8

Single-particle orbitals in deformed nuclei

For the spherical case we have discussed the isotropic harmonic-oscillator field. To amend for the radial deficiencies we have seen that the addition of a term proportional to $-\ell^2$ has the desired properties of giving rise to an effective interpolation between a harmonic oscillator and a square well. One thus obtains a fair reproduction of the spherical single-particle levels by the following Hamiltonian – the modified-oscillator (MO) Hamiltonian:

$$H_{\text{sph}} = -\frac{\hbar^2}{2M}\Delta + \frac{1}{2}M\omega_0^2 r^2 - C\boldsymbol{\ell}\cdot\mathbf{s} - D\left(\ell^2 - \left\langle \ell^2 \right\rangle_N\right)$$

As a secondary and undesirable effect of ℓ^2 alone, there is a general compression of the distance between the shells below $\hbar\omega_0$. This basic energy spacing is restored by the subtraction of the term $\left\langle \ell^2 \right\rangle_N = N(N+3)/2$ (see problem 6.7), which thus assumes a constant value within each shell. One argument for the introduction of the $\left\langle \ell^2 \right\rangle_N$ term is the following. Only the terms proportional to r^2 are conveniently included in the volume conservation condition (see below). In order not to upset volume conservation by the effective widening of the radial shape by the ℓ^2 term, it appears reasonable to subtract from this term the average value appropriate to each shell. A resulting level scheme is exhibited in fig. 6.3. In that figure, different strength parameters, κ and μ' are used. The relations $C = 2\kappa\hbar\omega_0$ and $D = \mu'\hbar\omega_0$ are straightforward to derive. The parameters κ and μ' (or μ where $\mu' = \kappa\mu$) are the standard parameters used together with dimensionless oscillator units.

This potential easily lends itself to a generalisation so as to be applicable to the deformed case. If we allow for the potential extension along the nuclear z-axis (3-axis) being different from the extension along the x- and

y-axes, we may write the single-particle Hamiltonian in the form

$$H = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+\frac{M}{2}\left[\omega_\perp^2\left(x^2+y^2\right)+\omega_z^2 z^2\right]-C\boldsymbol{\ell}\cdot\mathbf{s}$$

$$-D\left(\boldsymbol{\ell}^2-\left\langle\boldsymbol{\ell}^2\right\rangle_N\right)$$

The anisotropy corresponds to the difference introduced between $\omega_\perp$ and ω_z. It is convenient to introduce an elongation parameter ε (Nilsson, 1955):

$$\omega_z = \omega_0(\varepsilon)\left(1-\frac{2}{3}\varepsilon\right)$$

$$\omega_\perp = \omega_0(\varepsilon)\left(1+\frac{1}{3}\varepsilon\right)$$

where $\omega_0(\varepsilon)$ is weakly ε-dependent, enough to conserve the nuclear volume (see below). The distortion parameter ε is obtained as $\varepsilon = (\omega_\perp - \omega_z)/\omega_0$. It is defined so that $\varepsilon > 0$ and $\varepsilon < 0$ correspond to so-called prolate and oblate shapes, respectively.

8.1 Perturbation treatment for small ε

Let us first study the situation for very small ε-values. Expanding in ε we may write

$$H = H_0 + \varepsilon h' + 0\left(\varepsilon^2\right)+\ldots$$

where H_0 is the spherical shell model Hamiltonian. Furthermore $\varepsilon h'$ is given as

$$\varepsilon h' = \varepsilon\frac{M}{2}\omega_0^2\frac{2}{3}\left(x^2+y^2-2z^2\right) = -\frac{M}{2}\omega_0^2\frac{4}{3}\varepsilon r^2 P_2(\cos\theta)$$

As shown in preceding chapters we may write the eigenfunctions in the spherical case as

$$\phi(N\ell sj\Omega) = R_{N\ell}(r)\sum_{\Lambda\Sigma}\langle\ell s\Lambda\Sigma|\ell sj\Omega\rangle\, Y_{\ell\Lambda}\chi_{s\Sigma}$$

where the constants of the motion are $\mathbf{j}^2$ and Ω, the total angular momentum and its z-component, and furthermore $\boldsymbol{\ell}^2$ and $\mathbf{s}^2$, the orbital and spin angular momenta. The projections of the orbital and spin angular momenta are denoted by Λ and Σ, respectively.

In the spherical case each j state is $(2j+1)$-fold degenerate. This degeneracy is removed by the perturbation h' to first order as (see problem 8.1)

$$\langle N\ell sj\Omega|\varepsilon h'|N\ell sj\Omega\rangle = \frac{1}{6}\varepsilon M\omega_0^2\left\langle r^2\right\rangle\frac{3\Omega^2-j(j+1)}{j(j+1)}$$

This result of the deformation of the field is easily understood qualitatively. For a so-called prolate distortion ($\varepsilon > 0$) of the field, matter is removed from the 'waistline' and placed at the 'poles'. This corresponds to a softer potential in the z-direction and a steeper potential in the perpendicular x- and y-directions where the equatorial orbitals with $\Omega \simeq j$ are mainly located. Classically, this is understood from the fact that the $\Omega \simeq j$ angular momentum vector is almost parallel to the z-axis and the particle moves in a plane perpendicular to this vector. Consequently, the $\Omega \simeq j$ orbitals move up in energy. On the other hand, the polar orbitals with $\Omega << j$ are associated with a negative energy contribution for $\varepsilon > 0$. They are thus favoured by a prolate deformation, i.e. they move down in energy. For an oblate distortion the opposite is true, i.e. the large Ω-values are suppressed energywise (cf. the splitting of the j-shells for small distortions in fig. 8.3 below).

8.2 Asymptotic wave functions

Before we discuss the case of moderate deformations of $\varepsilon \simeq 0.2$–0.3, acquired by most deformed nuclei, we shall now consider the limit of very large ε-values. Beyond very small ε-values, say $\varepsilon \simeq 0.1$, the exhibited perturbation treatment of the ε-term is no longer applicable. Instead one may at large ε introduce a representation that exactly diagonalises the harmonic oscillator field while instead the ℓ^2 and $\ell \cdot \mathbf{s}$ terms are treated as perturbations.

Let us write

$$H = H_{\text{osc}} + H'$$

where

$$H_{\text{osc}} = -\frac{\hbar^2}{2M}\Delta + \frac{M}{2}\left[\omega_\perp^2\left(x^2 + y^2\right) + \omega_z^2 z^2\right]$$

It is now convenient to introduce what one may call 'stretched' coordinates (Nilsson, 1955)

$$\xi = x\left(\frac{M\omega_\perp}{\hbar}\right)^{1/2}, \quad \eta = y\left(\frac{M\omega_\perp}{\hbar}\right)^{1/2}, \quad \zeta = z\left(\frac{M\omega_z}{\hbar}\right)^{1/2}$$

Thus

$$H_{\text{osc}} = \frac{1}{2}\hbar\omega_\perp\left[-\left(\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2}\right) + \left(\xi^2 + \eta^2\right)\right] + \frac{1}{2}\hbar\omega_z\left(-\frac{\partial^2}{\partial\zeta^2} + \zeta^2\right)$$

In the spherical case we added correction terms of the type

$$H'_{\text{sph}} = -2\kappa\hbar\omega_0\,\ell \cdot \mathbf{s} - \mu'\hbar\omega_0\left(\ell^2 - \left\langle\ell^2\right\rangle_N\right)$$

Introducing an ℓ_t corresponding to the stretched coordinates ξ, η and ζ, where e.g.

$$(\ell_t)_x = -i\hbar\left(\eta\frac{\partial}{\partial\zeta} - \zeta\frac{\partial}{\partial\eta}\right)$$

it seems natural to generalise H' into

$$H'_{\text{def}} = -2\kappa\hbar\omega_0\ell_t\cdot\mathbf{s} - \mu'\hbar\omega_0\left(\ell_t^2 - \left\langle\ell_t^2\right\rangle_N\right)$$

One may show (Nilsson, 1955) that the difference terms between H'_{sph} and H'_{def} have no matrix elements within each N-shell. There exist alternatives but no really definite prescription for how the terms ℓ^2 and $\ell\cdot\mathbf{s}$ are to be generalised in going from the spherical to the distorted case (see e.g. Bengtsson, 1975). The presently employed recipe of simply replacing ℓ by ℓ_t is thus associated with a high degree of arbitrariness.

Consider first the oscillator part of H given above as H_{osc}. To proceed with the case of cylinder symmetry only, H_{osc} is transformed by going over to cylindrical coordinates (ρ,φ,ζ) where

$$\xi = \rho\cos\varphi$$
$$\eta = \rho\sin\varphi$$

(contrary to above, ρ is here the 'cylinder radius' $\rho = (\xi^2+\eta^2)^{1/2}$). We can write the Schrödinger equation in terms of these coordinates:

$$\left[\frac{1}{2}\hbar\omega_\perp\left(-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \rho^2\right) + \frac{1}{2}\hbar\omega_z\left(-\frac{\partial^2}{\partial\zeta^2} + \zeta^2\right) - E\right]\psi = 0$$

We separate off the φ-dependence by the assumption

$$\psi = U(\rho)Z(\zeta)\phi(\varphi)$$

where

$$-\frac{\partial^2}{\partial\varphi^2}\phi = \Lambda^2\phi$$

with the solution

$$\phi = e^{i\Lambda\varphi}$$

corresponding to the fact that $[L_z, H] = 0$ and thus $L_z = \Lambda$ a constant of the motion. We can also separate off the ζ-dependence and obtain

$$\hbar\omega_z\left(-\frac{\partial^2}{\partial\zeta^2} + \zeta^2\right)Z(\zeta) = E_zZ(\zeta)$$

with the usual one-dimensional harmonic oscillator solution where $E_z =$

$(n_z + 1/2)\,\hbar\omega_z$. Finally, with $E = E_\perp + E_z$, one ends up with the following equation for $U(\rho)$:

$$\frac{1}{2}\hbar\omega_\perp \left(-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{\Lambda^2}{\rho^2} + \rho^2 \right) U(\rho) = E_\perp U(\rho)$$

or

$$\frac{\mathrm{d}^2U}{\mathrm{d}\rho^2} + \frac{1}{\rho}\frac{\mathrm{d}U}{\mathrm{d}\rho} - \frac{\Lambda^2}{\rho^2}U - \rho^2 U = -\frac{2E_\perp}{\hbar\omega_\perp}\cdot U$$

From the behaviour in the limiting cases $\rho \to 0$ and $\rho \to \infty$ it is natural to assume

$$U = \rho^{|\Lambda|}\mathrm{e}^{-\rho^2/2}W(\rho)$$

Hence W fulfils

$$W'' + \left(\frac{2|\Lambda| + 1}{\rho} - 2\rho \right) W' - 2\left(|\Lambda| + 1 - \frac{E_\perp}{\hbar\omega_\perp} \right) W = 0$$

After the substitution

$$z = \rho^2$$

we obtain

$$zW'' + (|\Lambda| + 1 - z)\,W' - \frac{1}{2}\left(|\Lambda| + 1 - \frac{E_\perp}{\hbar\omega_\perp} \right) W = 0$$

