THE DENSITY MATRIX RENORMALIZATION GROUP AND THE NUCLEAR SHELL MODEL*

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We summarize the current status of a program to develop an angular-momentum-conserving variant of the Density Matrix Renormalization Group method into a practical truncation strategy for large-scale shell model calculations of atomic nuclei. Following a brief description of the method, we report the results of systematic test calculations for both even–even and odd-mass nuclei in the $2p$–$1f$ shell. In all, the nucleons are limited to the orbitals of the $2p$–$1f$ shell and interact via the GXPF1A interaction. The calculations systematically converge to the exact diagonalization results, where available. Most importantly, the fraction of the complete space required to achieve a high level of agreement is found to go down rapidly as the size of the full space grows.

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1. Introduction

In the traditional nuclear shell model, the low-energy structure of a nucleus is described by assuming an inert doubly-magic core and diagonalizing the effective nuclear Hamiltonian in an active space involving at most a few major shells. Despite the enormous truncation inherent in this approach, the method can still be only applied in very limited nuclear regimes. For most nuclei, further truncation is required to reduce the number of shell-model configurations to a manageable size.

An attractive truncation possibility is provided by the Density Matrix Renormalization Group (DMRG), a method introduced for low-dimensional quantum lattices [1] and later extended to finite Fermi systems. In the latter

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context, it has been applied to a variety of different strongly-correlated systems with great success [2]. This suggests that it might also prove useful as a dynamical truncation strategy for obtaining accurate approximate solutions to the nuclear shell model.

The DMRG method involves a systematic inclusion of the degrees of freedom of the many-body problem. When treating quantum lattices, real-space sites are included iteratively. In finite Fermi systems, these sites are replaced by single-particle levels. At each stage, the system (referred to as a *block*) is enlarged to include an additional site or level. This enlarged block is then coupled to the rest of the system (*the medium*) giving rise to the *superblock*. For a given eigenstate of the superblock or perhaps a group of important eigenstates, the reduced density matrix of the enlarged block in the presence of the medium is constructed and diagonalized and those eigenstates with the largest density eigenvalues are retained.

This process of systematically growing the system and determining the optimal structure within that enlarged block is carried out iteratively, by sweeping back and forth through the sites, at each stage using the results from the previous sweep to define the medium. Through this process, information on each block is iteratively updated until convergence from one sweep to the next is achieved. Finally, the calculations are carried out as a function of the number of states retained in each block, until the changes are acceptably small.

The traditional DMRG method, when applied in nuclei and elsewhere, works in a simple product space, whereby the enlarged block is obtained as a product of states in the block and the added site and likewise the superblock is obtained as a product of states in the enlarged block and the medium. In the nuclear context, this is equivalent to working in the m-scheme. A limitation of this algorithm is that it does not necessarily preserve symmetries throughout the iterative process. Since the density matrix procedure involves a truncation at each of the iterative stages, there is a potential to lose these symmetries and the associated correlations. For this reason, we proposed [2] the adoption of a strategy whereby angular momentum is preserved throughout the DMRG process. This method, called the JDMRG, was first applied in nuclear physics in the context of the Gamow Shell Model [3], where it was also tested extensively [4]. It was subsequently developed for application to the traditional shell model by Pittel and Sandulescu [5], where a first test application to ^{48}Cr was reported.

We have now dramatically improved the JDMRG algorithm, to the point where it can be applied to significantly heavier nuclei. The first such application was reported by Thakur, Pittel and Sandulescu [6] for ^{56}Ni. In this presentation, we report systematic test results for nuclei throughout the $2p$–$1f$ shell, including both even–even and odd-mass systems. Many of the new results have been reported recently in the PhD thesis of Thakur [7].

An outline of the paper is as follows. In Sec. 2, we provide an overview of the DMRG method including a discussion of the changes required to preserve angular-momentum conservation throughout. In Sec. 3, we report extensive test calculations of the method for both even–even and odd-mass nuclei in the $2p$–$1f$ shell. Finally in Sec. 4, we summarize the principal conclusions of this work and outline some of the work currently under investigation.

2. An overview of the DMRG method

2.1. DMRG truncation strategy

The DMRG method is based on an iterative inclusion of the degrees of freedom of the problem, represented as a chain of sites on a lattice (see Fig. 1).

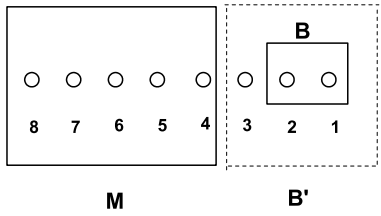

Fig. 1. Schematic illustration of the DMRG growth procedure. A block (B) consisting of sites 1 and 2 is enlarged to include site 3, forming B′. The medium (M) consists of all remaining sites.

