Particle-hole symmetry, F-spin, and r-process parameters

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We exploit approximate symmetry under particle-hole conjugation and the systematics associated with a classification scheme (inspired by the neutron-proton interacting boson model) to obtain estimates of binding energies and low-lying excitation energies for even-even r-process nuclei drawn from the major proton and neutron shells, $50 < Z < 82$ and $82 < N < 126$. We anticipate that our simple formalism for binding energies, depending on only six parameters, has an accuracy of ~ 0.8 MeV. We argue that the particular dual particle-hole conjugation symmetry required to relate excitation energies in neutron-rich nuclei to the known excitation energies of the corresponding conjugated nuclei holds to within 10% or so.

Among the various nuclear inputs into dynamical r-process calculations, the binding energies of neutron-rich nuclei are perhaps the most important (given the sensitivity of reaction rates to Q values), but it would seem that, in fact, the situation regarding level densities (required in the calculation of "astrophysical" neutron capture cross sections) remains the most unsatisfactory [1], the presently favored treatment being somewhat too ad hoc. Developments in fluctuation-free spectroscopic methods in the last decade [2] make feasible (and relatively straightforward) the calculation of level densities outside of the ground-state regime starting directly from a shell-model Hamiltonian. In this paper, we argue that an approximate symmetry under a dual particle-hole conjugation inspired, in part, by the neutron-proton interacting boson model (or IBM-2) [3], can be exploited to estimate excitation energies in the low-lying spectra of even-even neutron-rich nuclei. We also consider the systematics for binding energies that emerge within an IBM-2 F-spin [4] classification scheme. We take advantage of particle-hole symmetry within this scheme to deduce an extremely simple, yet reasonably accurate, expression for the binding energies of neutron-rich nuclei.

For reasons that will become apparent below, we study nuclei drawn from the major proton shell $50 < Z < 82$ and the major neutron shell $82 < N < 126$. The F-spin classification scheme on which our treatment is based is depicted in Fig. 1 (which also indicates the character of the data available to us). F spin was introduced [4] to facilitate the discussion of proton-neutron symmetry in the IBM-2: it is formally similar to the isospin, corresponding to the SU(2) symmetry group with generators (if we restrict ourselves to just s and d bosons)

$$\begin{aligned} \hat{F}_+ &= s_\pi^\dagger s_\nu + d_\pi^\dagger \cdot \tilde{d}_\nu = (\hat{F}_-)^\dagger , \\ \hat{F}_z &= \tfrac{1}{2}(s_\pi^\dagger s_\pi - s_\nu^\dagger s_\nu + d_\pi^\dagger \cdot \tilde{d}_\pi - d_\nu^\dagger \cdot \tilde{d}_\nu) , \end{aligned} \tag{1}$$

where s_π (s_ν) and $\tilde{d}_\pi$ ($\tilde{d}_\nu$) denote a proton (neutron) s and d boson annihilation operator, respectively, and μ runs over the five spherical components of the rank-2 d boson operator. For our purposes, we note that an even-even nucleus with N_π (N_ν) valence proton (neutron) bo-

