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Parity mixing in deformed Hartree-Fock approximation in $A \approx 70$ mass region

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Abstract. Parity mixing in defomred Hartree-Fock orbits preferentially lowers the energies of prolate deformed shapes and leads to a consistent description of the shapes of $A \approx 70$ nuclei.

Keywords. Parity mixing; Hartree-Fock calculation.

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1. Introduction

The region of the periodic table with mass $A = 60$–80 has been the subject of much research activity in the past several years (Ahalpara *et al* 1981, 1985; Ramayya and Hamilton 1987; Sahu *et al* 1987). Some of these nuclei are strongly deformed (Moller and Nix 1981; Lister *et al* 1982, 1987; Siewert *et al* 1984). The prolate deformation of these nuclei has been deduced by Lecomte *et al* (1977, 1978, 1980) from Coulomb excitation reorientation experiments.

Deformed Hartree-Fock calculations using realistic interaction matrix elements (Ahalpara and Bhatt 1982; Sahu and Pandya 1984; Ahalpara 1985; Sahu *et al* 1987; Praharaj 1988a) predict the oblate or spherical shape as lower in energy than the prolate shape for many of these nuclei and are unable to explain the shapes of these nuclei. In this work we have studied the structure of nuclei in this mass region and find that parity mixing lowers the energy of the prolate shape by several MeV, while leaving the energy of the oblate or spherical shape essentially unchanged. As examples we present the results for ^{72}Ge and ^{76}Se (Praharaj 1988b).

In §2 the active shell model space and the residual interaction used in the calculations are given. The results of Hartree-Fock calculations, both without and with parity mixing, are given in §3. Section 4 contains discussions about the mechanism of parity mixing and the concluding remarks.

2. Model space and residual interaction

We assume a ^{56}Ni core and use a shell model space spanning two major shells. The shell model orbits are shown in figure 1. The single-particle energies of the neutron $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ states are taken from ^{57}Ni spectrum (Fortier and Gales 1979). The energies of these single-particle states for protons are assumed to be the same as those for the neutrons. The $g_{9/2}$ orbits for the protons and neutrons are taken 3·78 MeV

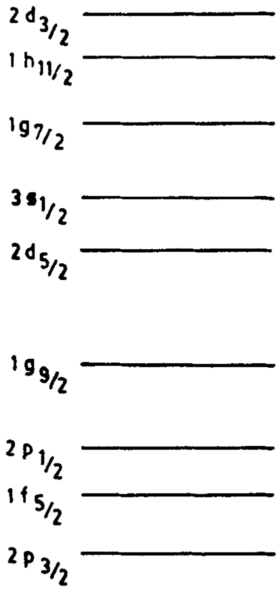

Figure 1. Spherical shell model orbits for protons and neutrons included in the present study. Note the large energy gap ($d_{5/2}$ and $g_{9/2}$ energy difference) above particle number 50.

Table 1. Single-particle energies (in MeV) for protons and neutrons.

Shell model orbit	$p_{3/2}$	$f_{5/2}$	$p_{1/2}$	$g_{9/2}$	$d_{5/2}$	$s_{1/2}$	$g_{7/2}$	$h_{11/2}$	$d_{3/2}$
Protons	0·0	0·78	1·08	3·78	12·78	18·18	12·78	18·18	15·18
Neutrons	0·0	0·78	1·08	3·78	12·28	14·28	12·88	15·68	14·78

above the $2p_{3/2}$ orbits. The shell gap above the $g_{9/2}$ orbit is taken as 9 MeV (approximately $40/A^{1/3}$ MeV and the energy splitting among the 3*s*, 2*d*, $1g_{7/2}$, $1h_{11/2}$ orbits are given reasonable values, consistent with the shell model energies in a Woods-Saxon potential well (Bertsch 1972). We remark that the general lowering of the prolate shape energy by parity mixing to be discussed in this work is independent of the fine details of these single-particle energies. The spherical single-particle energies used in our calculation are given in table 1.

