APPENDIX II

A. Single particle energies and two-body matrix elements of the $\bar{K}_s$ operator.

The operator involved in centroid calculation for particle removal strength for an orbit 's' is given by $A_s H B_s$. This can be expressed as :

$$A_s H B_s = \bar{K}_s + 1/2 \; (\; n_s H + H n_s \;) \; ; \quad n_s = A_s \; B_s . \tag{1}$$

$$\therefore \quad \bar{K}_s = A_s H B_s - 1/2 \; (A_s B_s H + H A_s B_s)$$

The (1+2) body hamiltonian can be written as

$$H = \sum_i \epsilon_i \; A_i B_i - 1/4 \sum_{i,j,k,l} W_{ijkl} \; A_i \; A_j \; B_k \; B_l \tag{2}$$

Where ϵ_i is the external single particle energy and W_{ijkl} is the antisymmetrized two body matrix element between s.p.states i, j, k and l.

(i) Single particle energy :

$$\bar{K}_s \; (1 - \text{body part}) = \sum_i \epsilon_i \{ A_s \; A_i \; B_i \; B_s - 1/2 \; (A_j B_j \; A_s B_s + A_s \; B_s \; A_i \; B_i) \}$$

$$= \sum_i \epsilon_i \{ - A_i A_s B_i B_s - 1/2 \; A_i (\delta_{is} - A_s B_i) \; B_s - 1/2 A_s \; (\delta_{is} - A_i B_s) \; B_i \}$$

$$= \sum_i \epsilon_i \{ - A_i A_s B_i B_s - 1/2 \; \delta_{is} \; A_i B_s + 1/2 \; A_i A_s B_i B_s - 1/2 \; A_s B_i \; \delta_{is} + 1/2 \; A_s A_i B_s B_i \}$$

$$= \sum_i \epsilon_i (-1/2\ \delta_{is}\ A_i B_s - 1/2\ \delta_{is}\ A_s B_i) = -\epsilon_s n_s$$

(ii) Two body matrix element:

$$\bar{K}_s \text{ (2+3-body part)} = 1/8 \sum_{i,j,k,l} W_{ijkl} \{ A_s B_s\ A_i A_j B_k B_l$$

$$A_i A_j B_k B_l A_s B_s \ - 2 A_s\ A_i A_j B_k B_l\ B_s \}$$

$$= 1/8 \sum_{i,j,k,l} W_{ijkl} \{ A_s\ (\delta_{is} - A_i B_s)\ A_j B_k B_l + A_i A_j B_k (\delta_{ls} - A_s B_l) B_s$$

$$- 2 A_s A_i A_j B_k B_l B_s \}$$

$$= 1/8 \sum_{i,j,k,l} W_{ijkl} \{ \delta_{is}\ A_s A_j B_k B_l - A_s A_i\ (\delta_{js} - A_j B_s)\ B_k B_l$$

$$+ \delta_{ls}\ A_i A_j B_k B_s - A_i A_j (\delta_{sk} - A_s B_k)\ B_l B_s$$

$$- 2 A_s A_i A_j B_k B_l B_s \}$$

$$= 1/8 \sum_{i,j,k,l} W_{ijkl} \{ [\delta_{is}\ A_s A_j B_k B_l - \delta_{js}\ A_s A_i B_k B_l + \delta_{is} A_i A_j B_k B_s$$

$$- \delta_{sk} A_i A_j B_l B_s\ ]_{\text{two-body}}$$

$$+ 2 [\, 1/2\ A_i A_j A_s B_k B_l B_s + 1/2\ A_s A_i A_j\ B_s B_k B_l$$

$$- A_s A_i A_j\ B_k B_l B_s\ ]_{\text{three-body}} \}$$

$$\therefore \bar{K}_s \text{(two body part)} = \frac{1}{2} (1/4 \sum_{i,j,k,l} W_{ijkl}\ (\delta_{is} + \delta_{js} + \delta_{ks} + \delta_{ls})$$
$$* A_i A_j B_k B_l \cdot$$

K_s^- (three body part)

$$= 1/4 \sum_{i,j,k,l} W_{ijkl} \left(-A_s A_i A_j B_k B_l B_s + 1/2 A_i A_j A_s B_k B_l B_s\right)$$

$$+ 1/2\ A_s A_i A_j B_s B_k B_l) = 0.$$

B. Single particle energies and two body matrix element for K_s^+ operator:

The operator involved in centroid calculation for particle addition strength for an orbit s is given by $B_s H A_s$. One defines a hermitian operator

$$K_s^+ = B_s H A_s - \frac{1}{2} (B_s A_s H + H B_s A_s)$$

(1) K_s^+ Single particle energy :

$$K_s^+ \text{ (1-body part)} = \sum_i \epsilon_i \{(B_s A_i B_i A_s - 1/2\ B_s A_s A_i B_i - 1/2\ A_i B_i B_s A_s)\}$$

$$= \sum_i \epsilon_i \{(\delta_{is} - A_i B_s)(\delta_{is} - A_s B_i) - 1/2\ (1 - A_s B_s) A_i B_i - 1/2 A_i B_i (1 - A_s B_s)\}$$

$$= \sum_i \epsilon_i \{\delta_{is}^2 - \delta_{is} (A_i B_s + A_s B_i) + A_i B_s A_s B_i - 1/2\ A_i B_i$$

$$+ 1/2\ A_s (\delta_{is} - A_i B_s) B_i - 1/2\ A_i B_i + 1/2\ A_i (\delta_{is} - A_s B_i) B_s\}$$

$$= \sum_i \epsilon_i \{\delta_{is}^2 - \delta_{is} (A_s B_s + A_s B_i) + A_i (1 - A_s B_s) B_i - A_i B_i - 1/2 A_i A_s B_i B_s$$

$$- 1/2\ A_i A_s B_i B_s\}$$

$$= \sum_i \epsilon_i \{\delta_{is}^2 - 1/2\ \delta_{is} (A_i B_s + A_s B_i)\}$$

$$= \epsilon_s + K_s^- \text{ (One-body part)}$$

(2) K_s^+ two body matrix element;

Now K_s^+ (2+3-body part)

$$= \frac{1}{4} \sum_{i,j,k,l} W_{ijkl} \{ B_s A_i A_j B_k B_l A_s - 1/2\ B_s A_s A_i A_j B_k B_l - 1/2\ A_i A_j B_k B_l B_s A_s \}$$

Let $T_1 = B_s A_i A_j B_k B_l A_s$

$$= (\delta_{is} - A_i B_s)\ A_j B_k\ (\delta_{ls} - A_s B_l)$$

$$= \delta_{is}\delta_{ls} A_j B_k - \delta_{is} A_j (\delta_{sk} - A_s B_k) B_l - A_i (\delta_{js} - A_j B_s) B_k \delta_{ls} + A_i (\delta_{js} - A_j B_s)(\delta_{sk} - A_s B_k) B_l$$

$$= \delta_{is}\delta_{ls} A_j B_k + \delta_{is} A_j A_s B_k B_l - \delta_{is}\delta_{sk} A_j B_l - \delta_{ls}\delta_{sj} A_i B_k + \delta_{ls} A_i A_j B_s B_k + A_i B_l \delta_{sj}\delta_{sk} - \delta_{sj} A_i A_s B_k B_l - \delta_{sk} A_i A_j B_s B_l + A_i A_j B_s A_s B_k B_l$$

$$= \delta_{is}\delta_{ls} A_j B_k - \delta_{is}\delta_{sk} A_j B_l - \delta_{ls}\delta_{sj} A_i B_k + \delta_{sj}\delta_{sk} A_i B_l - (\delta_{is} + \delta_{js} + \delta_{ks} + \delta_{is})\ A_i A_j B_k B_l + A_i A_j B_k B_l - A_i A_j A_s B_k B_l B_s$$

Let $T_2+T_3=-1/2\ (\ B_sA_sA_iA_jB_kB_l+\ A_iA_jB_kB_lB_sA_s)$

$= -1/2\ \{(1-A_sB_s)\ A_iA_jB_kB_l+\ A_iA_jB_kB_l\ (1-A_sB_s)\}$

$= -1/2\ \{\ A_iA_jB_kB_l-\ A_s(\ \delta_{is}-\ A_iB_s)\ A_jB_kB_l$

$+\ A_iA_jB_kB_l\ -\ A_i\ A_jB_k\ (\ \delta_{ls}\ -\ A_sB_l)\ B_s\ \}$

$= -\ A_iA_jB_kB_l\ +\ \frac{1}{2}\{(\ \delta_{is}\ A_sA_jB_kB_l-\ A_sA_i(\ \delta_{js}-\ A_jB_s)\ B_kB_l$

$+\ \delta_{ls}\ A_iA_jB_kB_s\ -\ A_iA_j\ (\ \delta_{sk}-A_sB_k)\ B_lB_s)\}$

$= -\ A_iA_jB_kB_l\ +\ \frac{1}{2}(\ \delta_{is}+\ \delta_{js}\ +\ \delta_{ks}\ +\ \delta_{ls})\ \ A_iA_jB_kB_l$

$+\ \frac{1}{2}\ (\ A_sA_iA_jB_sB_kB_l\ +\ A_iA_jA_sB_kB_lB_s).$

$\therefore\ K_s^+$ (two body part)$=1/4\ \sum_{ijkl}\ W_{ijkl}\ (T_1+T_2+T_3)_{\text{two body}}$

$= -1/4\ \sum_{i,j,k,l}\ W_{ijkl}\ (\ \delta_{is}\ \delta_{ls}\ A_jB_k-\ \delta_{is}\ \delta_{ks}A_jB_l$

$-\ \delta_{ls}\ \delta_{js}\ A_iB_k+\ \delta_{js}\ \delta_{ks}\ \ A_iB_l)$

$-\ \frac{1}{8}\ \sum_{i,j,k,l}\ W_{ijkl}\ (\ \delta_{is}+\ \delta_{js}\ +\ \delta_{ks}+\ \delta_{ls}\ )\ A_iA_jB_kB_l$

$-\ \frac{1}{4}\ \sum_{i,j,k,l}\ W_{ijkl}\ (-A_iA_jA_sB_sB_lB_k+\ \frac{1}{2}\ A_sA_iA_jB_sB_kB_l$

$+\ \ \frac{1}{2}\ A_iA_jA_sB_kB_lB_s)\ .$

$$= -\frac{1}{4}\Big(\sum_{j,k} W_{sjks} A_j B_k - \sum_{j,l} W_{sjls} A_j B_l - \sum_{i,k} W_{isks} A_i B_k$$

$$+ \sum_{i,l} W_{issl} A_i B_i \Big) + K_s^- \text{ (two body part)}$$

The first four terms being exactly equal, one finally has

$$K_s^+ \text{ (two body)} = K_s^- \text{ (two body)} + \sum_{i,j} W_{isjs} A_i B_j$$

