Pramāṇa – J. Phys., Vol. 25, No. 3, September 1985, pp. 251–258. © Printed in India.

Ground-state occupancies of f–p–g shell nuclei

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MS received 9 February 1985; revised 18 June 1985

Abstract. We have calculated the ground-state occupancies of various nuclei in the spectroscopic space of upper f–p shell and $g_{9/2}$ orbit using spectral distribution methods. The modified fully renormalised Kuo-Brown interaction has been used. The calculated values have been compared with the experimental results.

Keywords. Occupancy; f–p–g shell; spectral distribution method.

PACS No. 21·10.

1. Introduction

Orbit occupancies in the ground state of nuclei, are the simplest dynamical quantities that can be experimentally measured. Therefore, calculations of occupancies starting from effective two-body interactions, when compared with the experimental data, serve as a tool to investigate the relevance of various effective interactions. These calculations also allow one to study the systematic changes in the nuclear structure as the number of neutrons and protons changes. Several such calculations have been reported in the past. Various effective interactions in the s-d shell were studied by Potbhare and Pandya (1976). A similar analysis was done for the lower f-p shell nuclei by Kota and Potbhare (1979) and a few nuclei in the upper f-p shell were investigated by Kota *et al* (1982) using the fully renormalized Kuo-Brown interaction. Here, we present results for various nuclei in the upper f-p shell. The spectroscopic space for the present study consists of $p_{3/2}$, $f_{5/2}$, $p_{1/2}$ and $g_{9/2}$ orbitals. It is obvious that any shell model calculation of orbit occupancies, which requires exact ground-state wave function, would be impractical because of the large dimensionalities of the Hamiltonian matrices involved. We have therefore used the spectral distribution method (SDM) which allows one to evaluate occupancies without requiring the construction and diagonalisation of large Hamiltonian matrices.

The effective interaction in this study is derived by K H Bhatt and D P Ahalpara (Personal Communication, 1985) from the fully renormalised Kuo-Brown interaction. The following modifications were made empirically using the Hartree-Fock calculation:

(i) the $\langle g_{9/2}^2 | v | g_{9/2}^2 \rangle^{JT}$ matrix elements were changed so as to reproduce. ^{90}Zr and ^{92}Mo spectra, and

(ii) the centroid of $\langle g_{9/2} p_{1/2} | v | g_{9/2} p_{1/2} \rangle^{JT}$ matrix elements was adjusted to reproduce the separation of the $g_{9/2}$ and $p_{1/2}$ single particle states in ^{89}Y nucleus.

The single particle energies used are 0·0, 0·78, 1·08 and 3 MeV for $p_{3/2}, f_{5/2}, p_{1/2}$ and $g_{9/2}$ orbitals respectively; the first three values come from the experimental spectrum of ^{57}Ni, while the $g_{9/2}$ single particle energy is arbitrarily fixed at 3 MeV. In the next section we briefly outline the procedure for calculation. The results are analysed in §3.

2. Procedure

Occupancy calculation using SDM simplifies to a great extent if the space is decomposed according to proton-neutron (p–n) configurations. A p–n configuration $(\mathbf{m}_p, \mathbf{m}_n)$ is defined by assigning a fixed number of protons and neutrons to various proton and neutron orbitals such that

$$\sum_\alpha m_{\alpha,p} = \text{total number of protons;}$$

$$\sum_\alpha m_{\alpha,n} = \text{total number of neutrons,}$$

where α denotes the orbitals. Such a decomposition implies a fixed value of T_Z.

