Extended application of the DMRG methodology to nuclei in the $1f - 2p$ shell

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Abstract. In this paper, we present systematic results of the J-DMRG method (an angular-momentum-conserving version of the Density Matrix Renormalization Group) in truncated shell-model calculations of nuclei in the $1f - 2p$ shell. In contrast to earlier studies, these calculations consider both even-even and odd-mass nuclei. Comparison of the results of these calculations with those of exact shell-model treatments of the same nuclei shows that the method converges smoothly to the exact results in all cases and furthermore that the fraction of the full shell-model space required to obtain accurate agreement with the exact results decreases rapidly as the size of the full space grows. This latter result bodes well for the future applicability of the method to even larger nuclei with even larger shell-model spaces as is the ultimate goal of our development of this approach to large-scale shell model studies.

1. Introduction

The last few decades have witnessed a rapid growth in the capabilities of the Configuration Mixing Shell Model to treat complex atomic nuclei. Large-scale calculations with exact diagonalization can now be carried out for most of the nuclei in the $1f - 2p$ shell using sophisticated shell-model codes such as CMichSM, MSHELL, NATHAN, RedStick and the publicly available ANTOINE. Ideally one would like to extend the scope of shell-model calculations to even heavier nuclei. But with an exponentially increasing configuration space, any computational improvements realized in the foreseeable future might still be insufficient for larger calculations beyond the $1f - 2p$ shell. Over the years, a variety of approximate truncation strategies have been developed to address this limitation of the shell-model algorithm. One such method is provided by the Density Matrix Renormalization Group (DMRG), a method first introduced [1] for the study of quantum lattices and subsequently extended to finite Fermi systems [2]. In this context it has been suggested as a possible approach for use with the nuclear shell model. In this work, we focus on an issue crucial to its possible applicability to larger nuclear systems, how the method scales with the size of the shell-model problem.

2. Background and Motivation

The DMRG is a method for systematically including the degrees of freedom of a many-body problem. The algorithm begins by partitioning the complete space of the problem in terms of...
lattice sites, with each site hosting a small fraction of the complete space. In the nuclear context, these sites represent single-particle orbitals. The basic idea of the method is to systematically grow the system to include an additional site. At each stage of the iterative growth procedure, a truncation of the states in this enlarged system (called a block) is implemented through the use of density matrix considerations based on their importance within the complete space. The method is constructed so that the optimal set of states within each block is iteratively updated by sweeping over the various sites until convergence is achieved. For a comprehensive review of the DMRG procedure, we refer the reader to ref. \[2\].

The DMRG when applied to atomic nuclei has somewhat unique features, especially when compared with its more typical applications both to quantum lattices and in quantum chemistry. On the one hand, the fact that the lattice sites appropriate for nuclear applications are single-particle orbitals implies that they can have varying sizes, and this leads to computational difficulties in their iterative treatment. A second key difference is the presence of two kinds of fermions, making the choice of an appropriate order in which to iteratively include the associated orbitals more challenging. Our earlier applications of the DMRG methodology have addressed these issues and have come up with an optimal algorithm for their treatment. The algorithm we have adopted, the J-DMRG, also has the feature that it conserves angular momentum throughout the iterative procedure. A description of the algorithm we have developed and the associated terminology can be found in refs. \[3, 4\].

In our earlier applications of the J-DMRG method \[5, 6\], we focussed on two specific even-even nuclei in the $1f-2p$ shell, $^{48}$Cr and $^{56}$Ni. Those calculations indicated that the J-DMRG method indeed converges smoothly to the exact results for both nuclei and furthermore that the method seems to be scaling well with the size of the problem. In the current work, our goal is to see whether those results carry over to a broader range of nuclei and furthermore to better assess the scalability of the method. Towards that end we will discuss the application of the DMRG method to a wide range of nuclei in the $1f-2p$ shell, both even-even and with odd mass. We will assess how rapidly the method converges for these different types of nuclei and also how scalable is the method as a function of the size of the full shell-model problem.