Collecting both one and two body parts of K_s^+,

we have :

$$K_s^+ = K_s^- + \epsilon_s + \sum_{ij} W_{isjs} A_i B_j$$

C. Expression for correlation coefficient ζ_2 between the operators A_s H B_s and H in the scalar space.

We start with equation (39), chapter 4, which gives an expression for the correlation coefficient ζ_2 as :

$$\zeta_2 = \frac{< K_s^- H^{\nu=2} >^{m_p, m_n} + 1/2\sigma^2(m_p, m_n) + 1/2 < H^{\nu=2} n_s H^{\nu=2} >^{m_p, m_n}}{m_s \, \sigma^2 \, (m_p, m_n)}$$

where contribution comes from the rank-2 part of the hamiltonian, and the K_s^- operator. Since we are working in the proton-neutron space, we require $W^J_{ijkl}(p\text{-}p)$ and W^J_{ijkl} (p-n) which are the two body matrix elements between the proton-proton or neutron-neutron orbits and the proton-neutron orbits For spherical orbits, matrix elements could be defined a according to angular momentum-isospin (JT) symmetry. There is a straightforward manner of transforming matrix elements from one formalism to another :

$$W^J_{ijkl} \; (p\text{-}p \text{ or } n\text{-}n) = W^{J,T=1}_{ijkl}$$

$$W^J_{ijkl} \; (p\text{-}n) \; \frac{1}{\xi_{ij} \xi_{kl}} \left[W^{J,T=1}_{ijkl} - \xi_{ij} \, \xi_{kl} \, W^{J,T=1}_{ijkl} \right]$$

Where $\xi_{ij} = 1 / (1 + \delta_{ij})^{1/2}$

For convenience, let us denote W^{J}_{ijkl} (p-p) by A and W^{J}_{ijkl} (p-n) by B. The variance of the hamiltonian H in a space defined by (m_p, m_n) is :

$$\sigma^2 (m_p\ m_n) = PR(1) \sum_{i,j,k,\ell=1}^{NSEL} \sum_{J} (2J+1)\ A^2 /4$$

$$+ PR(2) \sum_{i,j,k,\ell=1}^{2*NSEL} \sum_{J} (2J+1)A^2 / 4$$

$$+ PR(3) \sum_{i,k=1}^{NSEL} \sum_{j,\ell=NSEL+1}^{2*NSEL} \sum_{J} (2J+1)\ B^2 .$$

Where NSEL = number of proton orbits, which is the same as the number of neutron orbits. The total number of orbits is given by 2 * NSEL. The factor 1/4 comes in the first two terms to take care of interchange of orbits. PR(i) are the propagators corresponding to operators P and R, given by:

$$PR(1) = \frac{m_p}{N} \frac{(m_p-1)}{(N-1)} \frac{(N - m_p)}{(N-2)} \frac{(N- m_p-1)}{(N-3)}$$

$$PR(2) = \frac{m_p}{N} \frac{(m_n-1)}{(N-1)} \frac{(N-m_n)}{(N-2)} \frac{(N- m_n-1)}{(N-3)}$$

$$PR(3) = \frac{m_p}{N} \frac{m_n}{N} \frac{(N - m_p)\ (N- m_n)}{(N-1)^2}$$

$N = \sum_{J} (2J+1)$ is the shell degeneracy.

Calculation of $\langle K_s^- H^{\nu=2} \rangle^{m_p, m_n}$ is similar to $\sigma^2 (m_p, m_n)$ with the matrix elements of K_s^- operator given in terms of those of H

$$\therefore \quad \langle K_s^- H \rangle^{m_p, m_n} = PR(1) \sum_{i,j,k,\ell=1}^{NSEL} \sum_J (2J+1)(-1/2)(\delta_{is}+\delta_{js}+\delta_{ks}+\delta_{ls})A^2/4$$

$$+ PR(2) \sum_{i,j,k,\ell=NSEL+1}^{2xNSEL} \sum_J (2J+1)(-1/2)(\delta_{is}+\delta_{js}+\delta_{ks}+\delta_{ls})A^2/4$$

$$+ PR(3) \sum_{i,k=1}^{NSEL} \sum_{j,\ell,=NSEL+1}^{2xNSEL} \sum_J (2J+1)(-1/2)[\delta_{is}+\delta_{ks})B^2 + (\delta_{js}+\delta_{ls})B^2]$$

The third term $\langle H^{\nu=2} n_s H^{\nu=2} \rangle^{m_p, m_n}$ is a three-operator product, and has to be treated carefully. The final expression turns out to be

$$\langle H^{\nu=2} n_s H^{\nu=2} \rangle^{m_p, m_n} = PQR(1) \sum_{i,j,k,\ell=1}^{NSEL} \sum_J (2J+1) C_{is} A^2/4$$

$$+ PQR(2) \sum_{i,j,k,\ell=NSEL+1}^{2xNSEL} \sum_J (2J+1) C_{is} A^2/4$$

$$+ PQR(3) \sum_{i,k=1}^{NSEL} \sum_{j,\ell=NSEL+1}^{2xNSEL} \sum_J (2J+1) C_{is} B^2 + \sum_{i,\ell=1}^{NSEL} \sum_{j,k=1}^{2*NSEL} \sum_J (2J+1) C_{is} B^2$$

$$+ PQR(4) \sum_{i,k=NSEL}^{2xNSEL} \sum_{j,\ell=1}^{NSEL} \sum_J (2J+1) C_{is} B^2$$

$$+ \sum_{i,\ell=1}^{NSEL} \sum_{j,k=NSEL+1}^{2xNSEL} \sum_J (2J+1) C_{is} B^2$$

Where PQR (i) are the propagators corresponding to three operators P, Q and R,

and $C_{is} = (1 - (2j_i+1)/N)\delta_{is} + (1-\delta_{is})\ (2j_s +1)/N,$

where j_i is the angular momentum of the ith orbit. This factor is the probability of a particle or a hole in the ith orbit.

The propogators PQR(i) are given by

$$PRQ\ (1) = 1/2 \binom{m_p}{2} - \binom{m_p}{3} + \frac{5}{2} \binom{m_p}{4} - \binom{m_p}{5}$$

$$PRQ(2) = \frac{1}{2} \binom{m_p}{2} - 2 \binom{m_n}{3} + \frac{5}{2} \binom{m_n}{4} - \binom{m_n}{5}$$

$$PRQ(3) = \frac{1}{2} \frac{m_p}{N} \frac{m_n}{N} - 3 \frac{m_n}{N} \binom{m_p}{2} + \frac{m_p}{N} \binom{m_n}{2} + 3 \binom{m_p}{2} \binom{m_n}{2}$$

$$+ 2 \frac{m_n}{N} \binom{m_p}{3} - 2 \binom{m_p}{3} \binom{m_n}{2}$$

$$\text{and } PQR\ (4) = \frac{1}{2} \frac{m_n}{N} \frac{m_p}{N} - 3 \frac{m_p}{N} \binom{m_n}{2} + \frac{m_n}{N} \binom{m_p}{2} + 3 \binom{m_p}{2} \binom{m_n}{2}$$

$$+ 2 \frac{m_p}{N} \binom{m_n}{3} - \binom{m_n}{3} \binom{m_p}{2} \quad ;$$

$$\text{where } \binom{m}{i} = \frac{m\ (m-1)\ (m-2)\ \ldots\ldots\ (m-i+1)}{N\ (N-1)\ (N-2)\ \ldots\ldots\ (N-i+1)}$$

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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.

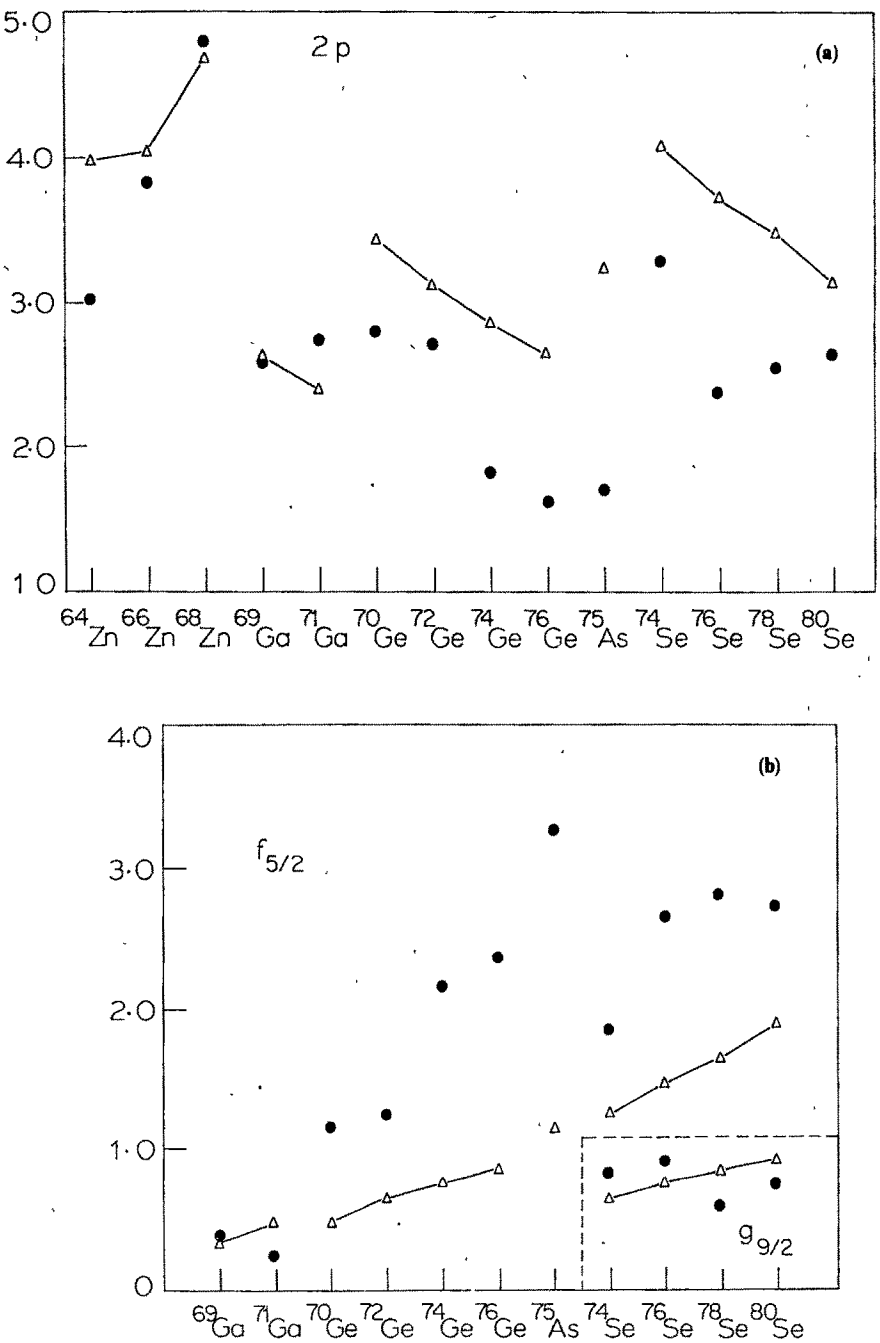

Figure 2. Occupancies vs nuclei. (Neutron occupancy for Zn and proton occupancy for other Nuclei.) Comparison of experimental results and calculated results. (a) *p*-orbit (b) $f_{5/2}$ and $g_{9/2}$ orbits Circles are around experimental values and triangles are around calculated occupancies.