The energy eigenvalue density $\rho(E)$ with respect to energy is defined as a sum of intensities of all configurations into which the space is subdivided, i.e.

$$\rho(E) = \sum_{\mathbf{m}_p, \mathbf{m}_n} \rho_{\mathbf{m}_p, \mathbf{m}_n}(E), \tag{1}$$

where each term in the summation corresponds to the intensity of configuration $(\mathbf{m}_p, \mathbf{m}_n)$, in the eigenvalue distribution at energy E. The intensity distribution of each configuration is assumed to be a gaussian and is given by

$$\rho(\mathbf{m}_p, \mathbf{m}_n) = \frac{d(\mathbf{m}_p, \mathbf{m}_n)}{\sqrt{2\pi}\,\sigma(\mathbf{m}_p, \mathbf{m}_n)} \exp\left\{-\tfrac{1}{2}\left(\frac{E - \langle H \rangle^{\mathbf{m}_p, \mathbf{m}_n}}{\sigma(\mathbf{m}_p, \mathbf{m}_n)}\right)^2\right\}, \tag{2}$$

where $d(\mathbf{m}_p, \mathbf{m}_n)$ is the dimensionality, $\langle H \rangle^{\mathbf{m}_p, \mathbf{m}_n}$ is the centroid, and $\sigma(\mathbf{m}_p, \mathbf{m}_n)$ is the width of the intensity distribution for the configuration $(\mathbf{m}_p, \mathbf{m}_n)$†. This assumption is partly based on the applicability of central limit theorem when the number of particles is large compared to the body rank of the effective interaction.

The ground state energy $E_{g.s}$ is calculated from the eigenvalue density $\rho(E)$ using the Ratcliff (1971) procedure,

$$\int_{-\infty}^{E_{g.s}} \rho(E)\,dE = \tfrac{1}{2} \times \text{ground state degeneracy} = \tfrac{1}{2}(2J+1). \tag{3}$$

It has been shown by Draayer *et al* (1977) that the expectation value of any operator O at x can be expanded in terms of orthogonal polynomials P_n

$$O(x) = \langle O \rangle + \sum_{n=1}^{\infty} \langle O P_n(H) \rangle P_n(x). \tag{4}$$

† It should be noted that $\langle O \rangle = \ll O \gg /\text{dimensionality}$, and $\ll O \gg$ is the trace and $\sigma = \langle H^2 \rangle - \{\langle H \rangle\}^2$.

These polynomials are defined by the eigenvalue density. When the space is decomposed according to *p-n* configurations, the expression can be written as

$$O(x) = \sum_{\mathbf{m}_p, \mathbf{m}_n} \frac{\rho_{\mathbf{m}_p, \mathbf{m}_n}(x)}{\rho(x)} \left(\langle O \rangle^{\mathbf{m}_p, \mathbf{m}_n} + \sum_{q=1}^{\infty} \langle O P_q^{\mathbf{m}_p, \mathbf{m}_n}(H) \rangle^{\mathbf{m}_p, \mathbf{m}_n} P_q^{\mathbf{m}_p, \mathbf{m}_n}(x) \right).$$

For occupancy calculations $O = n_{i,p}, n_{i,n}$ where n is the number operator and $x = E_{g.s}$. From (5), due to orthogonality properties of P_q's, and the scalar character of $n_{i,p}$ in the *p-n* configuration, it follows that

$$\langle n_{i,p} P_q(H) \rangle^{\mathbf{m}_p, \mathbf{m}_n} = \text{number of protons in the } i\text{th orbit}^* \, \delta_{q,0}$$
$$= m_{i,p}(\mathbf{m}_p, \mathbf{m}_n) * \delta_{q,0}.$$

Hence the expression for occupancy turns out to be

$$n_{i,p}(x) = \sum_{\mathbf{m}_p, \mathbf{m}_n} m_{i,p}(\mathbf{m}_p, \mathbf{m}_n) * \frac{\rho_{\mathbf{m}_p, \mathbf{m}_n}(x)}{\rho(x)}. \tag{6}$$

The above result follows directly and naturally from the polynomial expansion method. However, we feel that the polynomial method might not give very good results near the ground-state. Consider the expression

$$\rho(x) = \lim_{\Delta x \to 0} \frac{F(x) - F(x - \Delta x)}{\Delta x},$$

where $F(x) = \int_{-\infty}^{x} \rho(y)\,dy$ is the distribution function at x. If $x = E_{g.s}$ there will be no states below x, that is at $(x - \Delta x)$. Therefore, we propose to replace the density function by the distribution function for the ground-state occupancy expression which now reads,

$$n_{i,p}(E_{g.s}) = \sum_{\mathbf{m}_p, \mathbf{m}_n} m_{i,p}(\mathbf{m}_p, \mathbf{m}_n) * \frac{\int_{-\infty}^{E_{g.s}} \rho_{\mathbf{m}_p, \mathbf{m}_n}(x)\,dx}{\int_{-\infty}^{E_{g.s}} \rho(x)\,dx}. \tag{7}$$

The results of the occupancies calculated by both the methods are tabulated and analysed in the following section.