Assume that we have treated a group of these sites, referred to as the block and denoted B, and that we have retained a total number of states m within that block. We now wish to add to this block the next site, which we assume contains l states, thereby producing an enlarged block B′. For the moment, we will assume a product (or m-scheme) description, so that the enlarged block has $m \times l$ states

$$|i,j\rangle_{\mathrm{B}'} = |i\rangle_{\mathrm{B}}|j\rangle_{l}\,, \qquad i = 1,m\,, \qquad j = 1,l\,. \tag{1}$$

As typical in Renormalization Group methods, we would like to retain m states for the enlarged block, the same number as before the enlargement. How can we choose them in an *optimal* way?

In the DMRG method, we consider the enlarged block in the presence of a medium (M) that reflects all of the other sites of the system, referring to the full system as the superblock (SB). Assuming that the medium is likewise described by m states, the $m \times l \times m$ states of the superblock can be expressed as

$$|i,j,k\rangle_{\mathrm{SB}} = |i,j\rangle_{\mathrm{B}'}|k\rangle_{\mathrm{M}}\,. \tag{2}$$

We then diagonalize the full Hamiltonian of the system in the superblock, for now isolating on its ground state (GS)

$$|\mathrm{GS}\rangle_{\mathrm{SB}} = \sum_{i,j,k} \Psi_{ijk} |i,j,k\rangle_{\mathrm{SB}} \,. \tag{3}$$

If we construct the reduced density matrix of the enlarged block in the GS,

$$\rho_{ij,i'j'} = \sum_{k} \Psi^{*}_{ijk} \Psi_{i'j'k} \,, \tag{4}$$

diagonalize it and retain the m eigenstates with the largest eigenvalues we are *guaranteed* to have the m most important (or optimal) states of the enlarged block in the ground state (3) of the superblock.

It is straightforward to target a group of states of the system by constructing a mixed density matrix that contains information on all of them.

Once the optimal m states are chosen, we renormalize all required operators of the problem to the truncated space and store this information. This includes all sub-operators of the Hamiltonian, *viz.*: $a_i^\dagger$, $a_i^\dagger a_j$, $a_i^\dagger a_j^\dagger$, $a_i^\dagger a_j^\dagger a_k$, $a_i^\dagger a_j^\dagger a_k a_l$, + h.c. Having this information for the block and the additional level or site enables us to calculate all such matrix elements for the enlarged block as needed in the iterative growth procedure.

2.2. Steps of the DMRG method

With this as background, the DMRG procedure involves the following steps.

2.2.1. Choice of an order for the sites

Given a Hamiltonian and the set of sites on which it is to act, we need to define an order in which the sites are going to be iteratively included.

2.2.2. The warmup stage

The iterative process begins with a *warmup stage*, in which we make an initial guess on the optimal m states for each possible block that can be constructed. In our treatment, we do this by gradually growing blocks from each side of the chain, using those orbits already treated on the other end as the medium. This is illustrated in Fig. 2 for the enlargement of the right block from 2 to 3 sites, in the presence of a medium involving the two-site left block previously treated.

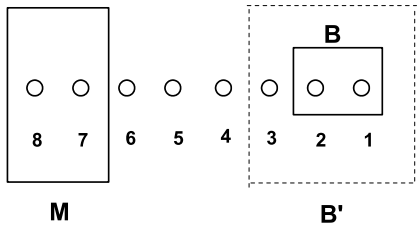

Fig. 2. Schematic illustration of the warmup stage as used in the calculations reported herein.

2.2.3. The sweep stage

Next, we gradually *sweep* through the sites of the chain, using for the medium the results either from the warmup phase in the first sweep or from the previous sweep stage. The sweeping process is done over and over until convergence is achieved from one sweep to the next.

2.2.4. As a function of m

The warmup and sweep steps are done for a given m. The calculations are then carried out as a function of m, until the changes that result are acceptably small.

2.3. The JDMRG approach

As noted earlier, most DMRG algorithms violate symmetries. In nuclei, for example, they typically work in the m-scheme. When imposing truncation in such a procedure, however, it is difficult to ensure that the states retained contain all the components required by the Clebsch–Gordan series to build states of good angular momentum. We have therefore chosen to use an angular-momentum-conserving variant of the DMRG method (called the JDMRG) in which angular momentum is preserved throughout the growth, truncation and renormalization stages.