This should be compared with the equation obtained in the spherical oscillator case (chapter 6) with the 'ansatz' $R_\ell(\rho) = \rho^\ell \mathrm{e}^{-\rho^2/2} f(\rho)$, where

$$\rho f'' + (\ell + 3/2 - z)\,f' + \frac{1}{2}\left(\frac{E}{\hbar\omega} - (\ell + 3/2) \right) f = 0$$

The differential equation for W is, similarly to the equation for f, a Kummer equation and the solution is a confluent hypergeometric function

$$W = F\left(\frac{1}{2}\left(|\Lambda| + 1 - E_\perp/\hbar\omega_\perp\right),\ |\Lambda| + 1\ ;\ z \right)$$

with the (finiteness) condition

$$\frac{1}{2}\left(|\Lambda| + 1 - E_\perp/\hbar\omega_\perp\right) = -n_\rho\ ;\ \ n_\rho = 0, 1, 2, \ldots$$

or

$$E_\perp = \hbar\omega_\perp\,(2n_\rho + |\Lambda| + 1) = \hbar\omega_\perp\,(n_\perp + 1)$$

The quantity n_ρ is thus the number of (cylinder) radial nodes and $n_\perp$ is the

total number of oscillator quanta in the x- and y-directions, $n_\perp = n_x + n_y$. Note that

$$2n_\rho + |\Lambda| = n_\perp$$

Thus

$$|\Lambda| = n_\perp,\ n_\perp - 2,\ n_\perp - 4 \ldots 0 \text{ or } 1$$

We may now sum up the final results for the cylindrical oscillator case

$$E(n_z, n_\perp) = \hbar\omega_z \left(n_z + \frac{1}{2}\right) + \hbar\omega_\perp (n_\perp + 1) = \hbar\omega_0 \left(N + \frac{3}{2} + (n_\perp - 2n_z)\frac{\varepsilon}{3}\right)$$

$$\psi(n_z, n_\perp, \Lambda) = C \cdot \mathrm{e}^{-\zeta^2/2} H_{n_z}(\zeta) \rho^{|\Lambda|} \mathrm{e}^{-\rho^2/2} F\left(-\frac{n_\perp - |\Lambda|}{2},\ |\Lambda| + 1;\ \rho^2\right) \cdot \mathrm{e}^{\mathrm{i}\Lambda\varphi}$$

Let us see how our oscillator levels look with distortion (fig. 8.1). Obviously each N shell, $N = n_\perp + n_z$, is split into $N + 1$ levels corresponding to $n_\perp = 0, 1, \ldots, N$. The degeneracy of each level is $2 \times (n_\perp + 1)$ corresponding to the two spin values $\Sigma = \pm 1/2$ and the $n_\perp + 1$ different Λ-values for each $n_\perp$ (for example $\Lambda = 2$, 0 and -2 for $n_\perp = 2$).

We may note in passing that, although the spherical shell structure is lost when $\varepsilon \neq 0$, new shells are re-appearing e.g. at $\varepsilon = 0.6$, $\varepsilon = 1$ and $\varepsilon = -0.75$ etc. Thus for $\varepsilon = 0.6$ we have $\hbar\omega_\perp = 2\hbar\omega_z$, i.e. we can replace one quantum $\hbar\omega_\perp$ with two quanta $\hbar\omega_z$ without change of energy just as for spherical symmetry $\hbar\omega_x$, $\hbar\omega_y$ and $\hbar\omega_z$ are interchangeable (cf. problem 5.1).

This covers the pure oscillator Hamiltonian. There remains, however, the $\boldsymbol{\ell}_t \cdot \mathbf{s}$ and ℓ_t^2 terms. One can actually treat these by first-order perturbation theory. The matrix elements of these terms are evaluated by operator methods in the last section of this chapter. For the perturbation treatment, we only need the diagonal terms:

$$\langle N n_z \Lambda\Sigma | \boldsymbol{\ell}_t \cdot \mathbf{s} | N n_z \Lambda\Sigma \rangle = \Lambda\Sigma$$

$$\left\langle N n_z \Lambda\Sigma \left| \ell_t^2 \right| N n_z \Lambda\Sigma \right\rangle = \Lambda^2 + 2n_\perp n_z + 2n_z + n_\perp$$

The diagonal value of the total Hamiltonian then becomes

$$\langle N n_z \Lambda\Sigma | H_{\mathrm{osc}} - 2\kappa\hbar\omega_0 \boldsymbol{\ell}_t \cdot \mathbf{s} - \mu'\hbar\omega_0 \left(\ell_t^2 - \left\langle \ell_t^2 \right\rangle_N\right) | N n_z \Lambda\Sigma \rangle$$

$$= \left(N + \frac{3}{2}\right)\hbar\omega_0 + \frac{1}{3}\varepsilon\hbar\omega_0 (N - 3n_z) - 2\kappa\hbar\omega_0 \Lambda\Sigma$$

$$-\mu'\hbar\omega_0 \left(\Lambda^2 + 2n_\perp n_z + 2n_z + n_\perp - \frac{N(N+3)}{2}\right)$$

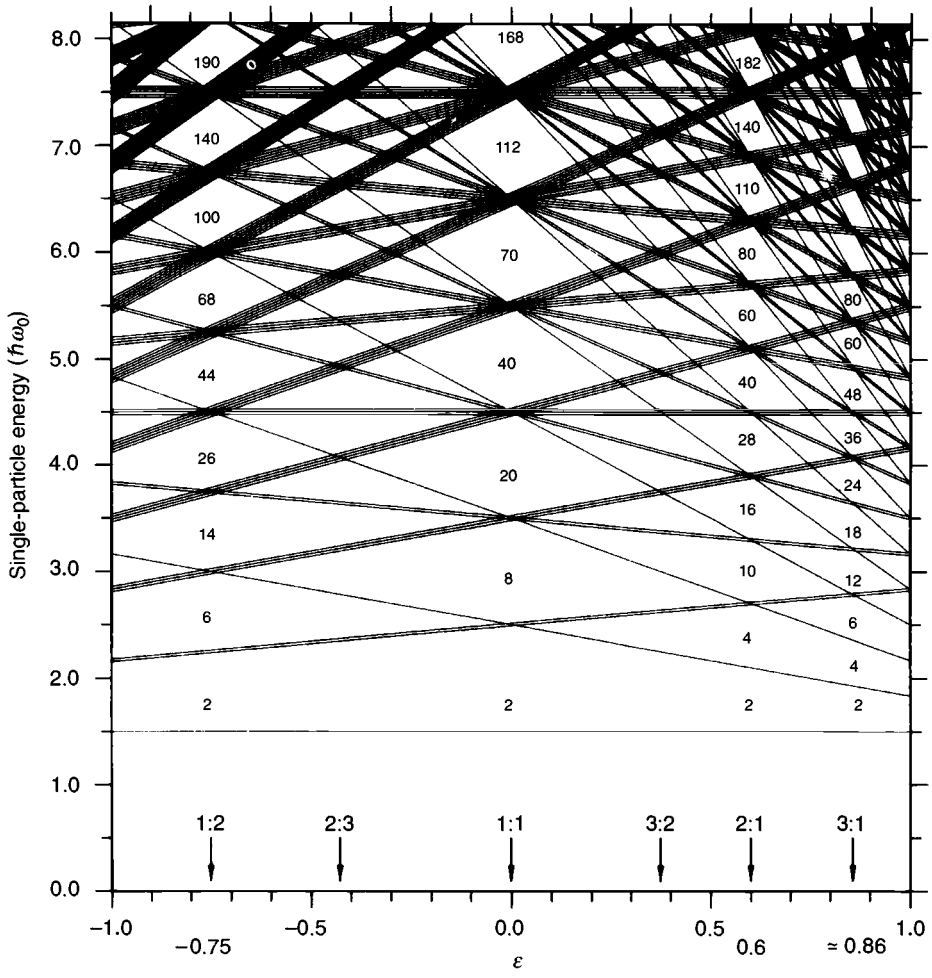

Fig. 8.1. Single-particle energies of the axially symmetric harmonic oscillator potential drawn as functions of the deformation parameter, $\varepsilon = (\omega_\perp - \omega_z)/\omega_0$. The orbitals that stay degenerate for all ε-values are drawn with a small spacing to indicate the total level density more clearly. The high degeneracy for spherical shape is partly broken for $\varepsilon \neq 0$ but is then largely regained for $\omega_\perp : \omega_z$ corresponding to small integer numbers where the most important ones are indicated in the lower part of the figure. For $\omega_\perp : \omega_z$ = 1:2, 1:1, 2:1, and 3:1, the corresponding magic numbers are given.

The effect of the inclusion of the $\ell_t \cdot \mathbf{s}$ and ℓ_t^2 terms in perturbation approximation is thus a lifting of the $2 \times (n_\perp + 1)$-fold degeneracy. After the inclusion of these terms only a two-fold degeneracy (the time-reversal degeneracy) remains. The splitting can be seen from fig. 8.2, where first the $\ell_t \cdot \mathbf{s}$ term and subsequently the ℓ_t^2 term have been added to an $N = 5$

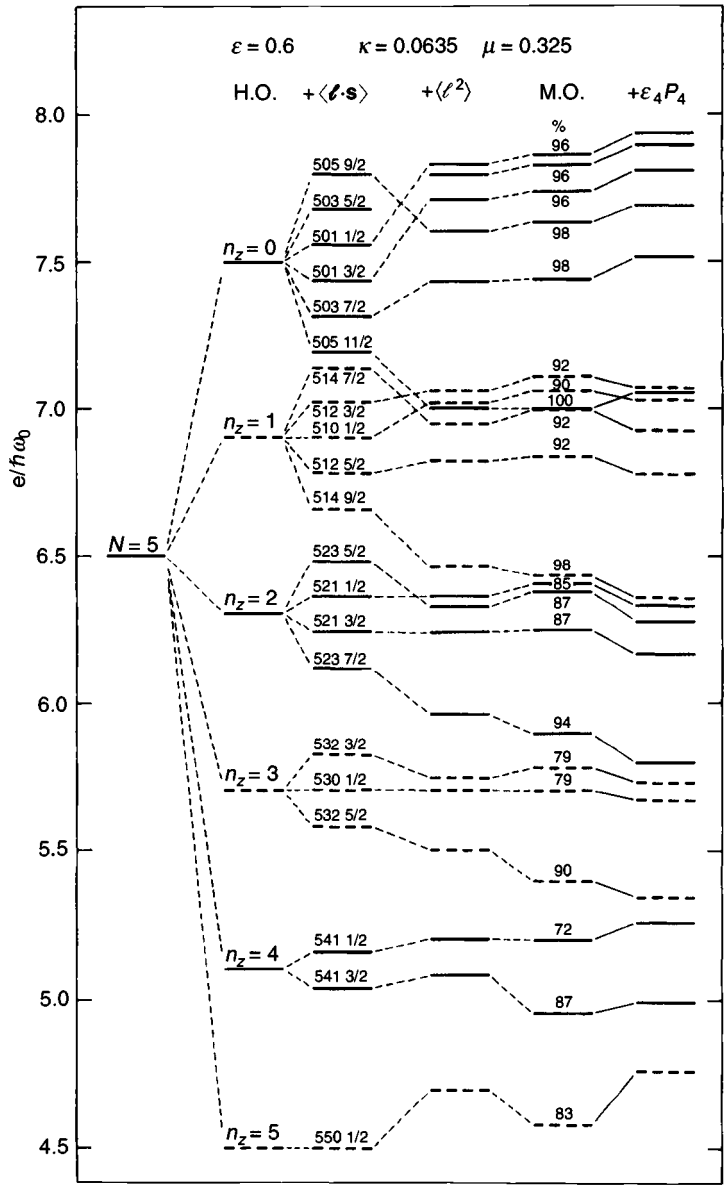

Fig. 8.2. Different contributions to the splitting of the $N = 5$ oscillator shell are illustrated. First the pure oscillator is deformed to $\varepsilon = 0.6$, then diagonal matrix elements of the $\ell \cdot \mathbf{s}$ and ℓ^2-terms are added to the $|Nn_z\Lambda\Omega\rangle$ basis. Finally, to the right, an exact diagonalisation was carried out, with $\varepsilon_4 = 0$ and 0.07 respectively. The latter value of ε_4 corresponds approximately to the liquid drop valley in the actinide region. The κ and μ parameters are chosen for neutrons in this same region. In the case of $\varepsilon_4 = 0$, the pureness of the asymptotic representation is indicated (from Ragnarsson *et al.*, 1978).

