

Density Matrix Renormalization Group: a new method for large scale shell model calculations

J. Dukelsky¹, S. Pittel², G. Sierra³, S. Dimitrova⁴ and M. Stoitsov⁴⁻⁶

¹ *Instituto de Estructura de la Materia, CSIC, Serrano 123, 28006 Madrid, Spain.*

² *Bartol Research Institute, University of Delaware, Newark, DE 19716 USA.*

³ *Instituto de Física Teórica, CSIC/UAM, Madrid, Spain.*

⁴ *Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia-1784, Bulgaria,*

⁵ *Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831, USA*

⁶ *Department of Physics & Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA,*

⁷ *Joint Institute for Heavy-Ion Research, Oak Ridge, Tennessee 37831, USA.*

Abstract

We present the basic ideas of the Density Matrix Renormalization Group and report on recent efforts to apply it in large scale nuclear structure calculations.

1 Introduction

The shell model (SM) is one of the most powerful approaches for a microscopic description of the low energy spectroscopic properties of nuclei. Its basic assumptions are: a doubly magic inert core, an active valence space usually consisting of a major shell each for neutrons and protons, and an effective hamiltonian within the valence space. In spite of the severe truncations imposed by the model, it is still only possible to treat limited nuclei in this way, namely those for which the hamiltonian matrices have a maximum dimension of order $10^7 - 10^8$ and can be treated with Lanczos or Davidson codes. By exploiting the symmetries of the hamiltonian, like rotational invariance, it is possible to reduce the dimension of the hamiltonian matrix for 0^+ states by roughly two orders of magnitude relative to the m -scheme dimension. This is done, e.g., by the code NATHAN developed by Caurier and collaborators [1]. Current computer limitations allow for exact SM diagonalization through the f - p shell. However, since the hamiltonian matrix dimension increases exponentially with the number of single particle states, it is not feasible to implement

the SM for heavier nuclei without drastic truncation.

Other fields of physics dealing with strongly correlated fermion systems face the same limitations. For instance, in condensed matter it is believed that the Hubbard hamiltonian on a two dimensional lattice is the microscopic model of high T_c superconductivity. Exploiting all possible symmetries, large scale diagonalizations (LSD) can be performed for lattices up to 20 sites, which is too small to meaningfully extrapolate to the physics of large systems. Analogously, in Quantum Chemistry a full Configuration Interaction diagonalization is limited to very small molecules.

About a decade ago, a very successful approach for going well beyond the limits of LSD, called the Density Matrix Renormalization Group (DMRG), was proposed by White [2] to treat one-dimensional lattice systems. In a first numerical application, he was able to calculate the ground state energy of the spin-1 Heisenberg chain to 12 significant figures, making clear the great accuracy of the method. Subsequently, the procedure was generalized for application to other strongly correlated systems, like electrons in 2-dimensional lattices, quantum Hall systems, molecules and ultrasmall superconducting grains. Very recently we began a program to apply the method to nuclear structure. In the following sections, we briefly introduce the DMRG method and then present some preliminary results that illustrate our progress in adapting it to large scale nuclear structure calculations.

2 The Density Matrix Renormalization Group

The DMRG is an iterative numerical procedure for diagonalizing a hamiltonian matrix whose dimension largely exceeds the limits of LSD. The method is based on Wilson's Renormalization Group (WRG), which subdivides the many body Hilbert space in small portions - called layers - and systematically grows the system from an initial core by adding layer after layer until the complete system is taken into account. Let us assume that we have already taken into account a small piece of the system consisting of several layers, which we call the block. The block is described in terms of m states. Next we add another layer with s states to the block. The enlarged block will then have $m \times s$ states. The basic idea of the renormalization group is to implement a truncation to the most important m states and then to add another layer, continuing until all layers have been exhausted. At the end of the procedure, we have a description of the low lying states of the system in terms of m states. Ideally we would like to perform several calculations with increasing m , stopping when we reach the desired accuracy. Therefore, a central point in the renormalization group is to

establish a criterion for the selection of the most important m states among the $m \times s$ states of the enlarged block.

In WRG, one simply diagonalizes the hamiltonian in the enlarged block and retains the lowest m eigenstates, dropping the other $m \times (s - 1)$. WRG had great success in application to the Kondo model, because the coupling between successive layers in that model decays exponentially. However, it failed to describe accurately other strongly correlated lattice systems, like the Heisenberg and Hubbard models.

In the DMRG method, the idea is quite different. One considers the enlarged block immersed in a medium that approximates the rest of the system. The entire system is referred as the superblock. The hamiltonian of the superblock is diagonalized yielding the ground state (GS) wave function Ψ . Assuming that the medium is described in terms of t states, the GS wave function can be expanded as a product of the states of the enlarged block and of the medium,

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

We may ask: Which are the optimal m states in the enlarged block? By optimal we mean that the approximate wave function Ψ'

$$|\Psi'\rangle = \sum_{a=1, m} \sum_{j=1, t} \Psi'_{aj} |a\rangle_B |j\rangle_M \quad (2)$$

has the maximum overlap with the exact wave function Ψ .

The solution to this problem is well known from linear algebra:

a) Construct the reduced density matrix of the enlarged block, contracting over the states of the medium

$$\rho_{ij} = \sum_{k=1, t} \Psi_{ik}^* \Psi_{jk} \quad (3)$$

b) Diagonalize the density matrix to obtain a set of $m \times s$ eigenstates

$$\sum_j \rho_{ij} u_j^a = \omega_a u_i^a \quad (4)$$

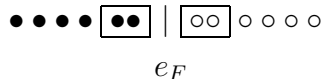
c) The eigenvalues of the density matrix give the probability of each state a in the full GS wave function Ψ . Thus, the DMRG prescription is to truncate to m states with the largest eigenvalues.

d) The corresponding m eigenvectors of the density matrix define a transformation to a truncated basis in which all operators, including the hamiltonian, should be expressed.

