Eur. Phys. J. A **22**, 13–16 (2004)
DOI 10.1140/epja/i2003-10226-8

THE EUROPEAN
PHYSICAL JOURNAL A

Study of N = Z nuclei in variation-after-projection framework

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Received: 28 April 2003 / Revised version: 20 March 2004 /
Published online: 14 September 2004 –
Communicated by A. Molinari

Abstract. Variation-after-projection (VAP) calculations in conjunction with the Hartree- Bogoliubov (HB) ansatz have been carried out for $A = 68$–88, $N = Z$ nuclei. In this framework, the yrast spectra with $J^\pi \leqslant 10^+$, $B(E2)$ transition probabilities and deformation parameter (β_2) have been obtained. A pairing interaction for like particles as well as protons and neutrons has been included in the model for a two-body interaction.

PACS. 21.10.-k Properties of nuclei; nuclear energy levels – 21.60.-n Nuclear structure models and methods – 27.50.+e $59 \leq A \leq 89$

1 Introduction

The study of nuclei with equal number of neutrons and protons ($N = Z$) present special interest due to the existence of unique characteristics in these nuclei. The observation of such characteristics has become possible due to advances in experimental measurement techniques [1–4]. The special feature of $N = Z$ nuclei up to ^{100}Sn, possibly the heaviest still bound among those nuclei, is that the protons and neutrons occupy the same shell model orbits. In these nuclei, the effects of shell gaps become very strong and determine rapid changes with N, Z and spin. Besides, in these nuclei the inclusion of np pairing effects is as important as the pairing between like particles. Therefore, any microscopic calculation for $N = Z$ nuclei with the inclusion of np pairing is very important.

The even-even nuclei with $N = Z$ which could be studied until now have revealed a rich variety of phenomena. For example, in ^{72}Kr there is a shape co-existence strongly manifesting itself in the lowest excited states [5]. ^{76}Sr and ^{80}Zr nuclei are observed to have the largest ground-state deformation [6,7]. The ^{84}Mo [8,9] nucleus appears much less deformed and the decreasing trend of this deformation continues with increasing values of $Z(= N)$. For example, the $N = Z$ nucleus ^{88}Ru [1] is weakly deformed with an E_2^+ energy of 0.616 MeV and E_4^+/E_2^+ ratio of 2.30, so ^{88}Ru continues the trend of decreasing collectivity already observed at ^{84}Mo.

The strongest motivation for studying the nuclear-structure properties of the $N = Z$ nuclei is to determine the importance of the effects of the inclusion of the np pairing interaction for these nuclei. It appears that pairing between like nucleons is extremely important in nuclei with $N \neq Z$, where it strongly overweighs the effects of np pairing due to the much larger number of like particle pairs. In the $N = Z$ nuclei the np pairing should be relatively enhanced, and it is likely that only here will it be possible to observe its effects on the nuclear properties. Recently some theoretical attempts [10,11] have been made to study some of $N = Z$ nuclei. Petrovici *et al.* [10] have studied ^{74}Rb and ^{72}Kr nuclei by using the Excited Vampir approach. They found that for the yrast states in ^{74}Rb the np correlations are found to be dominant. In ^{72}Kr all types of isovector pairs, nn, pp and np yield a similar contribution with increasing spin. Recently Patra *et al.* [11] have obtained the potential energy surfaces for $N = Z$, ^{72}Kr to ^{92}Pd nuclei in an axially deformed relativistic mean-field approach, using a quadratic constraint scheme. They have shown that $A = 72$–92 nuclei are in a region of multiple shape co-existence since more than two solutions of about the same intrinsic energy and different deformation are obtained.

Therefore, we have made an attempt to study the effects of inclusion of np pairing effects in $A = 68$–88, $N = Z$ nuclei in the framework of the variation-after-projection (VAP) technique in conjunction with the HB ansatz for the trial wave function resulting from the pairing plus quadrupole –quadrupole plus hexadecapole-hexadecapole (PQH) interaction operating in a large valence space. We have included pairing effects for both like particles as well as neutrons and protons.

