Full f-p Shell Calculation of ^{51}Ca and ^{51}Sc

A. Novoselsky,[1] M. Vallières,[2] and O. La'adan[3]
[1]*Racah Institute of Physics, Hebrew University, Jerusalem 91904, Israel*
[2]*Department of Physics and Atmospheric Science, Drexel University, Philadelphia, Pennsylvania*
[3]*Institute of Computer Science, Hebrew University, Jerusalem 91904, Israel*
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The spectra and the electromagnetic transitions of the nuclei ^{51}Ca and ^{51}Sc with 11 nucleons in the *f-p* shell are described in the nuclear shell-model approach by using two different two-body effective interactions. The full *f-p* shell basis functions are used with no truncation. The new parallel shell-model computer code DUPSM (Drexel University parallel shell model), that we recently developed, has been used. The calculations have been done on the MOSIX parallel machine at the Hebrew University of Jerusalem. [S0031-9007(97)04615-2]

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The nuclear shell model, introduced almost 50 years ago by Mayer [1] and by Haxel, Jensen, and Suess [2], has been very successful in describing the properties of nuclei with few valence nucleons [3]. These properties include the energy levels, magnetic and quadrupole moments, electromagnetic transition probabilities, β decay, and cross section for various reactions.

In order to describe nuclei in the framework of the nuclear shell model one has to know the effective one- and two-body interaction. Several approaches were proposed during the last 30 years for the derivation of the effective interaction for nuclei in the *s-d* and *f-p* shells. The first comprehensive method was proposed in the 1960s by Kuo and Brown, who used the Hamada-Johnston potential [4] in a systematic way to determine the effective two-body interaction in the *s-d* [5] and *f-p* [6] shells. Later, these two-body interactions were improved by using the folded-diagram methods [7].

Wildenthal [8] started from the Kuo and Brown effective interaction and introduced a nonlinear fit process to determine the 63 two-body matrix elements and the three single particle energies of the *s-d* shell from experimental data. He was able to reproduce a selection of 447 experimental excitation and binding energies of nuclei in the *s-d* shell with an rms deviation of 185 keV. He also used a simple mass dependence to improve the results. Later [9], a semiempirical interaction based on one-boson exchange potentials plus core-polarization correction terms of the multipole-multipole type was systematically developed by numerous least-squares fits to the same experimental data in the *s-d* shell.

Richter *et al.* [10] used similar approaches to determine the 195 two-body matrix elements and the four single particle energies of the *f-p* shell. In one approach—the model dependent potential method—a semiempirical interaction was obtained by using one-boson exchange potentials plus core polarization correction as in Ref. [9]. The final interaction obtained in this method was denoted FPD6 in Ref. [10]. Another approach—the model independent potential method—followed the original method of Wildenthal [8] in the *s-d* shell. They denoted this interaction as FPM13 [10]. The two interactions, i.e., FPD6 and FPM13, yield a good fit to the energy levels of nuclei in the lower part of the *f-p* shell, where the mass factor $(\frac{A}{42})^{-0.35}$ was used [10] (where A is the number of nucleons).

Other successful approaches to determine the effective interaction for the *f-p* shell were proposed by Zuker and his collaborators. Based on the Kuo and Brown interaction [6] they identified which matrix elements should be modified, while keeping the centroid of any two shells. This approach yielded the KB1 interaction [11]. Later, the KB3 interaction was obtained, by doing very mild changes in the KB1 interaction in order to improve the spectroscopy of some nuclei at the beginning of the *f-p* shell [12]. This interaction leads to fairly successful calculations in the *f-p* shell. However, because of bad saturation properties with KB3 [13] the Strasbourg Madrid shell-model collaboration—$(SM)^2$—introduced the modified realistic monopole interaction with the multipole Hamiltonian that contains "something" that is a normalized form of pairing plus quadrupole Hamiltonian [14].

The algorithm for describing nuclei in the shell-model framework, where the one- and two-body effective interaction is given, was first developed by Talmi and his collaborators who implemented the Racah's methods for atomic physics for nuclear shell-model calculations [3]. The Oak-Ridge shell-model code [15], which was written 30 years ago, was the first implementation of this method. It used a *j-j* coupled approach and became a very powerful tool to study nuclei in the *s-d* shell. Zwarts [16] recoded this approach (the RITSSCHIL code), 12 years ago, in a more flexible and powerful manner.

