Pittel, S.; Thakur, B.
The density matrix renormalization group and the nuclear shell model

The density matrix renormalization group and the nuclear shell model

S. Pittel and B. Thakur

Bartol Research Institute and Department of Physics and Astronomy,
University of Delaware, Newark, Delaware 19716, USA.

We summarize our recent efforts to develop the Density Matrix Renormalization Group (DMRG) method into a practical truncation strategy for large-scale nuclear shell model calculations. Following an overview of the essential features of the DMRG, we discuss the changes we have implemented for its use in nuclei. In particular, we have found it useful to develop an angular-momentum conserving variant of the method (the JDMRG). We then summarize the principal results we have obtained to date, first reporting test results for ^{48}Cr and then more recent test results for ^{56}Ni. In both cases we consider nucleons limited to the 2p-1f shell. While both calculations produce a high level of agreement with the exact shell model results, the fraction of the complete space required to achieve this high level of agreement is found to go down rapidly as the size of the full space grows.

Keywords: Nuclear physics; shell model; renormalization group methods.

Hacemos un resumen de nuestro intento reciente de desarrollar el método del Grupo de Renormalizacíon de la Matiz de Densidad (DMRG, por sus siglas en ingés) hacia una estrategia práctica de corte para cálculos amplios dentro del modelo de capas nucleares. Después de un resumen de las propiedades esenciales del DMRG, discutimos los cambios implementados por nosotros para su amplicación en núcleos. En particular, encontramos que es útil de desarrollar una variante de conservación de momento angular (el JDMRG). Entonces resumimos los resultados principales obtenidos hasta la fecha, primero reportando los resultados de prueba de ^{48}Cr y después los resultados de prueba más recientes para ^{56}Ni. En ambos casos consideramos núcleos limitados a la capa 2p-1f. Mientras ambos cálculos producen un acuerdo de alto grado con los cálculos exactos de modelo de capas, la fracción del espacio completo, necesario para obtener este alto grado de acuerdo, se encuentra que disminuye rápidamente con el aumento en tamaño del espacio completo.

Descriptores: Física nuclear; modelo de capas; métodos del grupo de renormalización.

PACS: 21.60.Cs; 05.10.Cc

1. Introduction

In the traditional nuclear shell model, the low-energy structure of a nucleus is described by diagonalizing the effective nuclear hamiltonian in an active space consisting of at most a few major shells outside/inside an assumed doubly-magic core. Despite the enormous truncation inherent in this approach, it can still only be applied in very limited nuclear regimes. For heavy nuclei or nuclei far from closed shells, further truncation of the shell-model space to a manageable size is required.

In this work, we discuss the use of the Density Matrix Renormalization Group (DMRG) as a truncation strategy for the nuclear shell model. Originally developed for the treatment of low-dimensional quantum lattices [1], the DMRG method was subsequently extended with impressive success [2–4] to finite Fermi systems, suggesting its possible usefulness for the nuclear shell model.

The DMRG method involves a systematic inclusion of the degrees of freedom of the problem. When treating quantum lattices, real-space sites are added iteratively. In finite Fermi systems, these sites are replaced by single-particle levels. At each stage, the group of sites that has been treated (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 (often the ground state) or perhaps for 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 states with the largest eigenvalues are retained. This method of truncation is guaranteed to be optimal in the sense that it maximizes the overlap of the truncated wave function with the superblock wave function prior to truncation.

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. In this way, the process iteratively updates the information on each block 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 works in a product space, whereby the enlarged block is obtained as a product of states in the block and the added site and the superblock is obtained as a product of states in the enlarged block and the medium. In the nuclear context, this means working in the m-scheme. This method was applied in nuclear physics by Papenbrock and Dean [5] and shown to provide an accurate description of the properties of ^{28}Si, but a much poorer description of ^{56}Ni where the converged solution was still energetically quite far from the exact ground state.

