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The density matrix renormalization group and nuclear structure

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We briefly review the Density Matrix Renormalization Group (DMRG) method and its potential use in large-scale nuclear shell-model calculations. We propose the use of an angular-momentum-conserving variant of the method (the JDMRG) and report the first test results of such an approach for the nucleus ^{48}Cr. The positive results of these calculations have motivated us to search for an even more efficient means of implementing the JDMRG strategy and the status of these efforts is also described.

Keywords: Shell model; renormalization group methods.

Se presenta un repaso del método DMRG y su posible aplicación en el modelo de capas nucleares. Se propone una versión del método que conserve el momento angular (JDMRG) y se discuten los primeros resultados para el núcleo ^{48}Cr. El éxito de estos calculós nos ha motivado buscar un método aún más efeciente para los cálculos JDMRG. Se describe brevemente el estatus de este esfuerzo.

Descriptores: Modelo de capas; métodos del grupo de renormalización

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1. Introduction

In this presentation, we describe an approach aimed at obtaining accurate solutions to the nuclear shell-model problem in cases where exact diagonalization is not feasible. The method is based on the use of the Density Matrix Renormalization Group (DMRG).

The DMRG was first introduced by White [1] in the early 1990s to treat quantum lattices through the iterative inclusion of real space lattice sites. Following the demonstration that it could describe lattice properties with extremely high precision, the method was subsequently reformulated to replace real-space lattice sites by energy (or momentum) levels. In this context, the method has proven very useful in describing a wide variety of finite Fermi systems (see ref. [2] for several recent reviews). These successes suggest the possible use of the DMRG in the description of another finite Fermi system, the atomic nucleus. In this presentation, we review the progress we have recently made in our efforts to build the DMRG into a viable approximation scheme for large-space shell-model calculations. There have been several other efforts to apply the DMRG in nuclear structure physics, and these are reported in Ref. 3.

Other methods for approximately solving the nuclear shell model in very large spaces have also been reported recently. Perhaps most promising has been the Quantum Monte Carlo approach [4], for which the most ambitious application to date has been a shell-model description of the even Ba isotopes. The approach described here will hopefully prove competitive with these other methods.

2. Brief overview of the DMRG method

The DMRG, like other renormalization group (RG) algorithms, is a method for systematically taking into account all of the degrees of freedom of a problem without letting the problem get computationally out of hand. Assume that we have treated a set of L sites/levels and that the total number of states we have kept to describe them is m. We refer to that portion of the system as the *block*. We then add the next site or level, the $L+1^{st}$, which admits s states. If we assume that the states in the resulting enlarged block are products of those in the original block and the extra site/level, the enlarged block would contain $m \times s$ states. All RG algorithms implement a truncation of the states of the enlarged block to the same number m as before the block enlargement.

This process, which involves truncation and the associated renormalization of operators in the truncated space, is continued by adding the next site/level and again truncating to m states and iterated until all sites or levels have been treated. The calculation is performed as a function of m, until the change with m is acceptably small.

A key step in the procedure is to calculate at each step the matrix elements of all hamiltonian sub-operators,

$$a_i^\dagger, \quad a_i^\dagger a_j, \quad a_i^\dagger a_j^\dagger, \quad a_i^\dagger a_j^\dagger a_k, \quad a_i^\dagger a_j^\dagger a_k a_l, \quad +h.c.,$$

and store them. Having this information for the block and the additional level or site enables us to calculate all such matrix elements for the enlarged block.

In the numerical RG procedure introduced by Wilson to solve the Kondo problem, the truncation involves diagonalizing the hamiltonian in the $m \times s$-dimensional space of the enlarged block and retaining its lowest m eigenstates.

In the DMRG approach of White, the truncation is implemented through a very different procedure, schematically illustrated in Fig. 1a. Consider the enlarged block B' in the presence of a medium M that approximates the rest of the system. White's truncation is carried out based on the importance of the states of the enlarged block in a selected set of target states of the full *superblock, i.e.*, the states of B' coupled to M.

Assume here that we target only the ground state of the superblock hamiltonian in the truncation,

$$|\Psi_{gs}\rangle = \sum_{i=1,\ m\times s} \ \sum_{j=1,\ t} \Psi_{ij}\ |i\rangle_B\ |j\rangle_M\ ,$$

where t denotes the number of states of the medium. We construct the ground-state density matrix for the enlarged block,

$$\rho^B_{ii'} \ = \ \sum_{j=1,\ t} \Psi^*_{ij}\Psi_{i'j}\ ,$$

diagonalize it, and truncate to the m states with the largest density-matrix eigenvalues. This is guaranteed to provide an optimal approximation to the superblock ground state.

To target a group of states and not just the ground state, we would construct a mixed density matrix containing information on the block content of all of them.

So far, we have described the infinite DMRG algorithm, in which we pass through the set of sites or levels once. This works well if the correlations between layers fall off sufficiently fast. Usually they do not, however, since the truncation in early layers has no way of knowing about coupling to subsequent layers.

This limitation can be avoided by using a sweeping algorithm, whereby after going through the layers the first time we reverse direction and update the blocks based on results from the previous sweep. This is done iteratively until acceptably small change from one sweep to the next is achieved.

This improved method, known as the finite algorithm, requires a first pass through the levels, called the warmup stage. One possibility is to use Wilson's RG diagonalization strategy to get a first approximation to the optimal structure in the various size blocks. In nuclei, as in other finite Fermi systems, the DMRG approach with sweeping is required.

