SHAPE TRANSITION AND COLLECTIVE DYNAMICS IN EVEN $^{94-100}$Zr NUCLEI

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ABSTRACT

Quadrupole and octupole excitations in even $^{94-100}$Zr nuclei are studied within the fully microscopic generator coordinate method using a basis generated by the selfconsistent Hartree-Fock method. Results relevant for the A=100 shape transition and for the octupole mode propertis are reported.

1. Introduction

The isotopic chain of neutron rich zirconium nuclei offers an example of a very rapid spherical to deformed shape transition: ^{96}Zr shows features typical of a spherical nucleus while the isotope ^{100}Zr has already one of the largest known ground state deformations, $\beta_2 \approx 0.35$ [1] [6]. There are also other unusual and interesting properties of these isotopes: 1) Shape coexistence - found in ^{98,100}Zr by extensive experimental studies, in particular, of low lying excited 0^+ states (see refs. [2,3,4] and references quoted therein). 2) The enhanced "sphericity" of ^{96}Zr with respect to the expected trend of losing spherical properties when going from the magic ^{90}Zr towards larger neutron numbers [3]. Since semimagic properties of Z=40 are neutron number dependent (e.g. enhanced in ^{96}Zr by a large $2d_{5/2}$-$3s_{1/2}$ neutron subshell spacing) the special role of the neutron-proton interaction was suggested to explain the latter effect [5]. 3) Relatively low lying 3^- states in $^{92-98}$Zr nuclei and unusually large $B(E3, 3^- \rightarrow 0^+)$ value of 65(±10) W.u. in ^{96}Zr [6], the largest B(E3) known.

A correct theoretical description of these data is difficult both due to frequently encountered troubles with the reproduction of single particle spectrum in A≈100 Zr nuclei by phenomenological potentials [7,8] or within the Hartree-Fock+BCS (HFBCS) method [9,10] and to the necessity of going beyond the static models, i.e., beyond the Strutinsky or HFBCS methods. Motivated especially by the latter point, we have used in the recent work [11] the fully microscopic generator coordinate method (GCM) based on the selfconsistent HF approach with the Skyrme force SkM* to describe the properties of $^{94-100}$Zr nuclei.

2. Method

As described in detail in the ref.[12], our GCM calculations start from the generation of the HFBCS states $|\Phi(q_i)\rangle$, having prescribed quadrupole/octupole moments. The GCM eigenstates $|\Psi_k\rangle$ result then from the diagonalization of the hamiltonian [7] within the nonorthogonal basis of HFBCS states $|\Phi(q_i)\rangle$ corresponding to different

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[6] An equally sharp shape transition is observed in Sr isotopes, while it becomes smooth in Mo, Ru and Pd elements.
[7] the same as the one used in the generation of HFBCS states.

deformations q_i:

$$| \Psi_k \rangle = \sum_{q_i} f(q_i) \mid \Phi(q_i) \rangle. \quad (1)$$

Quadrupole shapes are described by the quadrupole moment, $Q = < 2z^2 - x^2 - y^2 >$, and triaxiality γ. For such a shape we include its six orientations resulting from a relabelling of the principal axes of the nucleus. Working in so enlarged GCM basis we classify the GCM solutions according to the irreps of the group of permutations of three coordinate axes, S_3. This corresponds to a partial angular momentum projection [13]. Within this approach, the 0^+ and 2^+ states are represented by: the symmetric irrep containing all the I=0, and parts of the I=4 and I≥6 components, and the two-dimensional irrep containing all the I=2 and I=5, and parts of the I=4 and I≥6 components, respectively.

Separately, we study negative parity excitations introducing axial octupole deformation by means of the constraint on the octupole moment, $q_3 = < r^3 Y_{30} >$, of the HFBCS states [14].

3. Results

From the previous HF study of the A=80 and A=100 deformed regions [10] it is clear that with the the Skyrme force SIII one cannot account for any spherical-prolate shape coexistence in ^{98,100}Zr nuclei. We have found that the SkM* interaction [15] is better for the A≈100 Zr nuclei, in particular, its spherical spectrum is much closer to experimental suggestions. In the pairing channel we use the spin singlet pairing generated by the zero-range δ interaction, $V_0^T/4(1-\sigma_1\sigma_2)\delta(\mathbf{r}_1-\mathbf{r}_2)$, as described in the ref.[16]. This pairing interaction is state dependent, i.e., weaker between spatially different orbitals. The particle number projection (PNP) has been included in order to eliminate any smoothing of nuclear properties depending on particle numbers.

The obtained HF energy maps, Fig. 1, show that ^{94,96,98}Zr nuclei all have spherical minima with quadrupole softness increasing with A. The prolate secondary minimum around Q=8b appears in ^{98}Zr, 600 keV above the spherical one. In ^{100}Zr the deformed minimum, around 9b, becomes the absolute one, with the spherical point 1.65 MeV above. Along the prolate axis the minimum and the spherical point are separated by a small barrier, which can be bypassed via nonaxial shapes. The spherical point is not a minimum; the secondary oblate minimum appears instead. The obtained static HF results well agree with the known behaviour of zirconium isotopes.

