

## Spectral distribution studies of $fp$ shell nuclei with a modified Kuo-Brown interaction

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The structure of nuclei in the lower half of the  $fp$  shell is investigated by the spectral distribution method using the modified Kuo-Brown interaction. This interaction recently showed success in reproducing observed properties through detailed shell model studies. Spectral distribution studies avoid explicit diagonalization and hold promise for applications to astrophysics. [S0556-2813(97)06603-X]

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### I. INTRODUCTION

In recent years there has been substantial progress in the application of the shell model to study nuclear structure. Full  $fp$  shell calculations involving valence particles in all four orbits  $f_{7/2}$ ,  $f_{5/2}$ ,  $p_{3/2}$ , and  $p_{1/2}$  have been successfully completed [1,2]. New realistic interactions in the  $fp$  shell have been suggested in order to obtain a better agreement with experimental results for the binding energies, low-lying spectra, and excitation strengths. These studies are being carried further to understand many other microscopic features of the nuclei in this region. Some of these nuclei are also important in astrophysics, in particular for presupernova stellar evolution [3,4] and  $r$ - and  $s$ -process nucleosynthesis. But for astrophysical purposes, one often finds that average properties, like smoothed level densities and averaged strength functions, are adequate. Here, results of statistical models of nuclear structure are useful. Spectral distribution theory [5,6] is a theory which, given enough valence particles in large spaces, is able to give statistically smoothed average shell model values for the physical quantities of interest.

In this paper we shall be concerned with the applications of the spectral distribution theory to the  $fp$  shell. In all earlier such studies the major uncertainties arose from the interaction used and none of the interactions used could give results in good agreement with observed values over the whole lower/upper half of the shell. But recently, shell model studies of  $A=48$  nuclei [1] as well as some other heavier ones [7] in the lower half of the shell indicate that a mini-

mally modified Kuo-Brown interaction (KB3) is able to reproduce successfully experimental binding energies, excitation spectra, and transition strengths. Then the question that naturally arises is how well do the spectral distribution studies work with this interaction in the lower half of the  $fp$  shell. In this work, we compare the predictions of the spectral distribution methods with experimental and shell model values. Similar studies were carried out in the  $sd$  shell [8] after the spectacular success of shell model results with universal- $sd$  interaction [9].

In spectral distribution theory one produces smoothed fluctuation-free forms for the density of states by distributing  $m$  fermions over  $N$  single particle states which go asymptotically to Gaussians. One is also able to provide average expectation values of operators as polynomial expansions in terms of energy of the initial space. The partitioning of the full shell model space into configurations and the use of a Gaussian form for the density in each configuration improve the predictability of the position of discrete states as well as the expectation values of operators and other relevant quantities. In predicting the binding energy through spectral distributions, one often uses the experimental spectra and does integration of Gaussians up to an excited state, and then subtracts out the excitation energy to reduce the inaccuracy coming from the integration procedure. The other correction one should incorporate is the small but nonzero skewness and excess ( $\gamma_1, \gamma_2$ ) of the distribution coming from large but finite shell model spaces. All earlier studies of spectral distributions in the  $fp$  shell used the excited state correction, but in this paper for the first time we incorporate ( $\gamma_1, \gamma_2$ ) corrections for  $fp$  shell nuclei in evaluating binding energies, excitation spectra and orbit occupation probabilities. A comparison with experimental values shows the importance of taking into account this deviation from Gaussians in improv-

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TABLE I. Binding energies (BE) of nuclei in the lower half of  $fp$  shell by spectral distribution methods (SDM) with KB3 interaction compared to experimental binding energies. Column  $\bar{A}$  gives BE by Ratcliff procedure and columns  $\bar{B}$  and  $\bar{C}$  by Ratcliff procedure with  $(\gamma_1, \gamma_2)$  corrections with  $\gamma_1(m), \gamma_2(m)$  and  $\gamma_1(m), \gamma_2(m, T)$  values, respectively.