3. Results and discussion

Though the results of (7) were expected to be more appropriate than that of (6) for the ground states, it turns out that the results of two equations are not significantly different. This, we feel, is due to large dimensionalities of the spaces involved. Hence, in table 1, we present the calculated ground-state occupancies of various nuclei using (6) only. The results using (7) are given for Zn isotopes only (in brackets) for comparison. It should be noted that we have taken proper care of the ground-state parity, by choosing only those configurations which have the same parity as that of the ground state. Further, to reduce the enormous amount of computing time, we have restricted calculations to include only those configurations which do not have more than four

Table 1. Calculated ground-state occupancies.

Nucleus	Proton occupancy				Neutron occupancy			
	$p_{3/2}$	$f_{5/2}$	$p_{1/2}$	$g_{9/2}$	$p_{3/2}$	$f_{5/2}$	$p_{1/2}$	$g_{9/2}$
^{64}Zn	1·78 (1·81)	0·13 (0·11)	0·08 (0·08)	0·01 (0·00)	2·92 (3·01)	1·71 (1·65)	1·08 (1·12)	0·29 (0·22)
^{65}Zn	1·69 (1·73)	0·21 (0·18)	0·07 (0·07)	0·02 (0·02)	2·76 (2·84)	2·20 (2·19)	1·02 (1·07)	1·01 (0·90)
^{66}Zn	1·76 (1·79)	0·18 (0·15)	0·05 (0·05)	0·01 (0·01)	2·93 (2·98)	2·58 (2·60)	1·13 (1·17)	1·36 (1·27)
^{67}Zn	1·71 (1·75)	0·22 (0·20)	0·05 (0·05)	0·02 (0·01)	3·06 (3·08)	2·95 (2·96)	1·22 (1·24)	1·77 (1·73)
^{68}Zn	1·78 (1·81)	0·16 (0·15)	0·05 (0·04)	0·01 (0·01)	3·27 (3·27)	3·42 (3·44)	1·45 (1·46)	1·86 (1·83)
^{67}Ga	2·39	0·40	0·16	0·05	2·91	2·39	1·22	1·48
^{69}Ga	2·43	0·34	0·20	0·03	3·30	3·28	1·53	1·88
^{71}Ga	2·27	0·48	0·14	0·12	3·12	3·95	1·47	3·47
^{68}Ge	3·00	0·56	0·37	0·10	3·10	2·19	1·38	1·33
^{69}Ge	2·91	0·60	0·39	0·1	3·23	2·61	1·46	1·71
^{70}Ge	3·01	0·49	0·45	0·06	3·43	3·10	1·64	1·84
^{71}Ge	2·77	0·48	0·39	0·36	3·40	3·72	1·60	2·28
^{72}Ge	2·83	0·66	0·31	0·20	3·23	3·84	1·58	3·35
^{73}Ge	2·53	0·82	0·29	0·37	3·19	4·15	1·51	4·15
^{74}Ge	2·61	0·76	0·28	0·35	3·16	4·52	1·58	4·75
^{76}Ge	2·36	0·87	0·31	0·44	3·24	5·09	1·65	6·03
^{73}As	3·03	0·99	0·56	0·45	3·36	3·71	1·59	3·34
^{74}As	2·88	1·09	0·48	0·56	3·30	4·05	1·56	4·10
^{75}As	2·79	1·16	0·46	0·60	3·27	4·37	1·57	4·79
^{72}Se	3·54	1·05	1·07	0·34	3·63	2·92	1·73	1·72
^{73}Se	3·37	1·13	0·84	0·67	3·52	3·39	1·66	2·44
^{74}Se	3·32	1·26	0·78	0·65	3·48	3·63	1·64	3·26
^{75}Se	3·08	1·45	0·65	0·83	3·37	3·96	1·57	4·11
^{76}Se	3·09	1·48	0·66	0·77	3·38	4·27	1·62	4·73
^{77}Se	2·93	1·58	0·63	0·86	3·38	4·59	1·63	5·40
^{78}Se	2·85	1·66	0·65	0·85	3·46	4·88	1·68	6·03
^{79}Se	2·54	1·85	0·62	0·99	3·45	5·11	1·68	6·76
^{80}Se	2·50	1·91	0·67	0·93	3·53	5·37	1·75	7·35
^{77}Br	3·16	1·96	0·78	1·11	3·42	4·17	1·59	4·82
^{79}Br	2·92	2·16	0·77	1·15	3·46	4·77	1·66	6·11
^{81}Br	2·61	2·40	0·79	1·20	3·56	5·28	1·74	7·42
^{80}Kr	3·15	2·59	0·95	1·31	3·53	4·70	1·70	6·08
^{81}Kr	2·92	2·76	0·92	1·40	3·52	4·95	1·70	6·82
^{82}Kr	2·85	2·84	0·97	1·34	3·60	5·23	1·77	7·40
^{83}Kr	2·61	2·98	0·96	1·46	3·65	5·45	1·80	8·10
^{83}Rb	2·97	3·36	1·11	1·57	3·59	5·15	1·76	7·50
^{84}Rb	2·84	3·44	1·13	1·59	3·67	5·41	1·81	8·10