shell of orbitals. The effect of the inclusion of neglected off-diagonal terms (exact diagonalisation) is then illustrated and finally the importance of hexadecapole deformations (see below) is shown. As the $\ell_t \cdot \mathbf{s}$ term enters with a negative coefficient the resulting splitting is such that orbitals with Λ and Σ parallel are favoured. Furthermore the spin–orbit splitting is smaller than in the spherical case and proportional to 2Λ rather than $2\ell + 1$. (Note that Λ is at the most equal to ℓ_t.) The ℓ_t^2-term favours states of high Λ-values among those of given n_z and $n_\perp$.

To conclude this section, it may be stated that, although the splitting of the $n_\perp$ degeneracy involves energies of the order of $\hbar\omega_0$, i.e. the separation between spherical shells, still off-diagonal elements are so small that the so called *asymptotic quantum numbers* N, n_z, Λ and Σ remain essentially preserved even at intermediate ε. This holds also for the spectroscopic data. The *asymptotic wave functions* $Nn_z\Lambda\Sigma$ (or $Nn_z\Lambda\Omega$ where $\Omega = \Lambda + \Sigma$) have become a very useful labelling of orbitals in nuclear spectroscopy. In fact nowadays deformed single-particle states identified experimentally are usually labelled in terms of this classification (see e.g. Jain *et al.*, 1990).

8.3 The intermediate region

In the intermediate region of ε being neither very small nor very large one usually employs an expansion in either $\phi(N\ell j\Omega)$, $\phi(N\ell\Lambda\Sigma)$ or $\phi(Nn_z\Lambda\Omega)$. Let us, however, first briefly consider the general case with a complete set of basis states ϕ_ν. Every wave function ψ_α, which solves the Schrödinger equation:

$$H\psi_\alpha = E_\alpha\psi_\alpha$$

can now be expanded in terms of the ϕ_ν base functions

$$\psi_\alpha = \sum_\nu S_{\alpha\nu}\phi_\nu$$

We insert this expansion in the Schrödinger equation:

$$\sum_\nu S_{\alpha\nu}H\phi_\nu = E_\alpha \sum_\nu S_{\alpha\nu}\phi_\nu$$

Multiplying from the left by ϕ_μ^* and integrating (taking the scalar product) we obtain

$$\sum_\nu S_{\alpha\nu} \int \phi_\mu^* H\phi_\nu \, \mathrm{d}\tau = E_\alpha \sum_\nu S_{\alpha\nu}\delta_{\mu\nu}$$

Denoting

$$\int \phi_\mu^* H \phi_\nu \, d\tau = \langle \mu | H | \nu \rangle = H_{\mu\nu}$$

we have thus a set of equations, one for each μ

$$\sum_\nu S_{\alpha\nu} (H_{\mu\nu} - E_\alpha \delta_{\mu\nu}) = 0$$

The condition that a solution exists is that the determinant vanishes:

$$\text{Det } (H_{\mu\nu} - E_\alpha \delta_{\mu\nu}) = 0$$

The problem is two-fold, first to calculate the matrix elements $H_{\mu\nu} = \int \phi_\mu^* H \phi_\nu \, d\tau$ and second to 'diagonalise' the matrix or in principle find the roots that make Det $(H_{\mu\nu} - E_\alpha \delta_{\mu\nu})$ vanish. Technically the computer programs constructed find a transformation matrix $S_{\alpha\mu}$ such that the transformed H-matrix is diagonal.

The set of equations can be written:

$$E_\alpha S_{\alpha\mu} = \sum_\nu S_{\alpha\nu} H_{\mu\nu}$$

or in matrix form

$$\boldsymbol{E}\,\boldsymbol{S} = \boldsymbol{S}\,\boldsymbol{H}$$

where $\boldsymbol{E}$ is a diagonal matrix:

$$\boldsymbol{E} = \begin{pmatrix} E_1 & 0 & 0 & \dots \\ 0 & E_2 & 0 & \\ 0 & 0 & E_3 & \\ \vdots & & & \end{pmatrix}$$

The eigenvalues E_α are now given as

$$\boldsymbol{E} = \boldsymbol{S}\,\boldsymbol{H}\,\boldsymbol{S}^{-1}$$

and the eigenvectors are the rows of the transformation matrix $\boldsymbol{S}$.

Let us now return to the practical case. We assume a wave function

$$\psi_{\alpha N\Omega} = \sum_{\ell\Lambda\Sigma} a_{N\ell\Lambda\Sigma} R_{N\ell}(\rho) Y_{\ell\Lambda}(\theta_t, \varphi_t) \chi_{s\Sigma} = \sum_{\ell\Lambda\Sigma} a_{N\ell\Lambda\Sigma} |N\ell\Lambda\Sigma\rangle$$

where we assume that $R_{N\ell}$ is normalised. The spherical harmonics $Y_{\ell\Lambda}$ are already normalised. The spin wave function $\chi_{s\Sigma}$ is simply

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The quantity ρ is now defined (in contradistinction to the cylindrical case) as the radius in the stretched coordinates,

$$\rho^2 = \xi^2 + \eta^2 + \zeta^2$$

while θ_t and φ_t are the polar and azimuthal angles in these coordinates. Note also that all the quantum numbers, $N, \ell, \ldots$ are defined in the stretched coordinates and should more appropriately be denoted $N_t, \ell_t, \ldots$. In these cases, we will however drop the index 't'.

The coefficients $a_{N\ell\Lambda\Sigma}$ are our unknowns. The assumption is that any wave function can be expressed in terms of these basis vectors $|N\ell\Lambda\Sigma\rangle$. These vectors form a complete basis but the problem is that our computer can only accept a finite number of basis states. Usually, we limit ourselves to the lowest N-values.

There are restrictions on the sum fortunately. First we note that $j_z = \ell_z + s_z = (\ell_t)_z + s_z$ (with $\omega_x = \omega_y = \omega_\perp$, it follows that $\ell_z = (\ell_t)_z$) is a constant of the motion as (cf. problem 8.4)

$$[j_z, H] = 0$$

Indeed $(\ell_t)_z$ and s_z both commute with the cylindrically symmetrical H_{osc} and also with ℓ_t^2. With $\ell_t \cdot s$ only the sum $(\ell_t)_z + s_z$ commutes. In the wave function expansion only two Λ values can occur as we have to fulfill $\Lambda + \Sigma = \Omega$. Thus we can have $\Lambda = \Omega - l/2$ and $\Lambda = \Omega + l/2$ corresponding to $\Sigma = +1/2$ and $\Sigma = -1/2$.

It is convenient to rewrite the Hamiltonian in the following form

$$H = H_d + H_\varepsilon$$

where H_d is a part of the Hamiltonian that is rotationally symmetric, in the stretched coordinates, (ξ, η, ζ);

$$H_d = \frac{1}{2}\hbar\omega_0\left(-\Delta_\xi + \rho^2\right) - 2\kappa\hbar\omega_0 \ell_t \cdot \mathbf{s} - \mu'\hbar\omega_0\left(\ell_t^2 - \left\langle \ell_t^2 \right\rangle_N\right)$$

We have furthermore

$$H_\varepsilon = \frac{1}{6}\varepsilon\hbar\omega_0\left(-\frac{\partial^2}{\partial\xi^2} - \frac{\partial^2}{\partial\eta^2} + 2\frac{\partial^2}{\partial\zeta^2} + \xi^2 + \eta^2 - 2\zeta^2\right)$$

The quantity H_ε now has the remarkable property that its matrix elements vanish identically between base states with different N quantum numbers. Between *states belonging to one N-shell* (or rather one N_t-shell) one may prove (see appendix 8) that the matrix elements are identical to those of

$$H'_\varepsilon = \frac{1}{3}\varepsilon\hbar\omega_0\left(\xi^2 + \eta^2 - 2\zeta^2\right) = -\frac{2}{3}\varepsilon\hbar\omega_0\rho^2 P_2(\cos\theta_t)$$

In the expansion of $\psi_{\alpha N\Omega}$, we used the fact that there are no matrix elements between states of different N or different Ω. The sum thus runs only over ℓ and Λ (with Σ determined from $\Sigma = \Omega - \Lambda$) and we can limit our diagonalisation to one N-shell and one Ω-value at a time. The index α is used to distinguish states, $\psi_{\alpha N\Omega}$ having the same N- and Ω-values.

The matrix elements are simple to generate within the computer or to calculate by hand. We have thus

$$\langle N\ell\Lambda\Sigma\,|H_d|\,N\ell\Lambda\Sigma\rangle = \frac{1}{2}\hbar\omega_0\left(N+\frac{3}{2}\right) - 2\kappa\hbar\omega_0\Lambda\Sigma - \mu'\hbar\omega_0\left(\ell(\ell+1) - \frac{N(N+3)}{2}\right)$$

For the $\ell\cdot$s-term, we note that $\ell\cdot\mathbf{s} = \frac{1}{2}(\ell_+ s_- + \ell_- s_+) + \ell_z s_z$ and obtain

$$\langle N\,\ell\,\Lambda+1\,\Sigma-1\,|\ell_t\cdot\mathbf{s}|\,N\,\ell\,\Lambda\,\Sigma\rangle = \frac{1}{2}[(\ell-\Lambda)(\ell+\Lambda+1)]^{1/2}$$

$$\langle N\,\ell\,\Lambda-1\,\Sigma+1\,|\ell_t\cdot\mathbf{s}|\,N\,\ell\,\Lambda\,\Sigma\rangle = \frac{1}{2}[(\ell+\Lambda)(\ell-\Lambda+1)]^{1/2}$$

Noting that H'_ε may be written $H'_\varepsilon = -h\omega_0\varepsilon\frac{4}{3}(\pi/5)^{1/2}\rho^2 Y_{20}$:

$$\langle N\ell'\Lambda'\Sigma'\,|H_\varepsilon|\,N\ell\Lambda\Sigma\rangle = \langle N\ell'\Lambda'\Sigma'\,|H'_\varepsilon|\,N\ell\Lambda\Sigma\rangle$$

$$= -\frac{2}{3}\varepsilon\hbar\omega_0\delta_{\Lambda\Lambda'}\delta_{\Sigma\Sigma'}\int R_{N\ell'}R_{N\ell}\rho^2\,\mathrm{d}\rho\cdot\left(\frac{2\ell+1}{2\ell'+1}\right)^{1/2}C^{\ell 2\ell'}_{\Lambda 0\Lambda'}C^{\ell 2\ell'}_{000}$$

We can thus easily construct the matrix and use the computer to diagonalise it. As already stated, the eigenvalues and eigenvectors both come out as a result. An example of a calculated single-particle diagram is provided in fig. 8.3.

