been taken as a ring lying in the disc at a distance z from the origin, as depicted in Figure 35. Hence

$$eQ = 2\pi\rho_e \int_{-a}^{+a} dz \int_{0}^{y^2} (2z^2 - \tilde{r}'^2)\tilde{r}'\, d\tilde{r}',$$

where y^2 is defined by the equation of the generating ellipse, namely

$$\frac{z^2}{c^2} + \frac{y^2}{b^2} = 1.$$

On integrating we have

$$eQ = \tfrac{8}{15}\pi\rho_e c b^2 (c^2 - b^2)$$

$$= Ze\tfrac{2}{5}(c^2 - b^2),$$

since the volume of the ellipsoid is $\tfrac{4}{3}\pi c b^2$ and Ze is the total charge.

We thus have

$$Q = Z\tfrac{4}{5}\eta R^2,$$

where $\eta = \dfrac{c^2 - b^2}{c^2 + b^2}$ and $R^2 = \dfrac{c^2 + b^2}{2}$.

We note that the algebraic sign of Q depends on the relative lengths of c and b, and is positive for prolate spheroids and negative for oblate spheroids.

7.8 The interaction energy of a charge distribution with an electric field

We consider now the interaction energy of a charge distribution with an electric field. The field is assumed to be axially symmetric about an axis which we shall denote by Oz'. In the practical cases to which we shall wish to apply this theory, the field will be that at the nucleus arising from the Coulomb charge of the atomic electrons. In that circumstance Oz' will be in the direction of $\mathbf{J}$, where

$\mathbf{J} = \mathbf{L} + \mathbf{S}$,

$\mathbf{L}$ being the resultant of the orbital angular momenta of the electrons and $\mathbf{S}$ the resultant of their individual spins. We take an axis system Ox', Oy', Oz', symmetrical with respect to the field, and a system Ox, Oy, Oz symmetrical with respect to the charge distribution, as in Figure 36. The electric field we take

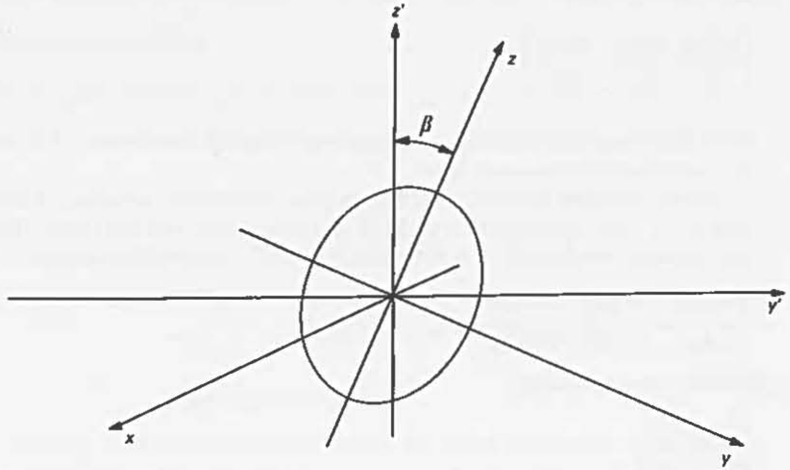

Figure 36 Ox', Oy', Oz' are fixed axes in an electric field which is symmetric about the z'-axis. Ox, Oy, Oz are axes fixed with respect to the spheroid. The x- and x'-axes instantaneously coincide

to be defined by an electrostatic potential $\phi(x, y', z')$. This function may be expanded in the neighbourhood of the origin, which we take to be the centre of mass of the nucleus and of the atom as a whole, to give

$$\phi(x, y', z') = \phi(0) + \left(x\frac{\partial\phi(0)}{\partial x} + y'\frac{\partial\phi(0)}{\partial y'} + z'\frac{\partial\phi(0)}{\partial z'}\right) +$$

$$+ \frac{1}{2}\left(x^2\frac{\partial^2\phi(0)}{\partial x^2} + 2xy'\frac{\partial^2\phi(0)}{\partial x\,\partial y'} + \ldots + z'^2\frac{\partial^2\phi(0)}{\partial z'^2}\right) + \ldots .$$