In the course of the study, we will also address other issues that were hinted at by our earlier investigations. One concerns which state or states of the full space to use in implementing the density matrix truncation algorithm. It is typical to focus on just the ground state and to build a reduced density matrix derived from that state only. Here we address the issue of whether it is better to include information on selected excited states as well by introducing mixed density matrices to define the optimal structure of each block.

3. **General features of our calculational apparatus**

All of the calculations to be described later are for nuclei in the $1f-2p$ shell. In all, we assume a description in terms of valence neutrons and protons outside a doubly-magic $^{40}$Ca core and restricted to the orbitals of that one major shell. The effective hamiltonian we use is based on the GXPF1A effective two-body interaction first proposed in reference \[7\], with the same set of single-particle energies as used in that work as well. This effective hamiltonian is known to provide a somewhat better description of nuclei in this region than the KB3 hamiltonian \[8\] used in our earlier investigations.

In all the calculations reported here, we use the so-called three-block growth strategy adopted in our earlier studies. The key features of this strategy are that (i) when we order our single-particle orbitals into a chain, we keep those for neutrons on one side of the chain and those for protons on the other side, and (ii) as we grow the system we only build blocks from orbitals of the same type. It was found in our earlier studies that this growth strategy has significant computational advantages to the more-traditional two-block approach in which mixed neutron-proton blocks would be constructed as well.
The order of orbitals used in all of the calculations reported herein are as illustrated in Figure 1. This has the feature that the maximally entangled orbits, the $1f_2^2$ and $2p_2^2$, are next to one another as is known to be important based on information theory considerations [9].

4. Calculations for the ground states of even-even nuclei
We first present results for the various even-even nuclei that we have studied, $^{48}\text{Cr}$, $^{50}\text{Cr}$, $^{52}\text{Fe}$, $^{54}\text{Fe}$ and $^{56}\text{Ni}$, focusing for now on their ground states only. In Table I, we compare the results of J-DMRG calculations with the exact ground state energies as a function of the parameter $m$ that defines how many states are retained in each block.

For $^{48}\text{Cr}$, we observe smooth convergence to the exact ground state energy as we increase the number of states $m$ retained. However, to achieve this level of accuracy we must retain roughly a quarter of the total number of 41,355 $J^\pi = 0^+$ shell-model configurations for the system. Even to get reproduction of the exact results to within about 60 keV requires of order 20% of the full space.

$^{50}\text{Cr}$, with two additional neutrons, displays similar features, likewise converging smoothly to the exact result with $m$ and likewise requiring almost 20% of the full space to obtain agreement to within roughly 60 keV.

Next we consider $^{52}\text{Fe}$, for which the full dimensionalities are much larger. Here the total number of $0^+$ configurations is 1,777,116. Once again the J-DMRG procedure converges smoothly to the exact result with increasing $m$. Here a calculation with $m = 200$, containing roughly 4% of the full space, was able to achieve agreement with the exact ground state energy to within 60 keV. $^{52}\text{Fe}$ is the largest even-even nucleus that can be solved exactly with the public version of the shell-model code ANTOINE.

Next we turn to $^{54}\text{Fe}$ which has an even larger space, containing 5,220,621 $J^\pi = 0^+$ states. Here too we see monotonic convergence with $m$. Furthermore, we find that to be able to achieve accuracy to within roughly 60 keV we now need roughly 3% of the full space.

Finally, we turn to $^{56}\text{Ni}$, which had been treated earlier, albeit with the KB3 hamiltonian. Here too we see smooth and rapid convergence to the exact results, with substantially less than 1% of the space required to achieve agreement to within 60 keV.

In Figure 2, we summarize results for the even-even nuclei $^{48}\text{Cr}$, $^{50}\text{Cr}$, $^{52}\text{Fe}$ and $^{56}\text{Ni}$, focussing on the number of states needed to obtain 60 keV accuracy as a function of the logarithm of the size of the shell-model basis. We also include a quadratic fit to the results. By extrapolating this fit, we conclude that the method can be used to treat systems with well in excess of $10^9$ $0^+$ configurations, using DMRG matrices of at most a few hundred thousand states.
Table 1. Calculated ground-state energies in MeV as a function of $m$ for several even-even nuclei in the $1f-2p$ shell. The maximum dimensions encountered in the sweep process are also given.