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-

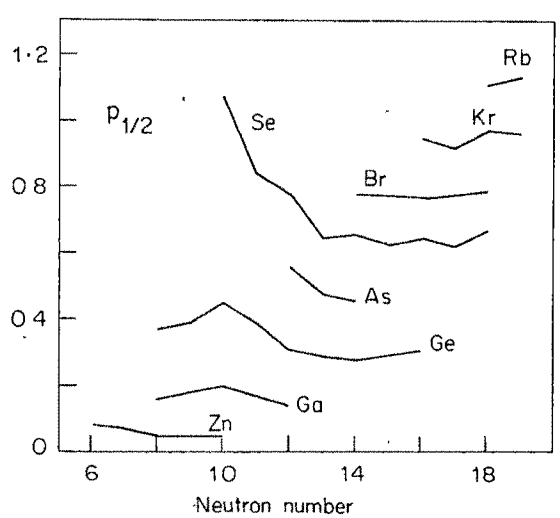

Figure 1. $p_{1/2}$-proton occupancy *vs* neutron number.

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	0·13	0·08	0·01	2·92	1·71	1·08	0·29
	(1·81)	(0·11)	(0·08)	(0·00)	(3·01)	(1·65)	(1·12)	(0·22)
^{65}Zn	1·69	0·21	0·07	0·02	2·76	2·20	1·02	1·01
	(1·73)	(0·18)	(0·07)	(0·02)	(2·84)	(2·19)	(1·07)	(0·90)
^{66}Zn	1·76	0·18	0·05	0·01	2·93	2·58	1·13	1·36
	(1·79)	(0·15)	(0·05)	(0·01)	(2·98)	(2·60)	(1·17)	(1·27)
^{67}Zn	1·71	0·22	0·05	0·02	3·06	2·95	1·22	1·77
	(1·75)	(0·20)	(0·05)	(0·01)	(3·08)	(2·96)	(1·24)	(1·73)
^{68}Zn	1·78	0·16	0·05	0·01	3·27	3·42	1·45	1·86
	(1·81)	(0·15)	(0·04)	(0·01)	(3·27)	(3·44)	(1·46)	(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

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

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 $\sigma = \langle H^2 \rangle - \{\langle H \rangle\}^2$.

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.

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Table 1. Ground-state energies for ^{20}Ne (in MeV)

Interaction	$E_g(H_M)$	$E_g(H_M)+\Delta E_g$(scalar)	$E_g(H_M)+\Delta E_g$(conf.)
HS1	−45·8	−44·9	−36·5
HS2	−43·8	−43·3	−40·1
HST1	−43·2	−42·4	−39·5
HST2	−47·0	−46·5	−40·8
HST3	−46·1	−45·6	−42·5
H_F	−40·6	—	—

The operator K is treated as a perturbation to the model Hamiltonian H_M. The scalar space result for such a correction is very easy to obtain;

$$S_1(E_g)+S_2(E_g)=-E_g/2(1-\zeta_{MF}^2)=\Delta E_g,$$

where E_g is the ground-state energy as given by H_M, ζ_{MF} is the correlation coefficient between H_M and H_F. Similar result using configuration space has been obtained in terms of averages of various combinations of H_M and H_F in each configuration. The ground-state energy corrections using these expressions have been displayed in table 1 for the case of ^{20}Ne in $d-s$ shell space using the PW interaction as the effective interaction, with ^{17}O single-particle energies.

The interactions HS1, HS2, HST1, HST2 and HST3 are various model interactions (Kota *et al* 1980). The ground-state energies in column 2 have been obtained using the shell-model programme; the third column gives the ground-state energies using the scalar space result while the last column corresponds to the corrected ground-state energies using the configuration space expressions for ΔE_g. It is immediately clear by looking at table 1 that the corrected ground-state energies are closer to the H_F ground-state energy and further that the configuration space result is much better than the scalar space result. Also the deviation from true ground-state is the largest in the case of HS1; the interaction derived using the least information input from the effective interaction.

In conclusion, we would like to point out that, we have a new derivation (8) of the expressions that are statistical in nature, for the inverse energy-weighted sums that appear in the Rayleigh Schrodinger perturbation theory. These expressions (especially (14) and its extensions) are useful in a wide variety of problems. As a simple example, we have applied them and calculated the ground-state energy corrections when the effective interaction is approximated by a model Hamiltonian.

Acknowlegement

We thank J B French for the valuable input that has come from him which lead to the derivation of equation (14).

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where $\varepsilon_0(c)$ and $\sigma_0(c)$ are the configuration density centroid and width respectively for unperturbed H. The introduction of perturbation αK to H shifts and scales each configuration differently, according to

$$\varepsilon_\alpha(c) = \varepsilon_0(c) + \alpha\langle K\rangle^c$$
$$\sigma_\alpha^2(c) = \sigma_0^2(c) + 2\zeta_c\sigma_K(c)\sigma_0(c) + \alpha^2\sigma_K^2(c).$$

Suffix 0 indicates unperturbed values which refer to H. Introducing these into the general expressions for $S_1(E)$ and $S_2(E)$ (equations (5) and (8) given above), though tedious, is quite straightforward. We merely indicate the final result here

$$S_1(E) = \frac{\sum_c d_c/D\,\rho^c(E)\{\langle K\rangle^c + \zeta_c\sigma_K^c x_c\}}{\rho(E)} \tag{13}$$

$$x_c = (E - \varepsilon_0(c))/\sigma_0(c)$$

$$\begin{aligned} S_2(E) = {} & \frac{1}{2\rho(E)}\left[\sum_c \frac{d_c}{D}\frac{\rho^c(x)}{\sigma_0(x)}\{\zeta_c^2\sigma_K^2(c)\mathrm{He}_3(x_c)\right. \\ & \left. + 2\langle K\rangle^c\sigma_K(c)\zeta_c\mathrm{He}_2(x_c) + [(\langle K\rangle^c)^2 + \sigma_K^2(c)]\mathrm{He}_1(x_c)\}\right] \\ & + \frac{1}{2[\rho(E)]^3}\left[\sum_c \frac{d_c}{D}\frac{x_c}{\sigma_0(c)}\rho^c(x_c)\right] * \left[\sum_c \frac{d_c}{D}\rho^c(x_c)[\langle K\rangle^c + \zeta_c\sigma_K(c)x_c]\right]^2 \\ & - \frac{1}{[\rho(E)]^2}\left[\sum_c \frac{d_c}{D}\rho^c(x_c)(\langle K\rangle^c + \zeta_c\sigma_K(c)x_c)\right] \\ & * \left[\sum_c \frac{d_c}{D}\frac{\rho^c(x_c)}{\sigma_0(c)}\{\langle K\rangle^c x_c + (x_c^2 - 1)\zeta_c\sigma_K(c)\}\right]; \end{aligned} \tag{14}$$

where He_i are the Hermite polynomials, and c in the above equations indicates that the corresponding quantity is calculated in configuration c. Note that in general, ζ_c cannot be called the correlation coefficient as the configuration partitioning does not correspond to good symmetry; however, it has the same structure and hence the same nomenclature is used;

$$\zeta_c = \langle (K - \langle K\rangle^c)(H - \langle H\rangle^c)\rangle^c/\sigma_K(c)\sigma_0(c).$$

4. Applications

Kota *et al* (1980) gave several model Hamiltonians H_M approximating the effective interaction H_F by linear combinations of various parts of the Q.Q operator and the pairing operator. It is clear that such a model interaction cannot completely represent H_F, as a part of the H_F will always be orthogonal to H_M. Hence, the ground-state energy calculated using H_M will not be the same as the true ground-state energy. We are now in a position to correct the ground-state energy estimate obtained using H_M, by taking into account the difference between H_F and H_M;

$$H_F = H_M + H_P = H_M + K.$$

This result was given by Halemane (1981). We have given a new and comparatively transparent derivation of the same using the Ratcliff's procedure. Further differentiation of (6) with respect to α would provide us expressions for $S_m(E)$, $(m > 2)$.

This result in the scalar space can be immediately applied whenever the strong action of the central limit theorem (CLT) renders the eigenvalue density function into a gaussian-defined by its centroid ε and width σ. The CLT also allows us to assume that the perturbed eigenvalue density due to small perturbation αK is gaussian too; however with centroid $\varepsilon(\alpha)$ and width $\sigma(\alpha)$. The change in the centroid merely shifts the eigenvalue spectrum while the width change corresponds to the scale change.

$$\varepsilon = \langle H \rangle; \quad \sigma^2 = \langle H^2 \rangle - \langle H \rangle^2, \quad \sigma_K^2 = \langle K^2 \rangle - \langle K^2 \rangle,$$
$$\varepsilon_\alpha = \langle H \rangle + \alpha \langle K \rangle, \quad \sigma^2(\alpha) = \sigma^2 + 2\alpha\zeta\sigma\sigma_K + \alpha^2\sigma_K^2,$$

where ζ is the correlation coefficient between H and K. The scale change parameter λ is defined by

$$\lambda = (\sigma(\alpha)/\sigma - 1) = (1 + 2\alpha\zeta\sigma_K/\sigma + \alpha^2\sigma_K^2/\sigma^2)^{1/2} - 1.$$

Taking into account these two changes, it is clear using the geometric picture that eigenvalue E_0 is shifted to E_α due to perturbation

$$E_\alpha = E_0 + \alpha\langle K \rangle + \lambda(E_0 - \varepsilon). \tag{9}$$

Expanding the parameter λ as a power series in α gives

$$E_\alpha = E_0 + \alpha\{\langle K \rangle + \zeta\sigma_K/\sigma * (E_0 - \varepsilon)\} + \alpha^2/2 * (E_0 - \varepsilon)(1 - \zeta^2)\sigma_K^2/\sigma^2. \tag{10}$$

Thus in the CLT limit we have,

$$S_1(E_0) = K(E_0) = \langle K \rangle + \zeta\sigma_K/\sigma * (E_0 - \varepsilon),$$
$$S_2(E_0) = 1/2(1 - \zeta^2)(E_0 - \varepsilon)\sigma_K^2/\sigma^2. \tag{11}$$

3. Extension to configurations

The arguments based on the centroid shift and scale change for calculating $S_1(E)$ and $S_2(E)$ are easily applicable in the scalar space. Usually, one partitions the space according to some symmetry group, in order to increase the accuracy of the results. If we decompose the space according to configurations (Chang *et al* 1971), the overall state density $\rho(E)$ is then expressed as the sum of intensities of all configurations into which the space has now been subdivided.

$$\rho(E) = 1/D \sum_c d_c * \rho^c(E) = \sum_c I_c(E) \tag{12}$$

where d_c is the configuration dimensionality and $D = \sum_c d_c$ is the total dimensionality. Each term in the summation above corresponds to the intensity of the configuration in the eigenvalue distribution at energy E. We assume that each configuration density is a gaussian,

$$\rho^c(E) = \frac{1}{[2\pi\sigma_0^2(c)]^{\frac{1}{2}}} \exp\left\{-\frac{1}{2}\left(\frac{E - \varepsilon_0(c)}{\sigma_0(c)}\right)^2\right\},$$

Rayleigh-Schrodinger perturbation theory

$$E_{n,\alpha} = E_{n,0} + \alpha S_1(E_{n,0}) + \alpha^2 S_2(E_{n,0}) + \cdots$$

$$= E_{n,0} + \alpha \langle E_{n,0}|K|E_{n,0}\rangle + \alpha^2 \sum_{m \neq n} \frac{|\langle E_{n,0}|K|E_{m,0}\rangle|^2}{(E_{m,0} - E_{n,0})}. \tag{2}$$

