Eur. Phys. J. A **25**, s01, 507–508 (2005)
DOI: 10.1140/epjad/i2005-06-059-3

EPJ A direct
electronic only

Wave function factorization of shell-model ground states

T. Papenbrock[a]

Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA and Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Received: 14 January 2005 /
Published online: 3 May 2005 –

Abstract. The wave function factorization method determines an optimal basis of correlated proton and neutron states, and accurately approximates low-lying shell-model states by a rather small number of suitable product states. The optimal basis states result from a variational principle and are the solution of relatively low-dimensional eigenvalue problems. The error involved in this truncation decreases exponentially fast as more basis states are included.

PACS. 21.60.Cs Shell model – 21.10.Dr Binding energies and masses

1 Introduction

The shell-model can now routinely be applied up to fp shell nuclei [1,2], and no-core shell-model calculations accurately describe p-shell nuclei [3]. In other mass regions, the dimensionality of the model space is often too large, and exact diagonalizations can only be carried out for a small number of nuclei in the region of interest. To deal with the increasingly large model-space sizes, various approximation techniques have been developed and applied. Some of them are based on extrapolation schemes [4], while others involve a basis state selection. In many methods, this selection is based on what are perceived to be the relevant states, *e.g.* low-energy eigenstates of the proton Hamiltonian and the neutron Hamiltonian [5], energy expectation values of configurations [6], or state selection based on symmetry arguments [7]. In other methods, the relevant states are selected by the Hamiltonian itself. In the Monte Carlo shell-model [8], for instance, a good basis is selected stochastically by random walks through the Hilbert space. In the density matrix renormalization group [9,10], relevant basis states are obtained from a density matrix. Recently, we proposed the wave function factorization [11]. In this method, the most important proton and neutron states are determined from a variational principle. This results in an accurate approximation of low-lying states states, and the dimensionality of the eigenvalue problem is reduced by orders of magnitudes. In this note, we briefly review the the wave function factorization and present future opportunities.

[a] Conference presenter;
e-mail: papenbro@mail.phy.ornl.gov

2 Wave function factorization

In the wave function factorization we approximate the shell-model ground state as a sum over Ω products of correlated proton states $|p_j\rangle$ and neutron states $|n_j\rangle$

$$|\Psi\rangle = \sum_{j=1}^{\Omega} |p_j\rangle|n_j\rangle. \tag{1}$$

The expansion (1) becomes exact for sufficiently large Ω and is based on the singular value decomposition of amplitude matrices [11]. The states $|p_j\rangle$ and $|n_j\rangle$ are not normalized. Variation of the energy yields the following set of eigenvalue equations that determine the states $|p_j\rangle$ and $|n_j\rangle$

$$\begin{aligned} \sum_{i=1}^{\Omega} \left(\langle n_j|\hat{H}|n_i\rangle - E\langle n_j|n_i\rangle \right) |p_i\rangle = 0, \\ \sum_{i=1}^{\Omega} \left(\langle p_j|\hat{H}|p_i\rangle - E\langle p_j|p_i\rangle \right) |n_i\rangle = 0. \end{aligned} \tag{2}$$

This system of equations is solved iteratively as follows. A random set of Ω neutron states is fixed and the eigenvalue problem for the proton states is solved for the lowest energy E. The resulting proton states are the input to the eigenvalue problem for the neutron states. Typically, the energy converges within 5–10 iterations for fixed Ω. Then, Ω is increased and the calculations are repeated. One empirically finds that the resulting function $E(\Omega)$ is of the form $E(\Omega) = E_0 + b\exp(-c\Omega)$, and a fit of the parameters E_0, b and c yields the estimate E_0 for the ground-state energy. For fp-shell nuclei, this estimate might deviate about

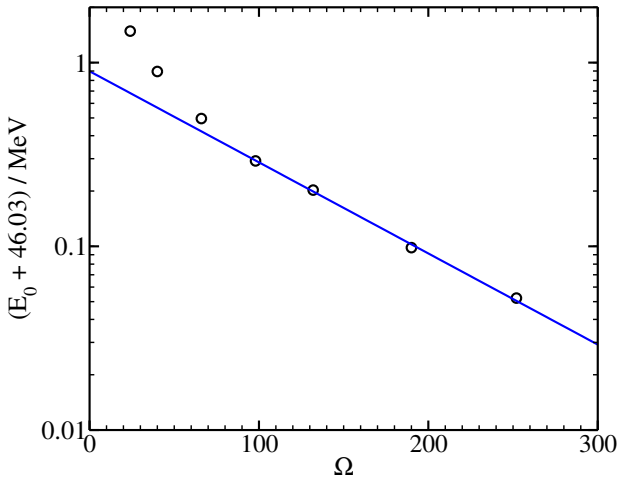

Fig. 1. Ground-state energy as a function of the number Ω of kept proton and neutron states obtained from the wave function factorization (data points) and exponential fit (line).

