Shell-model studies for the ¹³²Sn region. II. Exact and statistical results for multi-proton cases

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Level structures and level densities of nuclei consisting of a ¹³²Sn core plus as many as nine valence protons are calculated using a realistic effective interaction (*G* matrix) plus previously determined correction terms. The correction terms were determined so that the total interaction, when used in shell-model calculations, gave a fit to the observed ¹³⁴Te spectrum. Recently developed trace reduction methods are employed to determine the energy moments of the level densities for each spin value. Comparisons between these moments and results of exact shell-model diagonalizations show excellent agreement. Level density comparisons demonstrate that the effect of the necessary correction terms on the spectra is small and decreases as the number of allowed orbits increases. This level density method is also used to investigate the effects of the Coulomb force on the multi-proton spectra.

NUCLEAR STRUCTURE Exact and statistical shell-model structure of ¹³²Sn core plus valence protons; shell-model effective interaction consisting of Brueck-ner reaction matrix plus phenomenological multipole corrections; level densities via moment expansions.

I. INTRODUCTION

In the preceding paper (hereafter referred to as I), semirealistic shell-model studies for as many as five valence protons beyond a ¹³²Sn core were presented and discussed. The results of I have stimulated this extension to nuclei with larger numbers of valence protons using the same model spaces, two-body interactions, and single proton energies. The principal achievements of this extended investigation are threefold.

First, the shell-model spectra for nuclei consisting of six to nine valence protons outside a 132Sn core are calculated and shown to yield reasonable agreement with available experimental data. Because of practical limitations on the shell-model code, these calculations are made in the smaller of two model spaces used in I. This space allows only the orbits $0g_{7/2}$ and $1d_{5/2}$. The interaction used is the same semirealistic interaction employed in I for this small space. It consists of a bare G matrix from the Reid soft core potential plus a pairing, a P_2 and a P_4 multipole term. The three parameters for these added terms were adjusted in I so that the total interaction when used in the shell-model calculations fit the lowlying experimental spectrum of ¹³⁴Te. The basic idea or philosophy of such semirealistic interactions is that inadequacies of using solely a realistic bare G interaction defined in a finite space, can, to some extent, be compensated for by adding a small number of correction terms. In conjunction with this philosophy it is anticipated that the necessary number and magnitude of such terms

will decrease as the size of the model space is increased. However, some correction terms will always be needed at least to account for core polarization. The combined agreement obtained here and in I between experimental and theoretical spectra over a range of nine valence protons using the same fixed interaction supports this philosophy.

The second principal achievement of this extension of I is that the average magnitude of the necessary corrections to the bare interactions, and the extent to which these corrections compensate for model space truncation effects, are investigated further. In addition to the above mentioned interaction in the small model space, the present investigation involves a second but similarly constructed semirealistic interaction defined in a large model space $(0g_{7/2}, 1d_{5/2},$ $0h_{11/2}$, $1d_{3/2}$, and $2s_{1/2}$). This second interaction and space are also identical with a set used in I. The interactions in the large and small spaces differ from each other in that the added pairing P_2 and P_4 terms were adjusted separately in the two cases such that the calculated spectra gave fits to the observed ¹³⁴Te spectrum. A comparison between the strengths of the added terms for these two interactions is given in I.

To make this extended truncation study, statistical shell-model level densities¹⁻⁴ calculated from one-body and two-body interaction matrix elements are used (rather than detailed energy spectra), since shell-model level densities can be calculated in very large model spaces. By comparing the lower-energy portion of the level

densities calculated with different interactions (or different model spaces), one can easily assess the average effects on the energy spectra produced by changes in the interaction (or model space).²

In I a correlation of 0.93, (0.97) was obtained between the bare and corrected interactions for the small (large) model space. These values were interpreted as suggesting that the necessary corrections in the small space mainly account for model space truncation effects, since the phenomenological corrections become smaller relative to the bare interaction as the size of the model space increases. This latter feature is precisely in keeping with the philosophy of semirealistic interactions. Further support of this philosophy is obtained in Sec. III of this paper by comparing the level densities for several different angular momentum values. In addition, these comparisons imply that the correlation, defined in Eq. (1) of I for two-body matrix element comparisons, is a reasonable indicator of the average differences of spectra that will result from calculations using these matrix elements.