A limitation of the traditional algorithm is that it does not preserve symmetries throughout the iterative process. Since

the density matrix procedure involves a truncation at each iterative stage, there is the potential to lose these symmetries and the associated correlations. On this basis, we proposed [6] the adoption of a strategy in which angular momentum is preserved throughout the DMRG process. This method, called the JDMRG, was applied in nuclear physics for the first time in the context of the Gamow Shell Model [7] and then subsequently developed as a means of approximating the traditional nuclear shell model, with a preliminary application first reported [8] for ^{48}Cr. More recently, the algorithm was computationally improved and applied both to ^{48}Cr and to the ground state of ^{56}Ni [9]. In this work, we extend the results of Ref. 9 to include excited states of ^{56}Ni.

An outline of the presentation is as follows. We begin in Sec. 2 with a brief overview of the traditional DMRG method including a discussion of the changes required for exact angular-momentum conservation. In Sec. 3, we report our results for ^{48}Cr, which were first presented in Ref. 9, and then report our most recent results for ^{56}Ni, including those for excited states. Finally, in Sec. 4 we summarize the principal conclusions of this work and outline some directions for future investigation.

2. An overview of the DMRG method

2.1. The truncation strategy

The DMRG method is based on an iterative inclusion of the degrees of freedom of the problem, represented as sites on a lattice. This is illustrated schematically in Fig. 1 for a system with 8 *ordered* sites.

Assume that we have treated a group of sites, referred to as the block and denoted B, and that we have retained a total number of (optimal) states m within that block. We now wish to add to this block the next site (r) with 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,

$$|i,j >_{B'} = |i >_B |j >_r, \quad i = 1, m, \quad j = 1, l . \quad (1)$$

We wish to retain the optimal m states for the enlarged block. How do we choose them?

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 its optimum m states, the $m \times l \times m$ states of the superblock can be expressed as

$$|i,j,k >_{SB} = |i,j >_{B'} |k >_M . \quad (2)$$

We then diagonalize the full hamiltonian of the system in the superblock, isolating on its ground state,

$$|GS >_{SB} = \sum_{i,j,k} \Psi_{ijk} |i,j,k >_{SB} . \quad (3)$$

If we then construct the reduced density matrix of the enlarged block in the ground state,

$$\rho_{ij,i'j'} = \sum_k \Psi^*_{ijk} \Psi_{i'j'k} , \quad (4)$$

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.

FIGURE 2. Schematic illustration of two successive steps in the warmup procedure. (a) A block involving the site 8 is enlarged to include the next site 7, with the medium being a block involving the optimum states from the sites 1 and 2 obtained in the previous warmup step. (b) A block involving the sites 1 and 2 is enlarged to include the next site 3, with the medium being a block involving the optimum states from the sites 8 and 7 obtained in the warmup step of part (a).
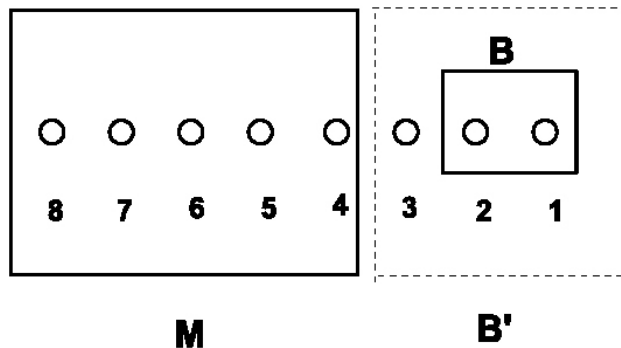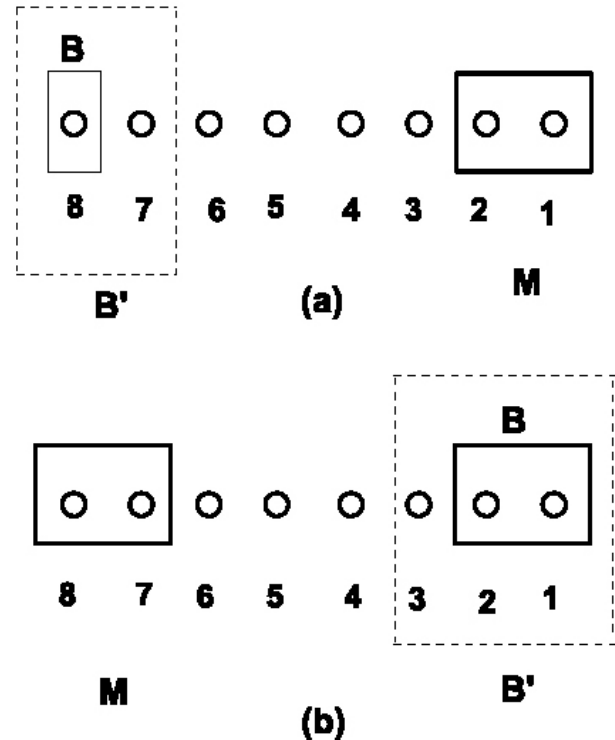

