

Effect of neutron orbitals on the nuclear shape in neutron-deficient and neutron-rich zirconium nuclei

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The neutron-deficient and neutron-rich zirconium nuclei are studied using statistical theory. The deformation dependence of occupation numbers of the neutron orbitals in these nuclei near the Fermi level is investigated. The preference of the neutrons to occupy or vacate a particular orbital is found to contribute a particular shape to the nucleus. [S0556-2813(97)02406-0]

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The study of nuclear deformation in both neutron-deficient and neutron-rich zirconium isotopes helps one to understand the nature of collective motion occurring in these nuclei. This collective motion is susceptible to modulation by shell structure. The transition from spherical to deformed shapes in these nuclei has been studied [1–9] extensively in the framework of the shell model [10]. The deformation and shape coexistence in zirconium nuclei are studied in the relativistic mean-field approach [11]. The development of collectivity in light zirconium isotopes with particle number and angular momentum has been analyzed experimentally [12] and also using interacting Boson model [13,14]. Hartree-Fock calculations with realistic forces [15,16] have also been used for a comprehensive understanding of the structure of the zirconium isotopes. The macroscopic-microscopic cranking calculations [17–19] have been useful in predicting the shapes and binding energies of these nuclei with deformed shapes. In our earlier calculations [20] the isospin fluctuations in nuclei around $A=90$ with triaxial deformation have been studied using the statistical formalism. In this paper the deformation dependence of the occupation numbers of the neutron orbitals in neutron-deficient and neutron-rich zirconium nuclei at low temperature is investigated. For this purpose the statistical theory [21] proposed by Moretto is used. The triaxial deformation is introduced into the picture by using the single-particle levels generated by diagonalizing [22] the triaxially deformed Nilsson Hamiltonian [23–25] in the cylindrical representation. The (k, μ) pair used for generating the single-particle levels are taken from [23] and are different for different oscillator shells. The occupation probability n_i of the i th shell is calculated using the conservation equation $\langle N \rangle = \sum n_i = \sum [1 + \exp(-\alpha + \beta \epsilon_i)]^{-1}$ for neutrons. The Lagrangian multiplier α conserves the neutron number for a given temperature $T=1/\beta$.

The aim of this paper is to calculate the occupation numbers of the various neutron orbitals in neutron-deficient and neutron-rich zirconium isotopes as a function of deformation and also to investigate the contribution to the nuclear shape

by the occupancy of the neutron orbitals above the Fermi level or the vacation of the neutron orbitals below the Fermi level. The occupancy or vacation of a particular orbital is found to contribute a particular shape to the nucleus in both neutron-deficient and neutron-rich zirconium isotopes. The percentage probability of a particular orbital among a number of active orbitals above the Fermi level being occupied as well as the percentage probability of a particular orbital among the active orbitals below the Fermi level being vacated is estimated. It is found that both these factors contribute to a particularly favored shape for the isotopes of zirconium nuclei.

The percentage occupation probability n^+ of a particular orbital means the percentage probability of that orbital being occupied among the active orbitals above the Fermi level due to transition of a particle from the active orbitals below the Fermi level. This percentage occupation probability is different from the conventional occupation probability of a level in the ordinary sense. Similarly the percentage vacation probability n^- of a particular orbital means the percentage probability of that orbital below the Fermi level being vacated among the active orbitals below the Fermi level. The occupation of a particular orbital above the Fermi level may be due to transitions from one or many active orbitals below the Fermi level. Similarly the vacation of a particular orbital among a number of active orbitals below the Fermi level may contribute to the occupation of one or many active orbitals above the Fermi level.