The third principal achievement of our extended work involves the approximate moment expansion techniques recently developed to obtain shellmodel level densities. These new techniques merit study in their own right through comparison with exact diagonalizations. We evaluate fixed angular momentum moments of operators using the approximate techniques of Ginocchio. 2,3,5,6 The accuracy of these calculated moments and average level densities is then demonstrated by comparing with exact shell-model moments and histograms for some cases in which exact diagonalizations are feasible. In view of recent incréasing interest⁷ in statistical methods, we emphasize results demonstrating the need for higher moment calculations as well as calculations of level densities via individual configurations.4

An additional feature we investigate in this paper is the average effects of the Coulomb force between the protons. The Coulomb force was not included in the present effective interaction. By comparing average level densities with and without the first order Coulomb interaction we conclude that the Coulomb force contributes very little relative splitting of the lowest levels. The main effect of the Coulomb force is to shift the centroid of the spectrum. These features are well accepted for few-particle spectra and we verify them for many-particle spectra.

As in I, all the multiproton shell model spectra were calculated with the help of the Rochester-Oak Ridge shell-model codes.⁸

II. SHELL-MODEL SPECTRA

Before presenting any results, we feel it is worthwhile to reiterate that the correction terms of the semirealistic effective interaction used here were completely determined in I by fitting the lowest levels of ¹³⁴Te. No parameters have been varied in any of the calculations presented here.

For the nuclei with 6-9 valence protons, shell-model calculations in the small space were carried out to investigate the question of how far into the open shell it is possible to push the semirealistic methods.

Experimental and theoretical spectra are shown

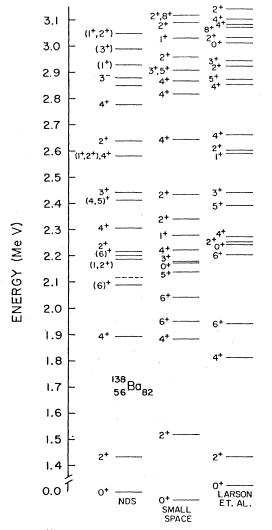


FIG. 1. ¹³⁸Ba spectra. NDS is experiment (Ref. 9). Center column is the present shell-model result in the $(0\,g_{7/2}$ and $1\,d_{5/2})$ space. Larson *et al*. (Ref. 10) is an MSDI shell-model calculation in the $(0\,g_{7/2},\ 1d_{5/2},\ 2s_{1/2},\ and\ 1\,d_{3/2})$ space with a maximum of one proton in each of the last two orbits.

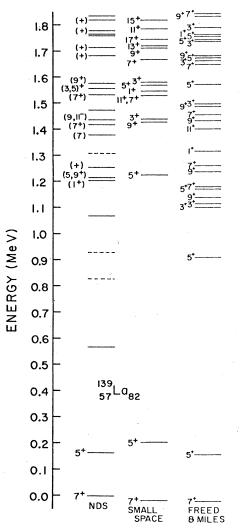


FIG. 2. 139 La spectra. NDS is experiment (Ref. 11). Center column is the present shell-model result in the $(0g_{7/2}, \text{ and } 1d_{5/2})$ space. Freed and Miles¹² is a QTDA calculation in the $(0g_{7/2}, 1d_{5/2}, 0h_{11/2}, 1d_{3/2}, \text{ and } 2s_{1/2})$ space.

in Figs. 1–4 for ¹³⁸Ba, ¹³⁹La, ¹⁴⁰Ce, and ¹⁴¹Pr respectively. In general the lowest few states are in reasonable agreement with experiment. Modified surface δ interaction (MSDI) calculations by Larson $et~al.^{10}$ and by Wildenthal¹⁴ are generally closer to experiment. In both articles the model space $(0g_{7/2},~1d_{5/2},~2s_{1/2},~$ and $1d_{3/2})$ was used but with a maximum of one proton per orbit in the $2s_{1/2}$ and $1d_{3/2}$ orbits. The better agreement with experiment is not unexpected since these authors employed a model space somewhat larger than our small space and adjusted phenomenological parameters to obtain overall agreement with experiment for these nuclei.