Nucleus		Expt. BE (in MeV)	BE by SDM (in MeV)			
$A$	$Z$		$\bar{A}$	$\bar{B}$	$\bar{C}$	BE by SDM (in MeV) (Haq and Parikh)
46	20	-56.79	-60.73	-56.70	-56.33	-58.93
46	21	-62.95	-66.36	-62.89	-62.89	-64.94
46	22	-71.49	-74.15	-69.08	-69.43	-70.53
46	23		-75.82	-71.01	-71.35	
48	20	-73.84	-77.70	-72.60	-72.31	-76.72
48	21	-81.71	-85.88	-81.32	-80.96	-81.56
48	22	-92.34	-98.16	-90.76	-91.05	-93.08
48	23	-94.94	-100.39	-94.15	-94.88	-96.36
48	24	-101.16	-104.96	-97.48	-98.64	-98.99
52	20	-95.18	-101.76	-97.05	-93.82	-100.61
52	21	-109.43	-120.35	-110.88	-108.78	-112.87
52	22	-126.02	-135.36	-125.96	-124.26	-127.37
52	23	-134.29	-144.70	-134.94	-134.94	-138.23
52	24	-145.63	-156.98	-143.71	-145.50	-146.25
52	25	-148.41	-158.37	-146.97	-149.54	-148.88
52	26	-154.22	-164.13	-150.49	-154.18	-153.18
56	20	-108.41	-112.25	-110.50	-108.79	-112.03
56	21	-126.95	-132.93	-130.10	-127.36	-133.27
56	22	-148.26	-157.94	-150.99	-146.71	-152.08
56	24	-177.96	-192.22	-177.24	-178.03	-180.18
56	25	-187.17	-201.80	-188.21	-189.48	-188.05
56	26	-198.93	-214.49	-196.62	-200.79	-198.63
56	27	-202.72	-216.51	-200.29	-205.60	-201.41
56	28	-208.66	-222.21	-203.46	-210.46	-207.29

ing predictions. This feature was also observed in the  $sd$  shell comparisons.

## II. FORMALISM

In the shell model space of  $m$  particles (called the scalar space) the density of states tends towards a Gaussian, which needs two quantities, the centroid  $E_c(m)$  [ $=\langle H \rangle^m$ ] and the variance  $\sigma^2(m)$  [ $=\langle \tilde{H}^2 \rangle^m = \langle (H - \langle H \rangle^m)^2 \rangle^m$ ], to be specified. Here the  $m$ -particle average is given by  $\langle H \rangle^m = \text{Tr}H/d(m)$  where  $\text{Tr}H$  is the trace of the Hamiltonian operator  $H$  and  $d(m)$  is the dimension of the shell model space. The skewness and excess are then given by

$$\begin{aligned}\gamma_1(m) &= \langle \tilde{H}^3 \rangle^m / \sigma^3(m), \\ \gamma_2(m) &= (\langle \tilde{H}^4 \rangle^m / \sigma^4(m)) - 3.\end{aligned}\quad (1)$$

Given the (1+2)-body realistic Hamiltonians, spectral distribution theory expresses the  $m$ -particle averages in terms of averaged 1- and 2-body matrix elements and propagators (which involve powers of  $m$  [6]). For application to real nuclei, one needs to work in  $(m, T)$  spaces where  $T$  stands for the isospin of the  $m$ -particle state. Spectral distributions also demonstrate the Gaussian forms for the  $(m, T)$  density

of states and give extensions of the propagation results for  $(m, T)$  as well as  $(\tilde{m}, T)$  spaces [5].  $(\tilde{m}, T)$  stands for configuration-isospin space where  $\tilde{m} = m_1, m_2, \dots, m_l$  are the particles in  $l$  orbits. The ground state energy  $\bar{E}_g$  is evaluated by a procedure suggested by Ratcliff [10] where one inverts the equation

$$\sum_{\tilde{m}} \int_{-\infty}^{\bar{E}_g} I_{\tilde{m}, T}(E) dE = d_0/2 \quad (2)$$

to get  $\bar{E}_g$  ( $d_0$  is the degeneracy of the ground state). Here  $I_{\tilde{m}, T}(E) = d(\tilde{m}, T) \rho(\tilde{m}, T)$ . The expression for the Gaussian density of states in  $(\tilde{m}, T)$  space is

$$\begin{aligned}\rho(\tilde{m}, T) &= \frac{1}{\sqrt{(2\pi)\sigma(\tilde{m}, T)}} \\ &\times \exp\left[-\frac{1}{2}(E - E_c(\tilde{m}, T))^2 / \sigma^2(\tilde{m}, T)\right].\end{aligned}\quad (3)$$