If $\psi_{\alpha N\Omega}$ is expanded in normal coordinates x, y, z instead of the stretched set ξ, η, ζ, there enter components with $N\pm 2$, $N\pm 4$. Their amplitude is not negligible and it is certainly only together with stretched coordinates that the use of pure N-shells (N_t-shells) can be justified.

8.4 The volume conservation condition

In the oscillator calculations the absolute energy scale is given by $\hbar\omega_0$. The energy scale is as well as its ε-dependence, however, irrelevant in establishing the single-particle level order. On the other hand, for a determination of the equilibrium distortion (chapter 9) the volume conservation condition is of primary importance. This condition is based on the empirical finding

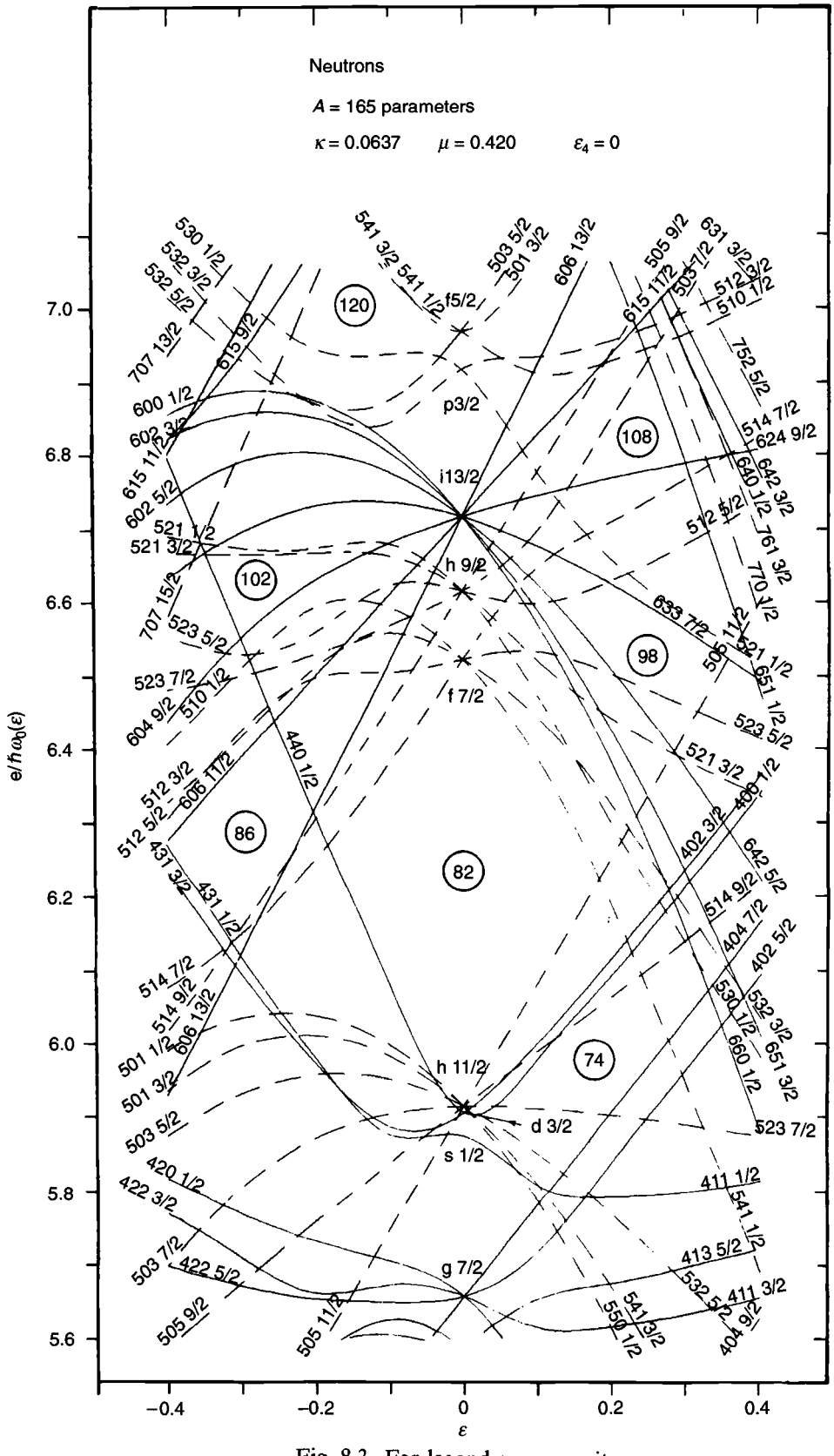

Fig. 8.3. For legend see opposite.

that nuclear matter is incompressible and the nuclear volume proportional to A. The short-range character of the nuclear force then appears to justify the condition that the volume enclosed by a given equipotential surface (the locus of points of the same nuclear potential) is preserved. For the simple harmonic oscillator potential an equipotential surface is obviously an ellipsoid.

$$V_{\mathrm{osc}} = \frac{1}{2}M\left(\frac{x^2+y^2}{1/\omega_\perp^2} + \frac{z^2}{1/\omega_z^2}\right) = V_0 = \text{constant}$$

The half-axes in this ellipsoid are given as proportional to $\omega_\perp^{-1}$ and ω_z^{-1} and the volume enclosed is thus proportional to $\omega_\perp^{-2}\omega_z^{-1}$. The remarkable feature for the pure oscillator is that for any equipotential surface (any value of V_0) we obtain the same volume conservation condition

$$\omega_\perp^2\omega_z = \text{constant} = (\omega_0(\varepsilon = 0))^3 = \left(\overset{0}{\omega}_0\right)^3$$

Using the definitions cited for ω_z and $\omega_\perp$ we obtain

$$\omega_0(\varepsilon) = \overset{0}{\omega}_0\left(1 - \frac{1}{3}\varepsilon^2 - \frac{2}{27}\varepsilon^3\right)^{-1/3} = \overset{0}{\omega}_0\left(1 + \frac{1}{9}\varepsilon^2 + \ldots\right)$$

All the energies in a level diagram such as fig. 8.3 are conveniently expressed in the ε-dependent energy unit $\hbar\omega_0(\varepsilon)$. Even though some energy levels appear wildly down-sloping as a function of ε in the $\hbar\omega_0$ scale, when expressed in the ε-independent unit $\hbar\overset{0}{\omega}_0$ they eventually bend upwards for large enough ε. Thus the ellipsoidal shape at very large distortions ultimately becomes unfavourable for any combination of nuclear orbitals filled.

Fig. 8.3. (*opposite*) Single-neutron orbitals calculated from the modified oscillator potential for nuclei in the mass region $150 < A < 190$ as a function of the ellipsoidal deformation parameter ε. Solid and dashed lines are used to distinguish between orbitals having even parity (even N) and odd parity (odd N), respectively. For large ε-values, the orbitals are labelled by the asymptotic quantum numbers $Nn_z\Lambda\Omega$, which, of course, are only approximate. N refers to the oscillator shell quantum number, n_z to the number of nodes along the z-axis, Λ to the value of the orbital angular momentum along the intrinsic z-axis and Ω to the value of the total angular momentum along the same axis. The spin projection along this axis is implied as $\Sigma = \Omega - \Lambda$.

8.5 Single-particle orbitals in an axially symmetric modified oscillator potential

The nuclear potential we have worked with so far can be written

$$V = V_{\text{osc}} + V'$$

$$V_{\text{osc}} = \frac{1}{2}\hbar\omega_0\rho^2\left(1 - \frac{2}{3}\varepsilon P_2(\cos\theta_t)\right)$$

$$V' = -2\kappa\hbar\overset{0}{\omega}_0\,\boldsymbol{\ell}_t\cdot\mathbf{s} - \mu'\hbar\overset{0}{\omega}_0\left(\ell_t^2 - \left\langle\ell_t^2\right\rangle_N\right)$$

Here, we have by convention (Nilsson, 1955) used the volume conserved frequency, $\overset{0}{\omega}_0$, together with the $\boldsymbol{\ell}_t\cdot\mathbf{s}$- and ℓ_t^2-terms. To be able to describe nuclear shapes other than ellipsoidal ones, the potential must be generalised in some way. A natural generalisation is (Nilsson *et al.*, 1969)†

$$V_{\text{osc}} = \frac{1}{2}\hbar\omega_0\rho^2\left(1 - \frac{2}{3}\varepsilon P_2(\cos\theta_t) + 2\sum_{\lambda=3,4,\ldots}\varepsilon_\lambda P_\lambda(\cos\theta_t)\right)$$

With this potential, we preserve the property that for any equipotential surface, $V_{\text{osc}} = V_0$, the same volume conservation condition is obtained. However, the ratio $\omega_0(\varepsilon,\varepsilon_3,\varepsilon_4,\ldots)/\overset{0}{\omega}_0$ must be calculated numerically (see e.g. Bengtsson, Ragnarsson and Åberg, 1991).

The shape of an equipotential surface is obtained as

$$\rho^2 = \frac{\text{constant}}{\left(1 - \frac{2}{3}\varepsilon P_2(\cos\theta_t) + 2\sum_\lambda \varepsilon_\lambda P_\lambda(\cos\theta_t)\right)}$$

Using the definition of the stretched coordinates, we obtain a relation between the stretched and unstretched radii:

$$\rho^2 = \frac{\omega_\perp M}{\hbar}\left(x^2 + y^2\right) + \frac{\omega_z M}{\hbar}z^2 = \frac{M\omega_0}{\hbar}r^2\left(1 - \frac{2\varepsilon}{3}P_2(\cos\theta)\right)$$

Here we will only calculate r to first order in the distortion coordinates. It is then possible to neglect the difference between $\cos\theta$ and $\cos\theta_t$ ($\cos\theta_t = (\xi^2+\eta^2)^{1/2}/\rho$) to obtain

$$r = r_0\left(1 + \frac{2\varepsilon}{3}P_2 - \sum_\lambda \varepsilon_\lambda P_\lambda + \ldots\right)$$

This expression, which should only be used for small values of ε, ε_3 and ε_4,

† The quadrupole deformation parameter is sometimes referred to as $\varepsilon_2 \equiv \varepsilon$. Here we have used ε to indicate that the constant of the εP_2 term is different from that of the $\varepsilon_\lambda P_\lambda$, $\lambda \geq 3$, terms. Furthermore, the 'Cartesian coordinates' in the (ε,γ) plane are sometimes denoted $(\varepsilon_2,\varepsilon_{22})$ see e.g. Larsson (1973).

