Microscopic description of the high-spin yrast spectra in some doubly even zinc, germanium, and selenium isotopes

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A microscopic description of the yrast levels in some doubly even isotopes of Zn, Ge, and Se is attempted by carrying out Hartree-Fock-Bogoliubov calculations employing realistic effective interactions. The level energies, static quadrupole moments, reduced transition probabilities for $E2$ transitions, as well as the occupation numbers for the spherical single-particle orbits are calculated for the yrast states. The overall agreement between the calculated and experimental results is reasonably good.

[NUCLEAR STRUCTURE Doubly even Zn, Ge, and Se isotopes: calculated yrast levels, static quadrupole moments, reduced transition probabilities for $E2$ transitions, and occupation numbers for $p_{3/2}$, $p_{1/2}$, $f_{5/2}$, and $g_{9/2}$ subshells. Hartree-Fock-Bogoliubov method with angular momentum projection.]

I. INTRODUCTION

The aim of this paper is to report on the calculation of the yrast spectra of the doubly even nuclei ^{62,64,66,68}Zn, ^{70,72,74,76}Ge, and ^{72,74,76,78}Se. Apart from the energy spectra we shall also discuss here the results of the calculations of the static quadrupole moments and the reduced transition probabilities for $E2$ transitions for the yrast states, as well as the occupancies of the $p_{3/2}$, $p_{1/2}$, $f_{5/2}$, and $g_{9/2}$ subshells in the ground states of these nuclei.

In recent years there has been a rapid increase in the experimental activity of measuring the properties of the yrast states in Zn, Ge, and Se isotopes.[1-19] However, despite the numerous efforts on the experimental side, only a few theoretical calculations exist at present.[20-25]

Some earlier theoretical studies on Zn isotopes[20,21] have described them in terms of an anharmonic vibrational picture. Kregar and Mihailović[22] were the first to point out that nuclei such as ^{72}Ge may be deformed in their ground states. A number of recent investigations have clearly demonstrated the necessity of the existence of sizable deformations in the $A = 60$–80 mass region. Thus, whereas Bruandet *et al.*[17] have established the quasirotational character of the yrast cascade (with $J^{\pi}_{\max} = 12^{+}$) in ^{66}Zn, the data obtained by Heits *et al.*[18] can quite reasonably be interpreted, at least qualitatively, in terms of a deformed picture. The experimental study of the nucleus ^{72}Se by Hamilton *et al.*[19] has emphasized the quasirotational aspects of its high-spin yrast spectrum.

The currently available data on the yrast states in the isotopes of Zn, Ge, and Se thus makes it desirable to have a consistent description of these nuclei in the framework of a microscopic model involving a reasonably large configuration space as well as employing realistic effective interactions. Particularly, the explicit involvement of an orbit such as the $g_{9/2}$ orbit, which has a large single-particle quadrupole content, is of crucial importance in any calculation of the properties of the high-spin yrast cascades in view of the overwhelming evidence of the quadrupole collectivity—and the associated quasirotational behavior—implied by the available data.[17-19] Here we must also point out that, whereas Couch *et al.*[26] as well as Von Ehrenstein and Schiffer[27] have found no firm experimental evidence from stripping experiments of $f_{7/2}$ holes in the nuclei in the $A > 60$ mass region, Betigeri *et al.*[28] as well as McIntyre[29] have identified the presence of the $g_{9/2}$ configurations at low excitation energies in the Zn isotopes.

The calculations carried out so far—and they have been attempted *only* for the Zn isotopes and the nuclei ^{72,74}Ge—do not quite satisfy the criteria just mentioned. Van Hienen, Chung, and Wildenthal have carried out extensive shell-model calculations[23] for the Zn isotopes, distributing the active particles only in the $p_{3/2}$, $p_{1/2}$, and $f_{5/2}$ orbits outside an inert ^{56}Ni core. The Hartree-Fock-Bogoliubov (HFB) calculations which were attempted earlier,[24] with the exception of the calculation by Didong *et al.*,[25] have also omitted the $g_{9/2}$ orbit from the valence space, although they did include the $f_{7/2}$ orbit. Didong *et al.*[25] computed the spectra of only the nuclei ^{70}Zn and ^{72,74}Ge using a modified surface-delta interaction and employing the generator coordinate formalism. The

calculation included the $g_{9/2}$ orbit in addition to the valence space of Ref. 23. Although the calculation was successful in explaining many of the features of the low-lying spectra, it was restricted to just three nuclei.