Thus S_1 corresponds to the expectation value of K and S_2 is the first inverse energy weighted sum. The SDM provide smoothened expressions for the coefficients $S_i(E)$. Differentiating (1a) with respect to α (from now on we drop the state index n)

$$\frac{dp}{d\alpha} = 0 = \frac{\partial E}{\partial \alpha}\rho_\alpha(E_\alpha) + \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx, \tag{3}$$

$$\frac{\partial E_\alpha}{\partial \alpha} = -\frac{1}{\rho_\alpha(E_\alpha)} \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx. \tag{4}$$

In the limit $\alpha \to 0$, as the integration limits do not depend upon α, interchanging the integration over x and differentiation with respect to α, we get

$$\frac{\partial E_\alpha}{\partial \alpha}\Big|_{\alpha=0} = S_1(E_0) = K(E_0) = -\frac{1}{\rho(E_0)}\left[\frac{\partial}{\partial \alpha}\int_{-\infty}^{E_0} \rho_\alpha(x)dx\right]_{\alpha=0}$$

$$= -\frac{1}{\rho(E_0)}\left[\frac{\partial}{\partial \alpha}F_\alpha(E_0)\right]_{\alpha=0}. \tag{5}$$

$F(x)$ here is the distribution function and suffix 0 indicates the unperturbed values. This result was originally given by Chang and French (1973). Differentiating (4) again with respect to α, we obtain,

$$\frac{\partial^2 E_\alpha}{(\partial \alpha)^2} = -\frac{1}{\rho_\alpha(E_\alpha)}\int_{-\infty}^{E_\alpha} \frac{\partial^2}{(\partial \alpha)^2}\rho_\alpha(x)dx + \frac{1}{\rho_\alpha^2(E_\alpha)}\frac{\partial \rho_\alpha(x)}{\partial \alpha}\Big|_{x=E_\alpha} * \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx$$

$$+ \frac{1}{\rho_\alpha^2(E_\alpha)}\frac{\partial \rho_\alpha(E_\alpha)}{\partial \alpha}\int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx. \tag{6}$$

Here, one has to be careful in keeping all terms which depend upon α. For example, $\partial \rho_\alpha(E_\alpha)/\partial \alpha$ can be written as,

$$\frac{\partial \rho_\alpha(E_\alpha)}{\partial \alpha} = \frac{\partial}{\partial \alpha}\left\{\rho_\alpha(E_0) + \frac{\partial \rho_\alpha(x)}{\partial x}\Big|_{x=E_0}(E_\alpha - E_0)\right.$$

$$\left. + \frac{(E_\alpha - E_0)^2}{2!}\frac{\partial^2 \rho_\alpha(x)}{(\partial x)^2}\Big|_{x=E_0} + \cdots\right. \tag{7}$$

Substituting (7) into (6) and then taking the limit as $\alpha \to 0$, we obtain the inverse energy-weighted sum $S_2(E)$ as

$$S_2(E) = \frac{1}{2}\frac{\partial^2 E_\alpha}{(\partial \alpha)^2}\Big|_{\alpha=0}$$

$$= -\frac{1}{2\rho(E_0)}\left[\left(\frac{\partial^2}{(\partial \alpha)^2}F_\alpha(E_0)\right)_{\alpha=0} - \frac{\partial}{\partial E_0}\left\{\frac{1}{\rho(E_0)}\left(\frac{\partial F_\alpha(E_0)}{\partial \alpha}\Big|_{\alpha=0}\right)^2\right\}\right]. \tag{8}$$

2. Inverse energy-weighted sum-rules

Sum-rules in SDM are encountered in two different ways. First, if an excitation operator O acts on an eigenstate of a hamiltonian H, with energy E; then the expectation value of O^+O as a function of E, that is $O^+O(E)$ corresponds to the non-energy weighted sum of strength with respect to the intermediate eigenstates E' and with starting state energy E. Thus $O^+O(E)$, the non-energy weighted sum is the total strength of the excitation operator, averaged with respect to all starting states with energy E. Similarly, the linear energy-weighted sum $O^+HO(E)$, the expectation value of O^+HO as a function of E, relates to the centroid of the strength distribution. The $O^+H^2O(E)$ (quadratically energy-weighted sum) has information about the spread of the strength with respect to the energy of the intermediate states. These sums have been used to study single nucleon transfer processes (non-energy-weighted sum $\Rightarrow$ occupancy, linear energy-weighted sum $\Rightarrow$ effective single particle energy of orbit from or to which a particle is transferred). Secondly, the sum-rules arise when a hamiltonian is perturbed by a small operator αK, here α being only a multiplicative parameter. In this case, the expectation value of K as a function of energy is related to the width of the eigenfunction of H at E, when expressed in terms of the eigenfunctions of K; such calculations have earlier been reported by Potbhare (1977). So far, not much attention has been paid to the inverse energy-weighted sums, partly due to the notion that one has to deal with Green's function and complete solutions of the problem in order to deal with inverse-energy-weighted sums. Recently, however, Halemane (1981) applied the SDM to Rayleigh-Schrodinger perturbation theory and obained expressions for varieties of inverse energy-weighted sums. We now give a simpler procedure for deriving these sums.

The eigenvalue density of H in a finite dimensional space is always discrete. However, as the spectral distribution methods deal only with few lower order moments, a density of states $\rho(E)$ characterized by these is assumed continuous. Ratcliff (1971) gave a procedure to generate a smoothened spectrum from such assumed continuous density function, the spectrum so obtained is the averaged spectrum, free from level-to-level fluctuations. The averaged position of E_n, the nth level starting from the ground-state is given by,

$$n - 1/2 = d \int_{-\infty}^{E_n} \rho(x)\,\mathrm{d}x = d * F(E_n) = p_n, \tag{1}$$

d here is the dimensionality of the space and F is the distribution function. If a small operator αK is added to H, this perturbation will shift the eigenvalues. The new set of eigenvalues $E_{n,\alpha}$ can be obtained similarly using $\rho_\alpha(x)$, characterized by the moments of $(H + \alpha K)$,

$$d * \int_{-\infty}^{E_{n,0}} \rho_{\alpha=0}(x)\mathrm{d}x = d * \int_{-\infty}^{E_{n,\alpha}} \rho_\alpha(x)\mathrm{d}x = n - 1/2 = p_n. \tag{1a}$$

The procedure adopted here is statistical in nature and hence is applicable when the spectrum is rigid (that is, it does not involve crossing of levels or large level motion due to collectivity). Series expansion of $E_{n,\alpha}$ in powers of α is given by the

Pramāṇa – J. Phys., Vol. 32, No. 4, April 1989, pp. 507–513. © Printed in India.

Inverse energy weighted sum-rules

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Abstract. A new derivation of the inverse energy-weighted sum-rules is given by applying the spectral distribution methods to the Rayleigh-Schrodinger perturbation theory. The scalar space result is then extended to the configurations. This is applied to obtain corrections to the ground-state energy estimates when the effective interaction is approximated by a model Hamiltonian obtained by taking linear combinations of various parts of the pairing and the Q.Q operators

Keywords. Spectral-distribution-methods; inverse-energy-weighted sum-rules; ground-state-energy; effective-interactions.

PACS Nos 21·10; 21·60

1. Introduction

Spectral distribution methods (Kota and Kar 1987; French and Kota 1982) (SDM), which make use of moments and averages of various operators in a given spectroscopic space, have been well established and used quite extensively to study average properties like level densities, spin cut-off factors, averaged-spectra (fluctuation part removed), averaged-expectation values, averaged-strength distributions etc. There are some reservations against applying these methods in the ground-state domain, as this region is too far removed from the centre of the distribution (many times more than three widths away from the centroid). Nevertheless, it turns out that these methods have been quite successful in calculating ground-state energies (Chang *et al* 1971) and ground-state occupancies (Potbhare and Pandya 1976), much better than other microscopic theories. A detailed study using Wildenthal's universal $s-d$ shell interaction, performed recently by Sarkar *et al* (1986), confirms the claim of applicability of SDM in the ground-state domain. Here, we deal with correction to the ground-state energy when the effective hamiltonian is approximated by various model hamiltonians based on linear combinations of pairing and Q.Q operators (Kota *et al* 1980). Such a correction involves taking care of the difference between H_{eff} and H_{model}, perturbatively via inverse energy-weighted sums. In the next section, we derive the inverse energy-weighted sum-rule in the scalar space. This was first derived by Halemane (1981); we provide here an alternative derivation. In the third section, this result is extended to configuration space and then its application for ground-state energy correction is given in the last section.

single-particle energies have been evaluated and compared with experimental values. Similar analysis of nuclei in fp-shell is in progress.

We would like to thank the University Grants Commission, New Delhi, India for the financial support.

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for universal sd-interaction. For $s_{1/2}$ orbit, the change is from −6.2 MeV to −18.1 MeV, while for $d_{3/2}$ orbit it varies from −2.4 MeV to −14.6 MeV. So the energy span between $d_{5/2}$ to $d_{3/2}$ orbits for the universal sd-interaction has increased from 6.1 MeV to 7.2 MeV. For the PW interaction, the corresponding increase in energy span between $d_{5/2}$ and $d_{3/2}$ orbits is more i.e., from 6.1 MeV in ^{20}Ne to 12.1 MeV in ^{36}Ar. Again the splitting increases much more rapidly for the PW interaction as compared to the universal sd-interaction. The proton and neutron energies are symmetric as the effective interactions are isospin conserving. The Coulomb interaction, however, breaks this symmetry and hence the calculated values have to be corrected in order to be compared with the experimental results. Ishkhanov *et al.* have evaluated values of these for proton orbits using experimental data. The calculated values given in table 4 have been corrected for Coulomb energy using the standard formula for Coulomb energy. The calculated values agree quite well with the experimental values, with minor deviations in few cases. This is remarkable considering the fact that the errors in experimental evaluation are compounded. The universal sd-interaction at this stage seems to be much superior than the PW interaction. This can be easily seen by comparing $d_{5/2}$ and $d_{3/2}$ splittings produced by the two interactions with the experimental values. The PW interaction gives too large values for the separation between $E_{d_{5/2}}$ and $E_{d_{3/2}}$. Experimentally, the addition of a neutron pair to isotopes of magnesium, silicon and sulphur weakens the splitting of 1d level [8]). Both the interactions fail to reproduce the trend. This can be traced to the nature of the $\nu = 1$ part of the interaction (the induced single-particle energies [14]) and is clearly an interaction-dependent result. For both the interactions splitting between induced single particle energies between $d_{5/2}$ and $d_{3/2}$ orbits (for protons as well as for neutrons) can be seen to be increasing with proton and neutron numbers. In the universal sd-interaction this increase is damped due to the factor of $(18/A)^{0.3}$ in the two-body matrix elements. However, one can conclusively see that the universal sd-interaction compares much better with the experimental data than the PW interaction. Thus the method provides a nice way of selecting a proper effective interaction.