Concurrently with the developments of these codes, other shell-model codes have been written (use Ref. [17]). The most recent code was written by the Strasbourg group (ANTOINE code) [18]. These codes used the *m* scheme and the similarity between the action of creation and annihilation operators and the logical AND and OR

operations on the bits of computer words. Although these codes were efficient, they have disadvantages; the matrices generated are generally enormous, the maximum number of orbitals is limited by the word length, and no truncation scheme can be applied.

The Oxford–Buenos Aires shell-model (OXBASCH) code [19] follows a hybrid algorithm between the *m* scheme and the *j-j* scheme. The code builds the states in the *m* scheme and the Hamiltonian matrix in the *j-j* scheme. Thus, it avoids the angular momentum coupling algebra and the matrices are not enormous. (There is also a new version of the code ANTOINE [20] that has diagonalized matrices with fixed angular momentum.) However, there is still a computational difficulty in the transition from the *m* scheme to the *j-j* coupling scheme.

All the codes mentioned above were extensively used for shell-model calculations in the *s-d* shell, as well as in the beginning of the *f-p* shell (i.e., 4–5 nucleons). Recently, by using the latest version of the ANTOINE code and a powerful computer, Caurier *et al.* were able to describe the nuclei in the *f-p* shell with eight nucleons [21], and Martinez-Pinedo *et al.* describe the nuclei with seven and nine nucleons [22]. For nuclei with more nucleons in the *f-p* shell the dimension of the Hilbert space becomes prohibitively large. However, this is not the reason why most of the shell-model codes could not calculate the nucleus ^{51}Ca, with 11 nucleons in the *f-p shell*, although its Hamiltonian dimensions are small. Even the dimensions related to the nucleus ^{51}Sc are not too big for strong computers (see Table I).

The main difficulties that prevented the shell-model calculations of these nuclei are inherent to the traditional methods and algorithms, used in the shell-model codes, for constructing antisymmetric multishell states in multiple angular momentum coupling scheme, and consequently, the algorithm for calculating the Hamiltonian matrix. The basic idea is to construct the antisymmetric states for each subshell, usually by using the coefficients of fractional parentages (cfps), and then to couple the states to a total antisymmetric state. This is a numerically unstable formalism which requires construction of an overcomplete set of states, followed by an orthogonalization to project out the proper physical states.

TABLE I. The number of odd parity states with angular momentum J for the nuclei ^{51}Ca and ^{51}Sc.

J	^{51}Ca	^{51}Sc
$\frac{1}{2}$	790	13 016
$\frac{3}{2}$	1484	24 474
$\frac{5}{2}$	1965	33 103
$\frac{7}{2}$	2215	38 138
$\frac{9}{2}$	2214	39 420
$\frac{11}{2}$	2017	37 371
$\frac{13}{2}$	1669	32 824

A new algorithm for doing calculations in the nuclear shell model was introduced ten years ago [23–25]. This algorithm is based on permutation group concepts. We first construct *arbitrary* permutational symmetry states for nucleons that carry the same single particle angular momentum j. The states are constructed recursively using the appropriate coefficients of fractional parentage (cfps) for *arbitrary* symmetry. The algorithm for calculating these cfps is based on the method of diagonalization of the second Casimir operator of the permutational group [23]. A similar method is used for calculating the outer-product and the inner-product isoscalar factors of the permutational group [25]. Then, by using the outer-product isoscalar factors we obtain multishell states with good total angular momentum that belong to an *arbitrary* permutational symmetry. In our method, the isospin of the nucleons is treated separately as one shell. The globally antisymmetric states are obtained from the states with the given total angular momentum that belong to a well defined *arbitrary* symmetry and the states with the given total isospin that belong to the conjugate symmetry, by using the inner-product isosclar factors [24,25].

The Drexel University shell-model (DUSM) computer code [17] implemented this new approach to perform shell-model calculations in the isospin scheme where the nucleons are distributed in several subshells. The first full version of the code was completed one year ago. It outperforms the OXBASCH code by a large (4 or 5) factor in CPU usage with much reduced disk space and I/O requirement for multisubshell calculations in the *s-d* shell. For the *f-p* shell there are even better achievements.

During the last year we developed a parallel version of the DUSM code—DUPSM. This version uses the message passing paradigm for distributed memory parallel computers (MIMD machines). Recall that the DUSM code involves two computational phases: building the Hamiltonian matrix and the Lanczos diagonalization procedure. The use of the permutational symmetry group introduces extra (unconserved) labels with which to label the basis; this splits the Hamiltonian matrix into independent submatrices. These submatrices are distributed to different processors, effectively giving a straightforward domain decomposition in Hilbert space. The building of the Hamiltonian matrix uses the bulk of the CPU time in large calculations. This part of the code scales almost perfectly with the number of processors. The Lanczos procedure in the second phase has also been parallelized using the same data decomposition, and is quite efficient, albeit the fact that it does not perfectly scale. The result is a flexible parallel DUSM code, which can efficiently utilize the parallel

computer, making it clearly the most efficient coupled shell-model code.

