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Full *fp* shell calculation of ^{52}Sc

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The spectra and electromagnetic transitions of the odd-odd nucleus ^{52}Sc are calculated in the nuclear shell model approach, using the full fp shell basis functions with no truncation. Two of the most used two-body effective interactions in the fp shell yield quite different nuclear spectra. The energy levels from the two interactions are compared, as well as the magnetic and quadrupole moments and the electromagnetic transitions. The available experimental data, mostly 1^+ levels, are not sufficient to conclude which interaction provides a better fit. [S0556-2813(98)50301-9]

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In a recent paper [1] we presented a shell model description of the nuclei ^{51}Ca and ^{51}Sc. The Hamiltonian matrix was calculated in the full fp shell basis functions. This was the first ever calculation with 11 valence nucleons in the fp shell with no truncation of the basis functions. This was achieved by using the new parallel shell model code—the DUPSM (Drexel University Parallel Shell Model) code. (This code was developed and executed on the MOSIX [2] Computing Cluster system at the Hebrew University of Jerusalem.)

In Ref. [1] we used two different effective interactions; FPD6 of Richter *et al.* [3] and KB3 of Poves and Zuker [4]. These two interactions are based on the Kuo and Brown two-body effective interactions [5] derived in the late 60's from the Hamada-Johnston potential [6]. Later, this Kuo and Brown interaction was improved by using the folded-diagram method [7]. Richter *et al.* determined their interaction by doing a nonlinear fit to the experimental data available at that time starting from the Kuo and Brown interaction. The fit was done for nuclei in the fp shell with few valence nucleons, a restriction due to the lack of computer power available at that time (early 90's) and to the limitations of the computer code they used. On the other hand, Poves and Zuker simply modified the monopole centroids in the Kuo and Brown interaction to cure the bad saturation properties characteristic of all the forces that describe adequately the nuclear phase shifts. The resulted KB3 interaction was found very successful in describing all nuclei up to nine valence nucleons in the fp shell [8,9]. Note that Poves and Zuker did not use a mass factor whereas Richter *et al.* used the factor $(A/42)^{-0.35}$ (where A is the number of nucleons).

In Ref. [1] we found that the FPD6 and the KB3 interactions gave reasonable fits to the first four excited states of ^{51}Sc, while KB3 yielded a slightly better fit to the higher excited states. In general, the nuclear spectra and the electromagnetic transitions obtained by using FPD6 and KB3 were similar for ^{51}Sc (as well as for ^{51}Ca).

One of the most challenging aspects in the nuclear shell model is to be able to give a good description of odd-odd nuclei, since their spectra are usually highly sensitive to slight changes in the effective interactions. The odd-odd nucleus ^{52}Sc which contains 12 valence nucleons in the fp shell is even more challenging, since no computer code was able to construct its Hamiltonian matrices in the full fp shell basis, until now. The main reason was because too many coupled states are involved in this construction. On the other hand, the dimensions of the Hamiltonian matrices are moderate; the largest dimension is 36 287 for $J=4$. With the DUPSM code, running on the MOSIX system, we are able to build the full fp shell basis for this nucleus. Experimentally, only few nuclear levels of ^{52}Sc were recently measured [10]; the 3^+ ground state, few 1^+ levels and one more level at 0.675 MeV for which the angular momentum is not yet identified. Nevertheless, it is important to check whether the most used effective interactions for the fp shell can describe these data, and what the shell model can predict for other nuclear quantities that, hopefully, will be measured in the near future.

We use the two effective interactions FPD6 and KB3 to calculate the low-lying energy levels for $J=0,1,2,\ldots,8$; we plot the levels, up to 5 MeV, for $J=0,1,2,3,4$ in Fig. 1 and the levels for $J=5,6,7,8$ in Fig. 2. Table I gives explicitly the experimental values of the 1^+ levels (in MeV) as well as the calculated ones. From Figs. 1 and 2 we conclude that FPD6 and KB3 definitely yield different spectra, despite some energy levels that are close by. Moreover, we can see that except for $J=1$ and $J=5$, the number of states below 5 MeV predicted by FPD6 and KB3 for each J is different. (Except for $J=2$, FPD6 predicts more states than KB3.)

The results for the 1^+ levels require quantitative examination since we can compare them to the experimental values. In Table I we list the experimental and predicted energy levels of the 1^+ states. We include the 0.675 Mev level; it might also be a 1^+ state since it was obtained from the analysis of the log ft values in ^{52}Ca β^- decay, from which all the experimental data for the 1^+ states were deduced

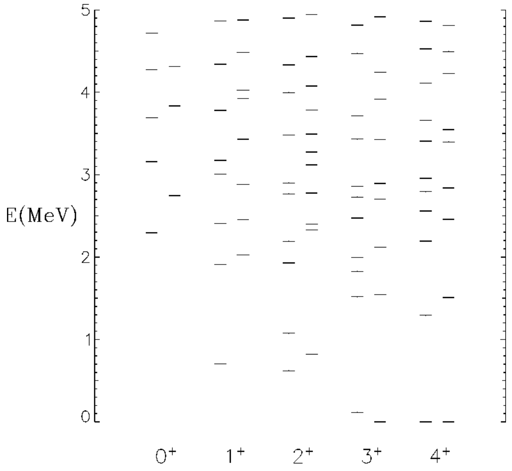

FIG. 1. The calculated low-lying energy levels (up to 5 MeV) of ^{52}Sc for $J=0,1,2,3,4$. The energy levels were obtained by using two different two-body interactions, FPD6—plotted to the left for each J value—and KB3—plotted to the right.

