and $i_{13/2}$ are the most easily polarisable for protons and neutrons, respectively. From these subshells, a one-particle–one-hole state can easily be excited as $\left(h_{11/2}\right)^{-1} h_{9/2}$ and $\left(i_{13/2}\right)^{-1} i_{11/2}$ respectively.

As a final remark on magnetic moments, let us mention that not only g_s but also g_ℓ might be subject to a modification relative to the 'free'-nucleon value. However, both experiment and theory point to a $|\delta g_\ell|$ not exceeding about 0.1 nuclear magnetons (see e.g. Häusser *et al.*, 1977, and references therein).

7.2 The electric quadrupole moment

Another nuclear quantity first observed on the basis of optical spectra is the electric quadrupole moment. One found certain deviations from Lande's interval rule for the hyperfine structure. These could be ascribed to the coupling between the electric quadrupole moment of the nucleus and the wave function of the electrons (Kopfermann, 1958).

Classically the electrostatic interaction energy due to the coupling between the electron cloud and the nucleus is given by the expression

$$W = e \int \rho_Z(\mathbf{r}) \phi(\mathbf{r})\, \mathrm{d}\tau$$

where ρ_Z is the electric charge density of the nucleus and ϕ the electrostatic potential due to the electrons. By expansion of $\phi(\mathbf{r})$ around the nuclear centre of gravity point one obtains

$$W = e \int \rho_Z \phi(0)\, \mathrm{d}\tau + e \int \rho_Z \nabla\phi \cdot \mathbf{r}\, \mathrm{d}\tau + \frac{e}{2} \int \rho_Z \left(\phi_{xx} x^2 + 2\phi_{xy} xy + \ldots\right) \mathrm{d}\tau + \ldots$$

where $\phi_{xy} = \partial^2\phi/\partial x\, \partial y$ etc., all derivatives assumed evaluated at the origin. The first integral corresponds to the case of a point charge at the origin. In the absence of a nuclear dipole moment, $\int \rho_Z \mathbf{r}\, \mathrm{d}\tau = 0$, the second term vanishes identically. Thus, the third integral gives the lowest order effect of the finite extension of the nucleus. With the coordinate system having its z-axis along the electronic axis of rotational symmetry (then excluding spherically symmetric $s_{1/2}$ and $p_{1/2}$ electrons for which such an axis cannot be defined, cf. fig. 7.6 below), the non-diagonal terms ϕ_{xy} etc. disappear leaving an energy contribution from the third term as

$$W_Q = \frac{e}{2} \left[\phi_{xx} \int \rho_Z x^2\, \mathrm{d}\tau + \phi_{yy} \int \rho_Z y^2\, \mathrm{d}\tau + \phi_{zz} \int \rho_Z z^2\, \mathrm{d}\tau\right]$$

The relation

$$\nabla^2\phi = 0$$

combined with the assumption of axial symmetry around the z-axis leads to

$$\phi_{zz} = -2\phi_{xx} = -2\phi_{yy}$$

We then obtain the third integral simplified to the following form

$$W_Q = -\frac{\phi_{xx}}{2} e \int \left(3z^2 - r^2\right) \rho_Z \, \mathrm{d}\tau$$

Assuming that the nucleus is rotationally symmetric, a new coordinate system (x', y', z') with the z'-axis along the nuclear symmetry axis is introduced. Now, if the angle between the z- and z'-axes is β, it is straightforward to make a coordinate transformation (cf. problem 7.2) to obtain:

$$W_Q = -\frac{\phi_{xx}}{2} e \int \left(3\,(z')^2 - r^2\right) \rho_Z \, \mathrm{d}\tau \left(\frac{3}{2}\cos^2\beta - \frac{1}{2}\right)$$

We now define the quadrupole moment (Q or Q_2) as the integral

$$Q = \int \left(3\,(z')^2 - r^2\right) \rho_Z \, \mathrm{d}\tau$$

or its quantum mechanical generalisation (dropping the 'primes' on the nuclear oriented coordinate system)

$$Q = \int \psi^* \sum_p \left(3z_p^2 - r_p^2\right) \psi \, \mathrm{d}\tau$$

where the sum is to be taken over the charge-carrying particles, i.e. in our case the protons in the nucleus. Note that the quadrupole moment, according to the standard definition, has the dimension of an area. The unit of charge thus does not enter. In terms of spherical coordinates we write for a single proton

$$Q_p = 3z_p^2 - r_p^2 = r_p^2 \left(\frac{16\pi}{5}\right)^{1/2} Y_{20}\left(\theta_p, \phi_p\right)$$