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Table 1. The experimental values of the E_2^+ energy, E_4^+/E_2^+ ratio and calculated quadrupole moments $\langle Q_0^2\rangle_{\rm HB}$ of intrinsic states associated with yrast levels in $N = Z$ nuclei. The intrinsic quadrupole moments have been computed in units of b^2, where $b = \sqrt{\hbar/m\omega}$ is the harmonic-oscillator parameter.

Nuclei	E_2^+ (in MeV)	E_4^+/E_2^+	$J^\pi_{\rm yrast}$					
	Exp.	Exp.	0^+	2^+	4^+	6^+	8^+	10^+
^{68}Se	0.85	2.28	46.68	49.91	52.85	52.85	52.85	52.85
^{72}Kr	0.71	1.85	52.04	56.38	59.84	59.84	59.84	59.84
^{76}Sr	0.26	2.86	96.09	96.09	96.09	96.09	96.09	96.09
^{80}Zr	0.29	2.79	95.80	95.80	95.80	95.80	95.80	95.80
^{84}Mo	0.44	2.54	87.41	87.41	87.41	87.41	87.41	87.41
^{88}Ru	0.61	2.31	71.25	71.25	85.90	85.90	95.90	91.06

2 Calculational details

2.1 The one- and two-body parts of the Hamiltonian

In our calculations presented here we have employed the valence space spanned by $3s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, $2d_{3/2}$, $2d_{5/2}$, $1f_{5/2}$, $1g_{7/2}$, $1g_{9/2}$ and $1h_{11/2}$ orbits for protons and neutrons under the assumption of $N = Z = 28$ sub-shell closure. The single-particle energies we have taken are (in MeV): $(3s_{1/2}) = 9.90$, $(2p_{1/2}) = 1.08$, $(2p_{3/2}) = 0.0$, $(2d_{3/2}) = 11.40$, $(2d_{5/2}) = 8.90$, $(1f_{5/2}) = 0.78$, $(1g_{7/2}) = 11.90$, $(1g_{9/2}) = 3.50$ and $(1h_{11/2}) = 12.90$. The energy values of single-particle orbits for $2p$-$1f$-$1g$ levels are the same as employed for ^{56}Ni core plus one nucleon. The energies of higher single-particle valence orbits are the same as used by Vergados and Kuo [12] relative to the $1g_{9/2}$ valence orbit.

The two-body effective interaction that has been employed is of PQH type. The parameters of the pairing–plus–quadrupole-quadrupole (PQ) part of the two-body interaction are also the same as used by Sharma *et al.* [13]. The relative magnitudes of the parameters of the hexadecapole-hexadecapole parts of the two-body interaction were calculated from a relation suggested by Bohr and Mottelson [14]. According to them the approximate magnitude of these coupling constants for isospin $T = 0$ is given by

$$\chi_\lambda = \frac{4\pi}{2\lambda+1}\,\frac{m\omega_0^2}{A\langle r^{2\lambda-2}\rangle}\,, \qquad \text{for } \lambda = 1,2,3,4 \tag{1}$$

and the parameters for the $T = 1$ case are approximately half the magnitude of their $T = 0$ counterparts. This relation was used to calculate the values of $\chi_{\rm pp4}$ relative to $\chi_{\rm pp2}$ by generating the wave function for $N = Z$ nuclei and then calculating the values of $\langle r^{2\lambda-2}\rangle$ for $\lambda = 2$ and 4.