To incorporate the  $(\gamma_1, \gamma_2)$  correction we use the Cornish-Fisher expansion [6]. In this expansion one transforms the variable  $x$  in  $\rho(x)$  by a series expansion onto a variable  $y$  so that the density in  $y$  is a Gaussian  $\rho_G(y)$ . Then for densities

TABLE II. Centroids, widths, and the correlation coefficient for the interactions modified Kuo-Brown (KB3) and MHW2.

Number of valence particles	Isospin	KB3		MHW2		Correlation coefficient between KB3 and MHW2
		Centroid (MeV)	Width (MeV)	Centroid (MeV)	Width (MeV)	
6	0	-42.04	8.33	-40.92	7.95	0.999
	1	-40.63	8.06	-39.72	7.72	0.999
	2	-37.81	7.49	-37.31	7.24	0.999
	3	-33.59	6.57	-33.70	6.48	1.000
8	0	-58.84	9.85	-57.01	9.32	0.998
	1	-57.44	9.61	-55.81	9.11	0.998
	2	-54.62	9.12	-53.40	8.69	0.998
	3	-50.40	8.35	-49.79	8.03	0.998
	4	-44.77	7.23	-44.98	7.10	1.000
12	0	-96.66	12.26	-92.86	11.42	0.997
	1	-95.24	12.06	-91.66	11.23	0.997
	2	-92.43	11.64	-89.25	10.85	0.997
	3	-88.21	11.01	-85.25	10.28	0.997
	4	-82.58	10.13	-80.83	9.51	0.997
	5	-75.54	8.97	-74.82	8.51	0.998
	6	-67.09	7.46	-67.60	7.24	0.999
16	0	-140.06	13.89	-133.61	12.73	0.996
	1	-138.65	13.71	-132.41	12.55	0.995
	2	-135.84	13.33	-130.00	12.20	0.995
	3	-131.61	12.76	-126.39	11.66	0.995
	4	-125.98	11.98	-121.58	10.94	0.995
	5	-118.94	10.98	-115.57	10.03	0.994
	6	-110.50	9.72	-108.35	8.90	0.995
	7	-100.64	8.14	-99.92	7.52	0.996
8	-89.38	6.06	-90.30	5.80	0.999	

in  $x$  and  $y$  both with zero centroid and unit width one obtains, including the  $(\gamma_1, \gamma_2)$  corrections,

$$y = x - \frac{\gamma_1}{6}(x^2 - 1) + \left[ -\frac{\gamma_2}{24}(x^3 - 3x) + \frac{\gamma_1^2}{36}(4x^3 - 7x) \right] \quad (4)$$

and conversely

$$x = y + \frac{\gamma_1}{6}(y^2 - 1) + \left[ \frac{\gamma_2}{24}(y^3 - 3y) - \frac{\gamma_1^2}{36}(2y^3 - 5y) \right] \quad (5)$$

so that  $\rho(x) = \rho_G(y)(dy/dx)$ . The orbit occupation probability for orbit  $s$  in the  $m$ -particle space is given by

$$n_s(E) = \sum_{\tilde{m}} \frac{I_{\tilde{m}T}(E)}{I_{mT}(E)} [m_s(\tilde{m})]. \quad (6)$$

This gives a simple dependence of the occupation probability on the energy  $E$  [11].

In spectral distribution theory, for comparison of different operators, an important quantity is the correlation coefficient between two operators  $G$  and  $H$  defined by

$$\zeta_{G-H} = \frac{\langle (G - \langle G \rangle)(H - \langle H \rangle) \rangle^m}{\sigma_G(m)\sigma_H(m)}, \quad (7)$$

where the  $m$ -particle trace  $\langle \tilde{G}\tilde{H} \rangle^m$  is calculated using propagation techniques and  $\sigma_G(m)$  ( $\sigma_H(m)$ ) are the widths of  $G$  ( $H$ ) in the  $m$ -particle space. The extension to  $(m, T)$  space also is easily carried out [5].