For ¹³⁸Ba the small space predicts better 0⁺ to

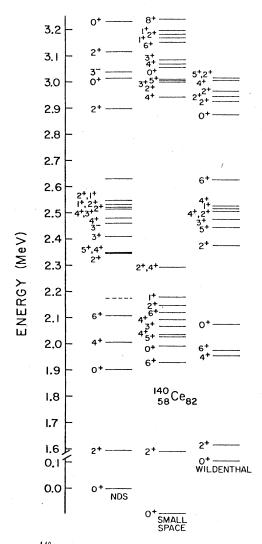


FIG. 3. 140 Ce spectra. NDS is experiment (Ref. 13). Center column is the present shell-model result in the $(0g_{7/2}$ and $1d_{5/2})$ space. Wildenthal (Ref. 14) is an MSDI shell-model calculation in the $(0g_{7/2}, 1d_{5/2}, 2s_{1/2},$ and $1d_{3/2})$ space with a maximum of one proton in each of the last two orbits.

 4_1^+ and 6_1^+ to 6_2^+ level splittings than those given by Larson $et\ al.$ Larson $et\ al.$, however, do seem to be in better agreement with the higherlying experimental levels. Both calculations have satisfactory overall agreement with experiment.

The seven-proton case ¹³⁹La is the first nuclide for which the small model space calculation fails to give a reasonable accounting of several low-lying levels. Most of the experimental levels from 0.5 to 1.5 MeV cannot be tentatively identified with any predicted level. It is possible that most of these levels lie outside the small model space. In fact, if one looks back to Fig. 1 of I it will be

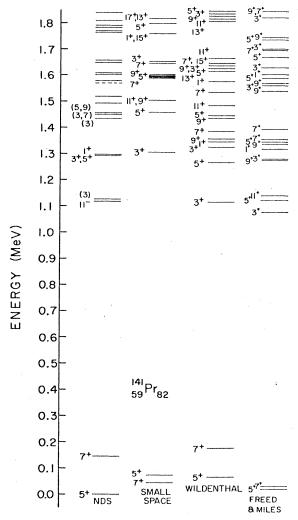


FIG. 4. 141 Pr spectra. NDS is experiment (Ref. 15). Second column is the present shell-model results in the $(0g_{7/2} \text{ and } 1d_{5/2})$ space. Wildenthal (Ref. 14) is an MSDI shell-model calculation in the $(0g_{7/2}, 1d_{5/2}, 2s_{1/2})$ and $(1d_{3/2})$ space with a maximum of one proton in either of the last two orbits. Freed and Miles (Ref. 12) is a QDTA calculation in the $(0g_{7/2}, 1d_{5/2}, 0h_{11/2}, 1d_{3/2}, 1d_{5/2})$ space.

noticed that the $\frac{1}{2}^+$ state near 1.2 MeV has been determined to have a significant single-particle transfer strength. The quasiparticle Tamm-Dancoff approximation (QDTA) results of Freed and Miles, who used the model space $(0g_{7/2}, 1d_{5/2}, 0h_{11/2}, 1d_{3/2},$ and $2s_{1/2})$, predict a lower $\frac{5}{2}^+$ state, but still do not yield predictions for some of the experimental levels. Further experimental data on the four levels between 0.5 and 1.1 MeV would be useful.

For 140 Ce the small model space overestimates the 0_1^+ to 2_1^+ level splitting by about 100 keV while

Wildenthal underestimates it by about the same amount. Since the experimental splitting is nearly 1.6 MeV (note broken energy scales for Figs. 1 and 3), these differences are not extreme. At slightly higher excitation it is seen that the small model space predicts the separation of the 2_1^+ and 0_2^+ levels somewhat better than Wildenthal's calculation. Also, if one allows the first 6^+ experimental level to correspond to the small model space's 6_2^+ level, then the small space calculation also predicts a better separation of the 4_1^+ and 6^+ levels. Wildenthal does, however, obtain better agreement with experiment from 2.3 to 2.7 MeV.

Finally, for ¹⁴¹Pr (nine protons) Withenthal's results are better in at least two ways. He gives the correct ground state and a more reasonable number of levels in the range of 1.1 to 1.8 MeV. The former is undoubtedly built into his selection of parameters and the latter may be due, at least in part, to his slightly larger model space. The results of Freed and Miles are generally similar to Wildenthal's. They do predict the correct ground state, but with considerably less splitting of the $\frac{7}{2}$ and $\frac{5}{2}$ levels than experimentally observed.