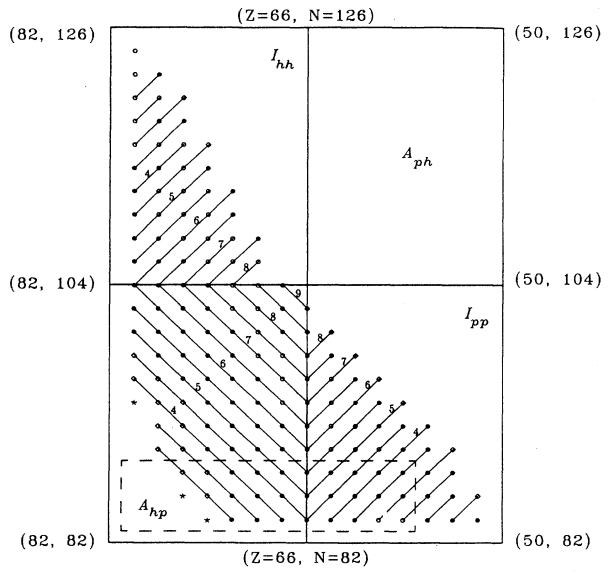

FIG. 1. F-spin classification scheme and definition of groups I_{pp}, I_{hh}, A_{hp}, and A_{ph}. The significance of the symbols employed is as follows: ○, stable nucleus; ●, unstable nucleus—binding energy and excitation spectrum data available; ◇, unstable nucleus—only binding energy available; ★, unstable nucleus (listed in Ref. [5])—no data available. The sources used in compiling our data ensemble are Refs. [6–8] and the interactive databank of the National Nuclear Data Center (NNDC), Brookhaven. The dashed box indicates the F-spin assignments that would be affected by adherence to Casten's $Z = 64$ subshell closure rule [9].

sons automatically has $F_z=(N_\pi-N_\nu)/2$, while the empirical success of the IBM-1 (in which no distinction between proton and neutron degrees of freedom is made) indicates that states in the ground-state band are predominantly of F spin $F=F_{\max}=(N_\pi+N_\nu)/2$ (corresponding to the configurations which are totally symmetric with respect to proton and neutron degrees of freedom). The observation that F spin is an approximate dynamical symmetry of the low-lying spectrum has motivated our classification in Fig. 1 of nuclei into formal F-spin multiplets—i.e., groupings for which $F_{\max}$ is fixed, but F_z takes on different values.

The identification of formal F-spin multiplets is predicated on the posture we adopt *vis-à-vis* the counting of valence boson numbers, N_π and N_ν: we ignore any subshell closures, taking N_π to be half the number of valence particle (hole) protons within the spherical shell model for $Z\leq 66$ ($Z\geq 66$) and N_ν to be half the number of valence particle (hole) neutrons for $N\leq 104$ ($N\geq 104$). (Another alternative would be to respect Casten's subshell closure rule [9]—i.e., for $N<90$ (and >82) there is a proton shell closure at $Z=64$. Since our binding-energy systematics (cf. below) do not show the effect of this subshell closure, we leave open in this paper the issue of whether or not Casten's rule should be adhered to.) The F-spin multiplets in our naive scheme are joined by unbroken lines in Fig. 1 and representative multiplets are labeled by the corresponding value of $F_{\max}$. It proves convenient to distinguish the four quadrants of Fig. 1: In A_{ph} (A_{hp}), the F-spin multiplets consist of alpha-different nuclei with particle p (hole h) proton bosons and hole (particle) neutron bosons; in I_{pp} (I_{hh}), the multiplets consists of isobaric nuclei with particle (hole) proton and neutron bosons. Following Ref. [10], we shall refer to the set of all the nuclei of a given $F_{\max}$ in groups A_{hp}, I_{hh}, and I_{pp} as an *extended* F-spin multiplet.

One advantage of this classification scheme becomes apparent when we plot the binding energies (BE) of nuclei (grouped according to these F-spin multiplets) against their value of F_z—cf., Figs. 2(a) and 2(b), which are representative. The remarkable regularity observed has encouraged us to attempt the fit

$$\mathrm{BE}(F,F_z)=C^{\mathrm{mid}}+a\tilde{F}+a'\tilde{F}_z+b\tilde{F}^2+b'\tilde{F}_z^2+c\tilde{F}\tilde{F}_z\ , \qquad (2)$$

where (for subsequent convenience) we work with $\tilde{F}=F-F^{\mathrm{mid}}$ and $\tilde{F}_z=F_z-F_z^{\mathrm{mid}}$, F^{mid} (F_z^{mid}) being the value F (F_z) takes on at the point of intersection of the four groups I_{pp}, I_{hh}, A_{hp}, and A_{ph}: $F^{\mathrm{mid}}=(\Omega_\pi+\Omega_\nu)/4=\frac{19}{2}$ and $F_z^{\mathrm{mid}}=(\Omega_\pi-\Omega_\nu)/4=-\frac{3}{2}$. This form is motivated by the standard IBM-2 result [3]

$$\mathrm{BE}(N_\pi,N_\nu)=C_0+a_\pi N_\pi+a_\nu N_\nu+b_\pi N_\pi^2+b_\nu N_\nu^2+c_{\pi\nu}N_\pi N_\nu+E_D(N_\pi,N_\nu)\ . \qquad (3)$$

