SPECTRAL DISTRIBUTION STUDIES OF fp SHELL NUCLEI WITH MODIFIED KUO–BROWN INTERACTION

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ABSTRACT

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1 INTRODUCTION

In recent years there has been substantial progress in the application of 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 for 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 minimally 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 does the spectral distribution studies do 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 improves 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 non-zero 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 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 improving
predictions. This feature was also observed in the sd shell comparisons.

2 FORMALISM

In the shell model space of \( m \) particles (called the scalar space) the density of states goes towards a Gaussian, which needs two quantities the centroid \( E_c(m) \) \( [= \langle H \rangle^m] \) and the width \( \sigma^2(m) \) \( [= \langle \tilde{H}^2 \rangle^m = \langle (H - \langle H \rangle^m)^2 \rangle^m ] \) to be specified. Here the \( m \)-particle average is given by \( \langle H \rangle^m = Tr \, H / d(m) \) where \( Tr \, H \) 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

\[
\gamma_1(m) = \langle \tilde{H}^3 \rangle^m / \sigma^3(m)
\]

\[
\gamma_2(m) = (\langle \tilde{H}^4 \rangle^m / \sigma^4(m)) - 3.
\]  \( \text{(1)} \)

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 \( \tilde{m} = m_1, m_2, ..., m_l \) are the particles in \( l \) orbits. The ground state energy \( \bar{E}_g \) is evaluated by a procedure due to Ratcliff [10] where one inverts the equation

\[
\sum_{\tilde{m}} \int_{-\infty}^{E_g} I_{\tilde{m}T}(E) dE = d_0 / 2
\]  \( \text{(2)} \)
to get $E_g$ ($d_0$ 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

$$\rho(\tilde{m},T) = \frac{1}{\sqrt{(2\pi)\sigma(\tilde{m},T)}} \exp\left[-\frac{1}{2}(E - E_c(\tilde{m},T))^2/\sigma^2(\tilde{m},T)\right]$$

(3)

To incorporate the $(\gamma_1, \gamma_2)$ correction we take recourse to 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 in $x$ and $y$ both with zero centroid and unit width one gets, including the $(\gamma_1, \gamma_2)$ corrections

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

(4)

and conversely

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

(5)

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

$$n_s(E) = \sum_{\tilde{m}} \frac{I_{\tilde{m},T}(E)}{I_m(T)} [m_s(\tilde{m})]$$

(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

$$\zeta_{G-H} = \frac{\langle(G - \langle G \rangle)(H - \langle H \rangle)\rangle}{\sigma_G(m)\sigma_H(m)}$$
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].

Our spectral distribution codes as yet 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 isospin space $n$ and $T^2$ and write $\gamma_2(n,T) = 0.04n - 0.04T^2$. 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.

3 RESULTS AND DISCUSSIONS

In Table 1 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 1 also gives the predictions of Haq and Parikh [12] using configuration isospin moment with excited state correction using MHW2 interaction. 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 Potb-
hare using SDM with excited state corrections with a phenomenological term involving neutron and proton numbers got the RMS deviation as 5.59, 2.19, 5.79, 8.39 and 3.60 MeV for KB, MHW2 KB10, bare and MWH interactions respectively [13]. So we see that incorporating the corrections in binding energies due to non-zero \((\gamma_1, \gamma_2)\) values make 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 Kuo-Brown interaction, we display in Table 2 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 behaviour 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 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.

The procedure for calculating the energy of states can be extended to excited states also. In Fig. 1 we compare for the nuclei \(^{46}Ti\) and \(^{48}Sc\) 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 $^{48}\text{Sc}$. Also in spectral distribution studies the spin sequence is assumed to locate each excited state. But we see that allowing for fluctuations of individual levels, the overall spectrum is reproduced quite well by spectral distributions for both the examples.

Finally in Table 3 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 probabilities of an orbit is related to the sum rule of stripping and pick-up strengths. But the analysis of the experimental results are not done for too many nuclei for direct comparison and even the data available have large uncertainties. We quote the experimental ground state occupancies given in Kota and Potbhare [12] 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 [3,14].

4 CONCLUSIONS

In conclusion, we stress that spectral distribution studies using corrections derived from a departure from Gaussians for the density of states through the
3rd and 4th moments of the Hamiltonian are quite successful in predicting binding energies, excitation spectra etc. These studies should be extended to the calculation of sum rules and transition strength distributions for different excitation operators and also to the upper half of the fp shell.

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Table 1

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, Column $\bar{B}$ and $\bar{C}$ by Ratcliff procedure with $(\gamma_1, \gamma_2)$ corrections with $\gamma_1(m), \gamma_2(m)$ and $\gamma_1(m, T), \gamma_2(m, T)$ values respectively.

| Nucleus | Expt BE (in MeV) | BE by SDM (in MeV) | BE by SDM (in MeV) |
|---------|------------------|--------------------|--------------------|
| A       | Z                | $\bar{A}$          | $\bar{B}$          | $\bar{C}$          | (Haq & 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             | -71.6       |
| 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 |
Table 1 (contd.)

| Nucleus | Expt BE (in MeV) | BE by SDM (in MeV) | BE by SDM (in MeV) |
|---------|------------------|--------------------|--------------------|
| A       | Z                | A                  | B                  | C                  |
| 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            |
Table 2

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

| Number of Iso-valence particles | KB3 | MHW2 | Correlation Coefficient between KB3&MHW2 |
|-------------------------------|-----|------|------------------------------------------|
|                               | Centroid | Width | Centroid | Width |                                |
|                               | (MeV)     | (MeV) | (MeV)     | (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 |
Table 3

Calculated occupancies for the fp - shell nuclei. The values in parenthesis are from experimental data† obtained by adding neutron and proton occupancies.

| Atomic Number | Number of valence particles | Isospin | $f_{7/2}$ | $f_{5/2}$ | $p_{3/2}$ | $p_{1/2}$ |
|---------------|-----------------------------|---------|-----------|-----------|-----------|-----------|
| 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 | 12.60 | 0.85 | 1.96 | 0.59 |
| 1 | 12.31 | 0.85 | 2.19 | 0.65 |
| 2 | 11.62 | 1.00 | 2.58 | 0.80 |
| 3 | 11.02 | 1.09 | 2.94 | 0.95 |
| 4 | 9.58 | 1.50 | 3.58 | 1.34 |
| 6 | 8.79 | 1.90 | 3.79 | 1.52 |
| 7 | 8.00 | 1.43 | 3.95 | 1.68 |

\[ t \] Ref. [13]
Figure Caption

Figure 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).