The percentage occupation and vacation probabilities n^+ and n^- are calculated for zirconium isotopes of even mass numbers from 74 to 104 for a temperature $T=0.4$ MeV and a spin $M=0$. The dependence of the percentage occupation probability or percentage vacation probability of different orbitals in these zirconium isotopes on deformation is studied. Calculations are performed for the deformation parameter $\delta=0.0-0.6$ with $\Delta\delta=0.1$ and for $\theta=-180^\circ$ and -120° . The deformation parameter $\theta=-180^\circ$ corresponds to the oblate shape rotating about the symmetry axis while $\theta=-120^\circ$ corresponds to the prolate shape rotating about an axis perpendicular to the symmetry axis. The deformation parameter $\delta=0.0$ corresponds to the spherical shape. The occupation numbers of the different neutron orbitals in spherical, oblate deformed, and prolate deformed neutron-deficient and neutron-rich zirconium isotopes are presented in Table I.

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TABLE I. Occupation numbers for the spherical (*s*), oblate deformed (*o*) and prolate deformed (*p*) neutron orbitals in neutron-deficient and neutron-rich zirconium isotodes.

Neutron		Mass number																
orbital	shape	δ	74	76	78	80	82	84	86	88	90	92	94	96	98	100	102	104
$1f_{7/2}$	<i>s</i>	0.0	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00
		0.2	5.99	6.00	6.03	6.28	7.08	7.69	7.92	7.99	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00
		0.4	4.00	4.06	4.79	5.42	5.81	5.97	6.01	6.11	6.54	7.15	7.65	7.83	7.96	8.00	8.00	8.00
	<i>p</i>	0.6	3.92	4.00	4.00	4.04	4.30	4.77	5.35	5.77	5.94	5.99	6.00	6.00	6.02	6.14	6.60	7.42
		0.2	6.01	6.15	6.63	7.17	7.67	7.92	7.99	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00
		0.4	6.00	6.00	6.00	6.07	6.29	6.69	7.27	7.91	7.99	8.00	8.00	8.00	8.00	8.00	8.00	8.00
$2p_{3/2}$	<i>s</i>	0.0	3.94	3.98	3.99	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00
		0.2	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00
		0.4	3.73	3.99	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00
	<i>p</i>	0.6	3.05	3.95	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00
		0.2	3.89	3.99	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00
		0.4	3.50	3.92	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00
$1f_{5/2}$	<i>s</i>	0.0	1.79	3.38	4.81	5.96	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
		0.2	2.16	3.94	5.48	5.95	5.99	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
		0.4	3.88	4.06	4.79	5.42	5.81	5.97	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
	<i>p</i>	0.6	3.21	3.96	4.00	4.02	4.11	4.35	4.83	5.45	5.83	5.98	6.00	6.00	6.00	6.00	6.00	6.00
		0.2	2.09	3.68	4.59	5.21	5.67	5.93	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
		0.4	2.79	3.66	3.99	4.06	4.29	4.69	5.27	5.91	5.99	6.00	6.00	6.00	6.00	6.00	6.00	6.00
$2p_{1/2}$	<i>s</i>	0.0	0.26	0.64	1.19	1.96	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
		0.2	1.84	1.98	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
		0.4	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
	<i>p</i>	0.6	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
		0.2	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
		0.4	0.00	0.01	0.23	1.39	1.83	1.94	1.98	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