Some results of GCM calculations in the Q-γ coordinates are compared to the experimental data in Table 1. As seen there, the agreement with experiment is much harder to obtain within the full dynamical calculation. The typical shell model configurations in ^{94}Zr are not reproduced within the GCM and the stiffnes against the quadrupole deformations seems to be overestimated. The calculated 0_2^+ energy in ^{96}Zr is not far from the experimental one and this GCM state has substantial deformed components, as required by experiment. The first 2^+ state is much worse reproduced. In ^{98}Zr, the GCM candidate for the first excited 0^+ state is deformed, so it could correspond nicely to the coexisting deformed band head. However, the GCM energy of the lowest 2^+ state and the ρ_{12} values, increasing rapidly at A=98, signal a problem of this calculation: the prominent shape coexistence pattern is predicted at A=98 instead of A=100. Indeed, the energy difference between the competing HF minima is the smallest for A=98. Therefore, the coexisting states can strongly mix and the large E0 strength occurs two mass units too early [17]. The first, mainly prolate, GCM 2^+ state in ^{100}Zr is degenerated with the ground state, which is not too bad representation of a rotational 2_1^+ state in a GCM calculation.

The 0_2^+ state comes out too high, as expected from what was said about ^{98}Zr results.

The calculated GCM octupole energy in ^{94}Zr, 3.0 MeV, is much too high. We have quite good agreement beteen the calculated and experimental 3^- energies in ^{96,98}Zr, and we predict very high, more than 3.9 MeV, octupole energy in ^{100}Zr. The most disturbing are the predicted B(E3) values which persistently come out eight times smaller than the one measured in ^{96}Zr. This is, in fact, independent of the forces used.

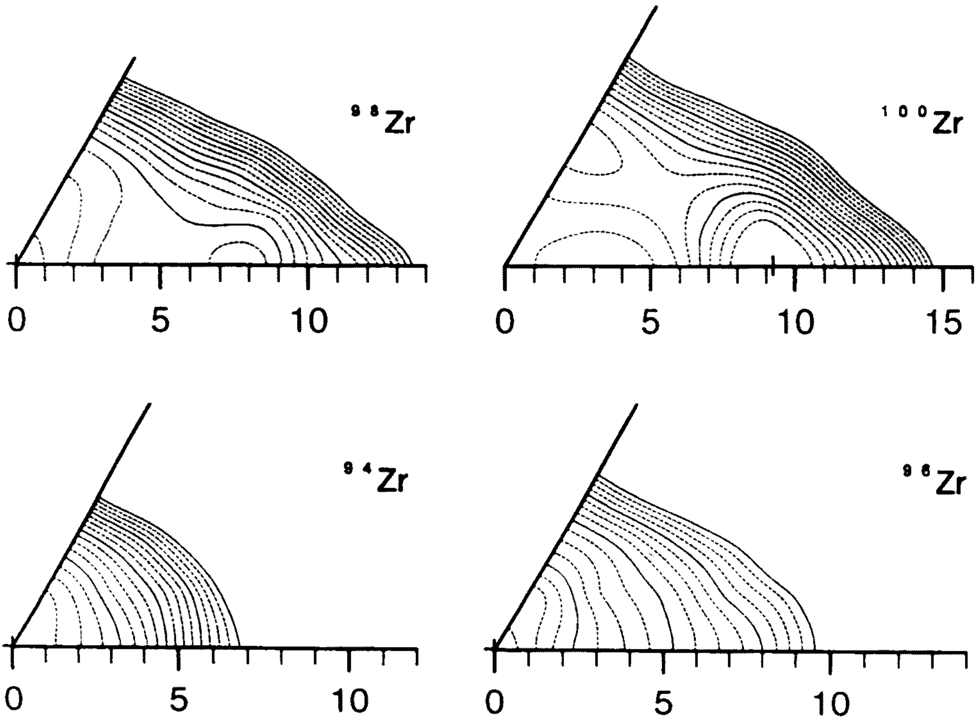

Figure 1

The HF energy, including PNP, of $^{94-100}$Zr in the Q-γ plane ($\beta_2 \approx 0.2$ at Q=5b) obtained with the Skyrme interaction SkM* and the state dependent pairing generated by the δ interaction with the strength V_0=240 MeV for ^{94,96}Zr and V_0=270 MeV for ^{98,100}Zr, both for neutrons and protons. The contour spacing is 250 keV.

One can hope that the full angular momentum projection which should be employed in this kind of analysis will solve some of the encountered descrepancies.

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Table 1

Nucleus	I^π	E_{exp} [MeV]	E_{GCM} [MeV]	$\rho^2_{exp} \times 10^3$	$\rho^2_{GCM} \times 10^3$
^{94}Zr	0^+	1.300	2.54	11.9	37
	2^+	0.919	1.35	-	-
^{96}Zr	0^+	1.582	1.83	7.4	32
	2^+	1.750	1.25	-	-
^{98}Zr	0^+	0.854	1.03	10	114
	2^+	1.223	0.64	-	-
^{100}Zr	0^+	0.331	0.99	92	118
	2^+	0.212	0.03	-	-

Experimental energies of the first excited 0^+ and 2^+ states and E0 strength $\rho^2_{12}(0^+_2 \rightarrow 0^+_1) \times 10^3$ values (from refs.[2,17]) are given vs. corresponding GCM results from the Q-γ calculation with parameters given in the figure caption.

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