For the extreme single-particle model, only the 'valence'-particle contributes to the quadrupole moment. Furthermore, by definition the quadrupole moment is calculated in the $m = j$ state and we thus obtain

$$Q = \begin{bmatrix} e_\mathrm{n} \\ e_\mathrm{p} \end{bmatrix} \left(\frac{16\pi}{5}\right)^{1/2} \left\langle r^2 \right\rangle_{N\ell} \left\langle \ell \frac{1}{2} jj \right| Y_{20} \left| \ell \frac{1}{2} jj \right\rangle = -\begin{bmatrix} e_\mathrm{n} \\ e_\mathrm{p} \end{bmatrix} \cdot \frac{2j-1}{2j+2} \left\langle r^2 \right\rangle_{N\ell}$$

where for the neutron and the proton we have $e_\mathrm{n} = 0$ and $e_\mathrm{p} = 1$, respectively. We shall derive this result for the case $j = \ell + \frac{1}{2}$ and will leave the proof that it holds also for $j = \ell - \frac{1}{2}$ to the exercises. We consider the matrix element

$$\left\langle \ell \frac{1}{2} jj \right| Y_{20} \left| \ell \frac{1}{2} jj \right\rangle$$

Let us here introduce the notation that bra- and ket-vectors, written with *rounded parentheses* imply that *only the angular integral* enters. The wave function in the $j = \ell + \frac{1}{2}$ case (corresponding to the case of parallel spin and orbital angular momentum),

$$\left| \ell\, s\, j = \ell + \frac{1}{2}\, m = j \right) = \sum_{m_\ell m_s} Y_{\ell m_\ell} \cdot \chi_{s m_s} C^{\ell\, s\, j=\ell+\frac{1}{2}}_{m_\ell\, m_s\, m=\ell+\frac{1}{2}} = Y_{\ell\ell}\chi_{\frac{1}{2}\frac{1}{2}}$$

comes out very simple because there is only one possibility of having $m_\ell + m_s = \ell + \frac{1}{2}$, namely $m_\ell = \ell, m_s = \frac{1}{2}$ (in the derivation of the magnetic moment above, this same fact was obtained from a direct evaluation of the Clebsch–Gordan coefficients obtained as 1 and 0, respectively). We now obtain

$$\left(\ell\, \frac{1}{2}\, j = \ell + \frac{1}{2}\, j \right| Y_{20} \left| \ell\, \frac{1}{2}\, j = \ell + \frac{1}{2}\, j \right) = \int \mathrm{d}\Omega\; Y^*_{\ell\ell}\, \chi^+_{\frac{1}{2}\frac{1}{2}} Y_{20}\, \chi_{\frac{1}{2}\frac{1}{2}} Y_{\ell\ell} \equiv \mathcal{I}$$

Note that

$$\chi^+_{\frac{1}{2}\frac{1}{2}}\chi_{\frac{1}{2}\frac{1}{2}} = (1 \quad 0)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1$$

and therefore

$$\mathcal{I} = \int Y^*_{\ell\ell}(\theta, \phi)\, Y_{20}(\theta, \phi)\, Y_{\ell\ell}(\theta, \phi)\, \mathrm{d}\Omega$$

In the preceding chapter, we quoted the addition formula for spherical harmonics

$$Y_{\ell m}(\theta, \phi)\, Y_{\ell' m'}(\theta, \phi) = \sum_{LM} \left(\frac{(2\ell + 1)(2\ell' + 1)}{4\pi(2L + 1)} \right)^{1/2} \cdot C^{\ell\ell' L}_{mm' M} \cdot C^{\ell\ell' L}_{000}\, Y_{LM}(\theta, \phi)$$

The sum over M obviously contains one term, $M = m + m'$ and consequently

$$Y_{20} Y_{\ell\ell} = \sum_L C^{\ell 2 L}_{\ell 0 \ell} Y_{L\ell} C^{\ell 2 L}_{000} \left(\frac{(2\ell + 1)(2 \cdot 2 + 1)}{4\pi(2L + 1)} \right)^{1/2}$$