particles excited to $g_{9/2}$ orbit compared to the lowest configuration obtained using non-interacting particles. In figures 1 and 2, we graphically present part of the information given in tables 1 and 2. We have not been able to gather enough experimental data due to scarcity of experiments in this region. However, those available are given in table 2. Comparison of the two tables shows that the two-body interaction used produces proper p-orbit ($l = 1$) occupancy as long as the neutron number is less than 12. However, for other nuclei, calculated occupancy is much larger than the observed p-orbit occupancy. The calculated occupancy for $g_{9/2}$ orbit turns out to be fairly close to the observed values for four selenium isotopes. The experimental $f_{5/2}$-neutron occupancy for Zn isotopes seems to be much larger than the calculated value. This may be due to the fact that the experimentally observed numbers have been obtained considering the spectroscopic space of f-p orbits only. In general the $f_{5/2}$-proton occupancy is not all reproduced properly by the interaction used.

The calculated results do show a change of proton occupancy structure, when the number of neutrons in the spectroscopic space crosses 12. Figure 1 shows such a change for germanium and selenium isotopes. However, this change is not as sharp as indicated by the experimental results. This failure of the interaction used is also responsible for the poor agreement of $f_{5/2}$-orbit proton occupancies with the experimental results. Change of structure of proton occupancies is also found for $f_{5/2}$ orbits, though to a lesser extent. If the $g_{9/2}$ orbit neutron occupancy is plotted against the neutron number, we can see that as the number of neutrons crosses 12, there is a distinct change in the gradient of the plot for all nuclei, and the $g_{9/2}$ orbit neutron occupancy increases linearly with the number of neutrons. We also see that the $g_{9/2}$ orbit neutron occupancy is independent of the number of protons; for example the $g_{9/2}$ orbit neutron occupancies of ^{71}Ga, ^{72}Ge, ^{73}As and ^{74}Se are 3·47, 3·35, 3·34 and 3·26 respectively; and those of ^{74}Ge, ^{75}As, ^{76}Se and ^{77}Br are 4·75, 4·79, 4·73 and 4·82 respectively.