5. Summary

We have evaluated the proton and neutron orbit occupancies using two standard sd-shell interactions and compared these with the experimentally observed values. Both these interactions do quite well. The particle transfer centroids and widths also have been calculated and their positions with respect to ground states of targets and final nuclei have been displayed. The widths are smaller than the average configuration width, indicating that the single-particle picture is quite good. Also it has been shown that the strength function when written as a sum of bivariate gaussians is a good approximation to the extent that sum-rule quantities seem to agree with the polynomial expansion results. Finally, the occupancy-dependent

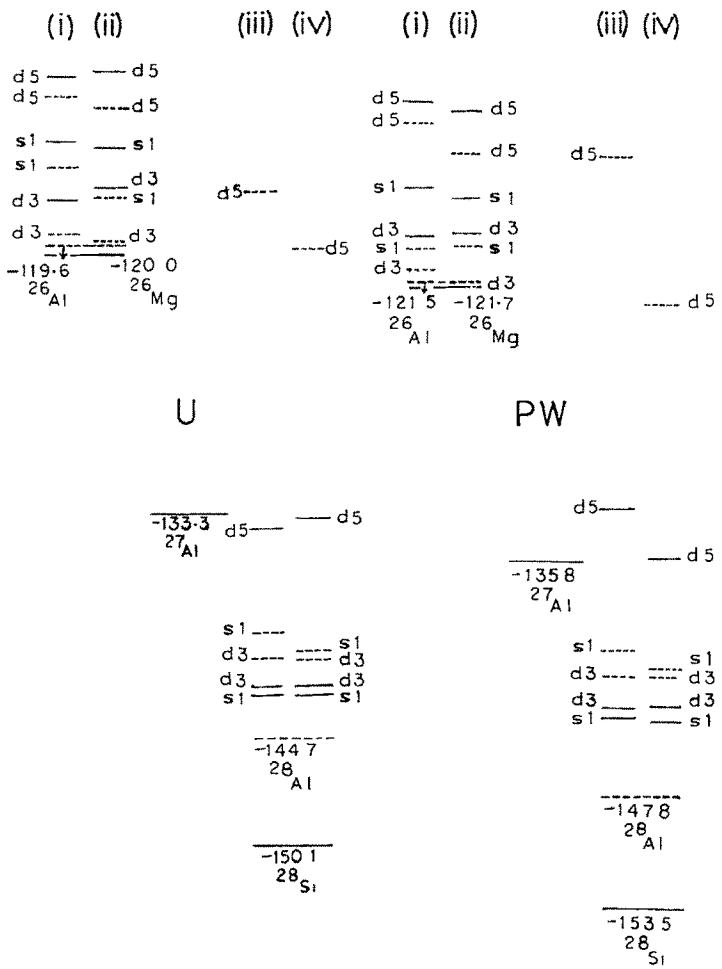

Fig. 2—continued

depend upon the excitation energy also, since the occupancies vary with energy. Their values in the ground-state region of the respective nuclei for proton and neutron orbits using both the interactions are presented in table 3. An analysis [13]) of this type in 2s1d and $f_{7/2}$ shell using PW interaction and cross-shell matrix elements from Kuo–Brown interaction was attempted without taking into account the ground-state occupancies properly. The energy span between $d_{5/2}$ and $d_{3/2}$ orbits seems to be slowly increasing as the shell is gradually being filled up. $E_{d_{5/2}}$ falls much faster than $E_{d_{3/2}}$. There is, however, no crossing of energy levels. Thus the $d_{5/2}$ (proton or neutron) gets progressively bound more and more as the shell is being filled. $E_{d_{5/2}}$ orbit energy falls from −8.5 MeV in ^{20}Ne to −21.8 MeV in ^{36}Ar

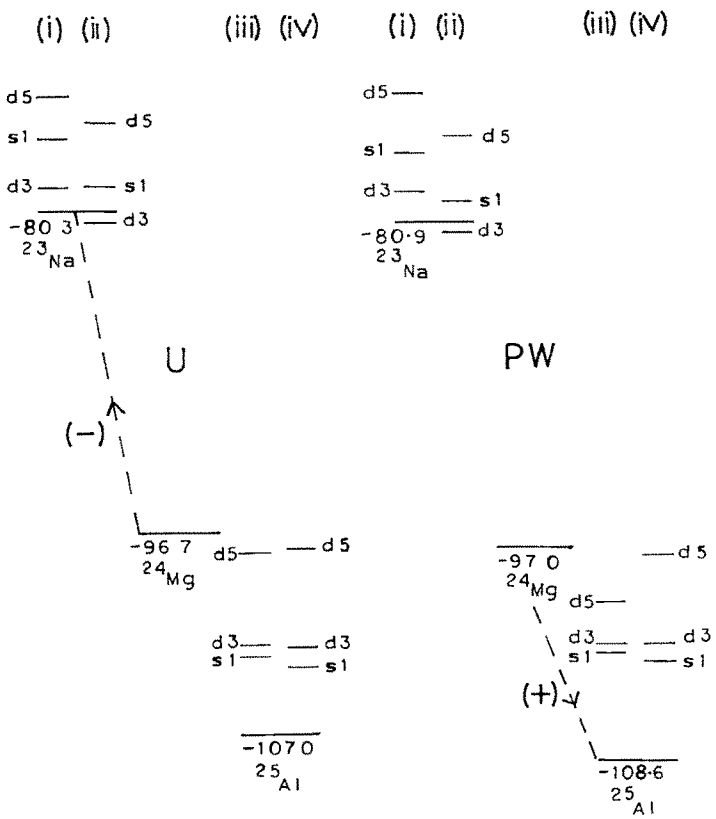

Fig 2. Locations of SNT centroids and ground-state energies of the target and final nuclei. Target nucleus in (a) is ^{24}Mg and in (b) is ^{27}Al, (i) particle removal using bivariate gaussian strength function, (ii) particle removal using polynomial expansion (iii) particle addition using bivariate gaussian strength function, (iv) particle addition using polynomial expansion. Proton transfer results are given by a solid line and the neutron transfer results by a dashed line. Coulomb correction has not been incorporated. Centroids are labelled by orbit angular momentum and $2j$ value of the orbit.

are small compared to the spread of the configuration intensity over the energy axis (average configuration width in ^{24}Mg = 8.2 MeV). This also indicates that the single-particle state is not spread over large energy domain, giving credence to the single-particle picture. The location and width together indicate the range of energy in which most of the particle transfer strength is concentrated, and hence gives an indication of the excitation energy to which an experiment must be conducted in order to exhaust most of the strength. As discussed earlier (eq. (7)), the particle addition centroids and the particle removal centroids with reference to a particular target state are related to one another through occupancies of the target state and average two-body matrix elements. The right-hand side of eq. (7) is the occupancy-dependent single-particle energy (Ej) of the target nucleus. These Ej's indirectly

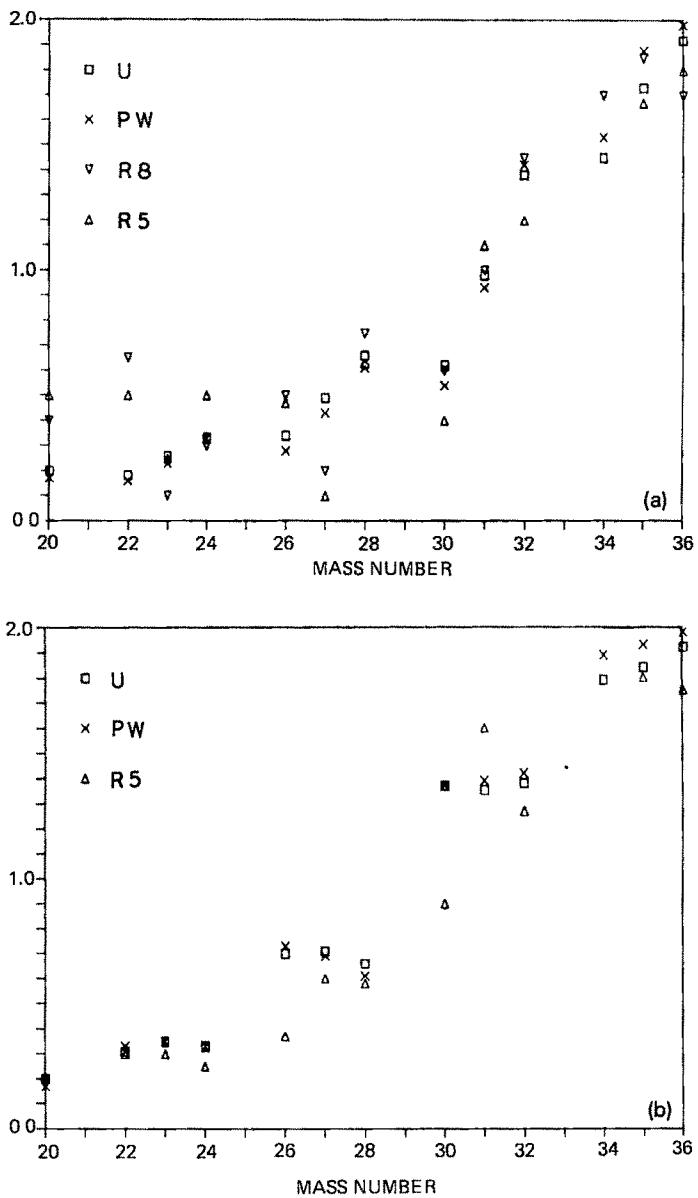

Fig. 1. Ground-state occupancies of $s_{1/2}$ orbit for various nuclei using the PW interaction and the universal sd-interaction along with experimental results. R5 and R8 refer to experimental results as given in refs. [5,8]), respectively.

TABLE 4

Coulomb corrected ($-Ej$) for proton orbits

Nucl.	$d_{5/2}$			$s_{1/2}$			$d_{3/2}$		
	U	PW	exp.	U	PW	exp.	U	PW	exp.
^{24}Mg	7.4	7.3	7.8	3.4	2.5	2.9	0.8	0.1	1.8
^{26}Mg	10.6	10.7	10.1	6.4	5.3	7.6	3.9	2.9	5.9
^{27}Al	10.5	10.7	11.5	6.0	4.9	5.1	3.7	2.5	4.5
^{28}Si	10.4	10.6	9 6	5.6	4.5	6.2	3.5	2.3	3.4
^{30}Si	13.2	13.7	12.1	8.8	7.9	8.9	6.2	4.4	6.5
^{31}P	13.0	13.5	13.3	8.7	8.0	7.5	5.9	4.0	4.2
^{32}S	12 6	13.1	12.6	8.5	8.1	8.2	5.6	3.4	3.7
^{34}S	15.4	16.2	12 5	11.3	10.9	10.0	8.1	5.1	6.6
^{35}Cl	15.1	15.9	12.4	11.2	10.9	9.2	7.9	4.4	5.7
^{36}Ar	14.8	15.9	12.8	11.1	10.5	8.9	7.6	3.8	5.9

Exp.: Experimental results from ref. [8]).

sd-interaction is 7.2 MeV while the same number for PW interaction is 13.3 MeV. This indicates large contribution of spin-orbit splitting in the PW interaction compared to the universal sd-interaction. For ^{22}Ne, ^{26}Mg, ^{32}S, ^{34}S, ^{35}Cl and ^{36}Ar, calculated values of the $d_{3/2}$ orbit occupancies match well with the experimental results.

