

Factorization of low-lying shell-model states

T. Papenbrock^{1,2} and D. J. Dean¹

¹*Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

²*Department of Physics and Astronomy, University of Tennessee, Knoxville TN 37996-1201, USA*

(Dated: January 30, 2003)

Shell-model ground-states may accurately be approximated by products of proton and neutron states. The optimal factors are determined by a variational principle and result from the solution of rather low-dimensional eigenvalue problems. Computations of the ground-state and low-lying excitations in ²⁸Si show that the method converges exponentially quickly as the number of retained factors is increased.

PACS numbers: 21.60.Cs, 21.10.Dr, 27.30.+t, 27.40.+z

Realistic nuclear structure problems are difficult to solve due to the complexity of the nucleon-nucleon interaction and the sheer sizes of the model spaces. In recent years, several approximations have been developed that truncate the model space while obtaining highly accurate approximations to low-lying states. Most truncation schemes are based on physical insights [1–3] or random searches in huge Hilbert spaces [4] but do not yield the optimal approximation. Exceptions are the density matrix renormalization group (DMRG) [5–8] and the factorization method [9] which yield optimal truncations. We describe the latter method in this talk.

Let us make the following ansatz for the shell-model ground-state

$$|\psi\rangle = \sum_{j=1}^{\Omega} |p_j\rangle |n_j\rangle. \quad (1)$$

This expansion is a factorization of the ground-state in terms of Ω proton states $|p_j\rangle$ and Ω neutron states $|n_j\rangle$. While this expansion is not unique, one can always obtain orthogonal factors $\langle p_i | p_j \rangle = 0 = \langle n_i | n_j \rangle$ for $i \neq j$, and order them such that the norms

$$s_j^2 \equiv \langle p_j | p_j \rangle \langle n_j | n_j \rangle \quad (2)$$

decrease with increasing index j . Normalization of the ground-state implies $\sum_{j=1}^{\Omega} s_j^2 = 1$. Note that the factorization (1) allows us to include the proton-proton and neutron-neutron correlations into the shell-model ground-state. The proton-neutron correlations are subsequently built in by increasing the number of retained factors Ω . Let d_P and d_N be the dimensions of the proton space and the neutron space, respectively. For $\Omega = \min(d_P, d_N)$, the ansatz (1) may yield the exact ground-state while smaller values of Ω result in an approximation.

We want to determine those proton states $|p_j\rangle$ and neutron states $|n_j\rangle$ that yield an optimal approximation to the true shell-model ground-state. To this purpose we vary the energy $E = \langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$ and find ($j = 1, \dots, \Omega$)

$$\sum_{i=1}^{\Omega} \left(\langle n_j | \hat{H} | n_i \rangle - E \langle n_j | n_i \rangle \right) |p_i\rangle = 0,$$

$$\sum_{i=1}^{\Omega} \left(\langle p_j | \hat{H} | p_i \rangle - E \langle p_j | p_i \rangle \right) |n_i\rangle = 0. \quad (3)$$

The optimal states are thus the solution of a nonlinear and coupled set of eigenvalue equations. Note however, that for fixed neutron (proton) states the first (second) set of these equations is a generalized eigenvalue problem for the protons (neutrons).

We have to explain the operators $\langle n_j | \hat{H} | n_i \rangle$ that enter Eq. (3). The shell-model Hamiltonian can be written as

$$\hat{H} = \hat{H}_N + \hat{H}_P + \hat{V}_{PN}, \quad (4)$$

where the neutron Hamiltonian \hat{H}_N , the proton Hamiltonian \hat{H}_P , and the proton-neutron interaction \hat{V}_{PN} are

$$\begin{aligned} \hat{H}_N &= \sum_n \varepsilon_n \hat{a}_n^\dagger \hat{a}_n + \frac{1}{4} \sum_{n,n',m,m'} v_{nn'm'm} \hat{a}_n^\dagger \hat{a}_{n'}^\dagger \hat{a}_m \hat{a}_{m'}, \\ \hat{H}_P &= \sum_p \varepsilon_p \hat{a}_p^\dagger \hat{a}_p + \frac{1}{4} \sum_{p,p',q,q'} v_{pp'q'q} \hat{a}_p^\dagger \hat{a}_{p'}^\dagger \hat{a}_q \hat{a}_{q'}, \\ \hat{V}_{PN} &= \sum_{p,n,n',p'} v_{pn p' n'} \hat{a}_p^\dagger \hat{a}_n^\dagger \hat{a}_{n'} \hat{a}_{p'}. \end{aligned} \quad (5)$$