$1g_{9/2}$	<i>s</i>	0.0	0.00	0.00	0.00	0.08	2.00	4.00	6.00	8.00	9.97	10.00	10.00	10.00	10.00	10.00	10.00	10.00
		0.2	0.01	0.08	0.50	1.77	2.87	4.06	5.15	5.75	5.98	6.00	6.00	6.00	6.00	6.00	6.01	6.02
		0.4	0.39	1.88	2.33	2.86	3.50	3.91	3.99	4.00	4.00	4.00	4.00	4.00	4.01	4.13	4.86	5.41
	<i>p</i>	0.6	1.82	1.99	2.00	2.00	2.00	2.05	2.16	2.50	3.17	3.83	3.98	4.00	4.00	4.01	4.05	4.28
		0.2	0.01	0.18	0.78	1.62	2.69	4.14	5.99	7.61	7.95	7.99	8.00	8.00	8.00	8.00	8.00	8.00
		0.4	1.71	2.40	3.78	4.33	5.00	5.52	5.82	5.98	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
$2d_{5/2}$	<i>s</i>	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	1.70	3.18	4.32	5.08	5.53	5.80	5.95
		0.2	0.00	0.00	0.00	0.01	0.05	0.25	0.93	2.27	3.97	5.24	5.83	5.96	5.99	5.99	6.00	6.00
		0.4	0.00	0.00	0.09	0.30	0.85	1.95	3.08	3.81	3.97	3.99	4.00	4.00	4.00	4.01	4.13	4.38
	<i>p</i>	0.6	0.00	0.05	0.95	1.81	1.97	1.99	2.00	2.00	2.01	2.09	2.60	3.39	3.89	3.98	4.00	4.01
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.17	0.14	0.68	2.13	3.88	5.19	5.74	5.90	5.96
		0.4	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.06	0.57	1.19	1.67	2.00	2.53	3.80	4.97	5.59
$1g_{7/2}$	<i>s</i>	0.0	0.00	0.00	0.00	0.00	0.00	0.01	0.17	0.58	1.06	1.45	1.74	1.92	1.98	2.00	2.01	2.17
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.30	0.82	1.66	2.90	4.40	6.02	7.38
		0.4	0.00	0.00	0.00	0.00	0.00	0.01	0.05	0.36	1.46	2.58	3.41	3.50	3.94	4.04	4.38	4.85
	<i>p</i>	0.6	0.00	0.05	1.01	1.83	1.97	1.99	2.00	2.01	2.05	2.31	3.24	3.79	3.97	4.00	4.00	4.03
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.23	1.07	1.73	1.96	2.09	2.57	3.37	4.08	4.71
		0.4	0.00	0.00	0.01	0.16	0.59	1.16	1.64	2.12	3.20	4.11	5.00	5.76	6.00	6.12	6.41	6.92
$3s_{1/2}$	<i>s</i>	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.04	0.10	0.34
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.30	0.90	1.43	1.73	1.89
		0.4	0.00	0.00	0.00	0.01	0.03	0.19	0.87	1.71	1.95	1.98	2.00	2.00	2.00	2.00	2.00	2.00
	<i>p</i>	0.6	0.00	0.00	0.02	0.16	0.79	1.39	1.76	1.93	1.98	2.00	2.00	2.00	2.00	2.00	2.00	2.00
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.07	0.26	0.61	1.03
		0.4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$2d_{3/2}$	<i>s</i>	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.03	0.08	0.29
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.25	0.81	1.44	1.99	2.54
		0.4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.15	0.49	1.30	2.50	3.79	3.98	3.99
	<i>p</i>	0.6	0.00	0.00	0.02	0.16	0.82	1.41	1.77	1.93	1.99	2.02	2.20	2.76	3.65	3.95	3.99	4.00
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.84	1.40	1.91	1.99	2.00	2.00	2.00	2.00
		0.4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$1h_{11/2}$	<i>s</i>	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.05
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.05	0.16	0.38	0.76
		0.4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.04	0.15	0.46	1.02	1.57	2.02	2.57	3.13
	<i>p</i>	0.6	0.00	0.00	0.00	0.00	0.01	0.04	0.13	0.40	1.03	1.75	1.97	1.99	2.00	2.00	2.00	2.02
		0.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.19	0.64	1.41
		0.4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.24	0.68	1.35	2.24	3.47	4.04	4.47	5.04
0.6	0.00	0.01	0.05	0.37	1.27	1.95	2.30	2.84	3.37	3.67	3.86	3.97	4.02	4.13	4.60	5.74		