For the semirealistic calculations, the first $\frac{5}{2}$ + state has been moving downward relative to the lowest $\frac{7}{2}$ + state as the number of valence protons increased. (See Fig. 5.) The systematics of the relative positions of the $\frac{5}{21}$ and $\frac{7}{21}$ levels must be regarded as a very sensitive test of the effective interaction. Thus, even though they are not quite correctly given, the systematics are sufficiently well reproduced that this result can be regarded as a strong confirmation of the semirealistic approach.

It appears that calculations for this relatively large number of protons (the small space holds at most 14 protons) are straining the limits of validity for the small model space. It is, however, not clear how much of the inadequacy of the seven or more proton cases is due to the truncation effects generated by using the small model space and how much is due to the possible need to adjust the semirealistic parameters. It is entirely possible that merely using the large model space would be sufficient.

III. STATISTICAL RESULTS

Moment expansion methods¹⁻⁷ developed in recent years make it possible to obtain excellent approximations to shell-model level densities directly from the one-body and two-body matrix elements without performing diagonalizations. The chief advantages of these "statistical" methods is that they can be carried out in very large configuration spaces and are relatively inexpen-

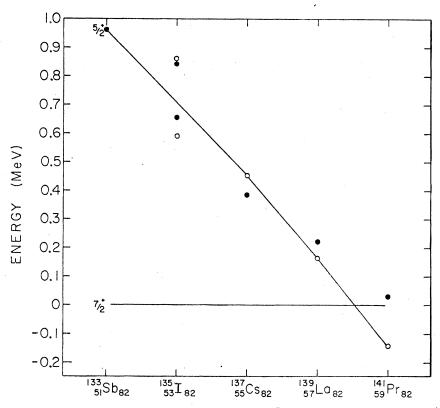


FIG. 5. Systematics of positions of $\frac{5}{2}$ + levels with respect to lowest $\frac{7}{2}$ + levels. The open and solid circles show, respectively, the experimental and shell-model excitations of lowest $\frac{5}{2}$ + levels with respect to the lowest $\frac{7}{2}$ + level. Experimentally observed systematics are well reproduced by the shell model, although inversion at nine protons is not quite predicted.

sive to utilize. In the present work we compute level densities for each total spin (J) and use them to demonstrate certain average effects of different matrix elements on the spectra.

To compute the level density for each total spin (J) we use the two moment (Gaussian) distribution and the m-scheme methods of Ginocchio $et\ al.^{2,3,5,6}$ to calculate the operator moments. These calculations were carried out using the computer code DENSJT developed at ORNL by one of the authors. ¹⁷

To promote better understanding of the inherent limitations on conclusions drawn from such statistical calculations, we first present some comparisons between exact shell-model results and results obtained using the statistical methods. In Figs. 6-9 discussed below, the solid lines indicate the statistical results and the dots indicate results obtained from exact shell-model diagonalizations. The shell-model and level-density calculations shown in Figs. 6-11 were carried out in the large model space using the semirealistic interaction discussed earlier. Comparisons for the number of states, energy centroids, and widths, each versus total spin J, are shown in Figs. 6 and

7 for ¹³⁵I (three valence protons). Similar comparisons are shown in Figs. 8 and 9 for ¹³⁶Xe (four valence protons). From these figures one can see that the *m*-scheme methods of Ginocchio give reasonable approximations for the number of states, energy centroids, and widths for each total spin value. Ginocchio and Yen³ have demonstrated that the inclusion of higher moments together with separate trace calculations for even and odd angular momentum projections (for even-even nuclei) improve the statistical results. Computer codes which include higher moment corrections for arbitrary orbitals are presently being developed.