Since $F=F_{\max}$ [$=(N_\pi+N_\nu)/2$] in Eq. (2), its use is tantamount to use of Eq. (3) under the assumption that the contribution of the deformation energy E_D is either negligible or can be mocked up by a second-order polynomial in N_π and N_ν (exactly this type of dependence is found in the various special symmetry limits of the IBM-2), modulo the distinction that in Eq. (2) we admit both particle and hole boson numbers, whereas in Eq. (3), N_π and N_ν refer (conventionally) only to numbers of particle bosons. We note that we can relax this restriction if we impose the following particle-hole symmetries on the coefficients in Eq. (3): for a_π and a_ν,

$$a_\pi\rightarrow -a_\pi-2\Omega_\pi b_\pi\ ,\qquad a_\nu\rightarrow a_\nu+\Omega_\pi c_{\pi\nu}\ , \qquad (4)$$

under *proton* particle-hole conjugation (here, $2\Omega_\pi$ is the degeneracy of the proton major shell), with analogous relations under *neutron* particle-hole conjugation, and

$$a_\pi\rightarrow -a_\pi-2\Omega_\pi b_\pi-\Omega_\nu c_{\pi\nu}\ ,\qquad a_\nu\rightarrow -a_\nu-2\Omega_\nu b_\nu-\Omega_\pi c_{\pi\nu}\ , \qquad (5)$$

under particle-hole conjugation of both protons and neutrons; for the other coefficients,

$$b_\pi=b_{\bar{\pi}},\quad b_\nu=b_{\bar{\nu}},\quad c_{\pi\nu}=-c_{\bar{\pi}\nu}=-c_{\pi\bar{\nu}}=c_{\bar{\pi}\bar{\nu}}\ , \qquad (6)$$

where the bar denotes particle-hole conjugation.

Under the assumption that E_D is negligible, these relations translate into the scheme of interrelationships for the coefficients of Eq. (2) given in Table I. Here, α

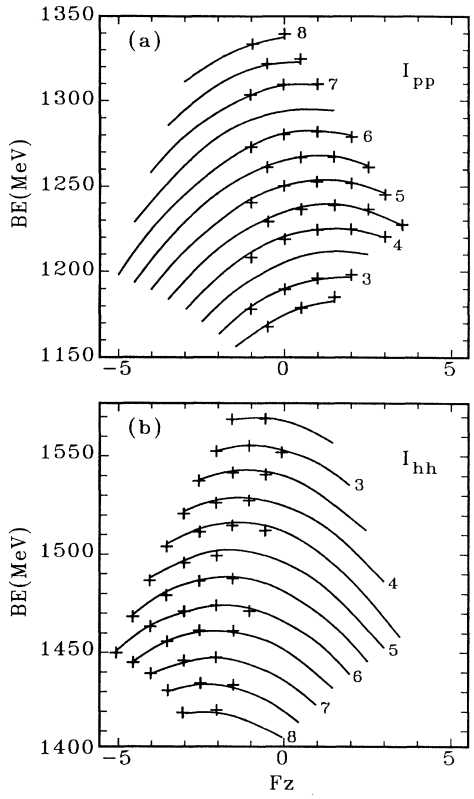

FIG. 2. Binding energies in F-spin multiplets of groups I_{pp} and I_{hh}. (Only multiplets with four or more members are represented.) The unbroken curves correspond to the extrapolation of the global fit based on Eq. (2) over the full extent of the various F-spin multiplets (representative values of F indicated).

TABLE I. Conjectured interrelationship between parameters of Eq. (2).

Group	a	a'	b	b'	c
I_{pp}	α	α'	β	β'	2γ
I_{hh}	$-\alpha$	$-\alpha'$	β	β'	2γ
A_{hp}	$-\alpha'$	$-\alpha$	β'	β	2γ
A_{ph}	α'	α	β'	β	2γ

denotes the value of a for the group I_{pp}, α' the value of a', etc. We have applied Eq. (2) in fits to the binding energies of all the various combinations of groups I_{pp}, I_{hh}, and A_{hp} under the constraint that the scheme of interrelationships in Table I is rigorously obeyed. (In this way, we can hope to extrapolate to the group A_{ph}.) The results are listed in Table II. Coefficients to which the fits were insensitive are highlighted by an asterisk.