Table 2 gives the ground-state pickup and stripping centroids and widths. Here, due to the absence of any experimental data, we restrict to some general comments and hope that this would stimulate a thorough experimental analysis in this region. Also, there are no exact shell-model calculations available for testing the accuracy of the two methods employed. Due to these reasons, we feel it unnecessary to give extensive results and hence results for only a few representative cases are given. Fig. 2, which is a pictorial representation of the data in table 2, gives the locations of the particle removal and the addition centroids and the respective ground-state energies of the target and the final nuclei. Both the interactions employed give similar results (which deviate from one another by small amounts) pointing to the gross similarity of the two interactions. Also the two methods of evaluating the centroids of strength distributions (though not giving identical results) do not differ from one another appreciably; thereby giving us licence to use the heuristic formula for the strength function which can be described now as a superposition of bivariate gaussians with constant correlation coefficient as proposed in ref. [12]) by French. This approach will be of immense use in huge spaces extending over many harmonic-oscillator orbits. It is true that sometimes the calculated values of strength centroids lie below the respective final-nucleus ground states. This is because of the inherent limitation of the finite polynomial expansion resulting due to truncation of the expectation value expression. On the other hand, one can invert the argument and say that in such cases, most of the strength would be concentrated within few states near the final-nucleus ground state. Secondly, the widths of the strength distributions

TABLE 3

Occupancy-dependent s p.e.'s ($-Ej$) at ground state

Nucl	Int.	$-Ej$ (protons)			$-Ej$ (neutrons)			g.s. energies
		$d_{5/2}$	$s_{1/2}$	$d_{3/2}$	$d_{5/2}$	$s_{1/2}$	$d_{3/2}$	
^{20}Ne	U	8.5	6 2	2.4	8.5	6.2	2 4	−39 4
	PW	8.4	5 6	2.3	8.4	5.6	2 3	−39 4
^{22}Ne	U	12.1	8.9	5 9	9.3	5.9	2 9	−61.7
	PW	11.8	7 8	5.3	9.0	5.5	2 4	−62.1
^{23}Na	U	12 4	8.8	5 9	11 0	7.4	4.5	−75.4
	PW	12.2	7.8	5 3	10 7	6.6	3 8	−76.1
^{24}Mg	U	12.7	8.7	6 1	12 7	8 7	6.1	−91.4
	PW	12.5	7 8	5 3	12.5	7 8	5.3	−92.4
^{26}Mg	U	15.8	11 6	9.1	13.2	8 8	6 4	−114.8
	PW	15.9	10 5	8.1	13.0	7.9	5.3	−116 7
^{27}Al	U	16.0	11 5	9.2	14.7	10.2	7.9	−127.7
	PW	16 2	10.4	8 0	14.8	9.1	6 7	−130 3
^{28}Si	U	16 3	11.5	9 4	16 3	11.5	9 4	−144.3
	PW	16.5	10.4	8 2	16.5	10.4	8.2	−147.6
^{30}Si	U	19.0	14 6	12.0	16.4	11.9	9.5	−163.6
	PW	19.5	13 7	10.2	16.8	10 8	7.9	−167.7
^{31}P	U	19.1	14 8	12.0	17.8	13.4	10 8	−179.4
	PW	19 6	14 1	10.1	18 3	12.6	9 0	−184 6
^{32}S	U	19 1	15.0	12 1	19.1	15 0	12.1	−190 1
	PW	19.6	14.6	9 9	19.6	14 6	9 9	−195.1
^{34}S	U	21.8	17.7	14 5	19.2	15.3	12.3	−206.5
	PW	22.6	17 3	11.5	19.8	14.9	9 3	−210.3
^{35}Cl	U	21 8	17.9	14.6	20 5	16.7	13 4	−218.1
	PW	22 6	17 6	11.1	21.2	16 5	10 1	−222.3
^{36}Ar	U	21.8	18.1	14 6	21 8	18 1	14 6	−230.3
	PW	22.9	17.5	10.8	22.9	17 5	10 8	−232.8

with the calculated results (within acceptable error limits) except in the case of light nuclei (^{20}Ne and ^{22}Ne) where the calculated values are considerably higher than the experimental results. The low occupancy of $d_{3/2}$ orbit would provide a tough test. The universal sd-interaction gives rise to slightly higher $d_{3/2}$ occupancy in upper sd-shell compared to the values given by the PW interaction. The trend is reversed in the lower sd-shell. This is the result of larger $d_{5/2}$–$d_{3/2}$ difference (spin–orbit splitting) in the external single-particle energies for the universal sd-interaction (5.60 MeV) as compared to the 5.08 MeV in the case of PW interaction. Induced single-particle energies [14]), however, reverse the situation in upper sd-shell; for example the spin–orbit splitting in $\nu = 1$ part of the interaction at ^{36}Ar for universal

TABLE 2

Centroids and widths for particle removal(−) and addition(+) for protons and neutrons

Nucl.			(1) EM1		(2) EM2		(3) SG−		(4) EP1		(5) EP2		(6) SG+	
			U	PW	U	PW	U	PW	U	PW	U	PW	U	PW
$^{20}_{10}$Ne		d5	18 2	18.0	20 5	20 7	3 4	3 3	−4 4	−4 2	−3.5	−3.0	5.3	5.3
		s1	17 7	17.3	20.5	20.0	3.4	3 3	−4.9	−4.5	−4.6	−4 2	5 3	5 3
		d3	15 6	15 5	18 7	18.7	3.4	3 3	−2.4	−2 2	−2.4	−2 2	5 2	5 4
$^{23}_{11}$Na	(p)	d5	20.8	20 9	21.9	22.7	4.7	4 8	−5.7	−5.3	−4.9	−3.9	5 7	5 9
		s1	18 5	18.4	20 3	20 1	4 8	4.7	−7 3	−6.5	−7.1	−6.3	5 8	5.9
		d3	17 0	17.1	15 1	18 6	4 8	4.7	−5 7	−4.9	−5.7	−4.9	5.7	6.0
	(n)	d5	18.7	18.7	21.0	21 8	5 1	5.3	0.1	0.4	3.6	4 9	5 9	6 2
		s1	15.5	15.4	19.0	19.1	5.2	5 2	−5.7	−4.8	−4.9	−4 0	5 9	6 1
		d3	13.6	13.6	16 6	17.0	5.2	5 2	−4.3	−3.5	−4 2	−3 4	5 7	6 1
$^{24}_{12}$Mg		d5	20.8	21 0	22 3	23 3	5.1	5 3	−1.0	−0.4	1 2	2 8	5 8	6 1
		s1	17 6	17.7	20.1	20 2	5 2	5.2	−6.9	−5.9	−6.4	−5.4	5 9	6 0
		d3	15.9	16.1	17 6	18.2	5.2	5.2	−5.9	−4.9	−5.8	−4.9	5.7	6.1
$^{27}_{13}$Al	(p)	d5	22 5	23.0	22.3	23.6	4.9	5.2	−0.2	1.1	−0 8	2 6	5 4	5.7
		s1	18.6	18.5	18 9	19.1	5.1	5.1	−9 3	−8.3	−9.2	−8 1	5 3	5 5
		d3	16.6	16 7	15 9	16 6	5 1	5.0	−8.8	−7.4	−8.8	−7.4	5 1	5.5
	(n)	d5	20 6	20.8	21.3	22.5	5.4	5.8	13.6	13.1	16 6	20 8	5 6	6 0
		s1	16.1	16.1	17 6	17 9	5 6	5 6	−6.9	−5.5	−6 1	−4 5	5 6	5 8
		d3	13 8	14 0	14 2	14 9	5.6	5.6	−7 4	−5.9	−7.3	−5 9	5 3	5 8
$^{28}_{14}$Si		d5	22.3	22.7	22 1	23 5	5 1	5.4	15 5	16 5	14 7	20.9	5.3	5.7
		s1	17 6	17.7	18.2	18.5	5.3	5 3	−8 4	−7.2	−8.2	−6.8	5 3	5 5
		d3	15 3	15.7	14.7	15 5	5 3	5 2	−8.9	−7.4	−9.0	−7.5	5 0	5 4
$^{31}_{15}$P	(p)	d5	24 1	24.8	22.3	24.1	4.2	4 6	50 7	61 4	25 0	49 3	4.1	4.6
		s1	18.8	18.5	17 5	17.6	4.3	4.5	−10.9	−10.3	−12.2	−11 1	4 1	4.1
		d3	16.3	15 7	13 4	13.5	4.3	4.3	−11.5	−9.4	−11 9	−9 7	3.8	4.1
	(n)	d5	21 9	22.4	20.9	22.7	4.7	5 2	72.0	87 1	51 0	95.3	4 4	4.9
		s1	16 6	16.5	16.4	16 7	5 0	5 1	−6.5	−3.7	−7 1	−3 4	4 4	4 7
		d3	14 0	13.7	12 3	12 2	4 9	4 9	−10.0	−7.8	−10 4	−8 1	4.2	4 5
$^{32}_{16}$S		d5	23 1	23 7	21 2	23 0	4 1	4.7	86 5	108 1	36 7	88.9	3.8	4.3
		s1	17 8	17 6	16.5	16.8	4 4	4 5	−8.9	−7 3	−11.8	−9.1	3.8	4.2
		d3	15.1	14.2	12.3	11 9	4 2	4 2	−11 3	−8.8	−12.0	−9 4	3.6	3 8

better than the PW interaction. Fig. 1b is a similar plot for $s_{1/2}$ neutron occupancies, experimental values in this case have been taken from ref. [5]). It seems that the calculated neutron occupancies agree much better with the experimental values again within the limits of error values mentioned. Here also, the universal sd-interaction is marginally better than the PW interaction. A comparison of calculated $l=2$ occupancy with experimental results is redundant, once the $s_{1/2}$ occupancy results have been analysed. However, we can still talk about decomposition of the strength into $d_{5/2}$ and $d_{3/2}$ components, but not with the same confidence as in the case of $s_{1/2}$ orbit, due to ambiguity in experimental identification of the strength bifurcation into these orbits. High occupancy values of $d_{5/2}$ orbit seem to agree well

TABLE 1—continued

Nucl.	Int.	Proton occupancy			Neutron occupancy		
		$d_{5/2}$	$s_{1/2}$	$d_{3/2}$	$d_{5/2}$	$s_{1/2}$	$d_{3/2}$
^{35}Cl	U	5 98	1 73	1.29	5 97	1.84	2 19
	PW	6.00	1.88	1.13	5.99	1 93	2.07
	R8	6 00	1 85	1 15			
	R5	6 00	1 67	1.33	6.00	1 80	2 20
^{36}Ar	U	6.00	1.92	2.08	6 00	1.92	2.08
	PW	6.00	1 98	2 02	6.00	1.98	2.02
	R8	5.80	1 70	2.30			
	R5	5 90	1 80	2 30	5 75	1.75	2.45

R5 Ref. [5]), R8 Ref. [8]).

for completeness of information. Table 3 gives the values of occupancy-dependent single-particle energy as defined in eq. (7). The first row for each nucleus corresponds to values obtained using the universal sd-interaction, while the PW interaction results are given in the second row. Table 4 gives the Coulomb corrected values of occupancy dependent single-particle energies for protons and the experimental values taken from a recent paper by Ishkhanov *et al.* [8]).