TABLE I. The energies (in MeV) of the calculated 1^+ states (up to 5 MeV) and the corresponding experimental values taken from [10]. The angular momentum of the state at 0.675 MeV is not determined yet, but might be 1^+.

Exp.	FPD6	KB3
(0.675)	0.701	-
1.636	1.910	2.027
-	2.405	2.455
2.745	3.007	2.881
3.458	3.172	3.430
-	3.782	3.923
-	-	4.024
4.265	4.338	4.485
-	4.864	4.878

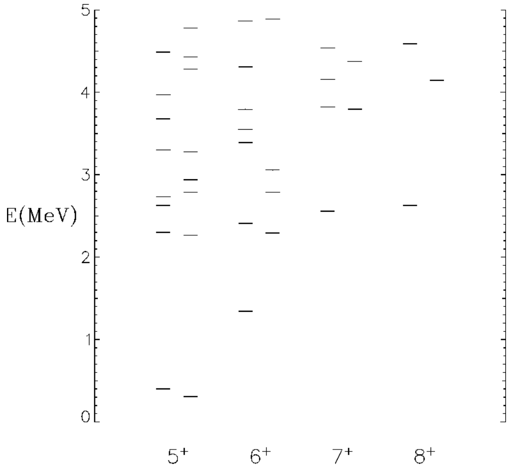

FIG. 2. The same as in Fig. 1 for $J=5,6,7,8$.

[10]. The FPD6 interaction predicts a 1^+ state at roughly this energy, while the KB3 interaction does not. Table I shows that FPD6 and KB3 reproduce reasonably the experimental levels at 1.636, 2.745, 3.458, and 4.265 MeV. We also predict more 1^+ states in ^{52}Sc at around 2.43, 3.85, and 4.87 MeV and maybe one more around 4 MeV, according to KB3 only.

The measured angular momentum of the ground state is 3_1^+. However, FPD6 and KB3 predict a doublet of 3_1^+ and 4_1^+. Actually, FPD6 predicts a 4_1^+ ground state and an excitation energy for the 3_1^+ at 0.11 MeV, whereas for KB3 the 3_1^+ and 4_1^+ have almost the same energy. Moreover, there are more doublet states among the 3^+ and 4^+ excited states as predicted by both FPD6 and KB3 (see Fig. 1).

Much can be learned about nuclear structure within the shell model by calculating electromagnetic transitions and moments. We compared the magnetic and quadrupole moments of the 3_1^+ and 4_1^+ levels. Using the bare electromagnetic factors for the magnetic moments, we obtain for FPD6 the values 3.6053 and 3.9606μ_N for the 3_1^+ and 4_1^+ states, respectively. For KB3 the values are 3.6178 and 4.3453μ_N, almost the same values. Using standard effective charges, i.e., 1.5e for protons and 0.5e for neutrons, in the electric quadrupole moment operator, we calculated quadrupole moment values of -14.507 e fm^2 using FPD6 and -15.119 e fm^2 using KB3 for the 3_1^+ state. Getting approximately the same values for the magnetic and quadrupole moments for the 3_1^+ energy level is a strong indication that the two different effective interactions yield almost the same wave functions for these states. The two effective interactions also predict similar wave functions for the 4_1^+ level; the quadrupole moment of this state is -15.186 e fm^2 using FPD6 and -15.204 e fm^2 using KB3.

We have calculated the magnetic and the quadrupole moments of the 1^+ states presented in Table I; we do not get in general similar results for the corresponding energy levels obtained from the FPD6 and KB3 interactions. We did, however, obtain close values for the first 1^+ states obtained from the FPD6 and KB3, although their energies are different, i.e., 0.701 and 2.027 MeV. The values are, respectively, 2.899 μ_N and -5.599 e fm^2 using FPD6 and 3.086μ_N and -6.974 e fm^2 using KB3.