Inspection of Table II indicates that the conjectured particle-hole symmetry of Table I is reasonably well satisfied. It would seem that we are in possession of a remarkably simple yet accurate ansatz for A_{ph} binding energies, based on the global fit (the last row in Table II), i.e., Eq. (2) with $C^{\rm mid}=1\,373.582$, $a=6.501$, $a'=29.243$, $b=-2.387$, $b'=-0.251$, and $c=-1.389$ (all in MeV). For completeness, a Haustein plot [11] of the residuals (i.e., $\mathrm{BE_{expt}}-\mathrm{BE_{fit}}$) corresponding to the global fit is given for all three groups in Fig 3 and a plot of the predicted mass excesses of A_{ph} nuclei is given in Fig. 4. We note the encouraging absence, for neutron-rich nuclei, of any significant bias towards either underbinding or overbinding in the residuals. No significance should be attached to the fact that, of the mass excess predictions appearing in a recent tabulation [12], we have chosen in Fig. 4 to compare ours with those of Spanier and Johansson [13].

We now consider whether we can exploit the systematics of *extended* F-spin multiplets to predict energy levels in neutron-rich nuclei relevant to the r process. More specifically, we want to relate the known excitation spectra of nuclei in group A_{hp} to those of the r-process nuclei in group A_{ph} (a successful N_pN_n-interpolation scheme exists for the excitation spectra of unstable nuclei within groups I_{pp}, I_{hh}, and A_{hp} [14]), so that we investigate the particular dual particle-hole symmetry involving the simultaneous particle-hole conjugation of both proton and neutron degrees of freedom.

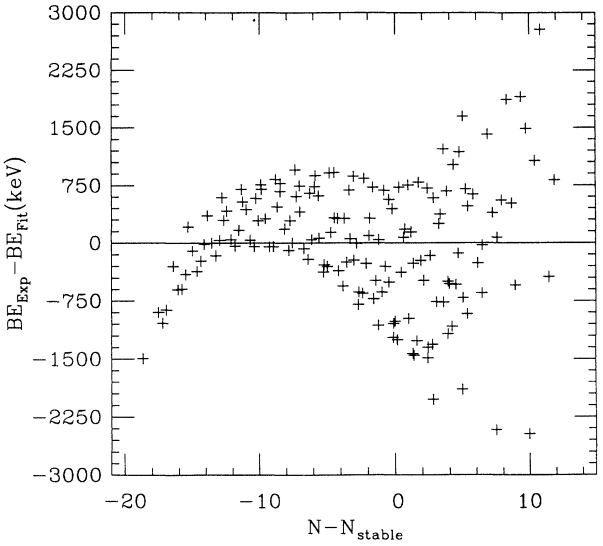

FIG. 3. Residuals $\mathrm{BE_{exp}}-\mathrm{BE_{fit}}$ with the global fit (last row of Table II) for all nuclei in groups I_{pp}, I_{hh}, and A_{hp}. (N denotes the neutron number, and, following Ref. [11], we parametrize $N_{\rm stable}$ as $Z+0.4A^2/(200+A)$.)

Our interest is in low-lying members of the excitation spectrum with energies of the order of a few hundred keV, which dominate the Boltzmann sum for temperatures relevant to the r process. We shall assume that these states arise predominantly from the mixing of different configurations of valence nucleons in the shells $50<Z<82$ and $82<N<126$. The lynchpin of our considerations is the observation that, within this model space, the matrix elements of the residual interaction (within, for definiteness, the spherical shell model) with respect to a particle-particle basis coincide with the corresponding matrix elements with respect to the hole-hole basis obtained by dual particle-hole conjugation. (A relationship of this simplicity does not hold for all manner of particle-hole conjugation—viz., particle-hole and particle-particle matrix elements are related [15] by a Racah transform (the Pandya relations).) In view of this assertion, the source of deviations from the desired dual symmetry lies in the nondegeneracy of the proton and neutron single-particle energies. For the major shells of interest, we estimate that these nondegeneracies should imply deviations of the order of 10%.