Owing to orthogonality it follows that the only non-vanishing contributions to the angular integral above are those with $L = \ell$. We have thus

$$\mathcal{I} = \left(\frac{5}{4\pi} \right)^{1/2} C^{\ell 2 \ell}_{\ell 0 \ell} C^{\ell 2 \ell}_{000}$$

and if the values of the Clebsch–Gordan coefficients (available e.g. from table 6B.1) are inserted, one obtains

$$Q = -\begin{bmatrix} e_{\mathrm{n}} \\ e_{\mathrm{p}} \end{bmatrix} \frac{2\ell}{2\ell + 3} \left\langle r^2 \right\rangle_{N\ell}$$

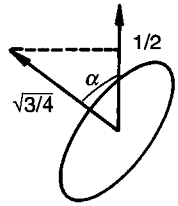

Fig. 7.6. Vector model of a spin $\frac{1}{2}$ particle. The angle α is quite large. This leads to a wave function that is smeared over all angles in such a way that the quadrupole moment Q vanishes.

which can be transformed to

$$Q = -\begin{bmatrix} e_n \\ e_p \end{bmatrix} \frac{2j-1}{2j+2} \left\langle r^2 \right\rangle_{N\ell}$$

This relation has thus been proven for $j = \ell + \frac{1}{2}$. In the exercises it is shown that this expression, with Q expressed in terms of j, also holds for $j = \ell - \frac{1}{2}$. This means that the quadrupole moment depends only on j and not on ℓ.

Note that directly from the expression for Q in terms of j it is apparent that $Q = 0$ for $j = \frac{1}{2}$. The quantum fluctuations are then so large that no deviation from sphericity can be observed. The picture provided by the vector model for these relations is illustrated in fig. 7.6. The length of the vector is $[j(j+1)]^{1/2} = \sqrt{\frac{3}{4}}$ (in units of $\hbar$) and the length of the z-component is $\frac{1}{2}$. In terms of this model the orbit precesses around the z-axis. This precession smears the charge distribution in space relative to that of the orbital by the smearing factor $(2j-1)/(2j+2)$. For $j = \frac{1}{2}$ the angle α is so large and the smearing as a consequence so severe that Q vanishes exactly.

We have derived an expression for the quadrupole moment valid for closed shells plus 1 particle. For the case of closed shells plus 1 hole the corresponding formula holds but with the opposite sign. We have thus

$$Q(\text{hole}) = -Q(\text{particle})$$

The situation is thus opposite to that for the magnetic moment. The reason for the change of sign for the quadrupole moment can be understood from an inspection of fig. 7.7. We have thus replaced the hole with cancelling + and – charge clouds. The + charge completes the closed shell. The – charge is subsequently responsible for the shift in sign of the quadrupole moment for a hole state relative to a particle state.

Let us estimate the magnitude of Q. We assume that the orbital of the

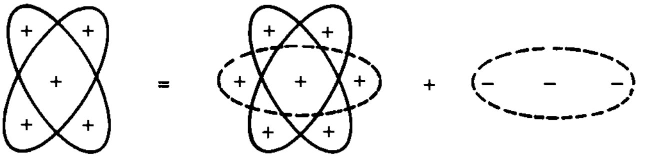

Fig. 7.7. Schematic addition of wave functions showing that a hole gives a quadrupole moment with a different sign than that of a particle (cf. fig. 7.3).

Table 7.1. *Experimental quadrupole moments compared with theoretical 'one-proton values' for nuclei with one proton or one neutron outside closed shells. Also given are the corresponding effective charges and polarisation factors.*

	Nucleus (doubly magic +1)		
	$^{17}_{8}O_9$	$^{17}_{9}F_8$	$^{209}_{83}Bi_{126}$
Orbital	$d_{5/2}$	$d_{5/2}$	$h_{9/2}$
Q^{exp} (barn)	–0.026	–0.10	–0.46
$\langle Q^{\text{one proton}}\rangle$ (barn)	–0.051	–0.051	–0.30
$e^{\text{eff}} = Q^{\text{exp}} / \langle Q^{\text{one proton}}\rangle$	0.51	2.0	1.5
$\alpha = \left(e^{\text{eff}} - e_{(n,p)}\right) / \left(Ze_p/A\right)$	1.1	1.8	1.3

valence nucleon lies near the surface of the nucleus. This leads to

$$|Q| \approx \left\langle r^2 \right\rangle \approx R^2 \approx 1.2^2 \cdot A^{2/3} \cdot 10^{-26}\,\text{cm}^2 = 1.44 \cdot A^{2/3} \cdot 10^{-2} \quad \text{barns}$$
$$(1\ \text{barn} = 10^{-24}\,\text{cm}^2)$$