In the present work we attempt a microscopic description of the yrast spectra in some doubly even Zn, Ge, and Se isotopes in the framework of the HFB approach, employing the valence space spanned by the $p_{3/2}$, $p_{1/2}$, $f_{5/2}$, and $g_{9/2}$ orbits. The doubly closed nucleus ^{56}Ni is treated as an inert core. The relevant effective two-body interaction that we have employed is a renormalized G matrix due to Kuo[30] which is the sum of G_{bare}, $G_{\text{3p-1h}}$, and $G_{\text{2p-2h}}$ in the ^{56}Ni core. The single particle energies we have taken are (in MeV) $e(p_{3/2})=0.0$, $e(p_{1/2})=1.08$, $e(f_{5/2})=0.78$, and $e(g_{9/2})=3.0$.

In Sec. II we discuss some details of the calculational framework. Section III discusses the comparison of the theoretical yrast spectra, static quadrupole moments as well as the inter-cascade $E2$ transition strengths with the available experimental results. The results for the calculation of the occupation numbers of the various subshells involved in the ground states of the Zn, Ge, and Se isotopes are also presented and compared with the transfer reaction data available from the studies of (d,p), (d,n), (p,d), and (t,α) reactions. Section IV contains some concluding remarks.

II. METHOD OF CALCULATION

We have obtained first the HFB intrinsic states employing the Kuo interaction and following the procedure discussed in Refs. 31–33. Only pairing correlations between the like particles were allowed in the present calculation. This assumption is quite justified here because the Fermi surfaces for the protons and neutrons are quite different in the present case owing to the neutron excesses in the nuclei considered.

The intrinsic deformed HFB state with $K=0$ can be written, in the usual notation, as

$$|\phi_0\rangle = \prod_m (u_i^m + v_i^m b_{i\,m}^\dagger b_{i\,\bar{m}}^\dagger)|0\rangle\,, \tag{1}$$

where the operators $b_{i\,m}^\dagger$ are written as

$$b_{i\,m}^\dagger = \sum_j c_{ji}^m a_{jm}^\dagger, \quad b_{i\,\bar{m}}^\dagger = \sum_j (-1)^{l+j-m} c_{ji}^m a_{j-m}^\dagger\,, \tag{2}$$

where j labels the spherical single-particle orbits $p_{3/2}$, $p_{1/2}$, $f_{5/2}$, and $g_{9/2}$.

The energy of a state with angular momentum J is given as[33]

$$E_J = \frac{\langle\phi_0|HP_{00}^J|\phi_0\rangle}{\langle\phi_0|P_{00}^J|\phi_0\rangle} = \frac{\int_0^\pi h(\theta) d_{00}^J(\theta)\sin\theta\, d\theta}{\int_0^\pi n(\theta) d_{00}^J(\theta)\sin\theta\, d\theta}\,.$$

Here P_{KK}^J is the angular momentum projection operator. The explicit expressions for $h(\theta)$ and $n(\theta)$ are given in Refs. 32 and 33. Using the angular momentum projected wave functions $|\Psi_{MK}^J\rangle = P_{MK}^J|\phi_K\rangle$ we have computed the static moments and the reduced transition probabilities for inter-band transitions with the help of the expressions given in Ref. 33. In computing the electromagnetic properties, the values of the oscillator constant have been obtained from the rms radii using the uniform density model.[34] Further, the effective charges have been used such that for protons the effective charge is $e_p=1+e$ and for the neutrons it is $e_n=e$.

III. RESULTS AND DISCUSSION

A. Yrast spectra

The experimental as well as theoretical yrast spectra for the Zn isotopes have been presented in Fig. 1.