As the residual interaction among nucleons in the model space, we take a surface delta interaction (Faessler *et al* 1967)

$$V(r_{12}) = -2F(R_0u_0)^{-4}\delta(r_1 - R_0)\delta(r_2 - R_0)\delta(\cos w_{12} - 1)$$

$$= -V_0 \sum_{lm} Y^*_{lm}(\Omega_1)Y_{lm}(\Omega_2). \quad (1)$$

Here R_0 is the nuclear radius and the radial wave functions u are approximated to be the same at the nuclear surface. The strength V_0 is taken to be 0·42 MeV and is assumed to be the same for the proton-proton, proton-neutron and neutron-neutron interactions. This is a reasonable approximation, since the protons and neutrons are filling the same major shell and the neutron-proton asymmetry $N-Z$ is small. The surface delta is a reasonable interaction for nuclear structure calculations (Brussard and Glaudemans 1977). In the present case the matrix elements $\langle g_{9/2}^2|V|g_{9/2}^2\rangle_J$ calculated with this interaction are similar to the modified matrix elements used by Bhatt *et al* (Ahalpara *et al* 1985) in this mass region.

3. Hartree-Fock calculations and parity mixing

We confine ourselves to axially symmetric deformed shape and calculate for both prolate and oblate shapes. We also look for spherical solutions. Two kinds of deformed HF-solutions are looked for: (1) solutions with good parity and (2) parity-mixed solutions. For good parity solutions we start the Hartree-Fock iteration with the Nilsson Hamiltonian

$$h = H_0 - \chi_2 \sum_i r_i^2 Y_{20}(\theta_i). \tag{2a}$$

Here H_0 is the spherical shell model Hamiltonian and the second term is the one-body quadrupole field (Bohr and Mottelson 1975). For the parity-mixed solutions we start the Hartree-Fock iteration with an octupole field added to the above Nilsson Hamiltonian

$$h' = H_0 - \chi_2 \sum_i r_i^2 Y_{20}(\theta_i) - \chi_3 \sum_i r_i^3 Y_{30}(\theta_i). \tag{2b}$$

Starting with positive and negative χ_3 we find two degenerate parity-mixed solutions having the same even multipole moments and with the odd multipole moments differing in sign only. The results for the Hartree-Fock calculation for ^{72}Ge and ^{76}Se are given in table 2, where we list the Hartree-Fock energies and various intrinsic even multipole moments for $l = 2$, 4, 6 and 8. Effective charges of 1·2e and 0·2e for

Table 2. Hartree-Fock solutions for ^{72}Ge and ^{76}Se giving HF energies and even multipole moments $\langle \sum_i e_i r_i^l Y_{l0}(\Omega_i)\rangle$ $l = 4, 6, 8$ in units of eb^l (b is the length parameter). Effective charges are 1·2e for protons and 0·2e for neutrons. The column before the last one gives the quadrupole moment $(16\pi/5)^{1/2}\langle \sum_i e_i r_i^2 Y_{20}(\Omega_i)\rangle$ in efm^2. The last column gives the experimental intrinsic quadrupole moments using eqn. (4) (Lecomte *et al* 1977, 1980). The parity-mixed solutions, denoted by asterisks, are two-fold degenerate, with opposite signs of odd l moments (not listed in the table). The two-fold degenerate parity-mixed solutions have the same even l moments.

Nucleus	Shape	E_{HF} (MeV)	Multipole 4	Moments 6	(eb^l) 8	Q_2 (efm^2)	Q_2 expt. (efm^2)
^{72}Ge	Spherical	−30·12	0	0	0	0	45·5±21
	Prolate*	−32·02	22·2	56·2	−0·1	57·1	
^{76}Se	Oblate	−47·48	15·6	−9·8	35·5	−79·2	119±31·5
	Prolate	−46·48	−3·8	20·4	81·1	75·8	
	Oblate*	−47·98	11·4	21·1	−120·6	−72·3	
	Prolate*	−53·48	14·8	−6·1	−205·6	125·7	

the protons and the neutrons respectively are used in the enlarged model space. For $l = 4, 6, 8$ the multipole moments are defined as the HF expectation values of $\sum_i e_i r_i^l Y_{lo}(\Omega_i)$

$$Q_L = \langle \phi_{HF} | \sum_i e_i r_i^l Y_{lo}(\Omega_i) | \phi_{HF} \rangle. \quad (3)$$

We use an additional factor of $(16\pi/5)^{1/2}$ for $l = 2$ to make it agree with the usual definition of quadrupole moment.

In the last column of table 2 the experimental intrinsic quadrupole moments (Lightbody *et al* 1972; Grissmer *et al* 1972; Lecomte *et al* 1977, 1978 and 1980) are given. In calculating the intrinsic quadrupole moment Q_2 from the measured spectroscopic quadrupole moment Q of the 2^+ state we use the rotational model expression

$$Q = [3K^2 - J(J+1)]/[(J+1)(2J+3)]Q_2 \quad (4)$$

with $K = 0$ and $J = 2$.