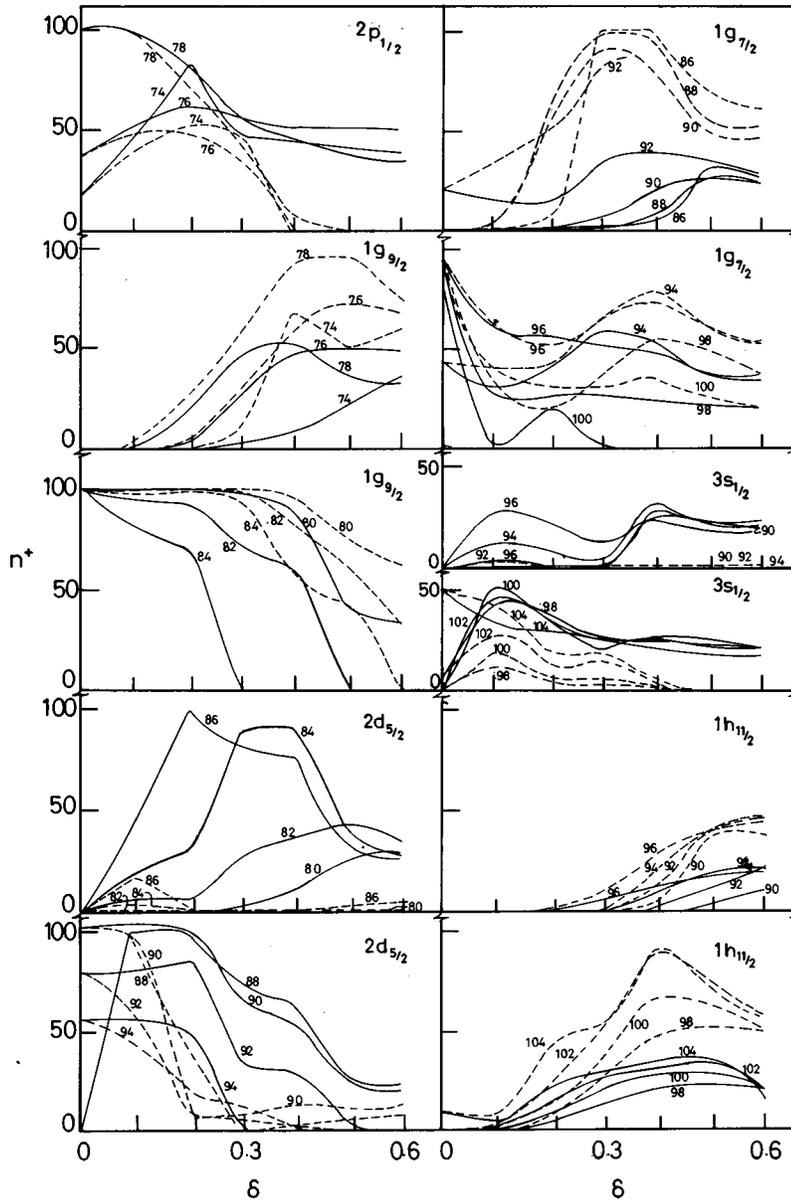


FIG. 1. The percentage occupation probability n^+ of the different neutron orbitals among the active orbitals above the Fermi level as a function of deformation parameters δ and θ . The solid line for $\theta = -180^\circ$ corresponds to oblate shape and the dashed line for $\theta = -120^\circ$ corresponds to the prolate shape. The numbers on the curves indicate the mass numbers of the nuclei.

Examination of the table reveals that the $1h_{11/2}$ orbital is preferred for occupation compared to the lower orbitals $3s_{1/2}$ and $2d_{3/2}$.

Figure 1 represents the percentage occupation probability n^+ of the orbitals $2p_{1/2}$, $1g_{9/2}$, $2d_{5/2}$, $1g_{7/2}$, $3s_{1/2}$, and $1h_{11/2}$ as a function of triaxial deformation parameters δ and θ for neutron-deficient and neutron-rich zirconium nuclei of even mass numbers from 74 to 104. It is found that when transitions to many orbitals take place each orbital has a tendency to favor a particular deformation character in all these nuclei. The transition to the $2p_{1/2}$ orbital among a number of active orbitals favors the oblate shape for $A = 74, 76,$ and 78 nuclei. For $A > 78$, transitions to higher orbitals only are possible. In a similar manner we find that the transition to the $1g_{9/2}$ orbital favors the prolate shape, the transition to the $2d_{5/2}$ orbital favors the oblate shape, the transition to the $1g_{7/2}$ orbital favors the prolate shape, and the transition to the $3s_{1/2}$ orbital favors the oblate shape for the neutron-deficient and neutron-rich zirconium nuclei. The $1h_{11/2}$ or-

bit, which becomes active in the neutron-rich Zr, region favors a prolate shape. It is obvious from Fig. 2 that the $2d_{3/2}$ orbital, which is hemmed in between the oblate favoring $3s_{1/2}$ orbital and prolate favoring $1h_{11/2}$ orbital, favors the oblate shape for $A = 102$ and 104 while for $A = 90, 92, 94, 96, 98,$ and 100 it exhibits a complex behavior.