The JDMRG approach follows the traditional DMRG approach outlined above in most respects. The most significant change is that now we must calculate and store throughout the iterative process the *reduced matrix elements* of all sub-operators of the Hamiltonian, as can be done using standard Racah algebra methods.

2.4. A three-block JDMRG strategy

In the calculations we report, we have adopted a three-block strategy for the enlargement and truncation process. The basic ideas are summarized in Fig. 3.

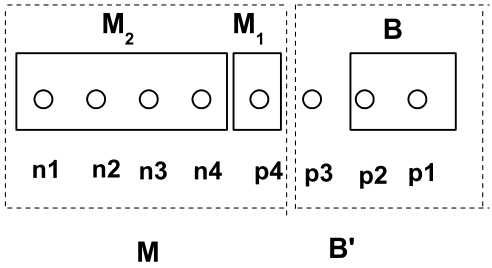

Fig. 3. Schematic illustration of the three-block DMRG growth procedure for a system with neutron and proton levels.

We begin by choosing our order of sites so that neutron and proton orbitals sit on opposite ends of the chain. We then gradually grow blocks of each type of particle only, namely we grow neutron blocks and proton blocks but no mixed blocks. Lastly, in the sweep stage we go to and fro through the orbits of a given type of particle only. The medium in this approach involves two components. When enlarging a proton block, as in the figure, the full medium (M) involves all of the remaining proton levels and all of the neutron levels.

This strategy, first proposed in Ref. [2], has been found to be computationally more efficient than the two-block approach that is customarily implemented when dealing with systems involving two types of particles.

3. Calculations

We have carried out systematic test calculations of the JDMRG method on both even–even and odd-mass nuclei in the $2p$–$1f$ shell through ^{56}Ni. We assume that these nuclei can be described in terms of valence neutrons and valence protons outside a doubly-magic ^{40}Ca core interacting via the GXPF1A effective shell-model Hamiltonian [8]. All calculations were carried out assuming the ordering of single-particle levels shown in Fig. 4.

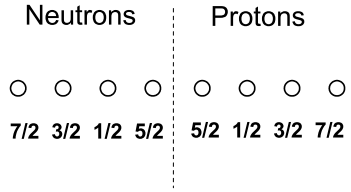

Fig. 4. Order of single-particle levels assumed in all calculations reported herein.

3.1. Results for even–even nuclei

Table I summarizes our results for the ground state of ^{48}Cr, with four active neutrons and four active protons. For this system the size of the full shell-model space contains 1,963,461 states, of which 41,355 are 0^+ states, 182,421 are 2^+ states, *etc.*

TABLE I

Results for the energy in MeV of the ground state of ^{48}Cr from JDMRG calculations. Max dim. refers to the maximum dimension of the superblock.

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

Our calculations converge smoothly to the exact ground state energy as m is increased, but require the inclusion of a substantial fraction of the full space to obtain a high level of accuracy. To achieve an accuracy of 50 keV, for example, we require roughly 20% of the full 0^+ space.

Next we turn to ^{56}Ni, the largest even–even calculation we have performed to date. Here the full space in the m-scheme contains 1,087,455,228 states. In an angular momentum basis, the number of 0^+ states is 15,443,684, the number of 2^+ states is 71,109,189 and the number of 4^+ states is 105,537,723.

The results for the ground-state energy as a function of m are shown in Table II, again in comparison with the exact result [9]. Here we are able to achieve roughly 60 keV accuracy with well below 1% of the full 0^+ space.

TABLE II

Results for the energy of the ground state of ^{56}Ni in MeV from JDMRG calculations. Max dim. refers to the maximum dimension of the superblock.

m	E_{GS}	Max dim.
80	−205.632	74,677
120	−205.651	106,383
160	−205.659	139,966
200	−205.670	199,274
Exact	−205.709	15,443,684

In Table III, we present the corresponding results for the lowest excited states, obtained using the blocks that derive from the ground state optimization. The results are clearly improving with m, but slowly. The agreement for $m = 100$ is not as good as we would like. We can improve the agreement for these states, without affecting significantly the description of the ground state, by targeting the ground state and the first excited 0^+ state through the use of a mixed density matrix [7].