Taking $\rho_e(x, y', z')$ as the charge density, the energy of the system can then be expressed as

$$W = \int \rho_e(x,y',z')\phi(x,y',z')\,d\tau$$

$$= \int \rho_e(x,y',z')\phi(0)\,d\tau + \int \rho_e(x,y',z')\left[x\frac{\partial\phi(0)}{\partial x} + y'\frac{\partial\phi(0)}{\partial y'} + z'\frac{\partial\phi(0)}{\partial z'}\right]d\tau +$$

$$+\frac{1}{2}\int \rho_e(x,y',z')\left[x^2\frac{\partial^2\phi(0)}{\partial x^2} + 2xy'\frac{\partial^2\phi(0)}{\partial x\,\partial y'} + \ldots + z'^2\frac{\partial^2\phi(0)}{\partial z'^2}\right]d\tau + \ldots$$

$$= W_{\mathrm{C}} + W_{\mathrm{D}} + W_Q + \ldots.$$

W_{C}, which is simply equal to

$$\phi(0)\int \rho_e(x,y',z')\,d\tau,$$

is seen to represent the Coulomb energy associated with the equivalent point charge. W_{D} represents the energy of the dipole moment of the charge distribution in the constant field

$$\left[\frac{\partial\phi(0)}{\partial x}, \frac{\partial\phi(0)}{\partial y'}, \frac{\partial\phi(0)}{\partial z'}\right].$$

When the charge distribution being considered is that of a nucleus $W_{\mathrm{D}} = 0$, since the electrical dipole moment is equal to zero.

We now consider the third term W_Q. Because of the axial symmetry, ϕ depends on x and y' only through its dependence on the distance from the z'-axis. Hence in ϕ, x and y' appear only in the combination $\sqrt{(x^2 + y'^2)}$. It follows that

$$\frac{\partial^2\phi(0)}{\partial x\,\partial y'} = \frac{\partial^2\phi(0)}{\partial x\,\partial z'} = \frac{\partial^2\phi(0)}{\partial y\,\partial z'} = 0.$$

Further, from symmetry,

$$\frac{\partial^2\phi}{\partial x^2} = \frac{\partial^2\phi}{\partial y'^2}.$$

Also, if we assume that ϕ arises from the atomic-electron Coulomb charge, and if we neglect the charge density of the orbital electrons within the nuclear volume, then ϕ satisfies Laplace's equation at the origin,

i.e. $$\frac{\partial^2\phi(0)}{\partial x^2} + \frac{\partial^2\phi(0)}{\partial y'^2} + \frac{\partial^2\phi(0)}{\partial z'^2} = 0,$$

and so $$\frac{\partial^2\phi(0)}{\partial z'^2} = -2\frac{\partial^2\phi(0)}{\partial x^2} = -2\frac{\partial^2\phi(0)}{\partial y'^2}.$$

Hence $$W_Q = \frac{1}{2}\int \rho_e(x,y',z')\left[z'^2\frac{\partial^2\phi(0)}{\partial z'^2} - \frac{1}{2}(x^2+y'^2)\frac{\partial^2\phi(0)}{\partial z'^2}\right]d\tau$$

$$= \frac{1}{4}\int \rho_e(x,y',z')(3z'^2 - r^2)\frac{\partial^2\phi(0)}{\partial z'^2}\,d\tau,$$

where $r = \sqrt{(x^2 + y'^2 + z'^2)}$. Thus finally we have

$$W_Q = \tfrac{1}{4}q\int \rho_e(x,y',z')(3z'^2 - r^2)\,d\tau,$$

where q is the gradient of the electric field intensity in the direction Oz'. We now express the integral in terms of the coordinates (x, y, z), which refer to the body axes Ox, Oy, Oz, noting that $z' = z\cos\beta - y\sin\beta$. Therefore

$$W_Q = \tfrac{1}{4}q\int \rho_e(x,y,z)(3z^2\cos^2\beta + 3y^2\sin^2\beta - 6yz\sin\beta\cos\beta - r^2)\,d\tau.$$

From the axial symmetry of the charge distribution,

$$\int yz\,\rho_e(x,y,z)\,d\tau = 0.$$

Also from symmetry

$$\int y^2\rho_e(x,y,z)\,d\tau = \int x^2\rho_e(x,y,z)\,d\tau$$

$$= \tfrac{1}{2}\int (x^2+y^2)\rho_e(x,y,z)\,d\tau$$

$$= \tfrac{1}{2}\int (r^2 - z^2)\rho_e(x,y,z)\,d\tau.$$

Therefore $$W_Q = \tfrac{1}{4}q\int \rho_e(x,y,z)\,[3z^2\cos^2\beta + \tfrac{3}{2}(r^2 - z^2)\sin^2\beta]\,d\tau$$

$$= \tfrac{1}{8}q\left[\int \rho_e(x,y,z)(3z^2 - r^2)\,d\tau\right](3\cos^2\beta - 1)$$

$$= \tfrac{1}{8}qeQ_0(3\cos^2\beta - 1), \qquad 7.13$$

where Q_0 is the quadrupole moment of the charge distribution as defined in section 7.6.