Previous calculations¹ have demonstrated that the total (summed over J) shell-model level density is very close to Gaussian in shape. In addition, the general shape of the shell-model spectra for each total spin also exhibits a Gaussian shape when the spectra involve a sufficient number of levels to justify the use of a statistical description. Unfortunately, this feature has usually been demonstrated¹⁸ by comparing the distribution function, which represents the number of states below a certain energy, with the integral up to the

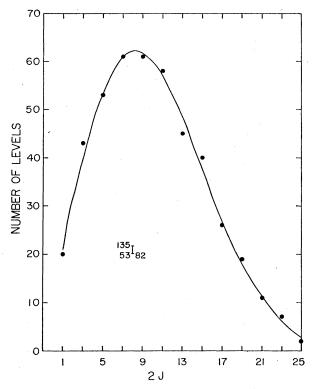


FIG. 6. Comparison of number of states versus angular momentum for 135 I. Solid line is obtained using the statistical methods. Dots represent the exact shell-model results. Both calculations were made in the $(0g_{7/2},\ 1d_{5/2},\ 0h_{11/2},\ 1d_{3/2},\ and\ 2s_{1/2})$ space.

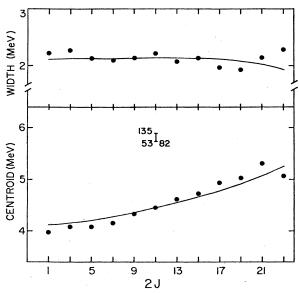


FIG. 7. Comparison of energy centroids and widths versus angular momentum for ^{135}I . Solid line is obtained using the statistical methods. Dots represent the exact shell-model results. Both calculations were made in the $(0g_{7/2},\ 1d_{5/2},\ 0h_{11/2},\ 1d_{3/2},\ \text{and}\ 2s_{1/2})$ space.

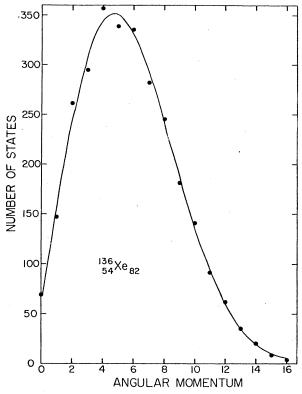


FIG. 8. Comparison of number of states versus angular momentum for 136 Xe. Solid line is obtained using the statistical methods. Dots represent exact shell-model results. Both calculations were made in the $(0g_{7/2}, 1d_{5/2}, 0h_{11/2}, 1d_{3/2}, and 2s_{1/2})$ space.

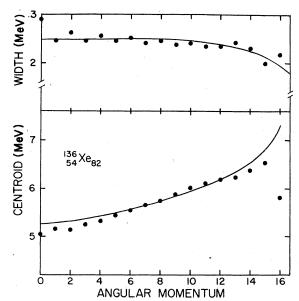


FIG. 9. Comparison of energy centroids and widths versus angular momentum for 136 Xe. Solid line is obtained using the statistical methods. Dots represent the exact shell-model results. Both calculations were made in the $(0g_{7/2},\ 1d_{5/2},\ 0h_{11/2},\ 1d_{3/2},\ and\ 2s_{1/2})$ space.

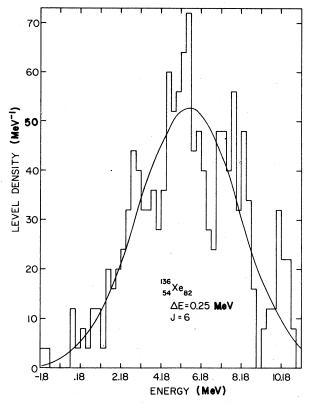


FIG. 10. Comparison of statistical level density with histogram from exact shell-model spectrum for 136 Xe J=6. The histogram interval is 0.25 MeV. Both calculations were made in the $(0g_{7/2},\ 1d_{5/2},\ 0h_{11/2},\ 1d_{3/2},\ and\ 2s_{1/2})$ space.

energy of interest of a Gaussian distribution. The relative effects of local fluctuations on the distribution function are small, so that comparing distribution functions is not the best method to exhibit particular features of the level densities themselves. In fact, a small fluctuation of the distribution usually represents a large fluctuation of the level density.