In table 2 the parity mixed solutions are denoted by asterisks. It is clear that parity-mixing in the Hartree-Fock orbits lowers the energy of the prolate shape, while the energy lowering for the oblate shape is quite negligible. In ^{72}Ge there is no oblate solution at all. Restricting ourselves to reflection symmetry we get only a spherical Hartree-Fock solution for ^{72}Ge which is known experimentally to have a large prolate deformation (Lecomte *et al* 1977, 1978, 1980). Allowing for parity-mixing in the Hartree-Fock orbits we get a lower energy prolate solution (Prolate*) which has a quadrupole moment with the correct sign and order of magnitude as in the experiment of Lecomte *et al* cited above. It is to be remarked that reflection symmetric Hartree-Fock calculations by Nazarewicz *et al* (Dobaczewski *et al* 1988) using Skyrme interaction predicts the oblate shape in ^{72}Ge as the lowest in energy, in contradiction with the above mentioned experiments.

In table 2 we find that the theoretical reflection symmetric oblate shape of ^{76}Se is lower in energy than the corresponding prolate shape, while experimentally the nucleus is known to be prolate deformed (Lecomte *et al* 1977). This conflict between theory and experiment is resolved by allowing for parity-mixing in the Hartree-Fock orbits. Parity-mixing lowers the energy of the prolate shape considerably, while the oblate shape energy is affected very little by such mixing.

The parity-mixed HF minima, obtained by starting with positive and negative χ_3 in eq. 2b, are degenerate in energy indicating that the nuclei are soft to odd multipole distortions. Strutinsky calculations by Nazarewicz *et al* (1984) also indicates octupole softness, but no permanent octupole deformation, for this region. Apart from lowering the energies of prolate Hartree-Fock solutions, parity mixing induces deformations of even multipolarity and the quadrupole moments of the prolate Hartree-Fock solutions increase substantially. By contrast, the energies and quadrupole moments of the oblate Hartree-Fock solutions are largely unaffected by parity-mixing.

4. Mixing mechanism and concluding remarks

Some of the lowest energy Hartree-Fock orbits of the various Hartree-Fock solutions (oblate, prolate, oblate* and prolate*) of ^{76}Se are plotted in figure 2. One clearly sees

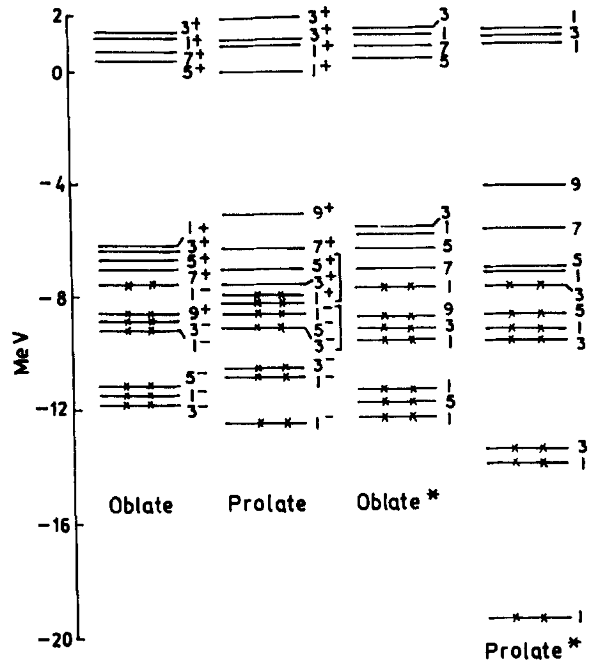

Figure 2. Lowest neutron orbits of deformed Hartree-Fock solutions for ^{76}Se. Asterisks denote parity-mixed solutions. The doubly degenerate orbits are denoted by $2|m|$ and crosses show the occupied orbits. Orbits with same m and different parities occur near the Fermi surface of the prolate HF.