Thus for light nuclei we expect in terms of the 'extreme' one-particle model a quadrupole moment of a few hundredths of a barn, and for heavier nuclei some tenths of a barn. A comparison with a few selected experimental values is shown in table 7.1.

Because $e = 1$ for protons and $e = 0$ for neutrons, one should expect to have $Q = 0$ for the odd-N case. Instead, the quadrupole moment turns out to be approximately equal to that expected for an odd proton. For the odd-proton case, Q comes out larger than the single-proton value by about a factor of 2. These deviations in the quadrupole moment are considered to represent matter polarisation as illustrated in fig. 7.8 (one often refers to the tidal waves caused on the surface of the earth by the orbiting moon).

Let us introduce the factor of polarisation α. This implies a charge $\alpha\cdot(Z/A)$

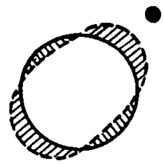

Fig. 7.8. Illustration of how a particle outside a spherical core polarises the core.

Table 7.2. *Quadrupole moments of nuclei removed from doubly closed shells. Subshells for protons and neutrons are denoted by π and ν, respectively. In the last five cases of the table, the polarisation factor α has no apparent meaning. These nuclei are deformed, permanently or momentarily through vibrations. The two In nuclei are so-called vibrational nuclei. The last three nuclei are permanently deformed. The quadrupole moment is 20–30 times larger than that of a single proton.*

Nucleus	State	$Q^{\rm exp}$ (barn)	$Q^{\rm one\ proton}$ (barn)	Polarisation factor	Comment
${}^{7}_{3}\mathrm{Li}_4$	$(\pi p_{3/2})$	−0.040	−0.020	$\alpha > 1$	
${}^{9}_{4}\mathrm{Be}_5$	$(\nu p_{3/2})^{-1}$	0.053	0.020	$\alpha > 1$	
${}^{35}_{17}\mathrm{Cl}_{18}$	$\pi d_{3/2}$	−0.082	−0.047	$\alpha > 1$	
${}^{37}_{17}\mathrm{Cl}_{20}$	$\pi d_{3/2}$	−0.065	−0.049	$\alpha > 1$	
${}^{113}_{49}\mathrm{In}_{64}$	$(\pi g_{9/2})^{-1}$	0.8	0.22	$(\alpha >> 1)$	Vibrational
${}^{115}_{49}\mathrm{In}_{66}$	$(\pi g_{9/2})^{-1}$	0.86	0.22	$(\alpha >> 1)$	nuclei $\alpha \simeq 10$
${}^{165}_{67}\mathrm{Ho}_{98}$	7/2	2.73	$\simeq 0.2$	$(\alpha >>> 1)$	Nuclei with
${}^{175}_{71}\mathrm{Lu}_{104}$	7/2	5.68	$\simeq 0.2$	$(\alpha >>> 1)$	stable deformations
${}^{181}_{73}\mathrm{Ta}_{108}$	7/2	3.9	$\simeq 0.2$	$(\alpha >>> 1)$	$\alpha \simeq 100$

from the polarisation. One thus obtains

$$e_{\rm n}^{\rm eff} = e_{\rm n} + \alpha_{\rm n}\frac{Z}{A}e_{\rm n} \approx 0 + \alpha_{\rm n}\cdot\frac{1}{2}$$
$$e_{\rm p}^{\rm eff} = e_{\rm p} + \alpha_{\rm p}\frac{Z}{A}e_{\rm p} \approx 1 + \alpha_{\rm p}\cdot\frac{1}{2}$$

As a very rough estimate, $\alpha_{\rm n}^{\rm exp} \approx 1$ and $\alpha_{\rm p}^{\rm exp} \approx 1-2$ (cf. table 7.1). The theoretical value obtained for the harmonic oscillator is $\alpha = 1$ and for the infinite square well potential $\alpha \approx 2$–4.