Equation 7.13 gives the interaction energy of a nucleus having a quadrupole moment Q_0 when its symmetry axis lies at an angle β to the symmetry axis of an axially symmetrical electric field with a field gradient q at the site of the nucleus.

7.9 Quadrupole moments in quantum-mechanical systems

The nucleus has as its axis of averaged symmetry the axis of the total angular momentum **I**. We now consider the nucleus to be placed in an electric field of axial symmetry at a point in the field where the gradient along the field symmetry axis Oz' is q. The couple arising from the interaction of the quadrupole moment with the field gradient will cause **I** to precess about Oz′. The usual quantum-mechanical conditions will require that the angle between **I** and Oz′ be such that the component of angular momentum parallel to Oz′ is $M_I\hbar$, where M_I is integral if I is integral, M_I is half-integral if I is half-integral, and where $|M_I| \leqslant I$. Since the angle of precession β can never be zero, the value of W_Q can never attain the value it would have in the classical case for a charge distribution with quadrupole moment Q_0, where the angle β could be zero. In the quantum-mechanical case the minimum value of the angle β will be

$$\cos^{-1}\frac{I}{\sqrt{[I(I+1)]}},$$

and the interaction energy for this orientation is given by

$$\begin{aligned} W_Q &= \tfrac{1}{8}qeQ_0\left[3\frac{I^2}{I(I+1)}-1\right] \\ &= \tfrac{1}{8}qeQ_0\left[\frac{2I-1}{I+1}\right]. \end{aligned} \qquad 7.14$$

We now introduce Q as the effective quadrupole moment, that is, the quadrupole moment which is observed experimentally. It will be less than the intrinsic quadrupole moment Q_0, because of the averaging of the charge distribution by the necessary precession of **I**. From 7.13, the maximum value of W_Q is

$$\tfrac{1}{8}qeQ(3\cos^2 0^\circ - 1) = \tfrac{1}{4}qeQ.$$

Comparing this expression with equation 7.14, we see that

$$Q = \frac{2I-1}{2(I+1)}Q_0.$$

We now consider the expressions for the interaction energies of the magnetic substates. The angle β is given by

$$\cos^{-1}\frac{M_I}{\sqrt{[I(I+1)]}}$$

and hence

$$\begin{aligned} (W_Q)_{M_I} &= \tfrac{1}{8}qeQ_0\left[\frac{3M_I^2}{I(I+1)}-1\right] \\ &= \tfrac{1}{8}qeQ\,\frac{2(I+1)}{2I-1}\left[\frac{3M_I^2-I(I+1)}{I(I+1)}\right] \\ &= \tfrac{1}{4}qeQ\left[\frac{3M_I^2-I(I+1)}{I(2I-1)}\right]. \end{aligned} \qquad 7.15$$

We now have to consider the two special cases $I = 0$ and $I = \frac{1}{2}$. Let us assume that we are dealing with a nucleus whose shape is that of an ellipsoid of revolution having an axis of symmetry Oz. When $I = 0$ there will be no rotation about the symmetry axis Oz. The lack of angular momentum about this axis enables the nucleus to lie with this axis orientated at random with respect to any specified direction. The arguments made above are then no longer valid for this case. The randomness of orientation of the nucleus will ensure its equivalence to a spherically symmetric charge distribution. Thus, although it has a finite intrinsic quadrupole moment Q_0, the effective quadrupole moment Q is zero. Turning to the case of $I = \frac{1}{2}$, we note that β must have the value $\cos^{-1}(1/\sqrt{3})$ and hence the nuclear orientation is always such that $(3\cos^2\beta - 1) = 0$. Hence, as is clear from the above expression for Q in terms of Q_0, again the effective quadrupole moment is zero despite the nucleus having an intrinsic quadrupole moment. We therefore arrive at the important conclusion that the measured quadrupole moment can only be finite for $I \geqslant 1$. This is found to be in accord with experimental measurements.

7.10 Summary

The theoretical concept of magnetic dipole moment was developed to establish, on the basis of the single-particle hypothesis, the relationship between the single-particle quantum numbers and the nuclear dipole moment.

The static electric moments of the nucleus were defined, particular attention being paid to the electric quadrupole moment and its role in connection with the classical interaction energy of the nucleus with an electric field. The modifications to these results arising from a quantum-mechanical treatment were discussed.