In Figs. 10 and 11 we show the Gaussian level density determined from the m-scheme techniques for the 136 Xe J=6 spectrum together with histograms obtained from the 340 exact shell-model levels with histogram interval widths of 0.25 and 1.5 MeV, respectively. This comparison demonstrates two worthwhile points. First, the shape of the shell-model level density histogram determined from diagonalization for a given J is reproduced on the average by the computed m-scheme Gaussian. Second, significant level clustering exists in the exact shell-model spectra. Obviously, these clustering effects cannot be described by the single Gaussian distribution; thus we refer to the latter as the "average" level density. It remains

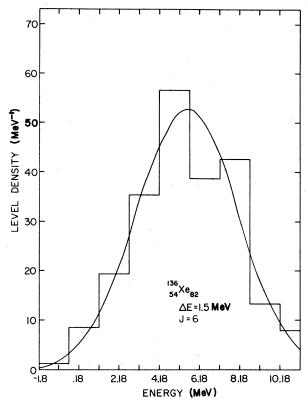


FIG. 11. Comparison of statistical level density with histogram interval is 1.5 MeV. Both calculations were made in the $(0g_{7/2}, 1d_{5/2}, 0h_{11/2}, 1d_{3/2}, and 2s_{1/2})$ space.

to be seen whether or not such fluctuations of the level density from the smooth average can be described by moment methods using configuration expansions.⁴

The statistically calculated average level density cannot be used to describe local clustering effects, but it can be used to compare the average effects on the shell-model spectra of different interactions. By comparing the calculated average level densities of several J values for two different interactions, one can readily determine, for instance, if changes in an interaction will produce overall shifts between the spectra for different spins. Below, the calculated average level densities are used to demonstrate several interesting features of the semirealistic interactions used here and in I.

One use of the average level density for each spin J is to demonstrate the effects of model space truncation on the average spectra. First, we recall that in I the parameters for the large and small model space were separately adjusted to fit the interlevel spacing for the two-particle ¹³⁴Te spectrum. In addition, correlations of 0.93 and 0.97 were obtained between the bare G matrix

and corrected interactions for the small and large model space, respectively. The stronger correlation in the large model space together with the magnitudes of these correlations clearly suggest that the adjustments mainly accounted for truncation effects.

In Fig. 12 we exhibit calculated average level densities versus energy for several total spin (*J*) values for ¹³⁷Cs which consists of five valence protons near the ¹³²Sn core. Curves A and C were determined from the semirealistic interactions in their small and large model space respectively. An overall energy shift was used in I to realign the spectra obtained using the small and large model spaces as in the average level density comparisons of Ayik and Ginocchio. To correspond to the spectrum shifts in I, curves A and C should be shifted to better align the extreme lower slopes for the spin value corresponding to the lowest-energy state. However, to better compare the

exact effects of different interactions on the average level densities, we have omitted this shift. Curves B in Fig. 12 represent the average level density calculated with the subset of the corrected large model space matrix elements corresponding to the small model space. In other words, only the matrix elements of the large model space interaction involving orbits of the small model space were used to establish curve B. Curves B thus represent the average level density for a truncated model space but without a readjusted interaction. The average level densities for the bare interaction differed so little from those using the corrected large model space interaction that curves B and C also represent well the 137Cs large and small model space results, respectively, for the bare interactions. If we gauge the needed strength of corrections by noting the discrepancy between densities calculated using corrected and bare interactions in the same space,

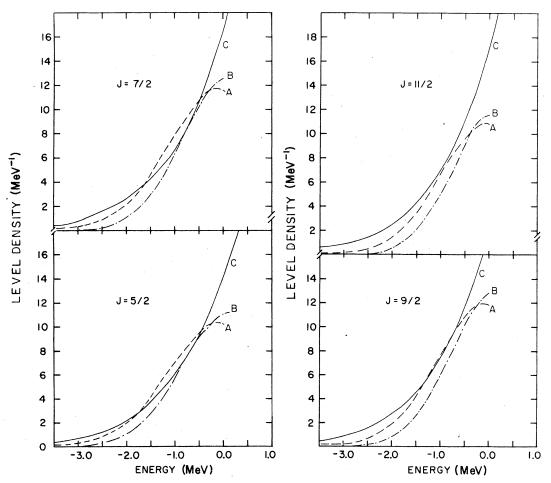


FIG. 12. Comparing 137 Cs $J = \frac{5}{2}$, $\frac{7}{2}$, $\frac{9}{2}$, and $\frac{11}{2}$ level densities for different interactions. Curves A and C were calculated in the small and large model spaces using the semirealistic interactions. Curve B was calculated in the small model space using the projection of the large space semirealistic interaction onto the small model space.