We first discuss here the nuclei ^{62,64}Zn. Van Hienen *et al.*[23] have employed in their exact shell-model calculations an effective interaction derived by Koops and Glaudemans[35] for a valence space formed by the $p_{3/2}$, $p_{1/2}$, and $f_{5/2}$ orbits. This interaction was labeled in Ref. 23 as the ASDI interaction. With a view to test the efficacy of the projected HFB (PHFB) method in the context of the calculation of the yrast spectra, we have obtained the yrast spectra for ^{62,64}Zn in the PHFB method using the same valence space as well as the set of input parameters (single particle energies and the effective interaction) as used in Ref. 23. The results thus obtained have been presented in Fig. 1 in the column labeled PHFB

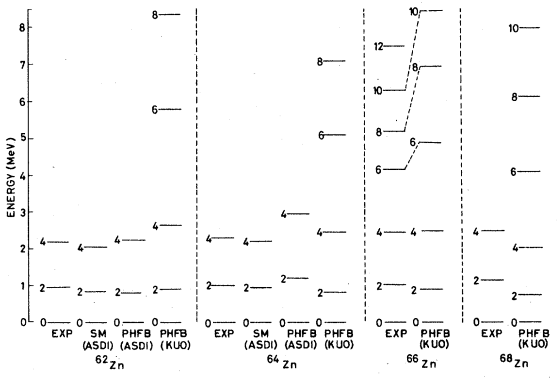

FIG. 1. Comparison of the experimental and calculated yrast spectra for some doubly even isotopes of Zn.

(ASDI), together with the exact shell model yrast spectra which have been labeled as SM (ASDI). We find that, whereas the SM and the PHFB spectra are in very good agreement in the case of the nucleus ^{62}Zn, the agreement is not so good for the nucleus ^{64}Zn. This can be attributed to the fact that the intrinsic state for ^{64}Zn resulting from the ASDI interaction has a small deformation, thus necessitating a mixing of more than one $K=0$ band in the calculation. However, for all the nuclei considered here the Kuo interaction yields deformations which are significantly larger than that obtained for the nucleus ^{64}Zn with the ASDI interaction. Thus the PHFB method, in conjunction with the Kuo interaction, can be considered fairly reliable.

From the results presented in Fig. 1 we note that, up to $J=4$, the PHFB results obtained with the Kuo interaction are not very different from those obtained with the ASDI interaction, although the latter operates in a smaller valence space. The present calculation in the extended space, however, predicts $J=6,8$ states in ^{62}Zn at excitation energies 5.8 and 8.4 MeV, respectively. In the nucleus ^{64}Zn, we predict $J=6,8$ states at energies 5.1 and 7.1 MeV, respectively.

Discussing next the nuclei ^{66,68}Zn, we notice from Fig. 1 that the observed level spacings in the lower part of the yrast cascade (with $J=0,2,4$) are reasonably well reproduced by the present calculation. In the nucleus ^{66}Zn, however, the positions of the states with $J=6,8,10$ are about 1.8 MeV too high compared to the experiment. This discrepancy may imply a necessity of using, for the Zn isotopes, a value for $e(g_{9/2})$ different from what we have used throughout in this paper, viz., $e(g_{9/2})=3.0$ MeV. However, in view of the lack of information on the high-spin levels in other Zn isotopes, we can not decide this point here. In the nucleus ^{68}Zn, although the calculation reproduces correctly the energy separation $(E_{J=4}-E_{J=2})$, the observed $J=2$ is calculated 0.4 MeV too low. Here we predict excited states with $J^\pi=6^+,8^+,10^+$ at energies 4.2, 6.2, and 8.0 MeV, respectively.