The code was implemented using PVM [26], a dynamic environment for parallel programming, supporting the message passing paradigm. It was developed and executed on the MOSIX [27] Computing Cluster (CC) system at the Hebrew University of Jerusalem. The MOSIX CC provides additional support for load balancing and redistribution of workload using preemptive process migration. The MOSIX CC configuration at Hebrew University consists of over 50 Pentium-Pro and Pentium PC's, connected by the Myrinet Gb/s LAN. The DUSM code was executed on a subcluster of 32 Pentium-Pro 200 MHz machines, each having 256 MB RAM.

By using the parallel DUSM code we are able to describe nuclei that have never been previously described in the full *f-p* shell basis. This enables us to examine various effective interactions, which yield good fits at the beginning of the *f-p* shell. In this paper we present the results for the nuclei ^{51}Ca and ^{51}Sc by using the two-body interactions KB3 [12] and FPD6 [10].

The energies of the low excited states of the nucleus ^{51}Ca (up to 2 MeV) are (in MeV) 1.24 and 1.96, whereas their angular momenta are unknown except the angular momentum for the ground state, which is probably $\frac{3}{2}^-$ [28]. By using the two-body interactions KB3 and FPD6 we confirm a ground-state spin of $\frac{3}{2}^-$. However, the energies of the first and the second excited states are 1.574 and 2.162 MeV for KB3 and 1.773 and 1.906 MeV for FPD6 with angular momentum $\frac{1}{2}^-$ and $\frac{5}{2}^-$, respectively.

We obtained a good description of ^{51}Sc. From Fig. 1 it can be seen that the first two excited states with angular momenta $\frac{3}{2}^-$ and $\frac{11}{2}^-$ are adequately obtained by KB3 and FPD6. In fact, KB3 gives a slightly better fit to these

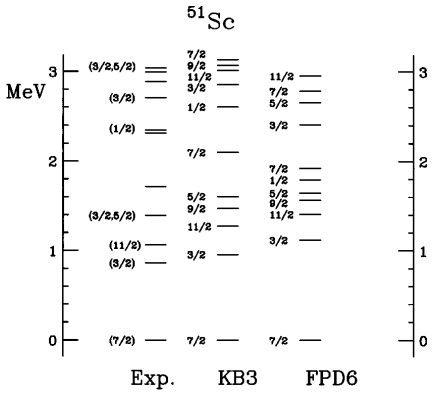

FIG. 1. The low lying energy levels (up to 3 MeV) of ^{51}Sc. The experimental data are taken from Ref. [28], and the calculated energy levels were obtained by using two different two-body interactions, KB3 and FPD6. All the states have odd parity. (We excluded the even parity state with excitation energy 1.167 MeV.) The experimental data that are not definitely determined are written in parentheses, as in Ref. [28].

energy levels, i.e., for $\frac{3}{2}^-$ ($\frac{11}{2}^-$) the experimental value is 0.862 (1.062) MeV and the calculated ones are 0.955 and 1.120 (1.271 and 1.408) MeV from KB3 and FPD6, respectively. Both shell-model calculations predict a pair of levels in ($\frac{9}{2}^-$, $\frac{5}{2}^-$) order, while experimentally only the first state of the doublet is known to be a $\frac{5}{2}^-$ state, the spin of the second state not being measured yet.

From the last six excited states in Fig. 1, the angular momentum of only two is possibly known, i.e., $\frac{1}{2}^-$ and $\frac{3}{2}^-$, and the last one might have either $\frac{3}{2}^-$ or $\frac{5}{2}^-$. From Fig. 1 it is easy to see that only KB3 reasonably yields the energy levels of $\frac{1}{2}^-$ and $\frac{3}{2}^-$. The prediction of FPD6 for these states is too high, with a wrong order level ordering. Therefore, using KB3 we predict the following angular momentum for the last six excited states in Fig. 1; $\frac{7}{2}^-$, $\frac{1}{2}^-$, $\frac{3}{2}^-$, $\frac{11}{2}^-$, $\frac{9}{2}^-$, and maybe also $\frac{7}{2}^-$ to the last one. (Note that the excitation energy of this level in KB3 is 3.133 MeV and the next excitation energy is 3.159 MeV with angular momentum $\frac{5}{2}^-$.) It would be interesting to determine the angular momentum of these levels, experimentally.