| $^{48}$Cr | $m$ | $E_{GS}$ | Max Dim |
|-----------|-----|---------|---------|
| 100       | -99.475 | 4,554 |
| 120       | -99.495 | 6,361 |
| 140       | -99.514 | 8,377 |
| 160       | -99.560 | 9,996 |
| 180       | -99.573 | 10,906 |
| Exact     | -99.578 | 41,355 |

| $^{50}$Cr | $m$ | $E_{GS}$ | Max Dim |
|-----------|-----|---------|---------|
| 100       | -122.807 | 34,454 |
| 120       | -122.814 | 42,669 |
| 140       | -122.821 | 51,408 |
| 160       | -122.839 | 62,440 |
| 180       | -122.850 | 73,830 |
| 200       | -122.873 | 83,393 |
| Exact     | -122.877 | 267,054 |

| $^{52}$Fe | $m$ | $E_{GS}$ | Max Dim |
|-----------|-----|---------|---------|
| 120       | -151.945 | 33,377 |
| 140       | -151.948 | 39,501 |
| 160       | -151.988 | 50,578 |
| 180       | -152.012 | 62,277 |
| 200       | -152.069 | 72,317 |
| Exact     | -152.129 | 1,777,116 |

| $^{54}$Fe | $m$ | $E_{GS}$ | Max Dim |
|-----------|-----|---------|---------|
| 140       | -175.653 | 123,639 |
| 160       | -175.656 | 141,397 |
| 180       | -175.665 | 168,026 |
| 200       | -175.680 | 198,253 |
| Exact     | -175.730 | 5,220,621 |

| $^{56}$Ni | $m$ | $E_{GS}$ | Max Dim |
|-----------|-----|---------|---------|
| 100       | -205.643 | 87,633 |
| 120       | -205.651 | 106,383 |
| 140       | -205.652 | 123,196 |
| 160       | -205.659 | 139,966 |
| 180       | -205.661 | 166,695 |
| 200       | -205.670 | 199,274 |
| Exact     | -205.709 | 15,443,684 |
The figure does not include our results for $^{54}$Fe, which as noted earlier we also treated but which lies somewhat above the curve. We have concluded that this is most likely a reflection of the difference in the number of active protons and neutrons in this case. We have found, however, that this can be improved substantially by choosing different $m$ values for neutron and protons, scaled in proportional to their respective number of $(nJ)$ partitions. In particular, if we assume the same number of partitions for both, we find that the fraction required for 60 keV accuracy is 0.031. When we scale $m_n$ and $m_p$ in accord with the relative number of neutron and proton partitions, respectively, the fraction goes down to 0.021. Such a procedure, which is now fully implemented in our J-DMRG algorithm, can be used for any problem with a different number of active neutrons and protons. Indeed, it is possible to improve our treatment even further through the use of a fully dynamical procedure for choosing $m$ values in a sweep [3].

**Figure 2.** Number of states required for 60 keV accuracy in DMRG calculations of even-even nuclei

5. Calculations for the ground states of odd-mass nuclei
In Table 2, we present the corresponding ground-state results for the odd-mass nuclei that we have studied, $^{47}$Cr, $^{49}$Cr, $^{51}$Fe, $^{53}$Fe and $^{55}$Ni.

For $^{47}$Cr, the results converge smoothly as a function of $m$ and we can achieve accuracy to within 25 keV. However, to achieve this level of agreement, we require inclusion of over 40% of the full space. In $^{49}$Cr, the convergence is again smooth and we achieve reproduction of the exact
Table 2. Calculated ground-state energies in MeV as a function of \( m \) for some odd-mass nuclei in the \( 1f - 2p \) shell. The maximum dimensions encountered in the sweep process are also given. The exact results for \(^{55}\text{Ni}\) were extracted from [10].