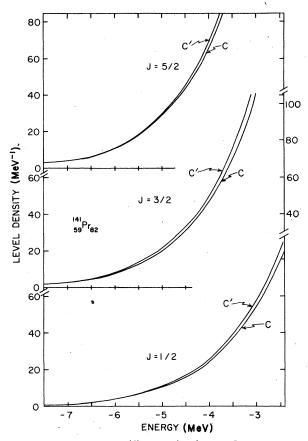


FIG. 13. Comparing ¹⁴¹Pr $J=\frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$ level densities for different interactions. Curves C and C' were calculated in the large model space using the semi-realistic and bare-G interactions, respectively.

then the differences between curves A and B in Fig. 12 clearly indicate that the corrections needed in the small model space are substantially greater than the corrections needed in the large model space. Therefore, these differences clearly suggest that the additional corrections mainly account for truncation effects.

The level densities for the different interactions in Fig. 12 also show the parameter adjustments to have different effects for different total spin values. We anticipate that adjustment of interaction parameters to simultaneously match lower slopes of level densities for several different total spin values would be an excellent way to adjust one interaction to match another.

To clearly exhibit the differences between the average level densities for the bare G matrix and corrected interactions in the large space, we consider the nine valence protons case. As is well known, differences between spectra due to differences in interactions are usually magnified as the number of valence particles, and hence the

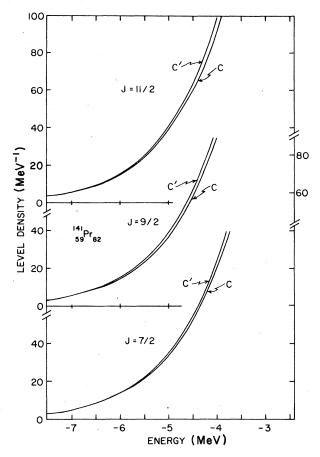


FIG. 14. Comparing ¹⁴¹Pr $J = \frac{7}{2}$, $\frac{9}{2}$, and $\frac{11}{2}$ level densities for different interactions. Curves C and C' were calculated in the large model space using the semi-realistic and bare-G interactions respectively.

number of interactions, is increased. Curves C and C' in Figs. 13 and 14 depict the average level densities calculated in the large model space for corrected and bare interactions, respectively. In keeping with the 0.97 correlation mentioned above, the nearness of these curves indicates that the corrected large model space interactions are, statistically speaking, very similar to the bare realistic reaction matrix elements. This observation and the demonstrated truncation effects suggest that for calculations carried out in sufficiently large model spaces, the bare G realistic interaction would give a reasonable account for the physical interaction between valence nucleons when core-polarization effects can be neglected.

Another feature investigated here with the average level density technique is the average effect of the Coulomb force between the protons. The Coulomb force was not included in the present effective interactions. A generally held conjec-

ture is that the Coulomb force will give an overall shift but will contribute very little to the relative splitting of the levels. To check this conjecture for multi-proton spectra, first-order matrix elements for the Coulomb force were computed in the harmonic oscillator basis of the large model space. Average level densities for six different J values of the ¹⁴¹Pr nine-particle case were calculated with this first-order Coulomb force added to the effective interaction. The centroids for each J increased by 7.3 MeV and the widths were decreased by about 100 keV. If the curves which include Coulomb effects are shifted downward by 7.75 MeV, their low-energy portions fall between curves C and C' in each case shown in Figs. 13 and 14. This indicates that, as expected, the Coulomb force has little effect on the low-energy portions of the level densities.

IV. SUMMARY AND CONCLUSIONS

The results of Sec. II extend and support the results and conclusions of I. Further confirma-

tion has been obtained for the semirealistic approach in general and specifically for the use of such shell-model studies near ¹³²Sn. Even for a small shell-model space, relatively minor corrections to a bare *G* matrix yield reasonable agreement with experiment. This suggests that the realistic interaction used here in a truncated space nearly accounts for the actual physical interaction between valence nucleons, and the combined effects of truncation and core polarization can be adequately handled by the semirealistic approach.

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