The values for the hexadecapole-hexadecapole part of the two-body interaction turn out to be

$$\chi_{\rm pp4}(=\chi_{\rm nn4}) = -0.00033\,{\rm MeV\,b^{-8}} \qquad \text{and}$$
$$\chi_{\rm pn4} = -0.00066\,{\rm MeV\,b^{-8}}\,.$$

The procedure for obtaining the axially symmetric Hartree Bogoliubov (HB) intrinsic states has been discussed in ref. [15]. The methods developed by Onishi and Yoshida [16] for carrying out projection of the states of good angular momentum from axially symmetric HB intrinsic states have been used for obtaining the spectra. The VAP calculations have been carried out as follows. We first generated the self-consistent HB solutions, $\Phi(\beta)$, by carrying out the HB calculations with the Hamiltonian $(H - \beta Q_0^2)$, where β is a parameter. The selection of the optimum intrinsic states, $\Phi_{\rm opt}(\beta_J)$, is then made by finding out the minimum of the projected energy

$$E_J(\beta) = \langle\Phi_0(\beta)|HP^J_{00}|\Phi_0(\beta)\rangle/\langle\Phi_0(\beta)|P^J_{00}|\Phi_0(\beta)\rangle \tag{2}$$

as a function of β. In other words, the optimum intrinsic state for each yrast J satisfies the condition.

$$\partial/\partial\beta[\langle\Phi_0(\beta)|HP^J_{00}|\Phi_0(\beta)\rangle/\langle\Phi_0(\beta)|P^J_{00}|\Phi_0(\beta)\rangle]\Big|_{\beta=\beta_J} = 0\,. \tag{3}$$

3 Results and discussion

3.1 Intrinsic states

In table 1 the values of E_2^+ and E_4^+/E_2^+ for $N = Z$ nuclei in the mass region $A = 68$–88, are given. It is observed that the E_2^+ energy decreases from its values of 0.85 MeV for ^{68}Se to 0.26 MeV for ^{76}Sr meaning thereby that there is an increase of deformation in going from ^{68}Se to ^{76}Sr. This fact is also confirmed by the increasing trend of the values of the ratio E_4^+/E_2^+. For example, the value of the ratio E_4^+/E_2^+ in ^{76}Sr is 2.86 whereas in ^{68}Se it is 2.28. As we know that the quadrupole moments have an inverse relationship with the E_2^+ energy. This means that the trend of the quadrupole moments of the ground states of these nuclei should be such that their quadrupole moments increase as one goes from ^{68}Se to ^{76}Sr and thereafter these values should show a decreasing trend. In table 1, the calculated results on quadrupole moments of the optimum intrinsic states associated with the yrast levels in the nuclei ^{68}Se, ^{72}Kr, ^{76}Sr, ^{80}Zr, ^{84}Mo and ^{88}Ru have also been presented. It may be noted that the intrinsic quadrupole moments of the optimum intrinsic states increase from their values of 46.68 units in ^{68}Se to 96.09 units in ^{76}Sr. Thereafter their values are found to decrease. Thus, the calculated trend of the intrinsic quadrupole moments is supporting the observed systematics of the E_2^+ energy states in these nuclei. Besides this, in the nuclei

Table 2. The sub-shell occupation numbers protons (neutrons) for $N = Z$ nuclei.

Nuclei	J^π	Sub-shell occupation number								
		$3s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$	$2d_{3/2}$	$2d_{5/2}$	$1f_{5/2}$	$1g_{7/2}$	$1g_{9/2}$	$1h_{11/2}$
^{68}Se	0^+	0.10	0.50	1.62	0.06	0.40	1.74	0.04	1.42	0.08
	2^+	0.13	0.49	1.54	0.08	0.48	1.63	0.05	1.47	0.08
	4^+–10^+	0.15	0.49	1.46	0.11	0.55	1.53	0.06	1.54	0.07
^{72}Kr	0^+	0.10	0.54	2.15	0.07	0.43	2.66	0.05	1.85	0.10
	2^+	0.12	0.53	2.08	0.08	0.52	2.60	0.06	1.89	0.08
	4^+–10^+	0.15	0.52	1.99	0.10	0.61	2.47	0.07	1.98	0.08
^{76}Sr	0^+–10^+	0.19	0.54	2.20	0.15	0.88	3.21	0.11	2.65	0.03
^{80}Zr	0^+–10^+	0.40	0.55	2.15	0.82	0.98	3.23	0.63	3.15	0.05
^{84}Mo	0^+–10^+	0.39	0.68	2.73	0.65	0.97	3.60	0.48	4.31	0.14
^{88}Ru	0^+–2^+	0.35	1.15	3.54	0.53	0.90	4.53	0.42	4.48	0.06
	4^+–8^+	0.42	0.87	3.31	0.74	1.02	4.08	0.57	4.87	0.07
	10^+	0.44	0.79	3.22	0.81	1.10	3.93	0.63	4.99	0.07