To confirm empirically whether or not these expecta-

TABLE II. Parameters of fits to binding energies.

Groups	No. BE's	$C^{\rm mid}$ (MeV)	α (MeV)	α' (MeV)	β (MeV)	β' (MeV)	γ (MeV)	rms error (keV)
A_{hp}	75	1375.9	28.9	5.3	−0.285	−2.24	−0.665	300
I_{pp}	49	1378.1	31.8	6.7	−0.02*	−2.56	−0.80	460
I_{hh}	44	1376.4	27.6	7.0	−0.06*	−2.49	−0.71	240
A_{hp} and I_{hh}	114	1375.1	28.8	5.6	−0.22	−2.26	−0.63	630
A_{hp} and I_{pp}	124	1374.5	29.6	6.1	−0.224	−2.35	−0.72	800
I_{pp} and I_{hh}	93	1372.6	29.4	7.3	−0.241	−2.60	−0.74	810
All 3	168	1373.6	29.2	6.5	−0.251	−2.39	−0.65	820

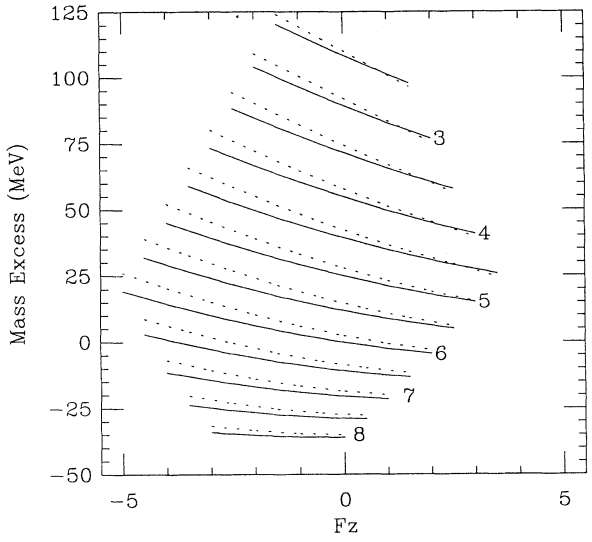

FIG. 4. Predicted mass excesses for the F-spin multiplets (of four or more members) in group A_{ph} on the basis of our global fit (unbroken lines) and the Spanier-Johansson formula [12,13] (dotted lines). Representative values of F are indicated.

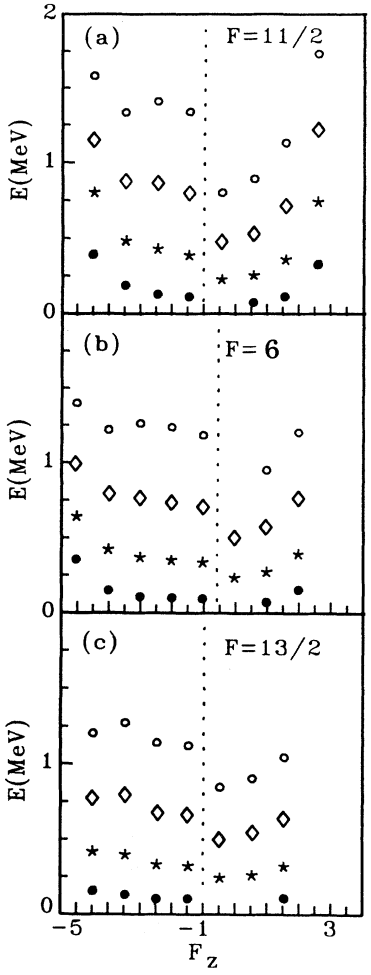

FIG. 5. gsb excitation spectra within naive F-spin multiplets of groups I_{pp} and I_{hh}. Points to the right (left) of the vertical dashed lines denote levels in nuclei belonging to I_{pp} (I_{hh}). The key to the symbols used is ●, 2^+ energy; ★, 4^+ energy; ◇, 6^+ energy; ○, 8^+ energy.