As yet, our spectral distribution codes can calculate up to third moments in  $(m, T)$  spaces exactly. The fourth moment of 2-body operators can be calculated only in scalar spaces. So for  $\gamma_2(m, T)$  we first make an approximation  $\gamma_2(m, T) = \gamma_2(m)$  to calculate the binding energies and spectra; then we improve this approximation by using a phenomenological correction term involving the two scalars of iso-

spin space  $n$  and  $T^2$  and write  $\gamma_2(n, T) = \gamma_2(n) + 0.04n - 0.04T^2$ . The correction coming from  $\gamma_1$  in the energy is small (a few percent); so changing the  $\gamma_1$  from its scalar to exact  $(m, T)$  values hardly makes any change in the corrected energy. Therefore we keep the scalar value for our calculation.

Spectral distribution theory also predicts simple forms for the sum rule strengths of transition operators. The sum rule strength, defined as the total strength for an excitation opera-

tor  $O$  from an initial state  $|i\rangle$  to all final states  $|f\rangle$ , is the expectation value  $\langle i|O^\dagger O|i\rangle$ . Spectral distributions give for the averaged sum rule strength a polynomial expansion in terms of the energy  $E$  of the initial state. Arguments based on the central limit theorem (CLT) in the shell model space inhibit terms beyond the first two in the expansion. This gives for nuclei with  $T=0$  the expression for the sum rule operator  $K = (O^{11} \times O^{11})^{00}$  with the excitation operator  $O^{11}$  which is a vector in both  $J$  and  $T$  [12],

$$K(E; m, T = M_T = 0 \rightarrow T' = 1, M_{T'} = \pm 1) = \langle m, T = 0 | K | m, T = 0 \rangle + \left\langle m, T = 0 \left| \frac{K(H - E_C(m, T = 0))}{\sigma(m, T = 0)} \right| m, T = 0 \right\rangle \frac{(E - E_C(m, T = 0))}{\sigma(m, T = 0)} = \langle m, T = 0 | K | m, T = 0 \rangle + \zeta_{H-K} \sigma_K(m, T = 0) \frac{(E - E_C(m, T = 0))}{\sigma(m, T = 0)}, \quad (8)$$

where  $\sigma_K(m, T)$  is the width of the operator  $K$  in the scalar- $T$  space. The extension of Eq. (8) to configuration averaged forms, as is done for occupancies in Eq. (6), is straightforward and is given by Eq. (5) of Ref. [12].

### III. RESULTS AND DISCUSSION

In Table I we compare the predictions for a number of nuclei in the lower half of the  $fp$  shell with the experimental binding energies (with the Coulomb contribution removed from it). Table I also gives the predictions of Haq and Parikh [13] using configuration isospin moments with excited state correction using MHW2 interaction. All the binding energies are relative to the  $^{40}\text{Ca}$  core. The exact shell model values are normally very close to the experimental values [1,2]. For the case of  $A=48$  nuclei the shell model with a small correction of 780 KeV in the centroid of KB3 interaction gives binding energies with respect to  $^{40}\text{Ca}$  core differing by  $-0.06, +0.03, +0.07, -0.04, +0.28, -0.10,$  and  $-0.05$  MeV from the experimental values for the Ca, Sc, Ti, V, Cr, Mn, and Fe nuclei [1]. We find that our procedure gives substantially better agreement with experimental values compared to earlier SDM applications particularly for nuclei with large ground state isospin values. The average and rms deviation of the corrected (column C) binding energies from the experimental values are 0.15 and 1.49 MeV, respectively. Kota and Potbhare, using SDM with excited state corrections with a phenomenological term involving neutron and proton numbers, obtained an RMS deviation of 5.59, 2.19, 5.79, 8.39, and 3.60 MeV for KB, MHW2 KB10, bare, and MWH interactions, respectively [14]. So we see that incorporating the corrections in binding energies due to nonzero  $(\gamma_1, \gamma_2)$  values makes substantial improvements compared to other methods using spectral distributions. Bearing in mind that fluctuations are of the order of 1 MeV, we find that this is a very satisfactory procedure.