| \(^{47}\text{Cr}\) | \( m \) | \( E_{GS} \) | Max Dim |
|-----------------|------|---------|--------|
| 30              | -83.722 | 12,229  |
| 40              | -83.735 | 12,567  |
| 50              | -83.749 | 13,455  |
| 60              | -83.754 | 15,914  |
| 70              | -83.757 | 18,578  |
| Exact           | -83.780 | 41,498  |

| \(^{49}\text{Cr}\) | \( m \) | \( E_{GS} \) | Max Dim |
|-----------------|------|---------|--------|
| 60              | -110.099 | 56,305  |
| 80              | -110.103 | 71,268  |
| 100             | -110.113 | 90,859  |
| 120             | -110.119 | 110,785 |
| Exact           | -110.169 | 595,314 |

| \(^{51}\text{Fe}\) | \( m \) | \( E_{GS} \) | Max Dim |
|-----------------|------|---------|--------|
| 60              | -136.286 | 161,315 |
| 80              | -136.297 | 230,126 |
| 100             | -136.306 | 217,328 |
| Exact           | -136.409 | 3,998,059 |

| \(^{53}\text{Fe}\) | \( m \) | \( E_{GS} \) | Max Dim |
|-----------------|------|---------|--------|
| 50              | -162.484 | 307,968 |
| 60              | -162.528 | 319,970 |
| 70              | -162.537 | 333,996 |
| Exact           | *     | 21,131,892 |

| \(^{53}\text{Ni}\) | \( m \) | \( E_{GS} \) | Max Dim |
|-----------------|------|---------|--------|
| 50              | -189.412 | 450,916 |
| 70              | -189.426 | 529,911 |
| 90              | -189.435 | 663,686 |
| Exact           | -189.534 | 63,268,915 |

result to within 50 keV using roughly 20\% of the full space. In comparison to their even-even neighbors, \(^{48}\text{Cr}\) and \(^{50}\text{Cr}\), the convergence is slightly slower. For \(^{51}\text{Fe}\) and \(^{53}\text{Fe}\), convergence is still smooth and the fraction of the full full space required to achieve accurate reproduction of the exact energies goes down rapidly.

\(^{55}\text{Ni}\) is the largest odd-mass calculation we report here, with the full space having a dimension of 63,268,915 states. While the results indeed converge smoothly, we are unable to achieve agreement to better than 100 keV in this case.

Note that in all of these nuclei, there are slightly different number of active neutrons and protons. The above results, which are based on equal \( m \) values for both neutrons and protons,
could be improved slightly by scaling them according to the relative numbers of partitions.

As for even-even systems, the fraction of the space required for a fairly high level of accuracy is seen to go down rapidly with the size of the problem. Though the results are not as striking as for even-even nuclei, they are still suggestive that we can go to somewhat larger odd-mass systems with the J-DMRG method.

6. Excited states

Once an optimal block structure has been determined, even if from properties of the ground state only, we can still use it to estimate excited states. To do this we simply couple the optimal blocks together to the desired angular momentum and then diagonalize the resulting hamiltonian.

We illustrate the results that would emerge from such a prescription for the lowest two $0^+$ states in $^{56}$Ni in Table 3. We also include for comparison the exact energies. What we see is that not surprisingly the description of the ground state is better than the description of the first excited $0^+$ state.

It is possible, however, to introduce a mixed density matrix in which we find the optimal block structures required to simultaneously describe more than one state. This at least in principle should enable us to get a comparable description of several states at the same time. In Table 4, we show results again for the two lowest $0^+$ states in $^{56}$Ni, this time targeting both states equally in building the requisite reduced density matrices. Now the description of the second $0^+$ state improves dramatically (by roughly 850 keV), without a significant loss of accuracy for the ground state.

Using the mixed density matrices that emerge from this and other calculations, we have evaluated other low-lying excited states in the various even-even nuclei we have treated, but we do not show those results here. In a more elaborate scheme, different weights, determined a priori or dynamically, could be associated with the different excited states to construct the

| $m$ | $E_{0_1^+}$ | $E_{0_2^+}$ |
|-----|-------------|-------------|
| 140 | -205.652    | -200.913    |
| 160 | -205.659    | -200.902    |
| Exact | -205.709    | -202.092    |

Table 3. Calculated energies for the ground state and the first excited $0^+$ state in $^{56}$Ni in MeV, for selected $m$ values. The calculations targeted the ground state alone to build the optimal block structures. The exact results are extracted from [11].

