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:

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

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

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

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 ℓ^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)

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

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

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