A new algorithm for large scale shell model calculations and its applicability to medium-heavy and neutron rich nuclei

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Abstract. An upgraded version of an algorithm developed few years ago for diagonalizing large matrices has been implemented for the nuclear shell model eigenvalue problem. The use of a spin uncoupled basis yields a quite sparse Hamiltonian matrix. Its dimensions are further reduced effectively by an importance sampling specific of the method. Some numerical examples emphasizes the potential of the revised algorithm.

1. Introduction

Lanczos algorithm provides a powerful tool for generating the lowest eigensolutions of large sized matrices [1]. For this reason, it has been widely adopted for solving the nuclear shell model eigenvalue problem. Some implementation codes use a spin-isospin \((J,T)\) \cite{2, 3} or a neutron-proton \(J\) (Nathan \cite{4, 5}) coupled basis. In those schemes, the Hamiltonian matrices have relatively small dimensions. On the other hand, they are quite dense and require lengthy calculations of coupling coefficients and fractional parentage coefficients.

The alternative \(m\)-scheme yields a Hamiltonian matrix of much larger dimensions. The matrix, however, is quite sparse and extremely easy to construct. These properties are exploited in Antoine \cite{4, 5}, maybe the most widely adopted shell model code.

Other methods, like shell model Monte Carlo (SMMC) \cite{6}, avoids the diagonalization of the Hamiltonian matrix and use a Monte Carlo technique to evaluate expectation values and strength functions of finite nuclei. The SSMC proved to be a powerful and efficient tool for studying thermal properties of medium-mass nuclei as well as electroweak nuclear properties. Its critical point resides in the famous sign problem which has not found yet a clear-cut solution. Moreover, it is not well suited for computing spectra.

This is done in the quantum Monte Carlo diagonalization (QMCD) method \cite{7, 8}, where the same technique is adopted to generate stochastically a truncated basis to be used for the diagonalization of the many-body Hamiltonian. This method, adopted with success for systematics in the \((s,d)\) and \((f,p)\) nuclear regions, has to face the problem of restoring the total spin and other symmetries.
Another method for effectively truncating the shell model space exploits \[9\] the density matrix renormalization group (DMRG) method, borrowed from condensed matter \[10\]. The method seems to be more performing in a \(J\)-coupled basis. In such a scheme, it was applied to nuclei in the \((f, p)\) shell, like \(^{48}\)Cr and \(^{56}\)Ni \[11, 12\].

Coming back to Lanczos, its numerical implementation deserves special care in order to eliminate numerical errors, whose propagation, during the iterative process, may lead to “ghost” states.

In the recent past, we have proposed a new diagonalization iterative algorithm \[13, 14\] which is of easy implementation and extremely stable. It is also endowed with an importance sampling that yields an effective drastic reduction of the space and allows to extrapolate to the exact eigenvalues.

The method was implemented in the coupled \(J\)-scheme only, which resulted to be too time consuming in the construction of the Hamiltonian matrix. We have now made a new version \[15\] which uses the \(m\)-scheme so as to exploit the sparsity of the Hamiltonian matrix. The sizes of such a matrix are further cut effectively by an importance sampling procedure similar to the one formulated in Ref. \[14\]. Here we will outline the procedure method, show how it is implemented numerically and present some illustrative results.

2. The algorithm

The algorithm deals with a matrix \(A\) assumed for simplicity to represent a self-adjoint operator \(A\) in an orthonormal basis \(\{|1\rangle, |2\rangle, |i\rangle, \ldots, |N\rangle\}\). It consists of several iteration loops. The first loop goes through the following steps: 1a) Construct and diagonalize the \(n_0 \times n_0\) \((n_0 << N)\) submatrix \(A_0 = (a_{ij})\), 1b) select the lowest \(v\) eigenvalues \(\lambda_1^{(0)}, \ldots, \lambda_k^{(0)}, \ldots, \lambda_v^{(0)}\) and the corresponding eigenvectors \(|\varphi_k^{(0)}\rangle = \sum_{i=1}^{n_0} c_i^{(0)} |i\rangle\),

\[
1c) \text{consider now the subspace spanned by the } v \text{ eigenvectors } |\varphi_k^{(0)}\rangle \text{ plus the basis states } |j\rangle = |n_0 + 1\rangle, \ldots, |n_1\rangle, \text{ compute } b_{k_j}^{(0)} = \langle \varphi_k^{(0)} | A | j \rangle \text{ and construct the new submatrix }
\]