To understand how the present interaction KB3 differs

from earlier interactions, like MHW2 which was also derived from the Kuo-Brown interaction, we show in Table II the centroid and width of the two interactions and their correlation coefficient in scalar-isospin  $fp$  spaces. These quantities, as one number estimates, give the overall behavior of the interactions. The interaction KB3 [1] is obtained by subtracting out 300 keV for  $J=1,3$  with  $T=0$  and 200 keV for  $J=2$  with  $T=1$  from the diagonal matrix elements of the  $f_{7/2}$  orbit of KB1. KB1 in turn is obtained by modifying some diagonal elements of the original Kuo-Brown interaction [1]. The centroids of KB3 and MHW2 are found to differ by up to 6 MeV for particle number ranging from 6 to

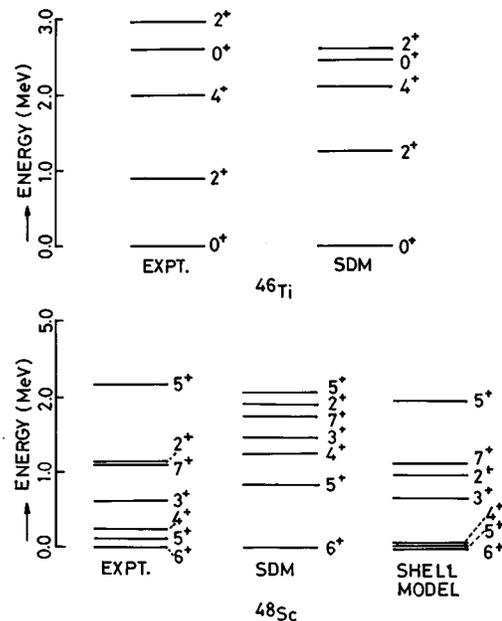


FIG. 1. The excitation spectrum of  $^{48}\text{Sc}$  and  $^{46}\text{Ti}$  calculated by spectral distributions (SDM) compared with the experimental and shell model (for  $^{48}\text{Sc}$ ) spectra. The interaction used for the SDM and shell model is the modified Kuo-Brown (KB3).

TABLE III. Calculated occupancies for the  $fp$ -shell nuclei. The values in parenthesis are from experimental data [13] obtained by adding neutron and proton occupancies.

Atomic number	Number of valence particles	Isospin	Occupancy			
			$f_{7/2}$	$f_{5/2}$	$p_{3/2}$	$p_{1/2}$
46	6	0	5.77	0.03	0.18	0.02
		1	5.79	0.01	0.18	0.02
			(4.89)	(0.23)	(0.88)	(0.00)
		2	5.66	0.01	0.30	0.03
		3	5.58	0.00	0.39	0.03
48	8	0	7.51	0.09	0.34	0.06
		1	7.39	0.09	0.44	0.08
		2	7.38	0.06	0.48	0.08
			(7.08)	(0.14)	(0.78)	(0.14)
		3	6.89	0.08	0.88	0.15
		4	6.62	0.06	1.14	0.18
52	12	0	10.58	0.36	0.84	0.22
		1	10.28	0.40	1.04	0.28
		2	10.13	0.35	1.21	0.31
			(9.98)	(0.06)	(1.96)	(0.00)
		3	9.50	0.42	1.65	0.43
		4	8.97	0.42	2.07	0.54
		5	8.18	0.57	2.52	0.73
		6	7.53	0.66	2.90	0.91
56	16	0	12.96	0.78	1.74	0.52
		1	12.60	0.85	1.96	0.59
		2	12.31	0.85	2.19	0.65
			(10.95)	(1.94)	(2.74)	(0.37)
		3	11.62	1.00	2.58	0.80
		4	11.02	1.09	2.94	0.95
		6	9.58	1.50	3.58	1.34
		7	8.79	1.90	3.79	1.52
		8	8.00	1.43	3.95	1.68

16. The width of MHW2 is seen to be consistently smaller than KB3 by a few percent, but as the correlation coefficient has the centroid subtracted and the widths divided out it has values very close to one for all particle numbers and isospins. A similar analysis using KB1 and KB3 interactions has also been performed by Poves and Zuker [15].