In Fig. 2 we have presented the observed[36] as well as the computed yrast spectra for the nuclei ^{70,72,74,76}Ge. In the calculated spectra, the $J=2$ states have been aligned with their observed position in all cases. A striking feature of the computed spectra which one notices here is the following: Whereas the calculation predicts the observed positions of the yrast states with $J>2$ in a reasonably accurate manner relative to those of the states with $J=2$, there is a discrepancy in the position of the calculated $J=0$ level. This discrepancy is seen to be systematically decreasing as one goes from ^{70}Ge

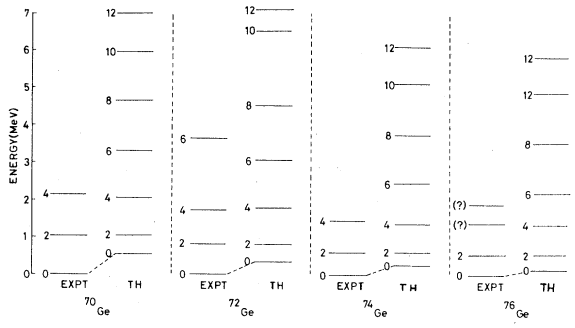

FIG. 2. Comparison of the experimental and calculated yrast spectra in Ge isotopes.

to ^{76}Ge. This trend of the discrepancy in the calculated position of the $J=0$ (relative to the remaining part of the spectra) may be due to the noninclusion of the $f_{7/2}$-excited, $J=0$ configurations—an effect which is expected to be of lesser significance in the higher isotopes as compared to that in the lighter ones.

The highest spin observed so far in the doubly even isotopes of Ge is $J=6$. The present calculation is successful in reproducing the energy separations between the $J=2$ and $J=4$ yrast levels in the nuclei ^{70,72,74}Ge; in the nucleus ^{76}Ge there is a level at 1.412 MeV which may be assigned a spin 4 in view of this success.

The present calculation predicts states with spin up to $J^\pi=12^+$ in the Ge isotopes considered here. An experimental study of the states with $J>6$ would not only be interesting in itself, it would help also very much in testing the assumptions underlying the present model, viz., the goodness of the doubly closed ^{56}Ni core.

The results for the calculated yrast spectra in the nuclei ^{72,74,76,78}Se are presented in Fig. 3 together with the observed ones. The computed yrast spectra again show a systematically decreasing discrepancy so far as the positions of the calculated $J=0$ states are

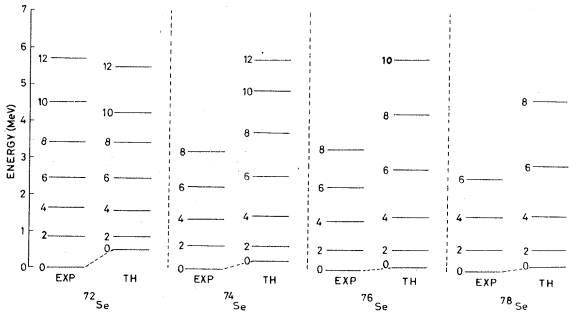

FIG. 3. Comparison of the experimental and calculated yrast spectra in Se isotopes.

TABLE I. The static quadrupole moments and the $B(E2)$ values for transitions involving the yrast states in some doubly even isotopes of Zn. The $B(E2)$ values are in units of 10^{-50} $e^2\,\mathrm{cm}^4$ and the static quadrupole moments have been given in units of $e\,\mathrm{fm}^2$. All the values have been computed with an effective charge $e=0.4$.

Nucleus	$\lvert E_i-E_f\rvert$	$J_i\rightarrow J_f$	$B(E2)$ Expt.	$B(E2)$ Theory	$Q(J_f^+)$ Expt.	$Q(J_f^+)$ Theory
^{62}Zn	0.950	$0\rightarrow 2$	14.0 ± 2.5	13.3		−24.9
	1.240	$2\rightarrow 4$		15.6		−26.8
	1.190	$4\rightarrow 6$		11.9		−32.8
^{64}Zn	0.990	$0\rightarrow 2$	15.8 ± 0.5	14.1		−31.7
	1.321	$2\rightarrow 4$		17.0		−33.6
	1.693	$4\rightarrow 6$		13.0		−30.5
^{66}Zn	1.039	$0\rightarrow 2$	13.7 ± 0.5	16.2		−23.9
	1.411	$2\rightarrow 4$	>09.6[a]	19.8		−33.4
	1.729	$4\rightarrow 6$	>01.18[a]	16.5		−30.3
^{68}Zn	1.080	$0\rightarrow 2$	13.6 ± 0.6	17.0		−19.3
	1.342	$2\rightarrow 4$		21.2		−37.0
	1.740	$4\rightarrow 6$		07.2		−14.9