\[
A_1 = \begin{pmatrix}
\lambda_1^{(0)} & 0 & 0 & 0 & b_{1j}^{(0)} & \cdots & b_{1n_1}^{(0)} \\
0 & 0 & 0 & 0 & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \lambda_2^{(0)} & \cdots & \cdots & \cdots \\
b_{(n_0+1)1}^{(0)} & \cdots & b_{(n_0+1)v}^{(0)} & a_{(n_0+1)(n_0+1)} & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
b_{n_11}^{(0)} & \cdots & b_{n_1v}^{(0)} & a_{n_1(n_0+1)} & \cdots & \cdots & a_{n_1n_1}
\end{pmatrix}
\]

1d) diagonalize \(A_1\), extract the new lowest \(v\) eigenvalues \(\lambda_k^{(1)}\) \((k = 1, v)\) and the corresponding eigenvectors \(|\varphi_1^{(1)}\rangle, \ldots, |\varphi_v^{(1)}\rangle\), 1e) add these updated eigenvectors to \(|j\rangle = |n_1 + 1\rangle, \ldots, |n_2\rangle\), compute \(b_{k_j}^{(1)} = \langle \varphi_k^{(1)} | A | j \rangle\) and construct and diagonalize the new submatrix \(A_2\).

The procedure, so outlined, is iterated until the full basis is exhausted. This zero approximation loop yields the approximate \(v\) eigenvalues and eigenvectors

\[
E_k^{(1)} = \lambda_k^{(N)}, \quad |\psi_k^{(1)}\rangle \equiv |\varphi_k^{(1)}\rangle = \sum_{i=1}^{N} c_k^{(N)} |i\rangle.
\]
These eigensolutions are the new entries for a new iteration loop. More specifically, we consider the basis composed of the eigenvectors $\psi_k^{(1)}$ plus the original basis states $\{ | j \rangle \}$. Since the vectors $\psi_k^{(1)}$ are linear combinations of the $| j \rangle$ states, this new basis is no longer orthonormal and may be even redundant. We have therefore to solve an eigenvalue problem of general form and resort to the Choleski decomposition method. With this modifications, the subsequent iteration loops proceed as the first one and generate a sequence of $v$ vectors that converge to the exact eigensolution $\psi_1, \ldots, \psi_v$[13].

3. New implementation
We consider the modified Hamiltonian

$$H_J = H + c[J^2 - J(J + 1)]^2,$$

(4)

where $H$ is a two-body Hamiltonian of general form, $J$ the total spin operator, and $c$ a positive constant. The shell model basis is composed of the states $|\{i\} \rangle = |\alpha_1, \alpha_2, \ldots, \alpha_v, M \rangle$, where $M = m_1 + \ldots + m_i + \ldots + m_v$ is the total magnetic quantum number of a system of $v$ valence nucleons, $\alpha_i = \{a_i, m_i\}$ denote the single particle (s.p.) quantum numbers and $a_i = \{n_i, l_i, j_i\}$ the s.p. shells.

Let us consider a subspace $M_0$ resulting from a given number of partitions $\{a_1^{n_1}, a_2^{n_2}, \ldots, a_i^{n_i}, \ldots, a_v^{n_v}\}$ of the $v$ valence nucleons, where $n_i$ is the occupation number of the s.p. shell $a_i$. Since $[J, J_i^2] = 0$, the states $|\{i\} \rangle$, spanning $M_0$, transform among themselves under the action of $J^2$.

Thus, for a given $J$, if the constant $c$ is chosen so as to push up in energy the eigenvalues with total spin $J' \neq J$, the diagonalization algorithm generates in $M_0$ $v$ lowest eigenvalues $E^{(0)}_1, \ldots, E^{(0)}_v$ and eigenvectors $\psi^{(0)}_1, \ldots, \psi^{(0)}_v$, all having the selected $J$. These eigensolutions are exact within $M_0$.

The Hamiltonian $H$ couples the eigenvectors $\psi^{(0)}_1, \ldots, \psi^{(0)}_v$ only to those basis states of the complementary subspace $M_0^{(C)}$ that differ from the ones in $M_0$ by at most two single particle states or, in the second quantization language, two particle-two holes $(2p - 2h)$. Let us add these states, denoted by by $|\{j\} \rangle >$ to the eigenvectors $\psi^{(0)}_1, \ldots, \psi^{(0)}_v$ and adopt the algorithm to diagonalize $H_J$ in this new subspace.