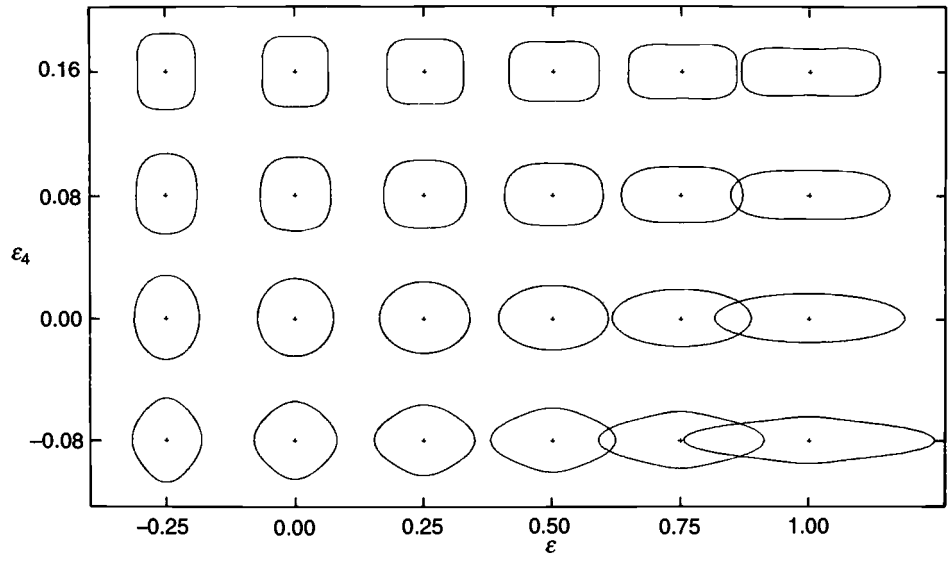

Fig. 8.4. The equipotential shapes generated by the parameters ε and ε_4 of the modified oscillator potential (from Nilsson *et al.*, 1969).

..., describes the same shapes as the coordinates β_λ (or $\alpha_{\lambda 0}$) used in chapter 4. Thus, to first order, one obtains for example

$$\varepsilon \approx \frac{3}{2}\left(\frac{5}{4\pi}\right)^{1/2}\beta_2 \approx 0.95\beta_2 \qquad \text{(quadrupole deformation)}$$

$$\varepsilon_3 \approx (-)\left(\frac{7}{4\pi}\right)^{1/2}\beta_3 \approx (-)0.75\beta_3 \qquad \text{(octupole deformation)}$$

$$\varepsilon_4 \approx -\left(\frac{9}{4\pi}\right)^{1/2}\beta_4 \approx -0.85\beta_4 \qquad \text{(hexadecapole deformation)}$$

Higher order expressions have been published e.g. by Bengtsson *et al.* (1989). At large distortions, the two parametrisations become rather different. The shapes generated in the $(\varepsilon, \varepsilon_4)$ parametrisation are illustrated in fig. 8.4. Observe that, if only $\varepsilon \neq 0$, one obtains pure spheroids, in contrast to the β_4-parametrisation with only $\beta_2 \neq 0$ (see problem 4.2).

In the Legendre polynomials, the coordinates ξ and η (or x and y) enter in a symmetric way (independence of φ_t or φ) and it follows that $[H, j_z] = 0$. Thus, Ω remains as a good quantum number. On the other hand, the different (stretched) N_t-shells are no longer uncoupled. One finds instead that, with λ even, P_4, P_6, ..., only the shells with $\Delta N_t = 2$ couple. This means that the even shells, $N_t = 0, 2, 4, \ldots$, do not mix with the odd shells, $N_t = 1, 3, 5,$

.... These shells are associated with even ℓ and odd ℓ, respectively, and thus with even and odd parity. The conservation of parity is associated with the fact that the potential is mirror symmetric, not only in the z–x and z–y-plane, but also in the x–y-plane. The analogous case in one dimension is a symmetric potential where the solutions separate in even and odd ones.

In fig. 8.5, we show the proton single-particle orbitals drawn along a path in the $(\varepsilon, \varepsilon_4)$-plane. A distinct difference compared with fig. 8.3 is that, for example, orbitals from $N = 5$ and $N = 7$, which have the same Ω-value, never intersect. This is a simple consequence of their interaction due to the ε_4-term. Two interacting orbitals never become degenerate in energy.

With odd λ, P_3, P_5, ... (and also P_1 which mainly corresponds to a shift of the centre of gravity of the potential), the mirror symmetry in the x–y-plane is lost and (intrinsic) parity is no longer a good quantum number. However, because of the rotational symmetry with respect to the z-axis, Ω remains well defined for the different single-particle orbitals. In addition, time-reversal symmetry (see chapter 13) leads to a double degeneracy of the single-particle energies. Thus, all orbitals are filled by two particles 'moving in different directions' (corresponding to $j_z = \Omega$ and $j_z = -\Omega$, respectively).

The calculation of the matrix elements of the $r^2 P_\lambda(\cos\theta_t)$ terms in a $|N\ell\Lambda\Sigma\rangle$ (or $|N\ell j\Omega\rangle$) basis involves one radial and one angular integral. The latter is solved exactly analogous to the $P_2(\cos\theta_t)$ term and results in a sum over Clebsch–Gordan coefficients. The matrix elements of ρ^2 can be given in closed form if the properties of the confluent hypergeometric functions are explored. The formula has been given for example by B. Nilsson (1969). When using such formulae, care must be taken that the same phase convention is used througout.

8.6 Triaxial nuclear shapes – the anisotropic harmonic oscillator potential

For description of the properties of really well-deformed nuclei, it seems to be a good approximation to consider only axially symmetric nuclear shapes. Thus, most of the early calculations (e.g. Mottelson and Nilsson, 1959a; Nilsson *et al.*, 1969; Brack *et al.*, 1972) on deformed nuclei were restricted to such shapes. However, for description of nuclei that are not so strongly deformed (transitional nuclei) it is in many cases necessary to consider also axially asymmetric (triaxial) shapes. Furthermore, it was pointed out in chapter 4 that the (inner) fission barrier of a large number of actinide nuclei is lowered by 1–2 MeV for a fission path involving triaxial shapes. It could also be mentioned that, even if a nucleus is axially symmetric in the ground state, it might change its deformation if it begins to rotate and thus

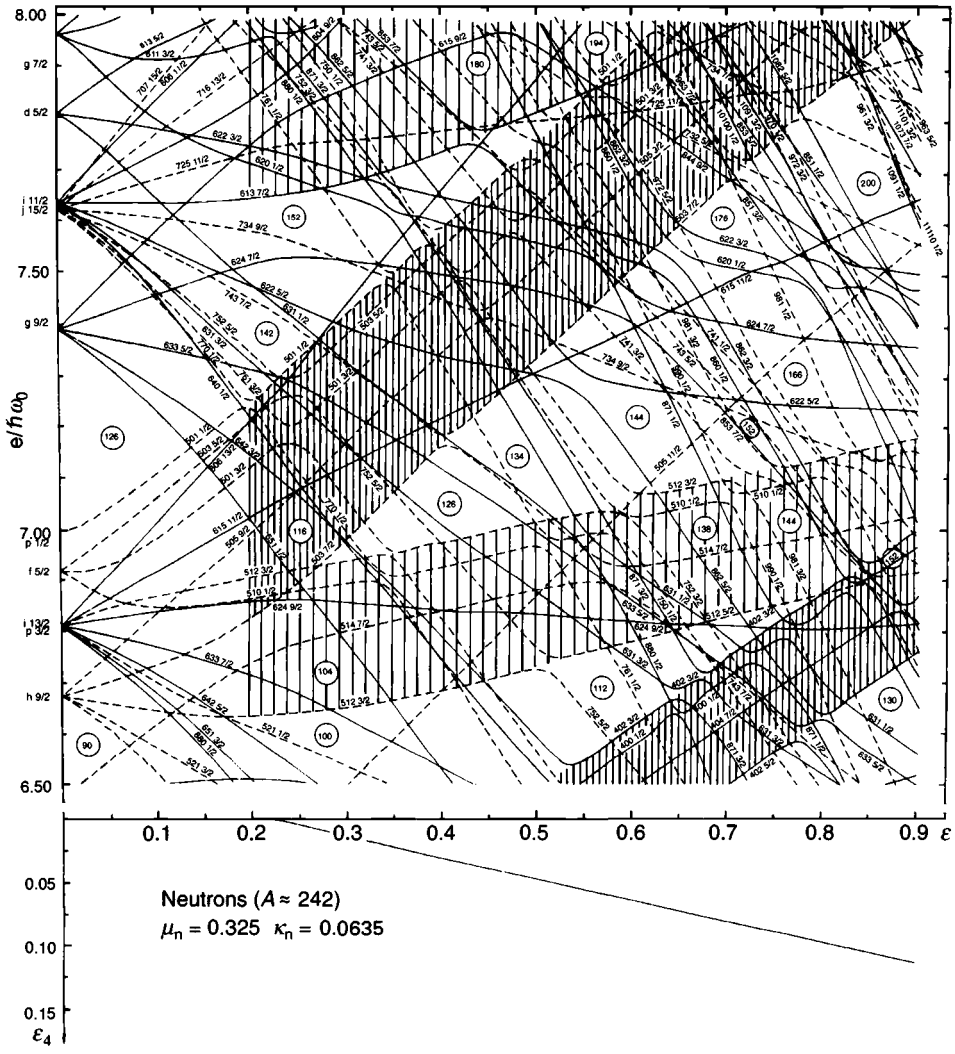

Fig. 8.5. Single-neutron levels in the actinide region drawn as functions of the set of prolate shapes defined in terms of ε and ε_4 as noted below the figure. The $\varepsilon_4\rho^2 Y_{40}$ term couples the different N-shells, $N' = N \pm 2$, which means that orbitals having the same parity and the same Ω-value never cross. Regions of almost degenerate orbitals with $n_z = 0$ and $n_z = 1$ are indicated. These orbitals lead to a high level density for special deformations and particle numbers and are largely responsible for the octupole ε_3-deformations at large ε-values as discussed in chapter 9 (from Ragnarsson *et al.*, 1978).

break the axial symmetry (chapter 12). Indeed, for a rotating nucleus, the special symmetry associated with the axial shape is broken. Thus, axial and non-axial deformations enter on exactly the same footing.