4. Discussion

Experimental values of ground-state proton occupancies have been reported recently by Ishkhanov *et al.* [8]). Similar compilation of experimental data has also been reported earlier [5]) for proton-neutron occupancies. It should be kept in mind that experimental spectroscopic factors are uncertain by about 20% to 30% in their relative values because of ambiguities in the optical model parameters, finite-range adjustments, nonlocality corrections etc. In addition, there is another source of ambiguity for sum-rule evaluation, the missing strength at high excitation energy. Secondly, it is not always possible to separate $l=2$ transfer strength into its $d_{5/2}$ and $d_{3/2}$ components. Fig. 1 is a partial representation of the data in table 1; we have plotted the ground-state proton and neutron occupancies for the $s_{1/2}$ orbit only. Similar plots for other orbits could be generated using table 1. Both the effective interactions used give almost similar results. For proton occupancies, the two sets of experimental compilations are at variance in several cases; this, however, is normal, providing justification for the comments on experimental uncertainty. Fig. 1a displays the variation of $s_{1/2}$-proton occupancy using the two effective interactions and the experimental values. Except for a few nuclei in the lower sd-shell, the calculated results seem to agree (within assumed experimental error of 25%) with the experimental values; the universal sd-interaction being slightly

TABLE 1

Ground-state proton and neutron occupancies

Nucl.	Int.	Proton occupancy			Neutron occupancy		
		$d_{5/2}$	$s_{1/2}$	$d_{3/2}$	$d_{5/2}$	$s_{1/2}$	$d_{3/2}$
^{20}Ne	U	1 79	0 20	0 01	1.79	0.20	0.01
	PW	1.81	0.17	0.02	1.81	0 17	0 02
	R8	1.20	0.40	0.40			
	R5	1 10	0.50	0 30	1 10	0.20	0.70
^{22}Ne	U	1 76	0 18	0.06	3 66	0.31	0.04
	PW	1.77	0.16	0.08	3.61	0.33	0.06
	R8	1.30	0 65	0 05			
	R5	1 30	0 50	0 10		0.30	
^{23}Na	U	2.64	0 26	0 10	3.56	0 35	0.09
	PW	2 65	0.23	0.12	3.52	0 35	0 13
	R8	2.90	0.10	0 00			
	R5		0.25			0.30	
^{24}Mg	U	3 57	0.33	0 10	3 57	0 33	0.10
	PW	3.52	0.33	0.15	3.52	0 33	0 15
	R8	3.20	0 30	0.50			
	R5	3 13	0 50	0 53	3.25	0 25	0.50
^{26}Mg	U	3 49	0.34	0 17	5.09	0 70	0.21
	PW	3.53	0.28	0.19	4.96	0 73	0 30
	R8	3.30	0.50	0 30			
	R5	3.28	0.47	0 25	5.10	0.37	0 57
^{27}Al	U	4.26	0 49	0.25	4.96	0.71	0.32
	PW	4.30	0.43	0.27	4.94	0 69	0.38
	R8	4 80	0 20	0 0			
	R5		0.1			0.6	
^{28}Si	U	5.04	0.66	0.29	5.04	0 66	0 29
	PW	5 05	0 61	0 34	5.05	0.61	0 34
	R8	4 50	0 75	0.75			
	R5	4 50	0.45	0.63	5.10	0 73	0 30
^{30}Si	U	5 11	0.62	0.27	5.69	1.37	0 93
	PW	5.20	0.54	0.26	5.70	1 37	0 94
	R8	4 80	0 60	0.60			
	R5	5.38	0.40	0 25	5 67	0.90	1.37
^{31}P	U	5.59	0.98	0.42	5 74	1.37	0.89
	PW	5 63	0 93	0.43	5.78	1.39	0.83
	R8	6.00	1 00	0 00			
	R5		1.10		6.00	1 60	0.50
^{32}S	U	5.79	1.38	0.83	5 79	1.38	0 83
	PW	5 82	1.42	0.76	5.82	1.42	0.76
	R8	5 75	1 45	0.80			
	R5	5.90	1.20	0 90	5.83	1.27	0 90
^{34}S	U	5.93	1.45	0.62	5.93	1.79	2.27
	PW	5.97	1.53	0 50	5.96	1 89	2.15
	R8	5.80	1.70	0.50			
	R5						

have been calculated again using the strength function in pn configuration space, in the form of a sum of bivariate gaussians as in the case of particle removal widths.

3. Results

As mentioned earlier, out of the many effective interactions designed for use in 2s1d shell, only the following two have been shown to agree [5,6]), within reasonable error limits, with the experimental results of $s_{1/2}$ orbit occupancy. The PW interaction [3]) is derived from Kuo–Brown interaction by adjusting certain two-body matrix elements to obtain a good fit to the levels of $A = 18$ to 22 nuclei and to give better predictions for excited rotational bands in these nuclei. The universal sd-interaction [4]) has been similarly obtained but in addition has the two-body matrix elements with a mild dependence on total number of nucleons in the nucleus. The calculation of necessary averages in case of the universal sd-interaction is a little more troublesome, as one has to start from square one for each new nucleus because of the number dependence of two-body matrix elements. The PW interaction employs the ^{17}O levels as the external single-particle energy levels (−4.15, −3.28 and 0.93 MeV for $d_{5/2}, s_{1/2}$ and $d_{3/2}$ orbits, respectively) and the corresponding single-particle energies for the universal sd-interaction are −3.95, −3.16 and 1.65 MeV, respectively. Earlier, calculations for occupancies in 2s1d shell using these two interactions have been performed in $\boldsymbol{m}$, T (configuration–isospin) formalism; while in this note, the space is decomposed according to proton–neutron configurations, so that one can talk directly about proton or neutron transfers.

Table 1 gives the orbit occupancies for various nuclei in the 2s1d shell along with the experimental values from refs. [5,8]). Table 2 gives the particle transfer centroids and widths for several nuclei. The results for other nuclei not listed in the table are available on request. For each nucleus in table 2, columns 1 to 6, respectively, give the following quantities: (i) proton/neutron removal centroid calculated using polynomial expansion upto the linear term in configuration space (ii) proton/neutron removal centroid with the assumption of bivariate gaussian strength function; (iii) proton/neutron removal width; (iv) proton/neutron addition centroid using polynomial expansion method; (v) proton/neutron addition centroid using bivariate gaussian strength function and (vi) proton/neutron addition width. Sub-columns for two interactions are labelled appropriately. For nuclei with equal number of protons and neutrons, both the proton and neutron transfer results are identical due to the proton–neutron symmetric nature of the effective interactions, hence only one set of results are given for these nulei. For other nuclei, proton transfer and neutron transfer results are given separately. All the results are in MeV and are with reference to the ground-state energy of the target nucleus. The ground-state energies are calculated using the well-known Ratcliff procedure [11]) with excited state correction [1]) whenever the identification of all excited states upto a certain energy is complete. These calculated ground-state energies for few nuclei are given in table 3

S_G in the above equation is a bivariate gaussian density function at E and E' parametrized by two configuration centroids $\varepsilon(m_p, m_n)$, $\varepsilon(m'_p, m'_n)$; two configuration widths $\sigma(m_p, m_n)$, $\sigma(m'_p, m'_n)$ and by a correlation coefficient ζ_2 in the space of m_p protons and m_n neutrons, $H^{\nu=2}$ being the irreducible rank-2 part of H, when the H is decomposed according to irreducible parts with respect to group $U(N/2)_p \oplus U(N/2)_n$, where the proton orbits and neutron orbits have been differentiated with; $\frac{1}{2}N$ being the total single-particle states for either protons or neutrons*. The primed configurations are those reached in the final nucleus as a result of excitation O from a state in unprimed configuration in the target state. Thus the density-weighted strength function is seen to be a superposition of bivariate gaussian forms, and hence can be easily used to evaluate its various moments, by integrating with respect to E'. All the necessary averages (as indicated earlier), when the excitation operator O is a particle removal operator B_s, have been calculated and used for evaluation of particle removal centroids ($\mathscr{E}_s^-(E)$) and particle removal widths $\sigma_s^-(E)$) as a function of energy in the target nucleus. Thus we have calculated $\mathscr{E}_s^-(E)$ in two different ways (i) by using the standard configuration linear expression for linearly energy-weighted sum rule and (ii) by exploiting the bivariate normal form of the density-weighted strength functions. The width estimate, however, is based only on the bivariate density form. In order to calculate the particle addition centroids $\mathscr{E}_s^+(E)$, we have used the well known identity [7])

$$\frac{(\mathscr{E}_s^+(E)-E)(2j_s+1-n_s(E))}{(2j_s+1)} - \frac{(\mathscr{E}_s^-(E)-E)n_s(E)}{(2j_s+1)}$$

$$= \varepsilon_s + \sum_t n_t(E)\{1-\delta_{st}/(2j_t+1)\}\bar{W}_{st}, \tag{7}$$

where s and t refer to spherical orbits for protons and neutrons, j_s is the angular momentum for spherical orbit labelled by s, ε_s is the external single-particle energy of orbit s and $\bar{W}_{st}$ is the average two-body matrix element between particles in spherical orbits s and t. The right-hand side of the equation is the occupancy-dependent single-particle energy for orbit s. The particle addition widths $\sigma_s^+(E)$

* Incidentally, the $\nu=1$ part of the interaction is given by $H^{\nu=1} = \sum_i \mathscr{E}_i(m_p, m_n)n_i$ with the summation over all proton and neutron orbits, n_i is the number operator for ith orbit and $\mathscr{E}_i(m_p, m_n)$ being the number-dependent traceless single-particle energy containing the contributions from external s.p.e. as well as from the two-body matrix elements [14]). For proton orbits,

$$\mathscr{E}_i(m_p, m_n) = \varepsilon_i - \bar{\varepsilon} + \left\{ \frac{m_p - 1}{\frac{1}{2}N - 2}\lambda_i^{pp} + \frac{m_n}{\frac{1}{2}N}\lambda_i^{pn} \right\}$$

where ε_i = external s.p.e. of orbit i, $\bar{\varepsilon}$ = average of external s.p.e.'s and the expression in curly brackets being the induced s.p.e. The expression for neutron orbits can be written down similarly keeping in mind $\lambda_i^{pp} = \lambda_i^{nn}$ due to the pn symmetric nature of effective interactions. The λ's can be expressed in terms of two-body matrix elements of the effective interactions; for the PW interaction λ^{pp} are (−1.77, 0.76, 2.27) MeV and λ^{pn} are (−2.63, 2.10, 2.90) MeV for $d_{5/2}$, $s_{1/2}$ and $d_{3/2}$ orbits, respectively. Similarly for the universal sd-interaction $\lambda^{pp} = (-0.74, 1.78, 0.22) \times (18/A)^{0.3}$ MeV and $\lambda^{pn} = (-0.85, 1.55, 0.49) \times (18/A)^{0.3}$ MeV for the corresponding orbits.

protons; m_n being defined similarly with $m_n = \sum_\alpha m_{\alpha,n}$ and $m = m_p + m_n$. With this decomposition, we get for fixed (m_p, m_n):

$$\rho^{m_p,m_n}(E) = \frac{1}{D(m_p, m_n)} \sum_{m_p,m_n} \rho^{m_p,m_n}(E) D(m_p, m_n),$$

$$\{O\}^{m_p,m_n}(E) = \sum_{m_p,m_n} (O)^{m_p,m_n}(E) \left[\frac{\rho^{m_p,m_n}(E) D(m_p, m_n)}{\rho^{m_p,m_n}(E) D(m_p, m_n)}\right], \tag{4}$$

the expression in square brackets in the last equation is the fractional intensity of configuration (m_p, m_n) at E. Following are the necessary averages (in each configuration) for the occupancy and particle removal centroid calculation in configuration linear approximation; $\langle n_s\rangle^{m_p,m_n}$, $\langle H\rangle^{m_p,m_n}$, $\langle H^2\rangle^{m_p,m_n}$, $\langle A_s H B_s\rangle^{m_p,m_n}$, $\langle A_s H B_s H\rangle^{m_p,m_n}$, $\langle n_s H\rangle^{m_p,m_n}$ and $\langle H n_s H\rangle^{m_p,m_n}$. Computer programmes for evaluation of these, when H is a (1+2)-body operator have been developed in spherical orbit formalism, s then represents a spherical orbit either for protons or for neutrons with angular momentum j_s.