The new set of lowest eigenvectors $\psi^{(1)}_1, \ldots, \psi^{(1)}_v$, of energies $E^{(1)}_1, \ldots, E^{(1)}_v$, are coupled only to the basis states, to be denoted by $|\{j\} \rangle >$, differing from the original $|\{j\} \rangle >$ by at most $4p - 4h$. The diagonalization of $H_J$ in the new subspace, spanned by $\varphi^{(1)}_1, \ldots, \varphi^{(1)}_v$ plus $|\{j\} \rangle >$, generates a new set of $v$ lowest eigensolution of good $J$.

By iterating the procedure just outlined, we cover eventually the full space and the set of $v$ eigensolutions tend to the exact ones.

3.1. Upgraded importance sampling
The above iterative procedure reduces effectively the dimensions of the Hamiltonian matrix by exploiting its sparsity. A further reduction is achieved by adopting an importance sampling, specific of the algorithm [14]. Here, a more efficient implementation of the sampling is proposed.

Let us fix a sequence of positive small numbers $\epsilon_i$ of decreasing values $\epsilon_0 > \epsilon_1 > \ldots > \epsilon_i > \ldots > \epsilon_n$. Once the diagonalization of $H_J$ in the initial subspace $M_0$ yields the lowest $v$ eigenvalues $E^{(0)}_1, \ldots, E^{(0)}_v$ with the corresponding eigenvectors $\psi^{(0)}_1, \ldots, \psi^{(0)}_v$, we pick only the $(2p, 2h)$ basis states $|j\rangle >$ that fulfill the condition

$$\frac{b_{ij}^{(1)}(kj)}{a_{jj} - E^{(0)}_k} > \epsilon_0,$$

(5)
where \( k = 1, v \) and \( a_{jj} (j = n_0 + 1, N, ) \) is the diagonal matrix element corresponding to the state \( |j\rangle \) coupled to \( \psi_k^{(0)} \) through the matrix element \( b_0(kj) = \langle j | H_j | \psi_k^{(0)} \rangle \).

The states \( \{|j\rangle\} \) so selected are added to the \( v \) eigenstates \( \{\psi_k^{(0)}\} \). These two sets of states are used to construct and diagonalize the Hamiltonian matrix. New eigenvalues \( E_1^{(1)}, \ldots, E_v^{(1)} \) and eigenvectors \( \psi_1^{(1)}, \ldots, \psi_v^{(1)} \) are generated. These eigenfunctions are linear combinations of the original \((0p - 0h)\) states of the subspace \( M_0 \) plus the \((2p - 2h)\) states selected according to the sampling condition (5).

We now select all the states \( |j\rangle \) that fulfill the updated condition

\[
\frac{b_1^2(kj)}{a_{jj} - E_k^{(1)}} > \epsilon_1
\]

where \( k = 1, v \) and \( b_1(kj) = \langle j | H_j | \psi_k^{(1)} \rangle \) (\( j = n_0 + 1, N \)).

The diagonalization algorithm, applied to the new subspace spanned by the \( v \) states \( \{\psi_k^{(1)}\} \) plus the set of states \( \{|j\rangle\} \), yields new eigensolutions \( E_1^{(2)}, \ldots, E_v^{(2)} \) and eigenvectors \( \psi_1^{(2)}, \ldots, \psi_v^{(2)} \). These updated eigenvectors include \( 2p - 2h \) states not admitted in the first run (since \( \epsilon_1 < \epsilon_0 \)) plus \( (4p - 4h) \) states. We now iterate the sampling procedure with decreasing values of \( \epsilon_i \), obtaining more and more accurate eigensolutions, until we exhaust the full basis. For \( \epsilon_n \to 0 \), the sampling yields the exact eigensolutions.