Figure 3 represents the percentage vacation probability n^- of the orbitals $2d_{5/2}$, $1g_{9/2}$, $1f_{5/2}$, and $1f_{7/2}$ as a function

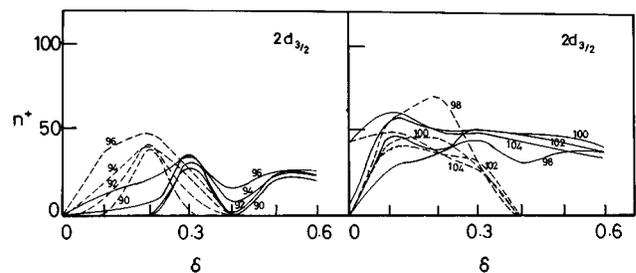


FIG. 2. Same as Fig. 1 for the $2d_{3/2}$ neutron orbital.

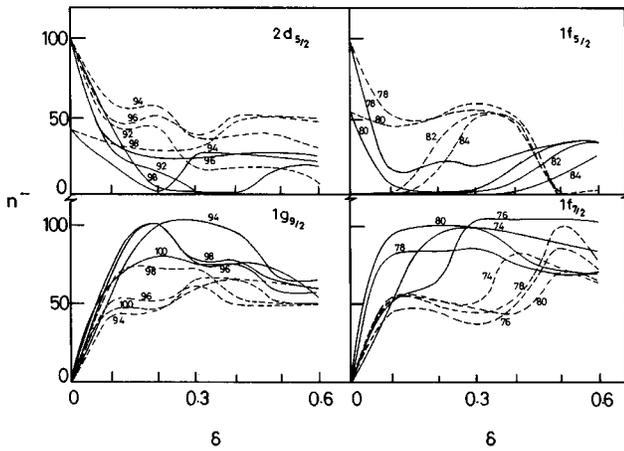


FIG. 3. Same as Fig. 1 for the percentage vacation probability n^- of the different neutron orbitals among the active orbitals below the Fermi level.

of triaxial deformation parameters δ and θ for neutron-deficient and neutron-rich Zr nuclei of even mass numbers from 74 to 104. It is found that when vacation of many orbitals below the Fermi level takes place each orbital has a tendency to favor a particular deformation character of the nucleus. Our calculations suggest that vacation of $2d_{5/2}$ and

$1g_{9/2}$ orbitals below the Fermi level which are active in the neutron-rich region favor prolate and oblate shapes, respectively, for the nucleus. Similarly, vacation of $1f_{5/2}$ and $1f_{7/2}$ orbitals below the Fermi level which are active in the neutron-deficient region show preponderance for prolate and oblate shapes, respectively, for the nucleus even though there is a deviation from this behavior at very large deformations for these two levels.

A study of $2d_{5/2}$ and $1g_{9/2}$ orbitals reveals that the occupation of the former contributes to oblate shape whereas its vacation contributes to the prolate shape while the reverse is the case for the latter. This implies that if the occupation of a particular orbit contributes to a prolate shape its vacation will contribute to an oblate shape and vice versa. The contribution of the proton orbitals to the nuclear shape is not dealt with here as the proton number is fixed for the Zr isotopes. It is hoped that the net contribution of the level character of all the active neutron orbitals and the proton orbitals will be determining the nuclear shape. An exhaustive calculation involving the effects of temperature and spin angular momentum on the optimum shape of these nuclei by minimizing the energy functional is in progress.

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