FIGURE 1. Schematic illustration of the DMRG growth procedure. A block B consisting of sites 1 and 2 is enlarged to include site 3, forming B'. The medium M consists of all of the remaining sites, $4 - 8$.
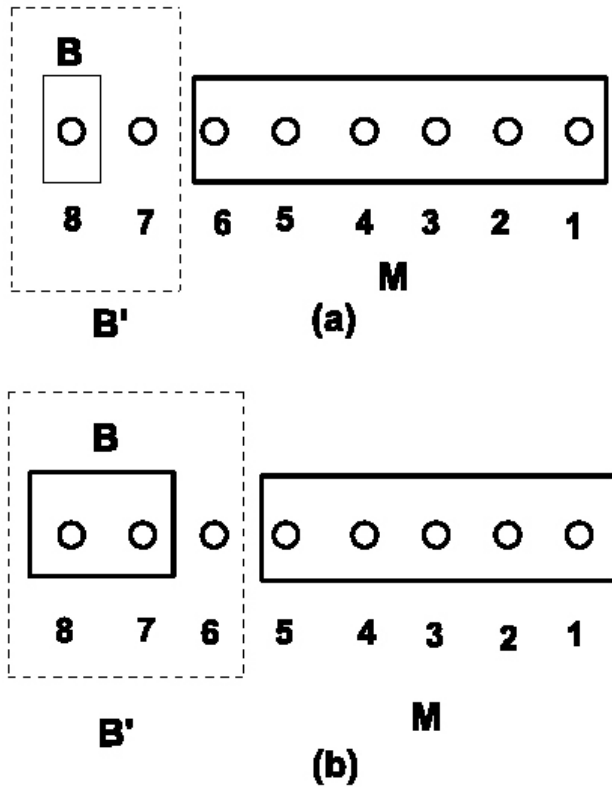
FIGURE 3. Schematic illustration of two successive steps in the sweep procedure. (a) A block involving the site 8 is enlarged to include the next site 7, with the medium being a block involving the optimum states from the sites $1-6$ obtined previously. (b) A block involving the sites 8 and 7 is enlarged to include the next site 6, with the medium being a block involving the optimum states from the sites $1-5$ obtained previously.

It is straightforward to target a group of states of the system, and not just the ground state, by constructing a mixed density matrix containing 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,

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

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. Stages of the DMRG method

With the above remarks as background, the DMRG procedure involves the following stages.

2.2.1. The warmup stage

In the warmup stage we make an initial guess on the optimal m states for each block. This choice is important in determining how rapidly the iterative procedure converges. In

our treatment, we do this by growing blocks from each side of the chain gradually, using those orbits that have already been treated on the other end as the medium. This is illustrated schematically in Fig. 2 for two successive steps of the warmup procedure.

2.2.2. The sweep stage

In this stage of the process, schematically illustrated in Fig. 3, we gradually sweep back and forth through the sites of the lattice, at each step of the sweep using for the medium the results either from the warmup phase (during the first sweep) or from the previous sweep stage. The sweep process is done over and over until convergence is achieved from one sweep to the next.

2.2.3. As a function of m

The above calculations are done for a given choice of m. The calculations are then done as a function of m, until the changes with increasing m are acceptably small.

2.3. The JDMRG approach

As noted earlier, most DMRG approaches violate symmetries. In nuclei, for example, they typically work in the m-scheme. Such a procedure is potentially problematic when imposing truncation, however, 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. The most significant difference between this (the JDMRG) approach and the more traditional DMRG approach is that now we must calculate and store the *reduced matrix elements* of all sub-operators of the hamiltonian,

$$a_i^\dagger,\; [a_i^\dagger \tilde{a}_j]^K,\; [a_i^\dagger a_j^\dagger]^K,\; \left([a_i^\dagger a_j^\dagger]^K \tilde{a}_k\right)^L,$$

$$\left([a_i^\dagger a_j^\dagger]^K [\tilde{a}_k \tilde{a}_l]^K\right)^0 + h.c.$$

This can be done using standard Racah techniques.