Comparing our results with those obtained by Kota *et al* (1982) for fully renormalised Kuo-Brown interaction, we conclude that (i) fully renormalised Kuo-

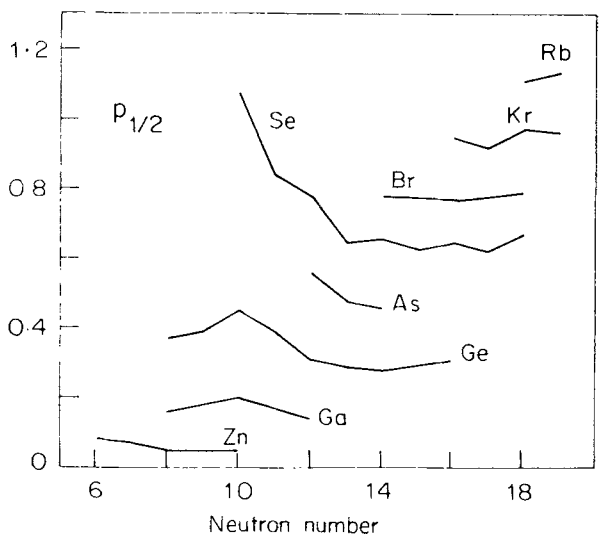

Figure 1. $p_{1/2}$-proton occupancy *vs* neutron number.