[a] Reference 17.

concerned. Hamiltonian *et al.*[19] had postulated the coexistence of spherical and deformed $J=0$ states in their experimental study of the high-spin yrast spectrum in ^{72}Se, while attempting to fit the observed spectrum empirically. The present work gives indications that this feature of coexistence may not be confined to the nucleus ^{72}Se alone; it may be a general characteristic of the spectra in the $A=70$–80 mass region. A consistent attempt to calculate the mixing of the two $J=0$ states, one with a deformed and the other with a spherical origin, may improve considerably the agreement between the calculated and the observed positions of the yrast $J=0$ states.

From the results presented in Fig. 3 we see that the observed yrast cascade in ^{72}Se (with $J_{max}=12$) is reasonably well reproduced in the present work. The observed spectra in ^{74,76,78}Se are also in fair agreement with the calculation. A notable exception, however, is the $J=8$ state in ^{76}Se; the calculated position shows a discrepancy of about 1 MeV.

To summarize, the overall agreement of the calculated yrast spectra in the doubly even isotopes of Zn, Ge, and Se with the experiment is surprisingly good, particularly in view of the fact that in the present model we have not considered the mixing of the ground state ($K=0$) band with other high-lying (quasiparticle-excited) bands.

B. Electromagnetic properties

In Tables I–III we have presented the results for the reduced transition probabilities for the

TABLE II. The static quadrupole moments and the $B(E2)$ values for the yrast states in Ge isotopes.

Nucleus	$\lvert E_i-E_f\rvert$	$J_i\rightarrow J_f$	$B(E2)$ Expt.	$B(E2)$ Theory	$Q(J_f^+)$ Expt.	$Q(J_f^+)$ Theory
^{70}Ge	1.040	$0\rightarrow 2$	17.9 ± 0.3	22.6	0 ± 10	−28.8
	1.114	$2\rightarrow 4$	09.6 ± 5.4[a]	21.4		−33.8
		$4\rightarrow 6$		07.3		−26.1
^{72}Ge	0.835	$0\rightarrow 2$	22.3 ± 0.5	23.2		−35.7
	0.895	$2\rightarrow 4$		32.7		−40.6
		$4\rightarrow 6$		34.8		−41.2
^{74}Ge	0.596	$0\rightarrow 2$	31.5 ± 2.5	22.6	-12 ± 16	−30.1
	0.869	$2\rightarrow 4$		31.4		−37.4
		$4\rightarrow 6$		33.4		−40.1
^{76}Ge	0.563	$0\rightarrow 2$	26.0 ± 0.5	21.8	-11 ± 14	−28.2
		$2\rightarrow 4$		28.1		−35.3
		$4\rightarrow 6$		30.2		−37.7

[a] Reference 18.

TABLE III. The static quadrupole moments and the $B(E2)$ values for the yrast states in Se isotopes.

Nucleus	$\lvert E_i - E_f \rvert$	$J_i \rightarrow J_f$	$B(E2)$ Expt.	$B(E2)$ Theory	$Q(J_f^+)$ Expt.	$Q(J_f^+)$ Theory
^{72}Se	0.862	$0 \rightarrow 2$		34.4		−48.8
	0.775	$2 \rightarrow 4$		48.5		−47.3
	0.830	$4 \rightarrow 6$		52.9		−54.2
^{74}Se	0.635	$0 \rightarrow 2$	37.0 ± 1.5	34.9		−36.8
	0.728	$2 \rightarrow 4$		49.1		−44.9
	0.868	$4 \rightarrow 6$		53.2		−51.7
^{76}Se	0.560	$0 \rightarrow 2$	42.0 ± 1.5	32.6		−33.8
	0.772	$2 \rightarrow 4$		45.9		−53.8
	0.932	$4 \rightarrow 6$		49.0		−51.9
^{78}Se	0.614	$0 \rightarrow 2$	32.0 ± 1.0	29.7		−33.3
	0.885	$2 \rightarrow 4$		57.0		−46.2
	1.040	$4 \rightarrow 6$		21.2		−55.7