**Figure 1.** Convergence of the lowest \( J^\pi = 0^+ \) eigenvalues in \(^{128}\)Te

4. **Numerical implementation**

We applied the algorithm to \(^{128}\)Te. We included the shells \( \{2d5/2, 1g7/2, 2d3/2, 3s1/2, 1h11/2\} \) for both valence neutrons and protons. The neutron single particle energies are the same as the
ones used in Ref. [18] to study $^{116}$Sn. The proton single particle energies are the ones adopted in Ref. [14] for $^{133}$Xe. A renormalized $G$-matrix [16] deduced from the CD-Bonn potential [17] was chosen as two-body interaction. The effective charges $e_p = 1.5$ and $e_n = 1.7$ were assigned to protons and neutrons, respectively.
The dimensions \( n_0 \) of the subspace \( M_0 \), necessary to generate the first \( v \) eigenvalues and eigenvectors of a given \( J \), depend on the number \( v \). In the present case, \( n_0 \approx 50 \) was sufficient to generate \( v = 5 \) lowest eigenstates. Once chosen \( M_0 \), we applied the iterative sampling procedure with decreasing values of \( \varepsilon_i (\leq \varepsilon_{i+1}) \). At the \( i_{th} \)-iteration, corresponding to a given \( \varepsilon_i \), the sampling picks up a set of states that differ from the \( 0p - 0h \) states of the original subspace \( M_0 \) by at most \( (k_i p, k_i h) \) configurations. As we move to the next iteration, the states differ from the starting \( 0p - 0h \) by at most \( (k_{i+1} p, k_{i+1} h) \) with \( k_{i+1} = k_i + 2 \). Each value \( \varepsilon_i \) determines uniquely the dimension \( n_i \) of the Hamiltonian matrix to be the diagonalized.

Figs. 1, 2 and 3 plot the lowest five eigenvalues, for \( J^\pi = 0^+, J^\pi = 2^+ \) and \( J^\pi = 4^+ \) respectively, versus the dimensions \( n/N \) of the sampled matrices, normalized to the dimensions \( N \) of the full matrix. As shown in the plots, all eigenvalues converge rapidly to the exact asymptotic levels. In general, less than 10\% of the basis states is sufficient to yield the exact eigenvalues.

A rapid convergence is achieved also for the \( E2 \) strengths (Figs. 4 and 5). The smooth behavior of both energies and strengths versus \( n/N \) is to be noticed. This allows to extrapolate the computed data asymptotically to the exact quantities.

5. Concluding remarks
As illustrated for \(^{128}\)Te, the iterative algorithm, implemented in the \( m \)-scheme, generates a large number of low-lying eigenstates for each \( J \) value.

Its convergence properties are greatly enhanced by an importance sampling, inherent the method, which induces an effective truncation of the Hamiltonian matrix. A rapid convergence is achieved also for the \( E2 \) transition strengths. Both energies and strengths behave smoothly and, therefore, can be extrapolated asymptotically to their exact values.

These convergence properties make us confident about the extension of the method to very large matrices and therefore to nuclei with a large number of valence nucleons.

We have already made a meaningful progress in this direction by succesfully applying the method to Hamiltonian matrices of dimensions close to one billion \([15]\). Thus, nuclei like \(^{140,142}\)Sn or \(^{138,140}\)Te are at reach.

References
[1] See, for instance, Golub G H and Van Loan C F 1996 Matrix Computations (Baltimore: John Hopkins University Press)
[2] Brown B A et al. 1985 OXBASH Code (MSU-NSCL: Technical Report No. 524)
[3] Vallieres M and Novoselsky A 1994 Nucl. Phys. A 570 345c
[4] Caurier E and Nowacki F 1999 Acta Physica Polonica 30 705
[5] Caurier E et al. 2005 Rev. Mod. Phys. 77 427
[6] Koozin S E Dean D J and Langanke K 1997 Phys. Rep. 278 1
[7] Otsuka T, Homma M and Mizusaki T 1998 Phys. Rev. Lett. 81 1588
[8] Otsuka T et al. 2001 Prog. Part. Nucl. Phys. 47 319
[9] Dukesky J and Pittel S 2001 Phys. Rev. C 63 061303
[10] White S R 1993 Phys. Rev. B 48 10345
[11] Pittel S and Sandulescu N 2006 Phys. Rev. C 73 014301
[12] Thakur B, Pittel S, Sandulescu N 2008 Phys. Rev. C 78 041303
[13] Andreozzi F, Porrino A and Lo Iudice N 2002 J. Phys. A: Math. Gen. 35 L61
[14] Andreozzi F, Lo Iudice N and Porrino A 2003 J. Phys. : Nucl. Part. Phys. 29 2319
[15] Bianco D, Andreozzi F, Lo Iudice N, Porrino A and Knapp F, to be submitted for publication
[16] Hjorth-Jensen M et al. 1995 Physics Reports 261 125
[17] Machleidt R 1989 Adv. Nucl. Phys. 19 189
[18] Dikmen E, Oztürk O, Valliere M 2009 J. Phys. : Nucl. Part. Phys. 36 045102