tions are borne out, we have attempted a comparison of the ground-state band excitation spectra of nuclei in groups I_{hh} and I_{pp}. (Observe that we expect deviations from our dual particle-hole symmetry to be larger for groups I_{pp} and I_{hh} than for groups A_{hp} and A_{ph}—the changes in the single-particle energies cancel to some extent in the latter case.) Unfortunately, the limitations of our data set mean that only for the $F=2$, $\frac{5}{2}$, $\frac{7}{2}$, and 4 extended multiplets is a direct comparison of dual particle-hole conjugated spectra possible and even that is restricted to the 2^+ and 4^+ energies. The relevant data are summarized in Table III (empty entries denote an absence of data). Observe that Casten's rule [9] does not affect the assignment of F and F_z, cf. Fig. 1. We take as a measure of the deviation from the desired particle-hole conjugation symmetry

$$\rho=|E_{pp}-E_{hh}|/(E_{pp}+E_{hh})\ , \tag{7}$$

where E_{pp} denotes an I_{pp} excitation energy and E_{hh} the corresponding I_{hh} excitation energy. It can be seen from Table III that, the $F=\frac{5}{2}$ multiplet excepted, dual particle-hole symmetry holds at the 10–20 % level. It is also noticeable that an I_{pp} excitation energy is always smaller than its I_{hh} counterpart. This is consistent with

TABLE III. Comparison of spectra related under dual particle-hole conjugation.

(F,F_z)	(2,0)		$(\frac{5}{2},-\frac{1}{2})$		$(\frac{7}{2},-\frac{1}{2})$		(4,−1)	
	E_{2^+}	E_{4^+}	E_{2^+}	E_{4^+}	E_{2^+}	E_{4^+}	E_{2^+}	E_{4^+}
	(keV)		(keV)		(keV)		(keV)	
I_{pp}	376.6	834.3	205.0		181.0	513.4	141.7	423.1
I_{hh}	466.0	1099	407.2	985.1	218.5	601	205.8	580.3
ρ	0.11	0.14	0.33		0.094	0.079	0.18	0.16

TABLE IV. Dual particle-hole symmetry violation implied by the discontinuities in Fig. 5.

F		$\frac{11}{2}$			6			$\frac{13}{2}$	
L	F_z	E_{L+} (keV)	$\rho_{\rm dis}(L)$	F_z	E_{L+} (keV)	$\rho_{\rm dis}(L)$	F_z	E_{L+} (keV)	$\rho_{\rm dis}(L)$
2	$-\frac{3}{2}$	122.6	0.25	-1	107.4	0.17	$-\frac{3}{2}$	97.9	0.15
	$-\frac{1}{2}$	72.8		0	76		$-\frac{1}{2}$	72.8	
4	$-\frac{3}{2}$	396.6	0.26	-1	349.8	0.17	$-\frac{3}{2}$	322.3	0.14
	$-\frac{1}{2}$	235.2		0	250.2		$-\frac{1}{2}$	240.3	
6	$-\frac{3}{2}$	808.6	0.26	-1	717.4	0.16	$-\frac{3}{2}$	666.4	0.14
	$-\frac{1}{2}$	478.9		0	517.3		$-\frac{1}{2}$	498.5	
8	$-\frac{3}{2}$	1348.6	0.25	-1	1199.3		$-\frac{3}{2}$	1122.5	0.14
	$-\frac{1}{2}$	807.0		0			$-\frac{1}{2}$	844.5	

our conjecture that the dual particle-hole symmetry breaking is related to the nondegeneracy of the single-particle spectrum: the single-particle states present in the dominant configurations contributing to an I_{hh} state are of higher energy than those present in the corresponding configurations of the I_{pp} counterpart.