Here, we use indices p, q and m, n to refer to proton and neutron orbitals, respectively. The antisymmetric two-body matrix elements are denoted as v_{ijkl} . Thus,

$$\begin{aligned} \langle n_i | \hat{H} | n_j \rangle &= \sum_{p,p'} \left(\sum_{n,n'} v_{pn p' n'} \langle n_i | \hat{a}_n^\dagger \hat{a}_{n'} | n_j \rangle \right) \hat{a}_p^\dagger \hat{a}_{p'} \\ &+ \langle n_i | \hat{H}_N | n_j \rangle + \langle n_i | n_j \rangle \hat{H}_P \end{aligned} \quad (6)$$

is an operator acting on the proton states. Note that the proton-neutron interaction becomes an effective one-body operator for the protons while the neutron Hamiltonian reduces to a constant. The structure of the remaining operators in Eq. (3) is similar and requires no further explanation.

We solve Eq. (3) as follows. We choose a random set of neutron states $|n_i\rangle$ as input and solve the first set of Eq. (3) for the protons. This requires us to solve a generalized eigenvalue problem of dimension Ωd_P . We

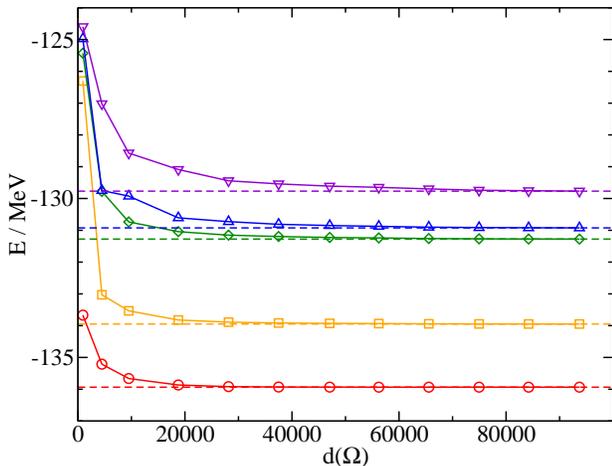


FIG. 1: Low-energy spectrum of the sd -shell nucleus ^{28}Si (USD interaction) versus the dimension of the eigenvalue problem. The dashed lines are the exact results and require the solution of a 93710 dimensional eigenvalue problem.

are only interested in the solution with lowest energy E since we are seeking an approximation for the shell-model ground-state. The resulting proton states $|n_i\rangle$ are input to the second set in Eq. (3). New neutron states are obtained from the lowest energy solution of the second set of Eq. (3). This generalized eigenvalue problem has dimension Ωd_N . We iterate this procedure until the energy E is converged sufficiently well, usually 5-20 times. The number of required iterations decreases with the increasing number of retained factors Ω . Note that one can maintain orthogonality between the proton states and between the neutron states during this iteration. This has the advantage that one has to solve standard eigenvalue problems instead of generalized eigenvalue problems. Details can be found in Ref. [9]. Note also that it is straightforward to include symmetries into the formalism. Our computations below are done in m -scheme and keep orthogonal sets of proton states and neutron states.

As an example, we consider the sd -shell nucleus ^{28}Si with the USD interaction [10]. The exact ground-state results from a diagonalization of an eigenvalue problem with m -scheme dimension $d_{\text{max}} = 93710$. We use the ansatz (1) to compute approximations of the ground-state and of low-lying excitations. We increase the number of retained factors up to $\Omega = \min(d_P, d_N)$ which yields the exact ground-state. The resulting eigenvalue problems (3) have a dimension $d(\Omega)$. Figure 1 shows the low-lying energy spectrum versus the dimension $d(\Omega)$ of the eigenvalue problem. The energies converge exponentially quickly as the number of retained factors is increased. The ground-state energy, for instance, deviates only 100 keV from the exact result at $d(\Omega) \approx 0.2d_{\text{max}}$. The level spacings are accurately reproduced already for relatively small dimensions $d(\Omega)$. To better understand the exponential convergence, we set $\Omega = \min(d_P, d_N)$,