It is straightforward to introduce triaxial shapes in connection with the harmonic oscillator potential, namely

$$V_{\rm osc} = \frac{1}{2}M\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right)$$

with $\omega_x \neq \omega_y \neq \omega_z$. It is then customary to describe the ratio of the frequencies by ε and γ (Bohr, 1952):

$$\omega_x = \omega_0(\varepsilon,\gamma)\left[1 - \frac{2}{3}\varepsilon\cos\left(\gamma + \frac{2\pi}{3}\right)\right]$$
$$\omega_y = \omega_0(\varepsilon,\gamma)\left[1 - \frac{2}{3}\varepsilon\cos\left(\gamma - \frac{2\pi}{3}\right)\right]$$
$$\omega_z = \omega_0(\varepsilon,\gamma)\left[1 - \frac{2}{3}\varepsilon\cos\gamma\right]$$

The parameter ε specifies the degree of deformation, and for $\gamma = 0°$, this parameter is the same as was introduced above. The parameter γ describes the departure from axial symmetry.† The deformation dependence of $\omega_0(\varepsilon,\gamma)$ is determined from volume conservation of the ellipsoidal equipotential surfaces. This is completely analogous to the case of axial symmetry and leads to

$$\omega_x\omega_y\omega_z = \left(\overset{0}{\omega}_0\right)^3$$

where the value of $\overset{0}{\omega}_0 \equiv \omega_0(\varepsilon = \gamma = 0)$ was discussed in chapter 6. It is thus evident that $\omega_0(\varepsilon,\gamma)$ can be given in closed analytic form.

The variation of the frequencies ω_x, ω_y and ω_z as functions of γ for a fixed ε is illustrated in fig. 8.6. One observes that one sector of 60°, e.g. $\gamma = 0$–$60°$, is enough to describe all ellipsoidal shapes. The different 60° sectors then only correspond to a different labelling of the three principal axes. Thus, for description of static nuclei we need only consider one sector, $\gamma = 0$–$60°$. The nucleus is prolate for $\gamma = 0°$, oblate for $\gamma = 60°$ and triaxial for intermediate γ-values. For a rotating nucleus, one often considers the case where the axis of rotation coincides with the x-axis. Then, to describe all possible situations, it is necessary to consider three sectors with the x-axis being the smaller ($\gamma = 0°$ to $60°$) the intermediate ($\gamma = 0°$ to $-60°$) and the larger ($\gamma = -60°$ to $-120°$) principal axis, respectively.

† Different conventions for the sign of γ are used in the literature. This has no importance for the shape of the nucleus but corresponds to a different labelling of the principal axes, see fig. 8.6.

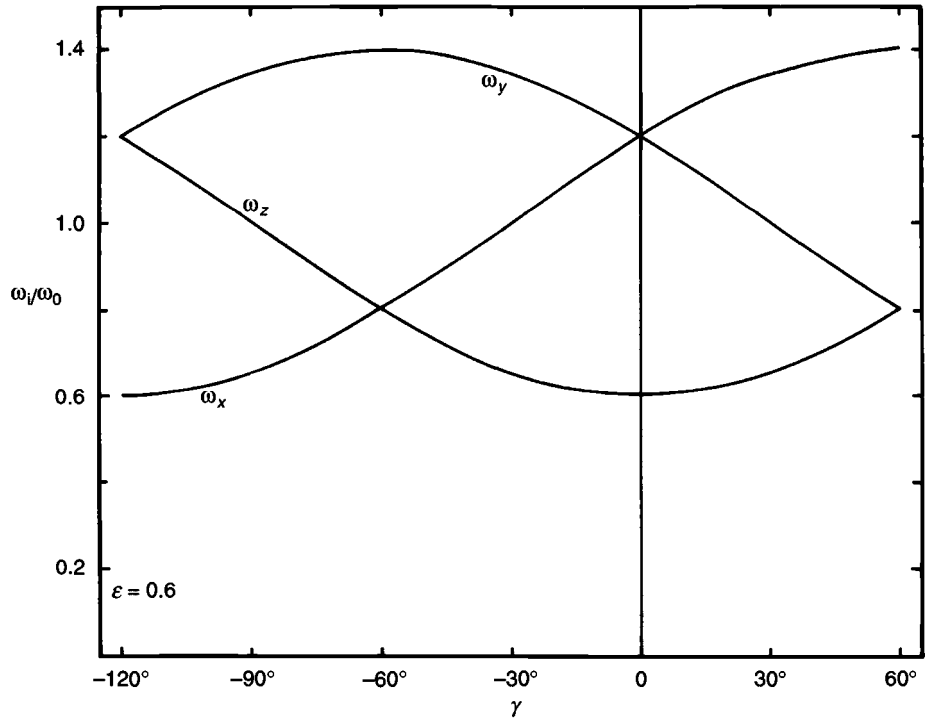

Fig. 8.6. The harmonic oscillator frequencies, ω_x, ω_y and ω_z, versus the asymmetry parameter γ for fixed value of ε, $\varepsilon = 0.6$.

With the introduction of stretched coordinates, $\xi = x(M\omega_x/\hbar)^{1/2}$ etc., the three-dimensional oscillator potential separates into three uncoupled oscillators

$$H_{\text{osc}} = H_x + H_y + H_z$$

where

$$H_x = \frac{1}{2}\hbar\omega_x\left(-\frac{\partial^2}{\partial\xi^2} + \xi^2\right)$$

and analogous expressions for H_y and H_z. The single-particle energies are thus obtained as

$$e_i = \hbar\omega_x\left(n_x + \frac{1}{2}\right) + \hbar\omega_y\left(n_y + \frac{1}{2}\right) + \hbar\omega_z\left(n_z + \frac{1}{2}\right)$$

In the case of $\omega_x = \omega_y = \omega_\perp$ ($\gamma = 0°$), these energies are exhibited in fig. 8.1. The present calculations thus show that the energies of fig. 8.1 are much easier to get out in Cartesian than in cylindrical coordinates. With the introduction of cylindrical coordinates, however, one takes advantage of

the symmetry of the Hamiltonian. The wave functions with corresponding (asymptotic) quantum numbers are thus more suited to deal with the $\ell \cdot \mathbf{s}$- and ℓ^2-terms and also axial deformations of a more general type (P_3, P_4, ...).

For axially symmetric shapes, we used Legendre polynomials, $P_\lambda(\cos\theta_t)$, to describe the potential. An obvious generalisation is to use spherical harmonics, $Y_{\lambda\mu}(\theta_t, \varphi_t)$, for triaxial shapes. The angles θ_t and φ_t are the polar and azimuthal angles in the stretched coordinates, ξ, η and ζ. In these coordinates, the potential takes the form

$$V_{\text{osc}} = \frac{1}{2}\hbar\omega_x\xi^2 + \frac{1}{2}\hbar\omega_y\eta^2 + \frac{1}{2}\hbar\omega_z\zeta^2$$

We now express the frequencies, ω_x, ω_y and ω_z in terms of ε and γ to obtain

$$V_{\text{osc}} = \frac{1}{2}\hbar\omega_0\rho^2\left[1 - \frac{2}{3}\varepsilon\left(\frac{4\pi}{5}\right)^{1/2}\left(\cos(\gamma Y_{20}) - \frac{\sin\gamma}{\sqrt{2}}(Y_{22} + Y_{2-2})\right)\right]$$

Our treatment in the stretched Cartesian basis shows that the corresponding Hamiltonian has no matrix elements that couple the different N-shells. The corresponding analysis in a 'stretched spherical basis' is carried out in appendix 8A. There, it is shown that those parts of the kinetic energy that break the 'spherical symmetry' *in the stretched coordinates* can be transformed to a potential energy term. This term cancels the $\Delta N = 2$ matrix elements of the original potential while it increases the matrix elements within an N-shell by a factor of two.

The triaxial potential, V_{osc}, can now easily be generalised by the addition of $\ell \cdot \mathbf{s}$- and ℓ^2-terms and also by deformations of higher order, $\rho^2\varepsilon_4 P_4(\cos\theta_t)$, etc. In addition it is straightforward, and in principle also necessary to introduce terms like $\rho^2\varepsilon_{42}(Y_{42} + Y_{4-2})$ and $\rho^2\varepsilon_{44}(Y_{44} + Y_{4-4})$ (Larsson *et al.*, 1976; Rohozinski and Sobiczewski, 1981; Nazarewicz and Rozmej, 1981). The importance of such terms can be understood from the fact that for triaxial shape, it is not clear with respect to which axis the angle θ_t should be defined.

The γ-deformation does not alter the fact that each orbital is filled by two particles 'moving in different directions' (due to the time-reversal symmetry). Also the parity is preserved as a good quantum number as long as no odd P_λ are introduced. Thus, the odd and even N-shells remain uncoupled. There are however no other exact quantum numbers and it is also difficult to find any approximate quantum numbers to compare with the asymptotic ones, $|Nn_z\Lambda\Omega\rangle$, which are used for axial symmetry.

The single-particle energies of the triaxial modified oscillator Hamiltonian

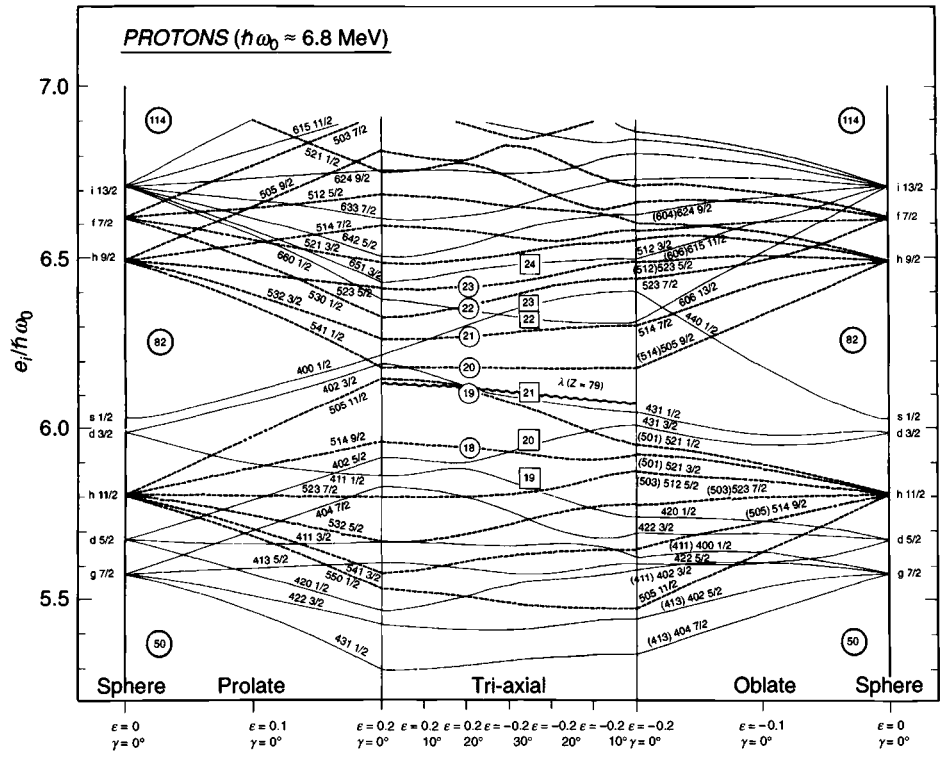

Fig. 8.7. Single-proton orbitals in the $Z \simeq 80$ region. The orbitals at the left edge and the right edge are identical and correspond to spherical shape. In between, ε and γ are varied in such a way that the left part of the figure is drawn for prolate shapes and ε-values up to 0.2, the middle part shows the orbitals for triaxial shape and in the right part of the figure, the orbitals corresponding to oblate shape are exhibited. The asymptotic quantum numbers for prolate and oblate shape, respectively, are given. At the small deformation of $\varepsilon = 0.2$, they are rather impure and in some cases, two alternatives are indicated. For γ-deformations, it is difficult to find any approximate quantum numbers, but the orbitals of different parity can be numbered from 'the bottom' as indicated in the figure. Furthermore, a calculated Fermi level, λ, (chapter 14) for $Z = 79$ is indicated by a wavy line (from C. Ekström *et al.*, 1989, *Nucl. Phys.* **A348**, 25).

are obtained from diagonalisation. An example of such energies, shown along a closed path in the (ε, γ)-plane, is provided in fig. 8.7. The orbitals are labelled by the asymptotic quantum numbers for oblate and prolate shape.