The width $(\sigma_s^-(E))$ calculation for SNT strength in configuration linear approximation requires evaluation of $\langle A_s H^2 B_s H\rangle^{m_p,m_n}$ (average of an operator involving third power of (1+2)-body H). The evaluation of this average involving H^3 is too much time consuming (due to two reasons: (i) the complexity and the number of operations increase very rapidly with increase in power of H, particularly if the number of single-particle spherical orbits is large and (ii) the number of configurations in the spaces of interest is also large). In addition, no experimental data is so far available for its comparison. Hence, at this stage, it is enough to engender its estimate using a simple approximation indicated by Kota and Kar [1]). Here the density weighted strength function

$$S(E, E') = d(m')\rho^{m'}(E')|\langle m', E'|O|m, E\rangle|^2 d(m)\rho^m(E)/\langle\langle O^+O\rangle\rangle^m$$

for an excitation operator O can be seen to be a bivariate density function which, under CLT, acquires a bivariate gaussian form [1,12]). Under partitioning of space, for better results near the ground state, it can be shown that in the space of (m_p, m_n)

$$|\langle E'|O|E\rangle|^2 = \sum_{\substack{m_p', m_n' \\ m_p, m_n}} \frac{I_{m_p,m_n}(E) I_{m_p',m_n'}(E')}{I_{m_p,m_n}(E) I_{m_p',m_n'}(E')} |\langle m_p', m_n'|O|m_p, m_n\rangle|^2$$
$$\times \frac{S_G(E, E', \varepsilon(m_p, m_n), \varepsilon(m_p', m_n'), \sigma(m_p, m_n), \sigma(m_p', m_n'), \zeta_2)}{\rho^{m_p',m_n'}(E')\rho^{m_p,m_n}(E)} \tag{5}$$

with $I(E) =$ Dimensionality $\times \rho(E)$,

$$|\langle m_p', m_n'|O|m_p, m_n\rangle|^2 = [D(m_p, m_n) D(m_p', m_n')]^{-1}$$
$$\sum_{\substack{\alpha\in(m_p, m_n) \\ \beta\in(m_p', m_n')}} |\langle m_p', m_n', \beta|O|m_p, m_n, \alpha\rangle|^2$$

$$\zeta_2 = \langle O^+ H^{\nu=2} O H^{\nu=2}\rangle^{m_p,m_n} / \{\langle O^+O\rangle^{m_p,m_n} \langle H^{\nu=2} H^{\nu=2}\rangle^{m_p,m_n}\}. \tag{6}$$

energy-weighted strength function with respect to the final-state energy E',

$$M_s^{\mathrm{p}}(E) = \frac{1}{D(m-1)} \sum_{E'} \langle E|A_s|E'\rangle (E')^{\mathrm{p}} \langle E'|B_s|E\rangle$$

$$= \int R_s(E, E')(E')^{\mathrm{p}} \rho^{m-1}(E')\, \mathrm{d}E'$$

$$= \langle E|A_s H^{\mathrm{p}} B_s|E\rangle = \{A_s H^{\mathrm{p}} B_s\}^m(E) \qquad (2)$$

where $\rho^m(E)$ is the normalized state density at E in m-particle space, $D(m)$ being the dimensionality (total number of states) in m-particle space and $\{O\}^m(E)$ is local expectation value of the operator O at E in m-particle space. It is known [9]) that the local expectation value can be expressed in the form of a series involving orthogonal polynomials in E defined with respect to the weight function $\rho^m(E)$. However, the action of the central limit theorem (CLT) in many-particle spaces (an important fact used in SDM and backed by several shell-model calculations and by extensive theory [10]) allows us to express the expectation values as a linear polynomial, with higher order terms providing corrections to the linear theory;

$$M_s^{\mathrm{p}}(E) = \langle A_s H^{\mathrm{p}} B_s\rangle^m + \langle A_s H^{\mathrm{p}} B_s \hat{H}\rangle^m \frac{(E-\varepsilon(m))}{\sigma^2(m)} + \text{higher order terms}. \qquad (3)$$

Here $\langle O\rangle^m$ is the averaged expectation value of O, averaged over all the states in m-particle space, $\varepsilon(m)$ and $\sigma(m)$ are the centroid and the width of normalized state density $\rho^m(E)$ and $\hat{H} = H - \langle H\rangle^m$. The total strength of particle removal starting from the target state at E is given by $M_s^0(E) = \{A_s B_s\}^m(E) = \{n_s\}^m(E)$ and it provides us the occupancy at energy E of a single-particle state s in the m-particle space. The centroid energy in the $m-1$ particle space of the corresponding strength is $\varepsilon_s^-(E) = M_s^1(E)/M_s^0(E)$ and the energy region (again in $m-1$ particle space) over which this strength is spread is given by

$$\sigma_s^-(E) = [M_s^2(E)/M_s^0(E) - (\varepsilon_s^-(E))^2]^{1/2}.$$

One can immediately write down the expressions for particle addition, similarly.

Due to large dimensionality of the spectroscopic spaces of interest, the ground state, which is the target state in all SNT reactions, lies too far below the centroid $\varepsilon(m)$, (in terms of $\sigma(m)$) to expect the linear expression of expectation values resulting from the CLT, to work well in the ground-state region. In order to rectify this situation, one can make use of higher order terms; but a more effective and satisfying procedure is to decompose the space of m-particles into configurations defined by distribution of particles in various spherical orbits. Following this standard procedure, we have decomposed the m-particle space into proton configurations $\boldsymbol{m}_{\mathrm{p}}$ and neutron configurations $\boldsymbol{m}_{\mathrm{n}}$, where $\boldsymbol{m}_{\mathrm{p}} = [m_{1,\mathrm{p}}, m_{2,\mathrm{p}}, \ldots]$ with $m_{\alpha,\mathrm{p}}$ indicating the number of protons in a spherical orbit α and $m_{\mathrm{p}} = \sum_\alpha m_{\alpha,\mathrm{p}} =$ total number of

provide information about the excitation energy in the final nucleus upto which the experiment must be conducted so as to exhaust most of the SNT strength.

The SDM are best suited for such calculations as these do not require the explicit construction of the exact target state (given by the conventional shell-model diagonalization procedure). In the second section, we review necessary theory for expectation values related to energy-weighted SNT sum-rules. In sect. 3, we present the results of calculations in 2s1d shell using two effective interactions; (i) the Preedom–Wildenthal interaction [3]) (PW) and (ii) the universal sd interaction [4]) (U). Both these effective interactions have been shown to agree well with the experimental $s_{1/2}$ occupancy data [5,6]). There are many other effective interactions in 2s1d shell. However, it has been conclusively shown [5,6]) that except for the two interactions (U and PW), other effective interactions fail to reproduce the ground-state occupancies and hence we have selected only these two effective interactions for further work. As we shall see below, both the interactions produce similar occupancy results but differ in their predictions of occupancy dependent single-particle energies [7]) (defined ahead). Also both are quite different in their nature; the PW interaction is independent of particle number while the universal sd interaction has particle dependence built into it. The calculated values of SNT centroids and widths are presented along with the respective occupancies. The occupancy dependent single-particle energies, calculated using the occupancies and the average two-body matrix elements, have been compared with the recent experimental results [8]).

2. Theory

Consider a single-particle transfer to and from a single-particle state labelled by s, with an m-particle target state at energy E; the final state reached in $m \pm 1$ particle space being at energy E'. The excitation operator for particle removal $(-)$ is the destruction operator B_s and corresponding operator for the particle addition being $A_s = B_s^\dagger$. In the following, we shall deal only with the particle removal, keeping in mind that the particle addition can be treated similarly. The strength function $R_s^-(E, E')$ for particle removal is given by

$$R_s^-(E, E') = |\langle m-1, E'|B_s|m, E\rangle|^2 , \tag{1}$$

where $|m, E\rangle$ and $|m-1, E'\rangle$ are respectively the target state and the final state reached as a result of excitation by the operator B_s; both states being the eigenstates of $(1+2)$-body hamiltonian H in m and $m-1$ particle spaces respectively. We shall henceforth drop the indices m and $m-1$ whenever that does not cause any confusion, similarly superfix$(-)$ indicating particle removal has also been dropped. In principle, the entire information about particle removal is contained in $R_s(E, E')$. As we are primarily interested here in the sum-rules (obtained by appropriately summing over all the final states) we define moments of the strength function by integrating the

Nuclear Physics A530 (1991) 171–186
North-Holland

SINGLE-NUCLEON TRANSFER SUM-RULES IN THE 2s1d SHELL

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Received 21 September 1990
(Revised 23 January 1991)

Abstract: Single-particle aspects of various nuclei in the 2s1d shell have been examined using the spectral distributions methods for two well-known effective interactions. Centroids and widths of single-nucleon transfer strength function have been calculated along with the proton–neutron occupancies. Results of our calculations have been compared with the available experimental data.

1. Introduction

Single-particle orbits and single-particle energies are the main concepts in any model based on the independent-particle approximation. Particularly, the nuclear shell model with its spherically symmetric potential, gives rise to single-particle orbitals and the corresponding single-particle energies. The self-consistent Hartree-Fock theory is also based on the existence of single-particle orbitals. In atomic shell models, the major part of the interaction corresponds to the Coulomb attraction of electrons by the central nucleus, leaving a small part (residual interaction), which can be treated perturbatively. However, in the nuclear shell model, due to absence of the domineering center and due to strong nature of the two-body interaction, the residual interaction cannot be treated perturbatively. This results into large configuration mixing for the description of nuclear states, leading to smearing out of the underlying single-particle picture and thereby spreading a single-particle state over a wide energy interval. In spite of large configuration mixing, the single-particle aspects of many-particle wave functions help us in understanding the structure and dynamics of nuclei. Many of the measured properties of nuclear states are expectation values of one-body operators in the ground state. For example, the orbit occupancies (which are measured via single-nucleon transfer (SNT) reactions) are the expectation values of number operators. These have been studied extensively using the spectral distribution methods (SDM) [1,2]) introduced and developed by French and his co-workers. In this note, we go beyond the occupancies and calculate further single-particle aspects, namely the centroids and the widths of SNT reaction strength functions. These numbers are of vital interest to an experimentalist, as they