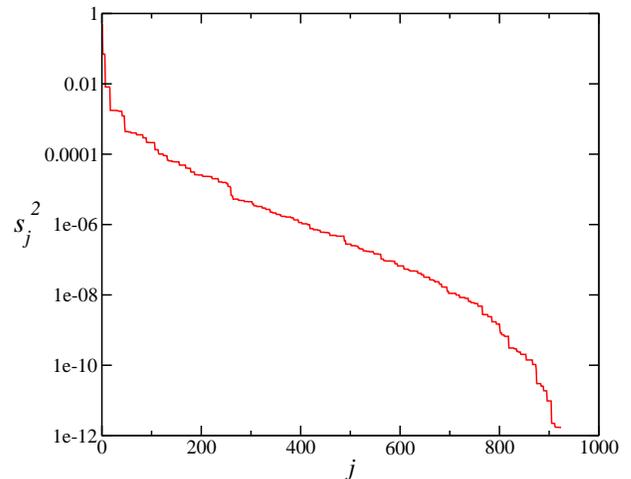


FIG. 2: Norms s_j^2 of the factors for the exact ground-state of ^{28}Si . The proton and neutron space have equal dimension $d_P = d_N = 924$.

i.e. $d(\Omega) = d_{\text{max}}$, and perform a factorization of the exact shell-model ground-state. The resulting norms (2) are plotted in Fig. 2. The norms decay exponentially quickly (degeneracies are due to spin and isospin symmetry), and this decay causes the exponential convergence of the factorization method. A similar behavior is found in DMRG calculations [5–7] of spin chains and pairing-plus-quadrupole Hamiltonians. While the origin of this exponential decay is not fully understood, it seems to be present in many systems of physical interest. The factorization method has successfully been applied to other sd -shell and pf -shell nuclei [9].

Let us also compare the factorization method presented in this work with the DMRG. Both methods rely on the exponential decay of the norms (2). While the DMRG is potentially able to treat huge Hilbert spaces, the factorization method can at best reduce the dimension of the eigenvalue problem by a square root from $d_P \times d_N$ to $\max(d_P, d_N)$. However, when applied to the sd -shell nucleus ^{24}Mg , the m -scheme factorization method converges much more quickly than the DMRG [8, 9].

Let us finally speculate about an extension of the factorization method. We have seen that a large-dimensional eigenvalue problem can approximately be solved by a factorization. The optimal factors themselves are solutions of lower-dimensional eigenvalue problems. One might thus speculate whether a recursive application of this method is possible, i.e. whether the lower-dimensional eigenvalue problems again might be solved approximately by a factorization. This might then lead to even lower-dimensional eigenvalue problems which might be solved with standard methods.

In summary, we have applied the factorization method to the sd -shell nucleus ^{28}Si . The method yields approximations for the ground-state and low-lying excitations

that converge exponentially quickly as the number of retained factors is increased.

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).

-
- [1] M. Horoi, B. A. Brown, and V. Zelevinsky, *Phys. Rev. C* **50**, R2274 (1994); [nucl-th/9406004].
 - [2] C. E. Vargas, J. G. Hirsch, and J. P. Draayer, *Nucl. Phys. A* **690**, 409 (2001); [nucl-th/0009050].
 - [3] F. Andreozzi and A. Porrino, *J. Phys. G* **27**, 845 (2001).
 - [4] M. Honma, T. Mizusaki, and T. Otsuka, *Phys. Rev. Lett.* **75**, 1284 (1995).
 - [5] S. R. White, *Phys. Rev. Lett.* **69**, 2863 (1992); *Phys. Rev. B* **48**, 10345 (1993).
 - [6] J. Dukelsky and S. Pittel, *Phys. Rev. C* **63**, 061303 (2001); [nucl-th/0101048].
 - [7] J. Dukelsky and S. Pittel, S. S. Dimitrova, and M. V. Stoitsov, *Phys. Rev. C* **65**, 054319 (2002); [nucl-th/0202048].
 - [8] S. S. Dimitrova, S. Pittel, J. Dukelsky, and M. V. Stoitsov, nucl-th/0207025.
 - [9] T. Papenbrock and D. J. Dean, nucl-th/0301006, submitted to *Phys. Rev. C*.
 - [10] B. A. Brown and B. H. Wildenthal, *Ann. Rev. Nucl. Part. Sci.* **38**, 29 (1988).