As we mentioned before, there are no experimental values to compare with for the electromagnetic transitions in ^{52}Sc. So, we can only compare the predictions of the two interactions. We have calculated the $BE(2)$ values for the electromagnetic transitions that usually are considered as the most important ones, i.e., the transitions to the ground doublet states 3_1^+ and 4_1^+. For the 3_1^+ state we have calculated the electromagnetic transitions from the first three 1^+ states using (as in the quadrupole moment calculations) effective charges of 1.5e for protons and 0.5e for neutrons. For FPD6 we obtain the following $B(E2)$ values

$$B(E2,1_1^+\rightarrow 3_1^+)=5.2373\,e^2\,\mathrm{fm}^4,$$

$$B(E2,1_2^+\rightarrow 3_1^+)=8.8234\,e^2\,\mathrm{fm}^4,$$

$$B(E2,1_3^+\rightarrow 3_1^+)=7.6041\,e^2\,\mathrm{fm}^4, \qquad (1)$$

and for KB3

$$B(E2,1_1^+\to 3_1^+)=8.5825\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,1_2^+\to 3_1^+)=26.945\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,1_2^+\to 3_1^+)=4.406\,e^2\,\mathrm{fm}^4\,. \tag{2}$$

Although the above $BE(2)$ values are different, it is interesting to note that the transition from the 1_2^+ state in FPD6 and the transition from the 1_1^+ state in KB3 are almost the same. This similarity might relate to the fact that the energies of these two states are close by (see Table I). However, the magnetic and quadrupole moments of these two states are not the same, as we mentioned before.

The other important transitions are those from the 2^+ and 6^+ levels to the 4_1^+. The $BE(2)$ values for the transitions from the first three 2^+ levels to the 4_1^+ state, using FPD6, are

$$B(E2,2_1^+\to 4_1^+)=7.4516\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,2_2^+\to 4_1^+)=0.4174\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,2_3^+\to 4_1^+)=13.055\,e^2\,\mathrm{fm}^4\,, \tag{3}$$

and, using KB3,

$$B(E2,2_1^+\to 4_1^+)=3.7576\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,2_2^+\to 4_1^+)=0.0448\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,2_3^+\to 4_1^+)=43.027\,e^2\,\mathrm{fm}^4\,. \tag{4}$$

The two interactions predict that the strongest transition is from the 2_3^+ level and that the transition from the 2_2^+ level is very weak. These results are different from what is usually expected, namely that the transition from the lowest 2^+ state should be stronger than those from the excited states.

The $BE(2)$ values for the transitions from the 6^+ levels to the 4_1^+ state, using FPD6, are

$$B(E2,6_1^+\to 4_1^+)=0.4459\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,6_2^+\to 4_1^+)=14.594\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,6_3^+\to 4_1^+)=0.0\,e^2\,\mathrm{fm}^4\,, \tag{5}$$

and, using KB3,

$$B(E2,6_1^+\to 4_1^+)=3.0899\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,6_2^+\to 4_1^+)=8.7489\,e^2\,\mathrm{fm}^4\,,$$

$$B(E2,6_3^+\to 4_1^+)=1.7889\,e^2\,\mathrm{fm}^4\,. \tag{6}$$

Here, the two effective interactions predict that the transition from the second 6^+ excited state be the strongest. On the other hand, FPD6 predicts that the transition from the 6_1^+ is weak and from the 6_3^+ actually negligible, whereas KB3 predicts these two transitions not to be so weak.

In conclusion, the DUPSM code—the first parallel shell model computer code—enables us to describe the odd-odd nucleus ^{52}Sc in the full fp shell basis. We used two different two-body effective interactions, FPD6 and KB3. Although these two interactions yield, more or less, the same nuclear spectra for ^{51}Ca and ^{51}Sc [1], they predict different spectra for ^{52}Sc. This result strongly supports the argument that the results of large-scale shell model calculations for odd-odd nuclei strongly depend on the effective interaction used, and are sensitive to the different features of the interaction [11]. However, the experimental data available so far is not sufficient to determine which interaction is more reliable for the description of the ^{52}Sc nucleus. We are anxiously waiting to compare our predictions with new experimental data that, hopefully, will be available in the near future.

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[1] A. Novoselsky, M. Vallières, and O. La'adan, Phys. Rev. Lett. (to be published).
[2] A. Barak and O. La'adan, in *Proceedings of the International Conference on High-Performance Computing and Networking (HPCN, Europe '97),* Vienna, Austria, 1997, Lecture Notes in Physics Vol. 1225, edited by B. Hertzbergr and P. Sloot (Springer, Berlin, 1997), pp. 624–635.
[3] W. A. Richter, M. J. Van Der Merwe, R. E. Julies, and B. A. Brown, Nucl. Phys. **A523**, 325 (1991).
[4] A. Poves and A. P. Zucker, Phys. Rep. **70**, 235 (1981).
[5] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **A114**, 241 (1968).
[6] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 382 (1962).
[7] T. T. S. Kuo, in *Contemporary Nuclear Shell Models* (Springer, Berlin, 1996), pp. 25–46.
[8] E. Caurier, A. P. Zuker, A. Poves, and G. Martinez-Pinedo, Phys. Rev. C **50**, 225 (1994).
[9] G. Martinez-Pinedo, A. P. Zuker, A. Poves, and E. Caurier, Phys. Rev. C **55**, 187 (1997).
[10] H. Junde, Nucl. Data Sheets **71**, 659 (1994).
[11] M. Kirson, in *Contemporary Nuclear Shell Models* (Springer, Berlin, 1996), pp. 289–291.