2.4. A three-block JDMRG strategy

In the nuclear shell-model calculations we will report here, we adopt a three-block strategy for the enlargement and truncation process, schematically summarized in Fig. 4.

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 back and forth through the orbits of a given type of particle only. As can be seen from the figure, the medium in this approach

TABLE I. Calculated ground-state energies in MeV as a function of m for ^{48}Cr. The maximum dimension encountered in the sweep process is also given.

m	E_{GS}	$Max\ Dim$
40	-32.698	1,985
60	-32.763	2,859
80	-32.788	4,494
100	-32.817	6,367
120	-32.840	6,367
140	-32.890	8,217
160	-32.902	9,978
180	-32.944	11,062
200	-32.947	12,076
Exact	-32.953	41,355

TABLE II. Results for the excitation energies in MeV of the lowest 2^+ and 4^+ states in ^{48}Cr from the JDMRG calculations described in the text. The dimensions of the associated hamiltonian matrices are given in parentheses.

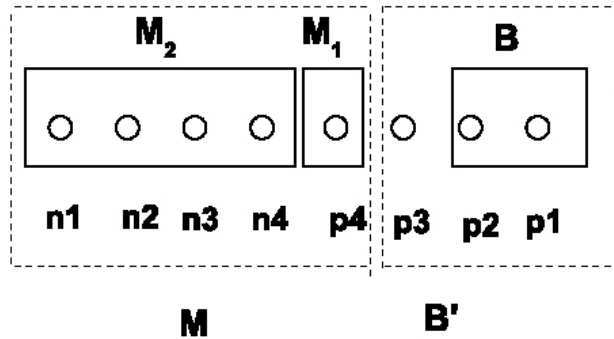| m	2_1^+	4_1^+
140	0.873 (9,191)	2.022 (12,442)
160	0.860 (12,038)	1.996 (16,553)
180	0.855 (15,148)	1.989 (21,628)
Exact	0.806 (182,421)	1.823 (246,979)

FIGURE 4. Schematic illustration of the three-block DMRG growth procedure for a system with neutron and proton levels.
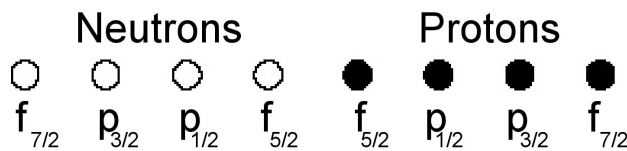

FIGURE 5. Order of single-particle levels used in the DMRG growth algorithm for both ^{48}Cr and ^{56}Ni.

involves two components. If, for example, we are enlarging a proton block, the full medium (M) involves all of the remaining proton levels (M_1) and all of the neutron levels (M_2).

3. Calculations

We have carried out test calculations of the JDMRG method described above on the nuclei ^{48}Cr and ^{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. In both, we use the order of single-particle levels shown in Fig. 5.

We report the results for these two applications in the following subsections.

3.1. Results for ^{48}Cr

We begin with our results for ^{48}Cr, for which there are four neutrons and four protons outside a ^{40}Ca core. In these calculations we assumed a KB3 effective interaction between valence nucleons and compared our results with those obtained for the same hamiltonian in Ref. 10. The size of the full shell-model space in this case involves 1,963,461 states, of which 41,355 are 0^+ states, 182,421 are 2^+ states, 246,979 are 4^+ states, etc.

Our results for the ground state are presented in Table I. The exact calculation produces a ground state energy of -32.953 MeV. The DMRG calculation converges smoothly to this result as m is increased, but requires the inclusion of a substantial fraction of the full space to obtain a high level of accuracy. With of order 25% of the full 0^+ space, we are able to achieve accuracy to only a few keV. To achieve an accuracy of better than 50 keV still requires, however, over 20% of the full 0^+ space.