100 keV from the results obtained from full space diagonalizations, while the dimension of the eigenvalue problem (2) is considerably smaller than in the full space matrix diagonalization. For the mid-shell fp-shell nuclei, for instance, the reduction in dimension reaches three orders of magnitude. For details we refer the reader to ref. [12].

As an example we consider ^{51}Mn in the $0f1p$-shell and use the KB3 interaction [13,14]. The Hilbert space consists of products of 38746 and 15504 Slater determinants for the neutrons and protons, respectively. The ground-state energy obtained from exact diagonalization is $E = -46.17$ MeV [1]. Figure 1 shows the result obtained from the wave function factorization. The estimate $E_0 = -46.03$ MeV deviates only 140 keV from the exact result and is obtained from $\Omega \approx 250$ proton and neutron states. This number is about a factor 60 smaller than the number of available proton states, and the 45×10^6 dimensional eigenvalue problem encountered in the exact diagonalization is reduced by the same factor in the wave function factorization. Note that the rotational symmetry is restored to a good approximation. The angular momentum expectation value of the approximated ground state is $\langle J^2 \rangle \approx 8.9$ compared to 8.75 (corresponding to spin $J = 5/2$) of the exact ground state. These results show that the method works quite well also for odd-mass nuclei. Our experience shows that shell-model states of odd mass systems and deformed nuclei are harder to factorize than their even-even neighbors or less deformed nuclei [12,15]. This is due to the fact that such systems exhibit stronger proton neutron correlations than more spherical and/or even-even nuclei. Note that low-lying excited states can also be computed by wave function factorization [12].

3 Summary and outlook

We have briefly reviewed the wave function factorization as an accurate approximation for large-scale nuclear structure calculations, and applied it to the fp-shell nucleus ^{51}Mn. Highly accurate approximations can be obtained from the solution of eigenvalue problems of relatively small dimension. Up to now, the wave function factorization has been tested mainly for sd-shell and fp-shell nuclei, and the results have been very encouraging. Studies of larger shell-model problems (with tens of billions of configurations) are currently under way. Such dimensions are out of reach for exact diagonalization methods and have so far been the realm of the Monte Carlo methods [8,16].

This research was supported in part by the U.S. Department of Energy under Contract Nos. DE-FG02-96ER40963 (University of Tennessee) and DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory).

References

1. E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves, J. Retamosa, A.P. Zuker, Phys. Rev. C **59**, 2033 (1999), nucl-th/9809068.
2. M. Honma, T. Otsuka, B.A. Brown, T. Mizusaki, Phys. Rev. C **65**, 061301(R) (2002), nucl-th/0205033.
3. P. Navrátil, J.P. Vary, B.R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000), nucl-th/0004058.
4. T. Mizusaki, M. Imada, Phys. Rev. C **65**, 064319 (2002), nucl-th/0203012.
5. F. Andreozzi, A. Porrino, J. Phys. G **27**, 845 (2001).
6. M. Horoi, B.A. Brown, V. Zelevinsky, Phys. Rev. C **50**, R2274 (1994), nucl-th/9406004.
7. V.G. Gueorguiev, W.E. Ormand, C.W. Johnson, J.P. Draayer, Phys. Rev. C **65**, 024314 (2002), nucl-th/0110047.
8. M. Honma, T. Mizusaki, T. Otsuka, Phys. Rev. Lett. **75**, 1284 (1995).
9. S.R. White, Phys. Rev. Lett. **69**, 2863 (1992).
10. J. Dukelsky, S. Pittel, Rep. Prog. Phys. **67**, 513 (2004), cond-mat/0404212.
11. T. Papenbrock, D.J. Dean, Phys. Rev. C **67**, 051303(R) (2003), nucl-th/0301006.
12. T. Papenbrock, A. Juodagalvis, D.J. Dean, Phys. Rev. C **69**, 024312 (2004), nucl-th/0308027.
13. T.T.S. Kuo, G.E. Brown, Nucl. Phys. A **114**, 241 (1968).
14. A. Poves, A.P. Zuker, Phys. Rep. **70**, 235 (1980).
15. T. Papenbrock, D.J. Dean, nucl-th/0412112.
16. S.E. Koonin, D.J. Dean, K. Langanke, Phys. Rep. **278**, 1 (1997), nucl-th/9602006.