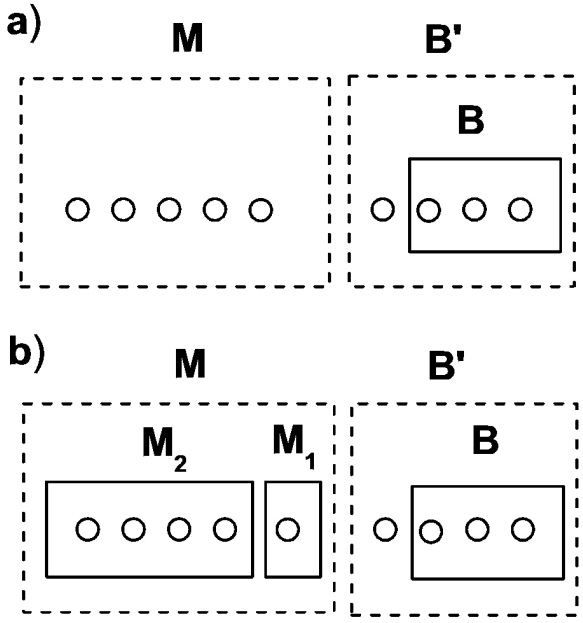

FIGURE 1. Schematic illustration of the DMRG growth procedure. (a) The standard two-block sweeping algorithm, with a block B that is enlarged to B' in the presence of a medium M. (b) A three-block algorithm, in which the medium M contains two components M_1 and M_2.

3. The JDMRG approach

Most DMRG approaches violate symmetries. In nuclei, for example, they typically work in the m-scheme. Such a procedure is potentially dangerous when imposing truncation, as 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. For this reason, we have chosen to develop an angular-momentum-conserving variant of the DMRG method in which angular momentum is preserved throughout the growth, truncation and renormalization stages. This method, which we refer to as the JDMRG, builds on earlier work by McCulloch and Gyulacsi [5], where it was shown that by not violating symmetries (*e.g.*, rotational symmetry) throughout the iterative process more accurate results could be realized with smaller bases.

In an angular-momentum-conserving approach we must instead calculate and store throughout the iterative process the *reduced matrix elements* of all sub-operators of the hamiltonian, namely

$$a^\dagger_i, \quad [a^\dagger_i \tilde{a}_j]^K, \quad [a^\dagger_i a^\dagger_j]^K, \quad \left([a^\dagger_i a^\dagger_j]^K \tilde{a}_k\right)^L,$$
$$\left([a^\dagger_i a^\dagger_j]^K \quad [\tilde{a}_k \tilde{a}_l]^K\right)^0 \quad + h.c.$$

This can be done using standard Racah algebra methods.

3.1. A three-block JDMRG strategy

In our first effort to build a JDMRG code for use in nuclear structure, we used a three-block strategy for density-matrix truncation during the sweep procedure (see Fig. 1b). In this strategy, we separate neutron from proton orbitals, rather than putting them in a single chain. As we grow the system for one type of particle, we carry out the truncation of that enlarged block in the presence of a medium containing the remainder of the orbits of that type of particle (a second block) and all of the orbits of the other type of particle (a third block).

Thus, the full medium in this strategy contains two components, denoted M_1 and M_2 in Fig. 1b. We initiate the process by growing the block for one type of particle in the presence of a medium that contains only the same set of orbits for the other type of particle. In this way, we bootstrap our way through the full set of orbits, generating the warmup information needed for the subsequent sweeping steps in which all orbits are included.

We have carried out a first set of test calculations of this three-block JDMRG code on the nucleus ^{48}Cr. As in the usual shell model approach, we assume that this nucleus can be described as four valence neutrons and four valence protons outside a doubly-magic ^{40}Ca core. We use the shell model hamiltonian KB3, for which exact results are available. The size of the full space for ^{48}Cr is 1,963,461 states. Of these, 41,355 are 0^+ states, 182,421 are 2^+ states, etc.

Our results for the ground state are presented in Table I. The exact calculation produces a ground state energy of $-32.95\ MeV$. The DMRG calculation with $m = 50$ produces a result of $-32.80\ MeV$, about $150\ keV$ from the exact result. In this case, the largest matrix that had to be diagonalized had a dimension of 3,657. The conclusion is that the three-block JDMRG algorithm gives a good reproduction of the exact results with a fairly small number of states retained in each block, but by calculating matrices with a substantial fraction of the full basis.

TABLE I. Results for the ground-state energy E_{GS} in MeV from the JDMRG calculations described in the text. *Max Dim* refers to the maximum dimension of the superblock hamiltonian matrix.

m	E_{GS}	$Max\ Dim$
20	-32.28	1,591
25	-32.47	1,893
30	-32.57	2,327
35	-32.66	2,685
40	-32.72	3,109
45	-32.76	3,403
50	-32.80	3,657
$Exact$	-32.95	41,355

Following convergence, we calculated excited states as well, using information on the optimized blocks. This requires much smaller matrices than the sweep process, since truncation has already been imposed. For $m = 50$, we obtain an excitation energy of the lowest 2^+ state of $0.84\ MeV$, to be compared with the exact result of $0.81\ MeV$. Thus, the method seems capable of producing reasonably accurate results for low-lying excited states as well, even when we target the ground state only.

3.2. A two-block JDMRG strategy

Our current efforts are focussed on replacing the three-block strategy described above with a more standard two-block strategy in which all single-particle orbits (neutrons and protons) are organized along a single chain and blocks containing both neutron and proton orbits are built. In such an approach (see Fig. 1a), there is but a single block in the medium, so that the size of the superblock scales as the square of the number of states in each block. This is to be compared with a cubic dependence in the three-block strategy previously used. This should enable us to significantly increase the number of states retained in a block for a given size of the full superblock matrix and could prove very helpful as we consider the application of these methods to heavier nuclei, the ultimate goal of the project. The code to implement this new JDMRG strategy is currently in its final throes of testing.

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