We will come back to the question of triaxial deformations in chapter 12. Now, we will, however, finish this chapter by discussing an operator method, which provides a concise method to calculate single-particle matrix elements in an oscillator basis.

8.7 Asymptotic wave functions by operator methods

We have earlier derived the wave function for the deformed harmonic oscillator with axial symmetry by the solution of the Schrödinger differential equation. We shall now utilise an operator method to generate the wave functions characterised by N, n_z and Λ being constants of the motion (Mottelson and Nilsson, 1959b).

From the study of the one-dimensional oscillator, the operator method is well known. Here we will briefly go through the necessary derivations. In terms of stretched coordinates, $\xi = x \cdot (M\omega_x/\hbar)^{1/2}$ etc., one may write

$$a_x = \frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right) = \frac{1}{\sqrt{2}}\left(\xi + \frac{\mathrm{i}}{\hbar}p_\xi\right)$$
$$a_x^+ = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right) = \frac{1}{\sqrt{2}}\left(\xi - \frac{\mathrm{i}}{\hbar}p_\xi\right)$$

where thus a_x^+ is the Hermitian adjoint of a_x. Inversely

$$\xi = \frac{1}{\sqrt{2}}(a_x + a_x^+)$$

$$\frac{\partial}{\partial\xi} = \frac{1}{\sqrt{2}}(a_x - a_x^+)$$

Similar definitions hold for a_y and a_z. It is easy to verify that the a_x operators fulfill the commutation relations

$$[a_x, a_x^+] = 1$$

Expressing

$$H_x = \frac{1}{2}\hbar\omega_x\left(-\frac{\partial^2}{\partial\xi^2} + \xi^2\right)$$

in terms of a_x^+ and a_x we obtain

$$H_x = \hbar\omega_x\left(a_x^+ a_x + \frac{1}{2}\right)$$

Thus H_x commutes with $a_x^+ a_x$, which means that these two operators can be assumed to have the same eigenvectors. We introduce eigenvectors ψ_k and eigenvalues λ_k

$$a_x^+ a_x \psi_k = \lambda_k \psi_k$$

Scalar multiplication with ψ_k leads to

$$\langle \psi_k \,|a_x^+ a_x \psi_k\rangle = \langle a_x\psi_k|\, a_x\psi_k\rangle = \lambda_k \,\langle \psi_k \,|\psi_k\rangle$$

Since $\langle a_x\psi_k \,|a_x\psi_k\rangle$ and $\langle \psi_k \,|\psi_k\rangle$ are non-negative, we conclude that

$$\lambda_k \geq 0$$

From the commutation relations we furthermore get

$$(a_x^+ a_x)\, a_x^+\psi_k = a_x^+\,(a_x^+ a_x + 1)\,\psi_k = (\lambda_k + 1)\, a_x^+\psi_k$$

which means that $a_x^+\psi_k$ is also an eigenvector of $a_x^+ a_x$, the corresponding eigenvalue being $\lambda_k + 1$. Similarly, one can show that $a_x\psi_k$ is an eigenvector with the eigenvalue $\lambda_k - 1$. The operator a_x^+ is thus called a raising operator, while a_x is a lowering operator. Since $\lambda_k \geq 0$, there must be a lowest value for λ_k:

$$a_x^+ a_x\psi_0 = \lambda_0\psi_0$$

The eigenvalue cannot become smaller and consequently

$$a_x\psi_0 = 0$$

This leads to

$$\lambda_0 = 0$$

and consequently $\lambda_1 = 1$, $\lambda_2 = 2$, etc., i.e.

$$a_x^+ a_x\psi_n \equiv a_x^+ a_x\,|n_x\rangle = n_x\,|n_x\rangle$$

We thus find for the oscillator Hamiltonian

$$H_x\,|n_x\rangle = \hbar\omega_x\left(a_x^+ a_x + \frac{1}{2}\right)|n_x\rangle = \hbar\omega_x\left(n_x + \frac{1}{2}\right)|n_x\rangle$$

The eigenvalue, n_x, of $a_x^+ a_x$ is referred to as the number of oscillator quanta. This justifies the designation of $a_x^+ a_x$ as a number operator, $\mathcal{N}_x$, with respect to the x quanta. The eigenvector Ψ_0 is of course the no-quantum ground state wave function

$$\psi_0 = |0\rangle = \pi^{-1/4}\mathrm{e}^{-\xi^2/2}$$

The one-quantum state is now easily calculated

$$a_x^+\,|0\rangle = \pi^{-1/4}\frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right)\mathrm{e}^{-\xi^2/2} = \pi^{-1/4}\sqrt{2}\cdot\xi\mathrm{e}^{-\xi^2/2}$$

Generally the normalised state with n_x quanta can be written

$$|n_x\rangle = \frac{1}{(n_x!)^{1/2}}\,(a_x^+)^{n_x}\,|0\rangle$$

The normalisation constant is obtained from the commutation relations. These lead to (see problem 8.7)

$$a_x^+ |n_x\rangle = (n_x + 1)^{1/2} |n_x + 1\rangle$$
$$a_x |n_x\rangle = \sqrt{n_x} |n_x - 1\rangle$$

After these general considerations in one dimension, we go back to the three-dimensional oscillator with cylinder symmetry. To exploit this symmetry between x and y we define

$$R^+ = \frac{1}{\sqrt{2}} \left(a_x^+ + \mathrm{i} a_y^+\right)$$
$$R = \frac{1}{\sqrt{2}} \left(a_x - \mathrm{i} a_y\right)$$
$$S^+ = \frac{1}{\sqrt{2}} \left(a_x^+ - \mathrm{i} a_y^+\right)$$
$$S = \frac{1}{\sqrt{2}} \left(a_x + \mathrm{i} a_y\right)$$

One can now verify the commutation rules

$$[R, R^+] = [S, S^+] = 1$$

while all other commutations vanish. It is apparent that one can subsequently construct eigenfunctions with the help of the R^+ and S^+ operators analogous to what is done in the a_x^+ case.

The operators R^+ and S^+ increase while R and S lower the quantum number $n_\perp$ by one unit. This corresponds to the fact that the number operator with respect to the quanta perpendicular to the z-axis can be written

$$\mathcal{N}_\perp = a_x^+ a_x + a_y^+ a_y = R^+ R + S^+ S$$

In terms of these new operators, the Hamiltonian of the cylindrically symmetrical harmonic oscillator can be written

$$H_{\text{cyl. osc}} = \hbar\omega_z \left(a_z^+ a_z + \frac{1}{2}\right) + \hbar\omega_\perp \left(a_x^+ a_x + a_y^+ a_y + 1\right)$$
$$= \hbar\omega_z \left(\mathcal{N}_z + \frac{1}{2}\right) + \hbar\omega_\perp (\mathcal{N}_\perp + 1)$$
$$= \hbar\omega_z \left(\mathcal{N}_z + \frac{1}{2}\right) + \hbar\omega_\perp (R^+ R + S^+ S + 1)$$

As we have seen in the earlier parts of this chapter, from the Schrödinger

equation we can find a solution to this Hamiltonian, which in addition has a good Λ quantum number, and is of the type

$$\psi = Z(\zeta)U(\rho)\phi(\varphi) = |n_z\rangle\,|n_\perp\Lambda\rangle$$

Alternatively using the operators we can write a solution

$$\psi = |n_z rs\rangle = \frac{1}{(n_z!r!s!)^{1/2}}\,(a_z^+)^{n_z}\,(R^+)^r\,(S^+)^s\,|0\rangle$$

It is easily seen that

$$H_{\text{cyl. osc}}\,|n_z rs\rangle = \left[\left(n_z + \frac{1}{2}\right)\hbar\omega_z + (n_\perp + 1)\,\hbar\omega_\perp\right]|n_z rs\rangle$$

where

$$n_\perp = r + s$$

Our next step is to express ℓ_z in terms of the R and S operators. We shall use the simplified notation ℓ_x etc. to denote $(\ell_t)_x$ etc. and furthermore assume the angular momentum vector to be expressed in units of $\hbar$ (thus set $\hbar = 1$)

$$\ell_z = \frac{1}{\mathrm{i}}\left(\xi\frac{\partial}{\partial\eta} - \eta\frac{\partial}{\partial\xi}\right) = \frac{1}{\mathrm{i}}\left(a_x^+ a_y - a_y^+ a_x\right) = (R^+R - S^+S)$$

Thus,

$$\ell_z\,|n_z rs\rangle = (r - s)\,|n_z rs\rangle = \Lambda\,|n_z rs\rangle$$

where

$$\Lambda = r - s$$

Hence $|n_z rs\rangle$ is an eigenfunction both of $H_{\text{cyl. osc}}$ and ℓ_z.

The operators R^+ and S increase the quantum number $\ell_z = \Lambda$ by one unit while R and S^+ lower Λ by one unit. This corresponds to commutation rules

$$[\ell_z, R^+] = R^+, \quad [\ell_z, S] = S, \quad [\ell_z, R] = -R, \quad [\ell_z, S^+] = -S^+$$

which are easily proven if the expression of ℓ_z in terms of the R- and S-operators is used.

For the ℓ_x and ℓ_y operators, we obtain

$$\mathrm{i}\ell_x = a_y^+ a_z - a_z^+ a_y = \frac{-\mathrm{i}}{\sqrt{2}}\left[a_z^+(R - S) + a_z\,(R^+ - S^+)\right]$$

$$\mathrm{i}\ell_y = a_z^+ a_x - a_x^+ a_z = \frac{-\mathrm{i}}{\sqrt{2}}\left[a_z\,(R^+ + S^+) - a_z^+\,(R + S)\right]$$

and furthermore

$$\ell_+ = \sqrt{2}\,(a_z^+ S - a_z R^+)$$
$$\ell_- = \sqrt{2}\,(a_z S^+ - a_z^+ R)$$

which latter expressions will prove useful later on.