that the oblate orbits are affected very little by parity-mixing, while the prolate shape is much more affected by it. Among the low energy positive parity deformed Hartree-Fock orbits are $|m = 9/2^+\rangle$ and $|m = 7/2^+\rangle$ for the oblate shape and there are no corresponding negative parity Hartree-Fock orbits with which these can mix if the conditions of parity-conservations is relaxed. In contrast to this, the positive parity $|m = 1/2^+\rangle$, $|m = 3/2^+\rangle$ and other orbits with small m are among the lowest in energy and are close enough to the negative parity orbits of the same m for the prolate solution. Hence, once parity mixing is allowed for, positive and negative parity orbits of the same m can mix via two-body interaction and this can lead to considerable energy lowering for the prolate* solution. The Hartree-Fock potential matrix for axial symmetry is given by

$$\Gamma_{j'mjm} = \sum_{j_2 j'_2 m_2} V(j'mj'_2m_2; jmj_2m_2)\rho_{j_2m_2j'_2m_2} \tag{5}$$

where

$$\rho_{j_2m_2j'_2m_2} = \langle \phi_{HF} | a^+_{j'_2m_2} a_{j_2m_2} | \phi_{HF} \rangle \tag{6}$$

are elements of the density matrix and $V(j'mj'_2m_2;jmj_2m_2)$ are the two-body matrix elements in the uncoupled representation.

In reflection symmetric solutions the density matrix ρ is diagonal in parity and hence has no matrix elements between single-particle states of different parities. For example,

$$\rho_{g_{9/2}m_2p_{3/2}m_2} = 0 \tag{7}$$

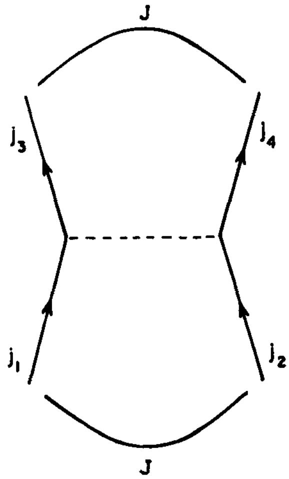

Figure 3. Diagram for the residual interaction matrix element $\langle j_3 j_4 J\pi | V_{12} | j_1 j_2 J\pi \rangle$. Interaction matrix elements that contribute to parity mixing in (5) and (6) are:

(a) $j_1, j_2 = pfh$ group; $j_3, j_4 = sdg$ group ($\pi = +1$),
(b) $j_1, j_2 = sdg$ group; $j_3, j_4 = pfh$ group ($\pi = +1$),
(c) $j_1, j_4 = pfh$ group; $j_2, j_3 = sdg$ group ($\pi = -1$) and
(d) $j_1, j_4 = sdg$ group; $j_2, j_3 = pfh$ group ($\pi = -1$).

Here *sdg* group denotes the $g_{9/2} d_{5/2}, s_{1/2} g_{7/2} d_{3/2}$ orbits and the *pfh* group stands for the $p_{3/2} f_{5/2} p_{1/2} h_{11/2}$ orbits.

for no parity-mixing and hence the uncoupled matrix elements $\langle g_{9/2} m g_{9/2} m_2 | V | p_{3/2} m p_{3/2} m_2 \rangle$ do not enter into calculations during Hartree-Fock iterations, although such matrix elements are large. When we allow for parity-mixing such matrix elements contribute and lead to mixing between $g_{9/2} m$ and $p_{3/2} m$ orbits.

In figure 3 the matrix elements of the residual interaction that can cause parity mixing in the Hartree-Fock potential of (5) are given. These matrix elements are numerous and do not enter the calculation in a parity-conserving Hartree-Fock theory. However in the parity-mixed theory discussed in this work these matrix elements cause mixing among single-particle states with opposite parities. This mixing in turn leads to a lowering of the energy of the parity-mixed Hartree-Fock solutions.

To summarise, parity mixing in deformed orbits seems to resolve the conflict between theory and experiment in the $A \approx 70$ region. We have dealt with, in this paper, two such nuclei, ^{72}Ge and ^{76}Se, and find that parity-mixing leads to far-reaching changes in the predictions for the shapes of these nuclei. Parity conserving Hartree-Fock calculations for these nuclei predict low energy for the oblate or spherical shape while parity-mixed Hartree-Fock calculations energetically favour the prolate shape. Small admixtures of *sdg* orbits with the *pf* and of $h_{11/2}$ orbits with the *sdg* orbits enhance the magnitude of the quadrupole moment and other even moments and lower the energy of the prolate Hartree-Fock minimum for many nuclei in this region. Deformed prolate orbits from above 50 gap are admixed with the less deformed orbits as a result of parity mixing which increases the prolate deformation. There is relatively little parity mixing for the oblate HF and hence the lowering of energy is much less. In many cases there is no parity mixing at all for the oblate shape. We have verified that these results are qualitatively independent of the details of the single-particle energies used. We have done calculations for a number of other even-even nuclei in this region and find similar lowering in energy and enhancement in deformation for the prolate shape due to parity mixing.

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