Some examples of other types of nuclei than closed-shells ± 1 nuclei are given in table 7.2. It is apparent that, in some cases, α becomes much larger than one. This must mean that the quadrupole moment is built from many nucleons and the whole nucleus is deformed, either vibrationally or more permanently (Bohr, 1976; Rainwater, 1976). In the coming chapters, we will consider the permanently deformed nuclei. As a preparation for the description of their measurable properties, we will study the single-particle orbitals of a deformed potential in chapter 8.

Exercises

7.1 Use the formula

$$\hbar^2 j(j+1)\langle jm|\mathbf{t}|jm'\rangle = \langle jm|\mathbf{j}|jm'\rangle\langle jm'|\mathbf{t}\cdot\mathbf{j}|jm'\rangle$$

where $\mathbf{t}$ represents a vector of type ℓ, s etc., to derive the formula for the magnetic moment:

$$\mu = \langle jj\,|g_s s_z + g_\ell \ell_z|\,jj\rangle = j\left(g_\ell \pm (g_s - g_\ell)\frac{1}{(2\ell+1)}\right)$$

The upper and lower signs are valid for $j = \ell \pm \frac{1}{2}$, respectively. Interpret the given formula in the case $m = m'$.

7.2 (a) Show that the quadrupole moment Q with regard to the symmetry axis of a homogeneously charged spheroid is $\frac{2}{5}Z\left(b^2 - a^2\right)$. The half-axes are given by a and b with b referring to the symmetry axis.

(b) If the symmetry axis of the spheroid is rotated by an angle β, show that the quadrupole moment with regard to the rotated axis is given by

$$Q' = Q\left(\frac{3}{2}\cos^2\beta - \frac{1}{2}\right)$$

7.3 Calculate the magnetic moment for the following closed shell ±1 nuclei (experimental values are given in square brackets)

^{15}N $\left(p_{1/2}\right)^{-1}$ [−0.28]
^{15}O $\left(p_{1/2}\right)^{-1}$ [0.719]
^{17}O $d_{5/2}$ [−1.894]
^{39}K $\left(d_{3/2}\right)^{-1}$ [0.391]
^{41}Ca $f_{7/2}$ [−1.595]
^{207}Pb $\left(p_{1/2}\right)^{-1}$ [0.590]
^{209}Bi $h_{9/2}$ [4.080]

Which g_s^{eff} is needed for the different nuclei to reproduce the experimental values? Use the formula $\mu^{\text{exp}} = j\left[g_\ell \pm \left(g_s^{\text{eff}} - g_\ell\right)/(2\ell+1)\right]$.

7.4 Because of the Coulomb field, the average potential for protons and neutrons becomes somewhat different. Estimate this difference due to the Coulomb energy for a $1g_{7/2}$ and a $2d_{5/2}$ proton, respectively in the following case.

(a) The wave function of the proton is of harmonic oscillator type
(b) The charge distribution in the nucleus is assumed homogeneous out to the radius $R = 1.2 \cdot A^{1/3}$ fm.

7.5 Calculate the quadrupole moment

$$Q = \left\langle \ell \frac{1}{2}\, jj \,|Q^{\text{op}}|\, \ell \frac{1}{2}\, jj \right\rangle$$

where $Q^{\text{op}} = e(16\pi/5)\langle r^2\rangle_{N\ell} Y_{20}$ is the quadrupole moment operator.

7.6 In the quark picture, the proton is described as being built from two u quarks and one d quark while the neutron is built from one u quark and two d quarks. The u quark has charge $(2/3)e$ and the d quark $(-1/3)e$. They both have an internal spin, $s = 1/2$. The magnetic moment operator for a quark with charge Q is now assumed to be given as $\mu_{\text{q}} = Q\mu_0 s_z$ where μ_0 is a constant. Furthermore, to fulfill the necessary symmetry relations, the two equal quarks in a proton or neutron must couple to spin 1. Through the coupling of the third quark, a total spin of $1/2$ is then obtained. Show that this leads to the relation $\mu_{\text{n}} = (-2/3)\mu_{\text{p}}$ for the neutron and proton magnetic moments. How does this relation compare with the experimental values?