intercascade $E2$ transitions in the doubly even isotopes of Zn, Ge, and Se. We have also calculated here the static quadrupole moments for the yrast states. As mentioned earlier, the effective charges employed are $1.4e$ and $0.4e$ for the valence protons and neutrons respectively.

We first discuss the results for the $B(E2)$ $(0^+ \rightarrow 2^+)$ values in various nuclei. These values are available from the half-life measurements for the first-excited $J^\pi = 2^+$ levels in most of the nuclei considered here. In Fig. 4 we have plotted the calculated and observed $B(E2)$ $(0 \rightarrow 2)$ values for 12 isotopes. From the results we see here that the calculation is quite successful in reproducing the general trend of variation with the mass number. Some significant discrepancies, however, occur for the nuclei ^{68}Zn, ^{74}Ge, and ^{76}Se. The computed values are very sensitive to the choice of the effective charges; it turns out that a change of the effective charges (e_p, e_n) from (1.4, 0.4) to (1.5, 0.5) can remove to a large extent the discrepancies in ^{74}Ge and ^{76}Se.

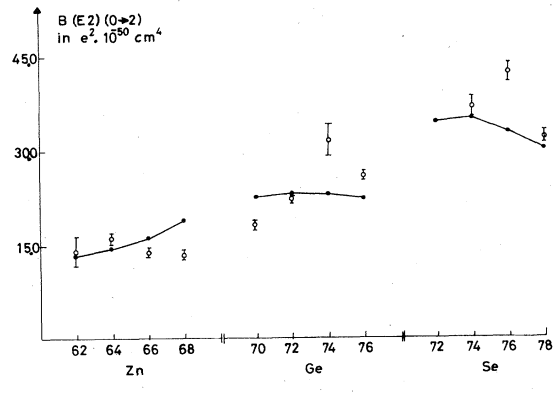

FIG. 4. Graphical presentation of some of the results presented in Tables I–III. The full line joins the points computed with the effective charges of 1.4 and 0.4 for the valence protons and neutrons respectively.

It is difficult to test the PHFB wave functions from the available data on the static quadrupole moments. Firstly the available results are very few in number, and secondly the experimental estimates have large error bars which arise due to the uncertainties associated with the effects of higher excited states in the Coulomb excitation processes.

It is clear from the present calculation that the PHFB wave functions for the Zn, Ge, and Se isotopes, which explain reasonably well the observed spectra in these nuclei, also give a good description of the electromagnetic properties, using the same set of effective charges throughout the mass region from $A = 62$ to $A = 78$.

C. Occupation numbers for shell-model orbits

In Table IV we have given the results for the occupation numbers of $p_{3/2}$, $f_{5/2}$, $p_{1/2}$, and $g_{9/2}$ orbits in the doubly even isotopes of Zn, Ge, and Se. The experimental numbers quoted here are

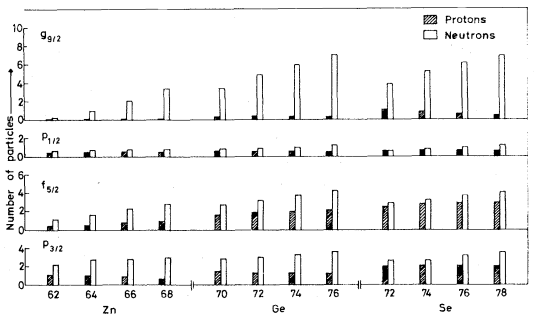

FIG. 5. Subshell occupation numbers for protons and neutrons in the ground states of doubly even Zn, Ge, and Se isotopes.