The procedure for calculating the energy of states can be extended to excited states. In Fig. 1 we compare for the nuclei  $^{46}\text{Ti}$  and  $^{48}\text{Sc}$  the calculated excitation spectrum with observed spectrum as well as shell model ones (for  $^{48}\text{Sc}$ ) obtained using the same KB3 interaction. The spectral distribution gives a globally averaged spacing and, as a result, does not reproduce well the clustering of states at low excitation energies for the odd-odd nucleus  $^{48}\text{Sc}$ . Moreover, in spectral distribution studies the spin sequence is assumed to locate each excited state. But we observe that, allowing for fluctuations of individual levels, the overall spectrum is reproduced quite well by spectral distributions for both the examples.

TABLE IV. The sum rule strength for Gamow-Teller (GT) transition for  $T=0$  nuclei in  $fp$  shell with KB3 interaction by spectral distribution using Eq. (8) which includes terms up to CLT. Column  $A$  gives the result for scalar space, whereas  $B$ ,  $C$ , and  $D$  are for configuration averaged values for one, six, and all configurations, respectively.

No. of valence particles	GT sum rule strength			
	$A$	$B$	$C$	$D$
6	7.51	7.05	7.23	7.21
8	9.39	8.53	9.04	8.97
12	11.88	10.00	11.72	11.51
16	13.94	12.50	12.77	13.22

Finally, in Table III we give the ground state occupation probabilities of the four orbits  $f_{7/2}$ ,  $p_{3/2}$ ,  $f_{5/2}$ , and  $p_{1/2}$  by our method. As is well known, the occupation probability of an orbit is related to the sum rule of stripping and pick-up strengths. A direct comparison with the experimental results is only possible in some cases and even the data available have large uncertainties. We quote the experimental ground state occupancies given in Kota and Potbhare [14] for nuclei  $^{46}\text{Ti}(T=1)$ ,  $^{48}\text{Ti}(T=2)$ ,  $^{52}\text{Cr}(T=2)$ , and  $^{56}\text{Fe}(T=2)$ . For  $^{48}\text{Ti}$  and  $^{52}\text{Cr}$  the  $f_{7/2}$  occupancies calculated by us agree reasonably well with experiments, but for  $^{46}\text{Ti}$  and  $^{56}\text{Fe}$  our values are higher. One feels the need for a more systematic analysis of present pick-up/stripping experiments and to perform further experiments for a more detailed comparison. The occupancies are quite useful for the estimation of Gamow-Teller sum rule strengths for  $\beta^-$  and  $\beta^+$  decays [3,12,16].

In Table IV we present the results for the sum rule strength for Gamow-Teller transitions for nuclei with  $T=0$  including terms up to the CLT limit. This is done to different levels of complexity in spectral distributions. The simplest is the scalar result and we also give the configuration averaged results including one, six, and all configurations. As the intensity of the higher configurations goes down fast, normally averaged results with a few low-lying configurations are very close to the ones with all configurations. Clearly, the Gamow-Teller sum rule probes the  $\hat{\sigma}\hat{\tau}\cdot\hat{\sigma}\hat{\tau}$  part of the interaction more sensitively. In future works we plan to calculate the sum rule strengths for  $E2$ ,  $M1$ , and other excitations which will probe some other parts of the total interaction Hamiltonian. We also intend to extend the calculations for nuclei with nonzero ground state isospin.

The actual strength distribution of the Gamow-Teller (GT) transitions has an important bearing on astrophysical problems like presupernova and supernova evolution [4,17,18]. Initial attempts at using the spectral distribution theory for the GT and isovector  $M1$  strength distribution for  $sd$  shell nuclei [19] need more detailed follow-up work and the extension to the  $fp$  shell.

#### IV. CONCLUSIONS

In conclusion, we stress that spectral distribution studies using corrections derived from a departure from Gaussians for the density of states through the third and fourth moments of the Hamiltonian are quite successful in predicting binding energies, excitation spectra, etc. These studies are extended to the calculation of sum rules and should be car-

ried out for transition strength distributions for different excitation operators and also to the upper half of the  $fp$  shell.

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