In Fig. 5, we show how the results converge as a function of the number of sweeps. As can be readily seen, after the first sweep we are extremely close to the final converged result. This is a direct consequence of our use of a warmup procedure that incorporates (in step 0) a significant part of the correlations.

In Table II, we present results for the lowest excited states, obtained using the blocks obtained at the ground state minimum. Here too convergence to the exact results is achieved, if a sufficiently large fraction of the full shell-model space is retained. This is true despite the fact that the density matrix truncation procedure implemented targeted the ground state only.

3.2. ^{56}Ni

Next we turn to ^{56}Ni, for which the size of the full shell-model space in the m-scheme contains 1,087,455,228 states, of which 15,443,685 have $J^\pi=0^+$, 71,109,189 have $J^\pi = 2^+$ and 105,537,723 have $J^\pi=4^+$, in all cases much larger than in ^{48}Cr.

TABLE III. Results for the ground-state energy of ^{56}Ni 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*
60	-205.603	64,397
80	-205.632	74,677
100	-205.643	87,633
120	-205.652	106,383
Exact	-205.709	15,443,685

TABLE IV. Results for the excitation energies in MeV of the lowest 2^+ and 4^+ states in ^{56}Ni from the JDMRG calculations described in the text. The dimensions of the associated hamiltonian matrices are shown in parentheses.

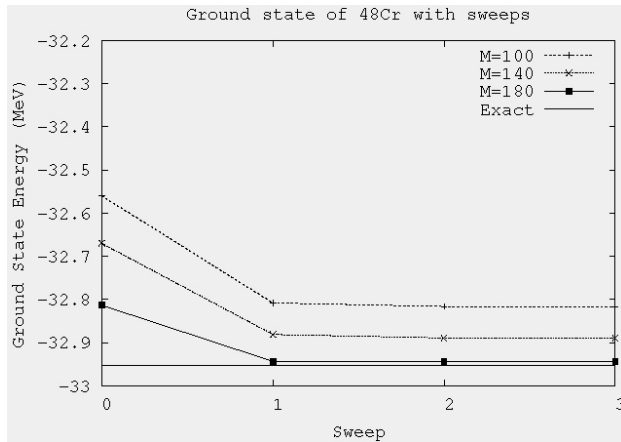| m	2_1^+	4_1^+
60	2.970 (296,633)	4.137 (445,898)
80	2.944 (345,213)	4.123 (556,572)
100	2.942 (423,265)	4.090 (701,502)
Exact	2.600 (71,109,189)	3.688 (105,537,723)

FIGURE 6. Convergence of the results for ^{48}Cr with the number of sweeps.

In our earlier published work on ^{56}Ni, we used the KB3 interaction for ^{56}Ni as well and compared the ground state energy with the results from Ref. 11. We only considered the ground state in those calculations, since those were the only exact results that had been reported in the literature. The reason for that is that KB3 is known to produce poor agreement with the experimental spectra for nuclei in this region of the $2p - 1f$ shell. Much better agreement can be obtained with the improved GXPF1A interaction [12]. Thus, we have redone our test calculations of ^{56}Ni with this interaction, now comparing with the exact results not only for the ground state but for low-lying excited states as well [13]. These are the largest test calculations we have carried out to date using the JDMRG method.

The results for the ground state energy as a function of m are shown in Table III. Here we are able to achieve roughly 60 keV accuracy with just 0.5% of the full 0^+ space. This is a significantly lower fraction of the full space than was required in ^{48}Cr to achieve the same level of accuracy.

This is perhaps the most encouraging result of our work to date. It suggests that the fraction of the space required to achieve a high level of accuracy with the JDMRG method goes down rapidly as the size of the space problem increases. If this is confirmed with extension to even larger problems it would bode very well for the future usefulness of the JDMRG method as a practical truncation approach for large-scale shell-model studies.

As noted above, exact results also exist with the GXPF1A interaction for excited states. In Table IV, we present our results for the lowest 2^+ and 4^+ states, again in comparison with the exact results. These results were obtained by diagonalizing the associated hamiltonian matrices that derive with the blocks obtained at the ground state minimum. Here too the results are getting better with m, albeit slowly. Agreement with the exact results for $m = 100$ is still not as good as we would like. It might be possible to improve the quality of the description of low-lying excited states by targeting both the ground state and the first excited state in the density matrix truncation procedure, hopefully without losing too much accuracy in our reproduction of the ground state.