TABLE III

Results for the energies in MeV of the lowest excited states from JDMRG calculations for ^{56}Ni. Dim. refers to the dimension of the superblock Hamiltonian.

m	$E_{2_1^+}$	(Dim.)	$E_{4_1^+}$	(Dim.)
60	2.977	(296,633)	4.137	(445,898)
80	2.944	(354,213)	4.123	(556,572)
100	2.942	(423,265)	4.090	(701,502)
Exact	2.600	(71,109,189)	3.688	(105,537,723)

In Fig. 5, we summarize our results for the even–even nuclei ^{48}Cr, ^{50}Cr, ^{52}Fe and ^{56}Ni, focusing on the number of states needed to obtain 60 keV accuracy as a function of the logarithm of the total size of the shell-model basis. We also include a quadratic fit to the results. Based on extrapolation of 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.

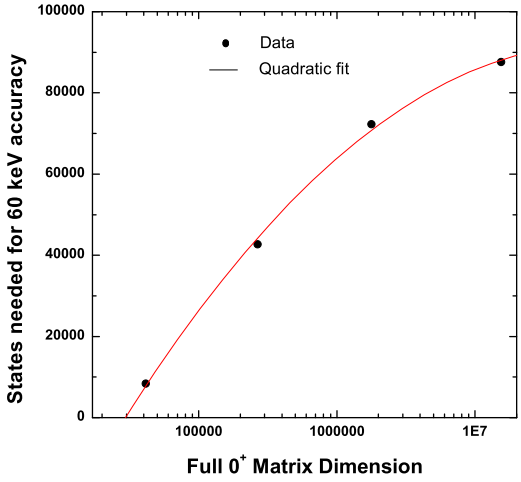

Fig. 5. Number of states required for 60 keV accuracy in DMRG calculations of even–even nuclei.

The figure does not include our results for ^{54}Fe, which 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 partitions, the fraction goes down to 0.021. Such a procedure, which is now fully implemented in our JDMRG 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 [7].

3.2. Results for odd-mass nuclei

We have also carried out test calculations on odd-mass nuclei in the same region of the $2p$–$1f$ shell. In Table IV we show the fraction of the space required to achieve a high level of accuracy for the ground state energies of ^{47}Cr, ^{49}Cr, ^{51}Fe and ^{55}Ni [10]. We also carried out calculations for ^{53}Fe but do not show those results since we do not have the exact ground state energy for that system. In all of these calculations, we have used the same value of m for both neutrons and protons despite differences in their respective numbers of partitions.

TABLE IV

Fraction of the full space required to achieve a high level of accuracy in the description of the ground state energy of odd-mass nuclei using the JDMRG method. Δ_E indicates the agreement achieved. Also shown are the m value at which this level of agreement was reached, the fraction of the full space required and the dimension of the full space. All energies are given in MeV.

Nucleus	m	Δ_E	Fraction	Dimension
^{47}Cr	40	0.058	0.295	(41,498)
^{49}Cr	120	0.056	0.153	(595,314)
^{51}Fe	100	0.095	0.056	(3,998,059)
^{55}Ni	90	0.099	0.010	(63,268,915)

Note that in the two heaviest nuclei we have treated we were only able to achieve accuracy to roughly 100 keV, because of the increased dimensionality. Odd-mass nuclei invariably have larger dimensions for their ground states than the neighboring even–even nuclei because of their non-zero angular momenta.

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 good as for even–even nuclei, they are still suggestive that we can go to somewhat larger odd-mass systems with the JDMRG method.

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 dimensionalities that arise in calculations of the ground state and (most) low-lying excited states, since most low-lying excitations 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 dimensionalities 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 [7].

4. Summary and outlook

In this paper, we have summarized the current status of our efforts to build the Density Matrix Renormalization Group Method into a practical dynamical truncation strategy for large-scale shell-model calculations of atomic nuclei. Following an overview of the essential features of the method, we discussed the changes we had to implement for its application to nuclei. Most importantly, we found it useful to develop an angular-momentum conserving version of the method, the JDMRG. We then summarized the principal results we have obtained to date with this method. We reported test calculations for both even–even and odd-mass nuclei in the $2p$–$1f$ shell 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. Most importantly we found that the problem 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. This was especially true for even–even systems, and to a lesser extent for odd-mass systems. 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.

There are several issues we are now in the process of exploring. One concerns how to treat the even larger single-particle orbitals that arise in the treatment of 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 [7]. We are also in the process of

including the calculation of other observables with the JDMRG. We have already applied it to electromagnetic observables and are now in the process of adapting the formalism to study observables that relate the properties of neighboring nuclei, *e.g.* beta decay. 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 where we can readily target several low-lying states.

Once these final stages have been fully implemented and tested, we expect to be in a position for many interesting applications of the method to problems of contemporary importance in nuclear structure physics.

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