TABLE IV. The calculated values of the occupation numbers for the various subshells in some Zn, Ge, and Se isotopes. The available experimental values (see Ref. 23) have been given in square brackets.

Nucleus	Protons				Neutrons			
	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$g_{9/2}$	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$g_{9/2}$
^{62}Zn	0.48	1.09	0.46	0.01	0.60	2.08	1.07	0.31
^{64}Zn	0.52	1.04	0.47	0.01	0.73	2.82	1.61	0.88
	[0.46±0.11]	[1.6±0.4]	[1.1±0.3]		[1.0±0.2]	[1.8±0.8]	[3.0±0.7]	
^{66}Zn	0.53	0.78	0.71	0.01	0.75	2.89	2.27	2.13
	[0.45±0.11]	[2.0±0.5]	[1.1±0.3]		[1.3±0.3]	[2.7±0.7]	[4.3±1.1]	[0.6±0.2]
^{68}Zn	0.52	0.60	0.87	0.01	0.76	2.99	2.85	3.42
					[0.7±0.2]	[2.3±0.6]	[5.1±1.3]	[0.9±0.2]
^{70}Ge	0.57	1.49	1.66	0.23	0.73	2.89	2.80	3.52
^{72}Ge	0.55	1.38	1.87	0.23	0.79	3.05	3.30	4.87
^{74}Ge	0.53	1.30	2.00	0.20	0.95	3.33	3.76	5.98
^{76}Ge	0.49	1.19	2.12	0.19	1.19	3.56	4.29	6.94
^{72}Se	0.57	1.99	2.49	0.97	0.65	2.59	2.91	3.89
^{74}Se	0.56	1.93	2.72	0.82	0.71	2.75	3.26	5.30
^{76}Se	0.57	2.00	2.83	0.63	0.89	3.23	3.67	6.24
^{78}Se	0.56	2.04	2.92	0.52	1.18	3.56	4.16	7.14

the lower limits on the observed values imposed in Ref. 23.

Here we see that the occupation numbers for $g_{9/2}$ orbit show a monotonic increase upon the addition of neutrons (Fig. 5). The neutron occupation numbers for $f_{5/2}$ orbit also display a similar trend. On the other hand the $p_{3/2}$ and $p_{1/2}$ occupation numbers do not change much along the isotopic sequences for neutrons. The available experimental values in the case of the nuclei ^{64,66}Zn are in fair agreement with the calculated ones.

In view of the scarcity of data on the single-nucleon spectroscopic factors in the isotopes of Ge and Se and the ambiguous nature of the available results in the Zn isotopes, we cannot conclude much at present from the results obtained here.

IV. CONCLUSIONS

We have presented here the results for the calculation of the energy spectra, electromagnetic observables as well as the subshell occupation numbers for the yrast states in some doubly even isotopes of Zn, Ge, and Se. It turns out that the structure of the yrast states in a majority of these nuclei can be successfully discussed in a parameter-free, microscopic manner, employing the projected HFB formalism and using the realistic effective interactions in a valence space spanned by the $p_{3/2}$, $p_{1/2}$, $f_{5/2}$, and $g_{9/2}$ orbits.

Present calculations, however, indicate the necessity of providing an improved description of the $J=0$ ground state in Ge and Se isotopes by incorporating more configurational admixtures within the $(p_{3/2},p_{1/2},f_{5/2},g_{9/2})$ space and/or by opening the $f_{7/2}$ core. We also find some significant discrepancies between the calculated and the experimental $B(E2)$ $(0\rightarrow 2)$ values in the nuclei ^{68}Zn, ^{74}Ge, and ^{76}Se. Importantly enough, our calculation has yielded large intrinsic quadrupole deformations for these nuclei even with the present small valence space; the calculated quasirotational spectra in these nuclei are characterized by relatively small (E_2-E_0) separation. Thus the assumption that ^{56}Ni can be regarded as an inert core may not be valid in the case of these nuclei. An explicit involvement of the $f_{7/2}$ orbit in the valence space is likely to improve considerably the theoretical $B(E2)$ estimates.

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