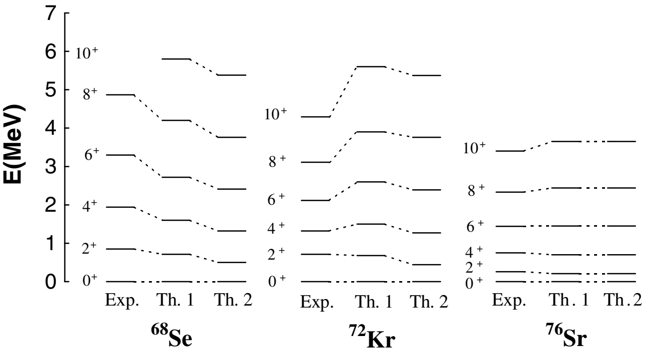

Fig. 1. Experimental and theoretical yrast spectra for $N = Z$, $A = 68$–76 nuclei.

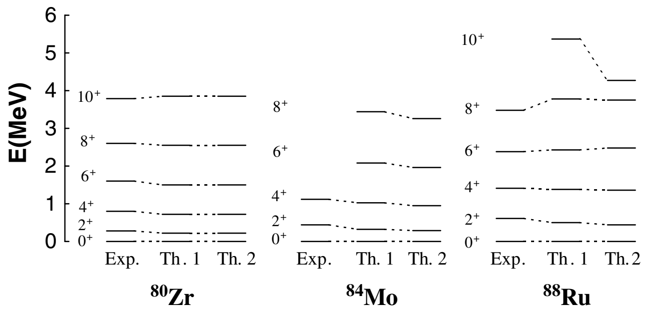

Fig. 2. Experimental and theoretical yrast spectra for $N = Z$, $A = 80$–88 nuclei.

^{68}Se, ^{72}Kr and ^{88}Ru the intrinsic state is found to change as one moves up along the yrast states. The excited states with $J^\pi \geqslant 4^+$ are found to have greater deformation than the states with lower spin.

In order to understand the observed systematics of the E_2^+ state in $N = Z$ nuclei from ^{68}Se to ^{88}Ru the sub-shell occupation numbers for protons and neutrons are presented in table 2. It may be noted that $1f_{5/2}$, $2p_{3/2}$ and $1g_{9/2}$ proton and neutron occupation numbers increase from their values of 1.74, 1.62 and 1.42 to 3.21, 2.20 and 2.65 as one moves from ^{68}Se to ^{76}Sr, respectively. Since protons and neutrons are occupying the down-sloping components of the Nilsson orbits $2p_{3/2}$, $1f_{5/2}$ and $1g_{9/2}$ in increasing order, there is an increase in the quadruople moments resulting from the HB calculation as one moves from ^{68}Se to ^{76}Sr. Thereafter the $1f_{5/2}$ and $2p_{3/2}$ orbits become more than half-full and the $k = 5/2$ component of the $1g_{9/2}$ orbit starts filling at ^{80}Zr, thus resulting in a decrease of the deformation as one moves to nuclei heavier than ^{76}Sr. Therefore, the observed trend, *i.e.*, an increase in deformation as one moves from ^{68}Se to ^{76}Sr and the next decrease of deformation for larger-mass $N = Z$ nuclei, is intrinsically related to the proton and neutron occupation probabilities for the sub-shells $2p_{3/2}$, $1f_{5/2}$ and $1g_{9/2}$.