Starting from the wave function $|n_z, n_\perp = r+s, \Lambda = r-s\rangle$, we may generate a wave function with $n_\perp \to n_\perp + 1$ and $\Lambda \to \Lambda + 1$ or $|n_z, n_\perp + 1, \Lambda + 1\rangle$ by operation with R^+. We utilise $[H_{\text{cyl. osc}}, R^+] = \hbar\omega_\perp R^+$ to obtain

$$\begin{aligned} H_{\text{cyl. osc}}\{R^+ |n_z rs\rangle\} &= R^+ (H_{\text{cyl. osc}} + \hbar\omega_\perp)\,|n_z rs\rangle \\ &= \left[\left(n_z + \frac{1}{2}\right)\hbar\omega_z + (r+s+2)\,\hbar\omega_\perp\right]\{R^+ |n_z rs\rangle\} \end{aligned}$$

Similarly

$$\begin{aligned} \ell_z\{R^+ |n_z rs\rangle\} &= R^+ (\ell_z + 1)\,|n_z rs\rangle = R^+(r-s+1)\,|n_z rs\rangle \\ &= (\Lambda + 1)\{R^+ |n_z rs\rangle\} \end{aligned}$$

Alternatively we may just exploit the fact that

$$R^+ |n_z rs\rangle = (r+1)^{1/2}\,|n_z\; r+1\; s\rangle$$

and the relations

$$n_\perp = r + s\,, \qquad \Lambda = r - s$$

With inclusion of spin the total wave function is

$$\psi = |n_z rs\rangle\,|\Sigma\rangle$$

We are now in a position to evaluate the matrix elements of $\ell_t \cdot \mathbf{s}$ and ℓ_t^2 in this asymptotic representation. Let us start with $\ell_t \cdot \mathbf{s}$. From the expansion

$$\ell_t \cdot \mathbf{s} = (\ell_t)_z\, s_z + \frac{1}{2}\,((\ell_t)_+ s_s + (\ell_t)_- s_+)$$

we obtain, simplifying the notation by leaving out t as is done above,

$$\ell \cdot \mathbf{s} = (R^+R - S^+S)\,s_z - \frac{1}{\sqrt{2}}\,(a_z R^+ - a_z^+ S)\,s_- - \frac{1}{\sqrt{2}}\,(a_z^+ R - a_z S^+)\,s_+$$

The first term is an eigenoperator of $|n_z rs\Sigma\rangle$

$$\ell_z s_z\,|n_z rs\Sigma\rangle = (r-s)\Sigma\,|n_z rs\Sigma\rangle = \Lambda\Sigma\,|n_z rs\Sigma\rangle$$

and

$$\langle n_z rs\Sigma\,|\ell \cdot \mathbf{s}|\,n_z rs\Sigma\rangle = \Lambda\Sigma$$

The next two terms of $(\ell \cdot \mathbf{s})$ give rise to non-diagonal coupling terms associated with selection rules

$$\Delta\Sigma = -1,\ \Delta\Lambda = 1,\ \Delta n_z = -\Delta n_\perp = \pm 1$$

and

$$\Delta\Sigma = 1,\ \Delta\Lambda = -1,\ \Delta n_z = -\Delta n_\perp = \pm 1$$

For the matrix elements, we get for example

$$\langle n_z - 1\, r + 1\, s\, \Sigma - 1 \,|\ell \cdot \mathbf{s}|\, n_z\, r\, s\, \Sigma\rangle = -\frac{1}{\sqrt{2}}\,[n_z(r+1)]^{1/2}$$

and thus

$$\langle n_z - 1\, n_\perp + 1\, \Lambda + 1\, \Sigma - 1 \,|\ell \cdot \mathbf{s}|\, n_z\, n_\perp\, \Lambda\, \Sigma\rangle = -\frac{1}{2}\,[n_z\,(n_\perp + \Lambda + 2)]^{1/2}$$

In a similar way, the other matrix elements are obtained as

$$\langle n_z + 1\, n_\perp - 1\, \Lambda + 1\, \Sigma - 1 \,|\ell \cdot \mathbf{s}|\, n_z\, n_\perp\, \Lambda\, \Sigma\rangle = \frac{1}{2}\,[(n_z+1)\,(n_\perp - \Lambda)]^{1/2}$$

$$\langle n_z + 1\, n_\perp - 1\, \Lambda - 1\, \Sigma + 1 \,|\ell \cdot \mathbf{s}|\, n_z\, n_\perp\, \Lambda\, \Sigma\rangle = -\frac{1}{2}\,[(n_z+1)\,(n_\perp + \Lambda)]^{1/2}$$

$$\langle n_z - 1\, n_\perp + 1\, \Lambda - 1\, \Sigma + 1 \,|\ell \cdot \mathbf{s}|\, n_z\, n_\perp\, \Lambda\, \Sigma\rangle = \frac{1}{2}\,[n_z\,(n_\perp - \Lambda + 2)]^{1/2}$$

From the expressions for ℓ_+ and ℓ_- it is easy to find an expression for $\ell_\perp^2 = \ell_x^2 + \ell_y^2$

$$\ell_\perp^2 = \frac{1}{2}\,(\ell_+\ell_- + \ell_-\ell_+) = 2a_z^+ a_z\,(R^+R + S^+S + 1) + R^+R + S^+S$$
$$-2\,(a_z^+)^2\,RS - 2\,(a_z)^2\,R^+S^+$$

The first three terms are an eigenoperator of $|n_z rs\rangle$ with the eigenvalue $2n_z\,(n_\perp + 1) + n_\perp$ while the last two terms have selection rules $\Delta\Lambda = 0$, $\Delta N = 0$, $\Delta n_z = -\Delta n_\perp = \pm 2$:

$$\left\langle n_z + 2\, r - 1\, s - 1 \left|\ell_\perp^2\right| n_z\, r\, s\right\rangle = -2\,[(n_z+2)\,(n_z+1)\cdot r \cdot s]^{1/2}$$

and

$$\left\langle n_z - 2\, r + 1\, s + 1 \left|\ell_\perp^2\right| n_z\, r\, s\right\rangle = -2\,[(n_z-1)\,n_z\,(r+1)\,(s+1)]^{1/2}$$

Thus with $\ell^2 = \ell_\perp^2 + \ell_z^2$:

$$\left\langle n_z\, n_\perp\, \Lambda\, \Sigma \left|\ell^2\right| n_z\, n_\perp\, \Lambda\, \Sigma\right\rangle = 2n_z\,(n_\perp + 1) + n_\perp + \Lambda^2$$

$$\left\langle n_z + 2\,n_\perp - 2\,\Lambda\,\Sigma \left| \ell^2 \right| n_z\, n_\perp\, \Lambda\, \Sigma \right\rangle$$

$$= -\left[(n_z+2)(n_z+1)(n_\perp+\Lambda)(n_\perp-\Lambda)\right]^{1/2}$$

$$\left\langle n_z - 2\,n_\perp + 2\,\Lambda\,\Sigma \left| \ell^2 \right| n_z n_\perp \Lambda\Sigma \right\rangle$$

$$= -\left[(n_z-1)\,n_z\,(n_\perp+\Lambda+2)(n_\perp-\Lambda+2)\right]^{1/2}$$

Exercises

8.1 Show that

$$\left\langle N\ell j\Omega \left| -M\omega_0^2 \frac{2}{3}\varepsilon r^2 P_2 \right| N\ell j\Omega \right\rangle = \frac{1}{6}\varepsilon M\omega_0^2 \left\langle r^2 \right\rangle \frac{3\Omega^2 - j(j+1)}{j(j+1)}$$

8.2 Find the solution in hypergeometrical functions of

$$\left(-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{\Lambda^2}{\rho^2} + \rho^2 - \frac{2E_\perp}{\hbar\omega_\perp}\right) U(\rho) = 0$$

Use the substitution

$$U(\rho) = \rho^{|\Lambda|} e^{-\rho^2/2} f(\rho)$$

8.3 Start from the harmonic oscillator Hamiltonian

$$H = -\frac{\hbar^2}{2M}\Delta_x + \frac{M}{2}\left[\omega_\perp^2\left(x^2+y^2\right) + \omega_z^2 z^2\right]$$

Make the substitution

$$\xi = x\left(M\omega_\perp/\hbar\right)^{1/2} \quad \text{etc.}; \qquad \rho^2 = \xi^2 + \eta^2 + \zeta^2$$

and show that H can be expressed as

$$H = H_d + H_\varepsilon$$

where

$$H_d = \frac{1}{2}\hbar\omega_0\left(-\Delta_\xi + \rho^2\right)$$

and

$$H_\varepsilon = \frac{1}{6}\varepsilon\hbar\omega_0\left(-\frac{\partial^2}{\partial\xi^2} - \frac{\partial^2}{\partial\eta^2} + 2\frac{\partial^2}{\partial\zeta^2} + \xi^2 + \eta^2 - 2\zeta^2\right)$$

8.4 Show that an axially symmetric modified oscillator Hamiltonian, H_{MO}, commutes with the j_z operator, $[H_{\mathrm{MO}}, j_z] = 0$. Calculate also $[\ell \cdot \mathbf{s}, \ell_z]$. Comments!

8.5 For the modified oscillator potential at small deformations, the energy levels can be calculated in first-order perturbation theory. At large deformations, a good approximation is to treat the harmonic oscillator exactly but only to consider diagonal contributions from the $\ell \cdot \mathbf{s}$- and ℓ^2-terms. Carry through these calculations for the $N = 2$ levels and sketch them for $|\varepsilon| \leq 0.75$. Put $\kappa = 0.1$ and $\mu' = 0.02$.

8.6 For the $\Omega = 3/2$, $N = 2$ levels of the modified oscillator potential, it is easy to make an exact diagonalisation. Carry through the calculations and compare with the approximate energies of problem 8.5.

8.7 Use the properties $[a, a^+] = 1$ and $a^+ a\,|n\rangle = n\,|n\rangle$ of the step operator a^+ to find the normalisation constant C_n in the formula

$$a^+\,|n\rangle = C_n\,|n+1\rangle$$

8.8 Prove that $[R, R^+] = 1$ and that $[R^+, S] = 0$.

8.9 Express ℓ_z in terms of R and S and their Hermitian conjugates.

8.10 Let $|A\rangle$ be an eigenvector of the operator A with the eigenvalue a, $A\,|A\rangle = a\,|A\rangle$. Show that, if $[A, B] = B$, then $B\,|A\rangle$ is an eigenvector of A with the eigenvalue $(a+1)$.

8.11 Prove

$$\langle n_z + 1\; n_\perp - 1\; \Lambda - 1\; \Sigma + 1\,|\ell \cdot \mathbf{s}|\, n_z n_\perp \Lambda\Sigma\rangle = \frac{-1}{2}\,[(n_z+1)(n_\perp+\Lambda)]^{1/2}$$

8.12 Use operator methods to calculate the radius of a triaxial harmonic oscillator wave function,

$$\left\langle n_x n_y n_z \left| r^2 \right| n_x n_y n_z \right\rangle$$

Specialise to spherical shape!