Another somewhat less direct measure of dual particle-hole symmetry is available to us for higher F ($F=\frac{11}{2}-\frac{13}{2}$). Figures 5(a)–5(c) contain a graphical comparison of the ground-state band (gsb) excitation spectra of nuclei in groups I_{hh} and I_{pp} based on our naive F-spin multiplet scheme: we plot, where available, the lowest 2^+ to 8^+ excitation energies (our "ground-state" band) of nuclei against the corresponding value of F_z. The feature of interest in these figures is the appearance of an apparent discontinuity at the interface between the I_{hh} and I_{pp} data. We can exploit this discontinuity to gauge the extent to which dual particle-hole symmetry is violated in these F-spin multiplets using

$$\rho_{\rm dis}(L)=|E_{L+}(F_z^>)-E_{L+}(F_z^<)|/[E_{L+}(F_z^>)+E_{L+}(F_z^<)], \tag{8}$$

where $F_z^<$ ($F_z^>$) is the largest (smallest) value of F_z within a multiplet corresponding to I_{hh} (I_{pp}) data ($F_z^>=F_z^<+1$ for these multiplets). The data and results are given in Table IV. We interpret the consistency of the values of $\rho_{\rm dis}(L)$ for different L as evidence that this measure is indeed meaningful. It also indicates that dual particle-hole symmetry holds at the 10–20 % level.

In summary, our shell-model considerations described above and the empirical data at our disposal together indicate that we are justified in assuming that our dual particle-hole symmetry holds at the 10–20 % level or better for groups A_{hp} and A_{ph}. Thus, if we identify the known excitation energies of low-lying levels in A_{hp} nuclei with the excitation energies of levels in the corresponding A_{ph} nuclei (one could also introduce a prescription which takes into account the fact that the dual particle-hole symmetry breaking is such that A_{ph} energies are systematically higher than A_{hp} energies), we expect to incur an error of typically a few tens of keV, which is as good as can be expected of any calculation. As with the binding energies discussed earlier, we have a very simple prescription for deriving nuclear r-process input. In principle, the same dual particle-hole symmetry can be invoked to infer from $N=82$ semimagic nuclei low-lying excitation energies in $N=126$ semimagic waiting-point nuclei. However, as these estimated excitation energies will typically be greater than 1 MeV, they are of little relevance to the r process.

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[1] F. K. Thielemann, in *Nuclear Astrophysics,* edited by M. Lozano, M. I. Gallardo, and J. M. Arias (Springer, Berlin, 1989), p. 106.

[2] J. B. French and V. K. B. Kota, Annu. Rev. Nucl. Sci. **32**, 35 (1982).

[3] F. Iachello and A. Arima, *The Interacting Boson Model*

(Cambridge University, Cambridge, 1987).
[4] A. Arima, T. Otsuka, F. Iachello, and I. Talmi, Phys. Lett. **66B**, 205 (1977).
[5] F. W. Walker, J. R. Perrington, and F. Feiner, *Nuclides and Isotopes,* 14th ed. (General Electric, San Jose, 1989).
[6] M. Sakai, At. Data Nucl. Data Tables **31**, 399 (1984).
[7] S. Raman, C. H. Malarkey, W. T. Milner, C. W. Nestor, Jr., and P. H. Stelson, At. Data Nucl. Data Tables **36**, 1 (1987); S. Raman, C. W. Nestor, Jr., S. Kahane, and K. H. Bhatt, *ibid.* **42**, 1 (1989).
[8] J. K. Tuli, *Nuclear Wallet Cards* (National Nuclear Data Center, Brookhaven, 1990).
[9] R. F. Casten, Nucl. Phys. **A443**, 1 (1985).
[10] P. O. Lipas, P. von Brentano, and A. Gelberg, Rep. Prog. Phys. **53**, 1355 (1990).
[11] P. E. Haustein, in *Nuclei Off the Line of Stability,* edited by R. A. Meyer and D. S. Brenner (American Chemical Society, Washington, 1986), p. 126.
[12] P. E. Haustein, At. Data Nucl. Data Tables **39**, 186 (1988); **39**, 289 (1988).
[13] L. Spanier and S. A. E. Johansson, At. Data Nucl. Data Tables **39**, 259 (1988).
[14] R. F. Casten, Phys. Rev. C **33**, 1819 (1986).
[15] P. J. Brussaard and P. W. M. Glaudemans, *Shell-model Applications in Nuclear Spectroscopy* (North-Holland, Amsterdam, 1977).