3.2 Yrast levels

In figs. 1 and 2 the yrast spectra for the $N = Z$ nuclei is displayed. The spectra corresponding to Th. 1 are obtained by including pairing effects for like particles and neutron-proton pairs. The spectra corresponding to Th. 2 have been obtained with the inclusion of pairing effects for like particles only. It may be noted that the spectra obtained with the inclusion of np pairing effects which are marked as Th. 1 for $N = Z$ nuclei have a satisfactory agreement with the observed [1–9] yrast spectra for these nuclei.

3.3 Quadrupole deformations (β_2) and B(E2) transition probabilities

The reliability and goodness of the HB wave function is examined by calculating the β_2 and $B(E2; 0_1^+ \rightarrow 2_1^+)$ values. In table 3, the calculated and experimental values for the deformation parameter (β_2) have been presented. The deformation parameter β_2 is related to $B(E2)\uparrow$ by the formula suggested by Raman *et al.* [17],

$$\beta_2 = (4\pi/3ZR_0^2)[B(E2)\uparrow/e^2]^{1/2}, \qquad (4)$$

where R_0 is usually taken to be $1.2A^{1/3}$ fm and $B(E2)\uparrow$ is in units of e^2b^2.

Table 3. Comparison of the calculated and experimental quadrupole deformation parameter (β_2) of the HB states in $N = Z$ nuclei. The theoretical $B(E2; 0_1^+ \rightarrow 2_1^+)$ are also given in units of e^2b^2.

Nuclei	(β_2)		$B(E2; 0_1^+ \rightarrow 2_1^+)$
	Th.	Exp.[(a)]	Th.
^{68}Se	0.25	0.27	0.25
^{72}Kr	0.29		0.42
^{76}Sr	0.43	> 0.40	1.06
^{80}Zr	0.40	> 0.40	1.05
^{84}Mo	0.37	0.30	0.97
^{88}Ru	0.26	0.24	0.64

([a]) Data taken from refs. [1,3,6,8].

From the systematics of the calculated β_2 values, it is noted that the set of values are in satisfactory agreement with the observed values.

A few years ago Bhatt *et al.* [18] developed an approach for the calculation of the $B(E2; 0_1^+ \rightarrow 2_1^+)$ transition probabilities from the values of intrinsic quadrupole moments of protons and neutrons. It has been justified by them that the $B(E2; 0_1^+ \rightarrow 2_1^+)$ in units of e^2b^2 are given by

$$B(E2; 0_1^+ \rightarrow 2_1^+) = (1.02 \times 10^{-5})A^{2/3} \times [e_\pi \langle Q_0^2 \rangle_\pi + e_\nu \langle Q_0^2 \rangle_\nu]^2 , \quad (5)$$

where $\langle Q_0^2 \rangle_\pi$, $(\langle Q_0^2 \rangle_\nu)$ are the intrinsic quadrupole moments of valence protons (neutrons), whereas e_π and e_ν are the effective charges of the protons and neutrons, respectively. The effective charges of the protons and neutrons are 1.3 and 0.3, respectively. We have used this formula for the calculation of the $B(E2)$ values for $N = Z$ nuclei. In view of non-availability of experimental $B(E2)$ values, we have given only theoretical values in table 3. Since the calculations for the $B(E2)$ values depend on the intrinsic quadrupole moments, the $B(E2)$ values should follow the same trend as that followed by the intrinsic quadrupole moments. This feature of the $N = Z$ nuclei has been reproduced by the present calculations.

4 Conclusions

From the results of the present calculations, the following broad conclusions can be drawn:

i) The results of HB calculations on yrast spectra clearly indicate that it is very important to include np pairing effects for $N = Z$ nuclei for determining the nuclear-structure properties.
ii) The hexadecapole interaction parameters employed by us are the appropriate ones for this mass region and produce accurate HB wave functions which yield values of β_2 in satisfactory agreement with experiment.
iii) The excited states with $J^\pi \geqslant 4^+$ are found to have greater deformation than the states with lower spin.

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