We can analyze the calculated energy levels in the simplest shell-model approach [3]. ^{51}Sc can be modeled as two valence neutrons occupying the $p_{\frac{3}{2}}$ subshell outside of ^{49}Sc. The latter has 21 protons and 28 neutrons—a closed (sub-) shell. This nucleus, which was well reproduced in the shell-model approach by using the KB3 interaction [22], has a ground state with angular momentum $\frac{7}{2}^-$ and its first excited state above 3 MeV. In first approximation, the lowest states of ^{51}Sc are obtained by coupling the two extra neutrons to the ground state of ^{49}Sc. These two neutrons can couple to $J = 0$ or $J = 2$ (antisymmetric states). Coupling the $J = 0$ pair to the ground state of ^{49}Sc produces the $\frac{7}{2}^-$ ground state of ^{51}Sc. Coupling the $J = 2$ pair to the ground state of ^{49}Sc produces the odd parity states with $J = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}$, and $\frac{11}{2}$. The latter states are clearly recognized among the states in the 1–2 MeV energy range in the calculated spectrum of KB3 and FPD6. This simple physical picture seems to also be present in the available experimental energy levels.

There are no experimental values, to compare with, for the electromagnetic transitions in ^{51}Sc. Nevertheless, we have calculated the electromagnetic transitions related to the first two excited states which are obtained with more or less the correct energies by KB3 and FPD6. Using the standard effective charges of $1.5e$ for protons and $0.5e$ for neutrons in the electric quadrupole transitions and moments, we obtain for KB3 the following $B(E2)$ values

$$B\left(E2, \frac{3}{2}^- \longrightarrow \frac{7}{2}^-\right) = 51.79e^2\ \mathrm{fm}^4,$$
$$B\left(E2, \frac{11}{2}^- \longrightarrow \frac{7}{2}^-\right) = 18.15e^2\ \mathrm{fm}^4, \quad (1)$$

and for FPD6

$$B\left(E2, \frac{3}{2}^- \longrightarrow \frac{7}{2}^-\right) = 68.1e^2\ \mathrm{fm}^4,$$
$$B\left(E2, \frac{11}{2}^- \longrightarrow \frac{7}{2}^-\right) = 20.99e^2\ \mathrm{fm}^4. \quad (2)$$

These $B(E2)$ values for the two different interactions are very similar. In addition, the calculated quadrupole moment of the ground state of ^{51}Sc is also very similar, i.e., $-22.18e$ fm^2 for KB3 and $-22.15e$ fm^2 for FPD6.

The FPD6 interaction was used in the shell-model Monte Carlo (SMMC) approach to describe nuclei in the middle of the *f-p* shell [29]. They found no need to use effective charges in fitting the $B(E2)$ transitions. A subsequent calculation in the SMMC approach based on the KB3 interaction did need effective charges [30]. This difference in the effective charges was attributed to the overly collective nature of the FPD6 interaction as compared to the KB3 interaction. Using the FPD6 and KB3 interactions we find that the same effective charges yield similar $B(E2)$ transitions in ^{51}Sc in full *f-p* shell-model calculations. The overly collective nature of the FPD6 interaction does not seem to manifest itself yet in this 11 valence nucleons (quarter of the shell) system.

In conclusion, DUPSM—the first parallel shell-model computer code—enables us to describe nuclei in the *f-p* shell that could not be described by other existing shell-model codes. In this paper we have demonstrated its ability by describing, in the full *f-p* shell basis, the nuclei ^{51}Ca and ^{51}Sc. We used two different two-body effective interactions, FPD6 and KB3. The interaction FPD6 was found very successful in the beginning of the *f-p* shell, but with a mass factor, and the interaction KB3 was found to give a good fit even to nuclei with nine nucleons in the *f-p* shell [22] with no mass factor. We find that both interactions give reasonable fits to the first four excited states of ^{51}Sc; KB3 yields a better fit to more excited states. We are anxiously waiting to compare our predictions using the KB3 interaction with new experimental data on ^{51}Sc that will be available in the near future.

We are now using the DUPSM code to describe nuclei in the *f-p* shell with more than 11 nucleons; these calculations yield huge Hamiltonian dimensions. We hope to complete these calculations in the near future. These results will help us to make a definite conclusion on the quality of the KB3 and FPD6 interactions for 11 or more nucleons in the *f-p* shell and might point us to possible improvements in these interactions.

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