4. Summary and outlook

In this talk, we have summarized the current status of our efforts to build the Density Matrix Renormalization Group Method method into a practical 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 results we have obtained for the nuclei ^{48}Cr and ^{56}Ni, in both cases comparing with the results of exact diagonalization. Both calculations were able to accurately reproduce the exact shell-model results. In the case of ^{48}Cr, however, this high level of accuracy required us to retain a very large fraction of the full space. In contrast, we were able to achieve comparably accurate results for ^{56}Ni with a much smaller fraction of the space. The fact that the fraction of the space goes down rapidly 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 that we intend to explore in the near future. One concerns the need to determine through additional calculations how rapidly the fraction of the space required for convergence scales with the size of the problem. Currently we only have two data points, ^{48}Cr and ^{56}Ni. More are needed to draw meaningful conclusions.

We are also looking into the question of whether we can obtain comparable agreement for both the ground state and

low-lying excited states by building a mixed density matrix that includes information not only on the ground state but also on the first excited 0^+ state.

We are also in the process of applying these methods to odd-mass nuclei around ^{56}Ni. Exact and Coupled Cluster results are now available for several such nuclei [14] and we are interested in seeing how well the JDMRG truncation strategy works on these nuclei and how well it compares with the Coupled Cluster method.

Another issue of current interest concerns the possibility of breaking up large single-particle orbitals, rather than adding them in a single stage. We have some thoughts on how this might be done without losing angular momentum conservation and we are now testing these ideas on the $f_{7/2}$ orbital for the same nuclei we have already studied. If successful, we will then consider the application of these ideas

to even larger shells, as will be critical for subsequent applications of the method to heavier nuclei, the ultimate goal of this project.

Acknowledgments

1. S.R. White, *Phys. Rev. Lett.* **69** (1992) 2863.

2. J. Dukelsky and G. Sierra, *Phys.Rev. Lett.* **83** (1999) 172; J. Dukelsky and G. Sierra, *Phys. Rev. B* **61** (2000) 12302.

3. S.R. White and R.L. Martin, *J. Chem. Phys.* **110** (1999) 4127; S. Daul, I. Ciofini, C. Daul, and S.R. White, *Int. J. Quantum Chem.* **79** (2000) 331.

4. N. Shibata and D. Yoshioka, *Phys. Rev. Lett.* **86** (2001) 5755; D. Yoshioka and N. Shibata, *Physica E* **12** (2002) 43; N. Shibata, *J. Phys. A* **36** (2003) R381.

5. T. Papenbrock and D.J. Dean, *J. Phys. G* **31** (2005) S1377.

6. J. Dukelsky and S. Pittel, *Rep. Prog. Phys.* **67** (2004) 513.

7. N. Michel, W. Nazarewicz, M. Ploszajczak, and J. Rotureau, *Rev. Mex. Fís.* **50** (2004) 74; J. Rotureau, N. Michel, W. Nazarewicz, M. Ploszajczak, and J. Dukelsky, *Phys. Rev. Lett.* **97** (2006) 110603.

8. S. Pittel and N. Sandulescu, *Phys. Rev. C* **73** (2006). 014301.

9. B. Thakur, S. Pittel, and N. Sandulescu, *Phys. Rev. C* **78** (2008) 041303.

10. E. Caurier, A.P. Zuker, A. Poves, and G. Martínez-Pinedo, *Phys. Rev. C* **5**0 (1994) 225.

11. E. Caurier *et al.*, *Phys. Rev. C* **5**9 (1999) 2033.

12. M. Honma, T. Otsuka, B.A. Brown, and T. Mizusaki, *Eur. Phys. J.A.* **25** (2005) 499.

13. M. Horoi, B.A. Brown, T. Otsuka, M. Honma, and T. Mizusaki, **73** (2006) 061305.

14. J.R. Gour, M. Horoi, P. Piecuch, and B.A. Brown, *Phys. Rev. Lett.* **101** (2008) 052501.