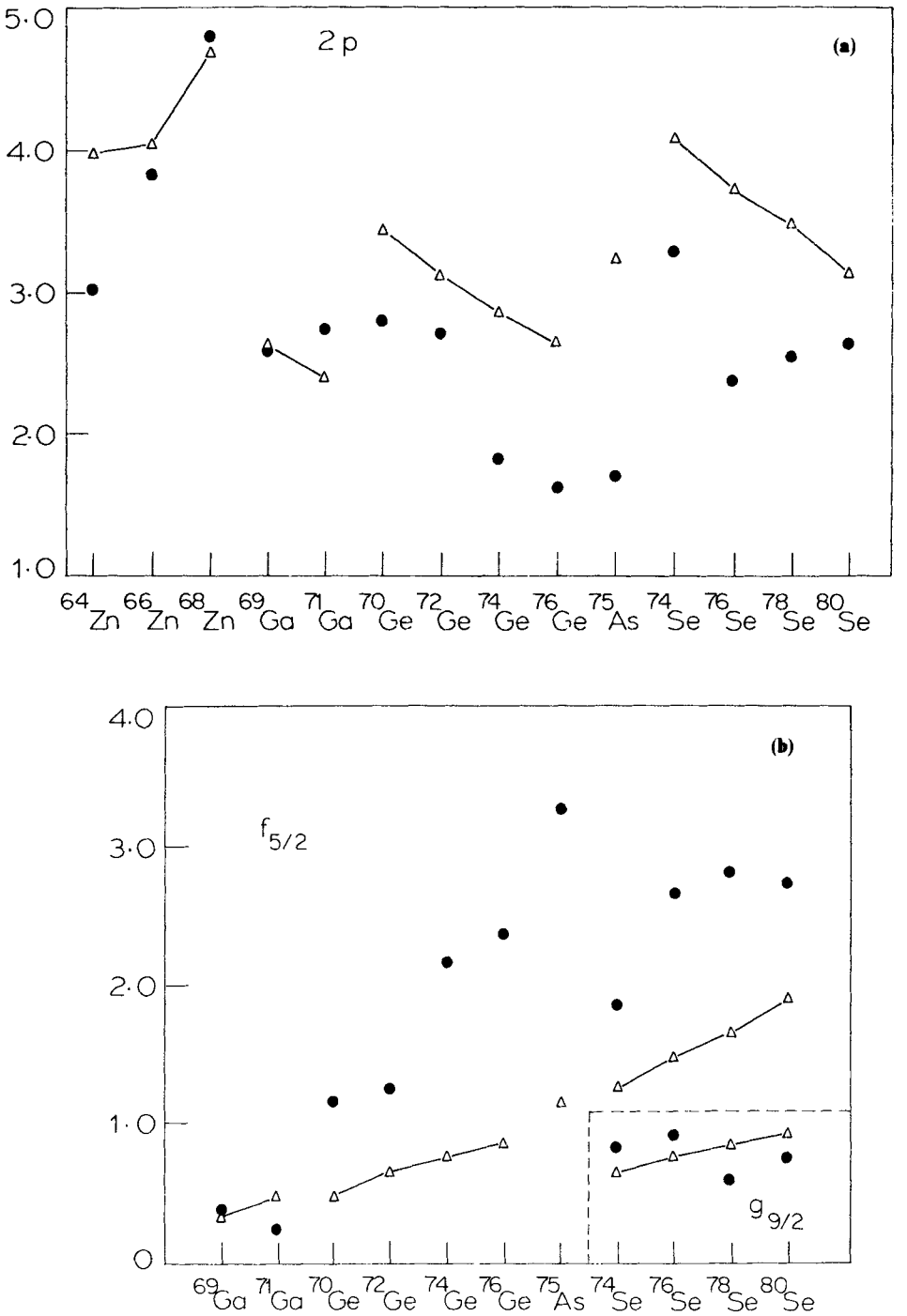

Figure 2. Occupancies vs nuclei. (Neutron occupancy for Zn and proton occupancy for other Nuclei.) Comparison of experimental results and calculated results. (**a**) p-orbit (**b**) $f_{5/2}$ and $g_{9/2}$ orbits. Circles are around experimental values and triangles are around calculated occupancies.

Table 2. Experimental ground-state occupancies.

Nucleus	Occupancies					Reference
	$p_{3/2}$	$p_{1/2}$	$2p$	$f_{5/2}$	$g_{9/2}$	
^{64}Zn			3·04	2·96		1
^{66}Zn			3·86	4·14		2
^{68}Zn			4·82	5·18		1
^{69}Ga			2·61	0·39		3
^{71}Ga			2·76	0·25		3
^{70}Ge			2·82	1·18		3
^{72}Ge			2·73	1·27		3
^{74}Ge			1·84	2·16		3
^{76}Ge			1·63	2·37		3
^{75}As			1·72	3·28		3
^{74}Se	2·78	0·53		1·86	0·83	4
^{76}Se	1·97	0·43		2·67	0·93	4
^{78}Se	2·25	0·32		2·82	0·61	4
^{80}Se	1·85	0·51		2·88	0·76	4

Notes: (i) The values for ^{64}Zn, ^{66}Zn, ^{68}Zn correspond to neutron occupancy. The rest are proton occupancies

(ii) References: 1. Von Ehrenstein and Schiffer (1967); 2. Abughazleh *et al.* (1977); 3. Rotbard *et al* (1978); 4. Rotbard *et al* (1982).

Brown interaction produces a sharper change in proton occupancy structure, and is in good agreement with the experimental results, (ii) interaction used here increases $g_{9/2}$ and $f_{5/2}$ orbit occupancies at the expense of mainly $P_{1/2}$ orbit occupancy. Increase in the $g_{9/2}$ orbit occupancy can, however, be attributed to the lowering of the $g_{9/2}$ orbit single particle energy by 1/2 MeV.

Modifications in the effective interaction matrix elements are usually done empirically to obtain a reasonably good agreement of the calculated eigenvalues with experimentally obtained energy eigenvalues spectra; this requires either extensive shell-model calculations or Hartree-Fock type calculations. We propose that an alternative method for modification of effective interaction matrix elements based on empirically fitting observed ground-state occupancies, which considers the experimentally observed trends, can be given. For example, the sudden change of proton occupancy structure for germanium isotopes when the neutron number in the space crosses 12 can be simulated by properly adjusting the induced proton-single-particle energies (Chang *et al* 1977) for p-orbits and $f_{5/2}$ orbit such that these cross-over when the number of neutrons becomes 12. The several advantages in the proposed scheme are listed below: (i) calculations involved are simple, (ii) only few parameters like induced single-particle energies (which depend on sums of two-body matrix elements) need to be varied and (iii) modification relates to the wavefunction of the ground state rather than the eigenvalues. This work will be reported in the near future.

Acknowledgement

The authors thank Dr V N Potbhare for his interest, help and guidance in this work.

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