| $m$ | $E_{0_1^+}$ | $E_{0_2^+}$ |
|-----|-------------|-------------|
| 140 | -205.641    | -201.739    |
| 160 | -205.645    | -201.752    |
| Exact | -205.709    | -202.092    |

Table 4. Calculated energies for the ground state and the first excited $0^+$ state in $^{56}$Ni in MeV, for selected $m$ values. The calculations targeted both the ground state and the first excited $0^+$ state to build the optimal block structures. The exact results are from [11].
Table 5. Calculated $7/2^-_1$ and $3/2^-_1$ energies of $^{53}$Fe in MeV as a function of $m$. In the first set of results only the $7/2^-_1$ ground state was targeted. In the second set of results both the ground state and the first excited state were targeted.

| $m$ | $E_{7/2^-_1}$ | $E_{3/2^-_1}$ | $E_{7/2^-_1}$ | $E_{3/2^-_1}$ |
|-----|---------------|---------------|---------------|---------------|
| 50  | -162.528      | -161.546      | -162.484      | -161.735      |
| 60  | -162.530      | -161.606      | -162.528      | -161.743      |

mixed density matrix.

There is a useful feature that arises when treating odd-mass systems as compared to even-even systems. In even-even systems, there is a large disparity between the dimensions that arise in calculations of the ground state and most low-lying excited states, notably those that do not have spin and parity $0^+$. It is for that reason that we targeted the ground state and the first excited $0^+$ state of $^{56}$Ni when we built mixed density matrices to improve our excited-state description. In odd-mass nuclei, the ground state and other low-lying excitations typically have similar dimensions and thus can be targeted simultaneously with no great computational burden. As such, we have been able to use mixed density matrices more effectively for odd-mass nuclei than for their even-even neighbors [3]. As an example, we illustrate in Table 5 our results for both the ground state and the first excited state of $^{53}$Fe. The first set of numbers arise when we target the $7/2^-_1$ ground state only in our truncation algorithm. The second set derives when we simultaneously target both the ground state and the first excited $3/2^-_1$ state. Targeting both lowers the $3/2^-_1$ state by almost 140 keV with essentially no impact on the energy of the ground state.

7. Summary and outlook

In this talk, we have summarized some of our most recent results obtained using the J-DMRG method for nuclei in the $1f - 2p$ shell. We reported systematic calculations of both even-even and odd-mass nuclei for nuclei ranging from $^{47}$Cr through $^{56}$Ni. Where possible, we compared with the results of exact diagonalization to assess the accuracy and applicability of the method. All calculations converged smoothly to the exact shell-model results. Furthermore, we found that the method scales very well with the size of the problem, with the fraction of the complete space required for a quantitative reproduction of the exact results going down rapidly with the full dimensionality. Though especially true for even-even systems, it was also found to be the case for odd-mass systems, albeit to a lesser extent. The fact that the fraction of the space goes down with the size of the problem bodes well for the future usefulness of the method in even larger shell-model problems.

We are also showed some first results to assess the usefulness of targeting more than just the ground state in the density matrix truncation algorithm. We found that such a method is particularly useful for odd-mass nuclei, where it is possible to simultaneously target several low-lying states with different values of the angular momentum.

There are several issues we are now exploring. One concerns how to treat even larger single-particle orbitals, as arise in heavier nuclei. We have developed a possible procedure for accomplishing this and preliminary application to the $g_{9/2}$ orbital in the Ni isotopes suggests it works well [3]. We are also in the process of including in our formalism the calculation of observables that relate the properties of neighboring nuclei, e.g. beta decay. Finally, we are also more systematically studying the usefulness of targeting more than just the ground state in the
density matrix truncation algorithm, especially for odd-mass nuclei.

The primary goal of this work has been to continue testing the J-DMRG method as a potentially practical dynamical truncation strategy for large-scale shell-model calculations of atomic nuclei. The results reported here are quite promising. Once we are able to implement the few improvements suggested above, we expect to be in position for many useful applications of the method to problems of contemporary importance in nuclear structure physics.

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