There are two important parameters that controls the accuracy of the procedure; the number of states m retained in each iteration and the probability of the discarded states defined as $1 - P_m = 1 - \sum_{a=1,m} \omega_a$.

3 The particle-hole DMRG

To now, we haven't established a procedure for constructing the block and the medium in each iteration. In finite Fermi systems, the Fermi energy separates the single particle states into a set that is mostly occupied (hole levels) from another mostly empty (particle levels). This can be viewed schematically as



where \circ denotes a particle level and \bullet denotes a hole level. In the particle-hole DMRG (p-h DMRG) one starts with the levels nearest to the Fermi energy, for example two particle levels and two hole levels, and then gradually adds to them levels farther away. The particle blocks serve as a medium for the hole blocks and the hole blocks serve as a medium for the particle blocks. The iterative procedure stops when all levels are treated.

One limitation of the present method is that in each iteration only the levels treated earlier are taken into account for implementing the truncation. In other words, the selection of the optimal states does not consider the coupling to the yet treated levels. Since the procedure starts at the Fermi energy, there is some hope that the correlations will decay with increasing distance from the Fermi energy and the effect of the levels not in the superblock can be neglected.

The first application of this methodology was carried out in the context of ultrasmall superconducting grains [3]. The model hamiltonian describing the physics of small grains is a pairing hamiltonian acting on a set of double degenerate single particle electronic states. The largest system we treated had 400 levels at half filling. The Hilbert space dimension of the hamiltonian matrix in the subspace of no broken pairs was 10^{119} . Keeping 60 states ($m = 60$) we obtained a ground state correlation energy $E_{GS} = -22.5168$ with a predicted relative error of 10^{-4} . Afterwards, we learned of an exact solution for the model given long ago by Richardson. For this specific case the exact energy is $E_{exact} = -22.5183$, confirming our results using the p-h DMRG.

In table I we show how the control parameters and the accuracy of the method evolve with increasing m for a system of 100 levels at half filling and with a pairing strength compatible with a well-defined superconducting regime. The matrix hamiltonian dimension of the Hilbert space in this case is 10^{29} .

| m | E_{GS} | dim | $1 - P_m$ |
|-----|-----------|------|-----------------------|
| 40 | -40.49884 | 1246 | 4.3×10^{-9} |
| 50 | -40.50014 | 2108 | 2.0×10^{-9} |
| 60 | -40.50061 | 3032 | 1.6×10^{-10} |
| 70 | -40.50068 | 3622 | 7.1×10^{-11} |
| 80 | -40.50072 | 4820 | 4.2×10^{-11} |
| 90 | -40.50074 | 6306 | 1.1×10^{-11} |
| 100 | -40.50075 | 7778 | 4.8×10^{-12} |
| 110 | -40.50075 | 9720 | 1.5×10^{-12} |

Table 1. Convergence properties of the p-h DMRG for a system with 100 levels. The first column gives the number of states m kept in each iteration, the second gives the ground state energy, the third gives the dimension of the largest superblock and the fourth gives the summed probability of discarded states.

The table clearly displays the variational character of the DMRG and the exponential convergence to the exact results with moderate computational effort, at least when the assumptions of the truncation approach are met by the model. as is the case of pairing. By looking at the Table we see that the first 7 significant figures in the correlation energy have converged by $m = 100$. The success of the p-h DMRG for this problem gave us hope that it might also work for problems in nuclear structure.

As a first test, we added to the pairing hamiltonian a quadrupole particle-hole interaction and studied the convergence properties of the p-h DMRG method in large single shell spaces [4]. For j shells as large as $99/2$ [5], we got similar convergence properties to the pairing model previously described.

As a first realistic application of the p-h DMRG in nuclear structure, we considered the nucleus ^{24}Mg with four protons and four neutrons in the $2s - 1d$ shell. In figure 1, we present the p-h DMRG results for the ground state and for the three lowest excites states as a function of the number of states retained m . It should be noted that the largest m for a full diagonalization without truncations is $m = 64$. The four energies indeed converge exponentially to the exact results, but the convergence is too slow for the method to be of practical use in light nuclei. Looking at the convergence properties of the angular momentum for the four states, we conclude that it is essential to conserve it in each iteration to significantly improve the accuracy of the procedure.

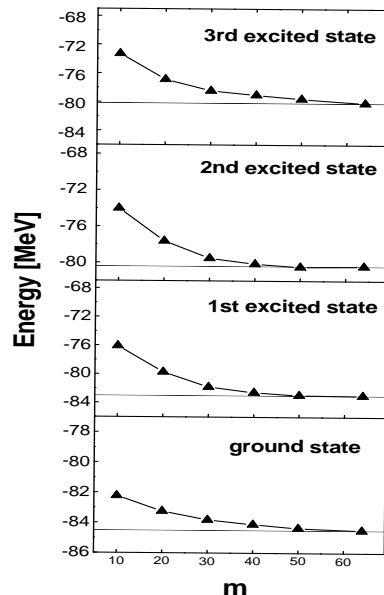


Fig. 1: Energies of the lowest four states in ^{24}Mg as a function of m . The horizontal lines refer to the exact results.

Currently, we are working on a new approach for applying the DMRG in nuclear structure [6]. The new procedure works in an angular momentum conserving basis. Furthermore, it implements a sweeping algorithm to overcome the aforementioned limitations of the one-way DMRG when correlations are not strongly concentrated around the Fermi surface. We hope that this new procedure, the J-DMRG, will provide a practical and efficient methodology for accurate large scale nuclear structure calculations.

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