An upgraded algorithm for shell model calculations and its implementation in medium-heavy nuclei

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Abstract. A matrix diagonalization algorithm we developed in the past years has been revised and implemented for large scale shell model calculations using a spin uncoupled basis so as to obtain a sparse Hamiltonian matrix. The dimensions of such a matrix are reduced drastically by a procedure that combines an effective projection of the good angular momentum with an importance sampling specific of the method. Its numerical implementation on 116Sn illustrates the simplicity of the method and the fast convergence of the iterative procedure.

1. Introduction
The standard methods [1] for diagonalizing matrices of very large dimensions are unmanageable even with the powerful computing facilities available now. On the other hand, one is mostly interested at generating the lowest eigenvalues and eigenstates.

Lanczos algorithm is the ideal tool for this purpose [2]. This algorithm has been implemented in several ways for performing large scale nuclear shell model calculations. Antoine [3, 4] is maybe the most widely adopted code in this field. It uses an uncoupled basis (m-scheme), which simplifies tremendously the construction of the Hamiltonian matrix and reduces effectively its dimensions by taking full advantage of its sparse nature.

Considerable effort has been devoted also at the attempt of reducing further the sizes of the Hamiltonian matrix. The quantum Monte Carlo diagonalization (QMCD) method [5, 6], adopted with success for systematics in the (s,d) and (f,p) nuclear regions, generates stochastically a truncated basis for the diagonalization of the many-body Hamiltonian. Specific procedures have been developed to restore the total spin and other symmetries, broken by the stochastic sampling procedure.

The Monte Carlo technique applied to shell model (SMMC) was first developed as a tool alternative to the direct diagonalization of the Hamiltonian [7, 8, 9]. The SMMC, indeed, evaluates expectation values and strength functions, providing important information on ground state properties and electromagnetic responses of medium-mass nuclei. The drawback of the SMMC approach is represented by the famous sign problem, not completely solved yet.

A method for achieving a drastic truncation of the shell model space is based on the density matrix renormalization group (DMRG) [10] borrowed from condensed matter [11]. In nuclear

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structure, this approach came out to be more effective in the coupled scheme and, in this form, was used to compute the low energy spectra of nuclei in the \((f,p)\) shell, like \(^{48}\)Cr and \(^{56}\)Ni [12, 13].

As pointed out already, all the above methods, apart from the SMMC, exploit the Lanczos algorithm. Although extremely powerful, this method presents some critical points. In fact, the states generated by the Lanczos iterative procedure, though mathematically orthogonal, might lose this property because of numerical errors that propagate rapidly with the number of iterations. It might happen, therefore, that the same state occurs more than once or states of unwanted angular momenta appear.

Few years ago, we developed a method [14, 15] that faces directly the diagonalization of the Hamiltonian. It is an iterative algorithm which generates a selected set of eigenvectors of a large matrix and is extremely simple to be implemented. It is also endowed with an importance sampling that yields a drastic reduction of the space and allows to extrapolate to the exact eigenvalues.

The method was implemented in the coupled \(j\)-scheme only, which is too time consuming in the construction of the Hamiltonian matrix. We have now implemented the algorithm in the \(m\)-scheme and developed a more efficient iterative procedure which allows to face matrices of much larger dimensions, especially when combined with an importance sampling [16]. A brief outline of the method together with illustrative results are presented here.

2. The algorithm

Let us consider an operator \(\hat{A}\), assumed for simplicity to be self-adjoint, and the matrix \(A = \{a_{ij}\}\) representing \(\hat{A}\) in an orthonormal basis \(\{|1\rangle, |2\rangle, \ldots, |i\rangle, \ldots, |N\rangle\}\). The diagonalization procedure goes through several iteration loops. The first loop is composed of the following steps:

1a) Consider the lowest \(n_0\) basis states \(|i > (n_0 << N)\), construct and diagonalize the \(n_0 \times n_0\) 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) consider the subspace spanned by the \(v\) eigenvectors \(|\varphi_k^{(0)}\rangle\) plus the basis states \(|j > = |n_0 + 1 >, \ldots |n_1 >\), compute \(b_{kji}^{(0)} = (\varphi_k^{(0)} \langle \hat{A} | j\rangle\) and construct the new submatrix

\[
A_1 = \begin{pmatrix}
\lambda_1^{(0)} & 0 & 0 & 0 & b_{11}^{(0)}(n_0+1) & \cdots & b_{1n_1}^{(0)} \\
0 & 0 & 0 & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & \lambda_v^{(0)} & b_{v1}^{(0)}(n_0+1) & \cdots & b_{vn_1}^{(0)} \\
b_{11}^{(0)}(n_0+1) & \cdots & b_{1v}^{(0)}(n_0+1) & a_{n_0+1}(n_0+1) & \cdots & a_{n_0+1}n_1 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
b_{n_1}^{(0)} & \cdots & b_{n_1v}^{(0)} & a_{n_0+1}(n_0+1) & \cdots & a_{n_0+1}n_1
\end{pmatrix},
\]

1d) diagonalize \(A_1\) and extract the new lowest \(v\) eigenvalues \(\lambda_k^{(1)}\) \((k = 1, v)\) and the corresponding eigenvectors \(|\varphi_k^{(1)}\rangle, \ldots, |\varphi_v^{(1)}\rangle\),

1e) consider now the new subspace spanned by \(|\varphi_k^{(1)}\rangle, \ldots, |\varphi_v^{(1)}\rangle\) plus the basis states \(|j > = |n_1 + 1 >, \ldots |n_2 >\), construct the new submatrix \(A_2\) just as done in point 1c) for \(A_1\) and,
after its diagonalization, extract the new lowest \( v \) eigenvalues \( \lambda_{1}^{(2)}, \ldots, \lambda_{v}^{(2)} \) and the corresponding eigenvectors \( | \varphi_{1}^{(2)} \rangle, \ldots, | \varphi_{v}^{(2)} \rangle \).

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

\[
E_k^{(1)} \equiv \lambda_k^{(N)}, \quad | \psi_k^{(1)} \rangle \equiv | \varphi_k^{(N)} \rangle = \sum_{i=1}^{N} c_k^{(N)} (i) | i \rangle. \tag{3}
\]

These eigensolutions are the new entries for a new iteration. More specifically, we consider the basis composed of the eigenvectors \( | \psi_k^{(1)} \rangle \) plus the original basis states \( \{ | j \rangle \} \). Since the vectors \( | \psi_k^{(1)} \rangle \) 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 the 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 \( \psi_1^{(i)}, \ldots, \psi_v^{(i)} \) that converge to the exact eigensolutions [14].

3. Implementation of the algorithm in the \( m \)-scheme

We start with the modified Hamiltonian

\[
H_J = H + c[J^2 - J(J + 1)]^2, \tag{4}
\]

where \( H \) is a two-body Hamiltonian of general form, \( J \) the total spin operator, and \( c \) a positive constant. The Hamiltonian acts in a model space spanned by the states \( | i \rangle = | \alpha_1, \alpha_2, \ldots, \alpha_p \rangle \), where \( p \) denotes the number of valence nucleons, \( \alpha_i = \{ a_i m_i \} \) the single particle (s.p.) quantum numbers and \( a_i = \{ n_i l_i j_i \} \) the s.p. shells. The states \( | i \rangle \) have a good magnetic quantum number \( M = m_1 + \ldots + m_i + \ldots + m_p \).

We define a subspace \( M_0 \) spanned by a set of configurations \( \{ a_i^{n_i} \} = \{ a_1^{n_1}, a_2^{n_2}, \ldots, a_i^{n_i}, \ldots \} \), where \( n_i \) is the occupation number of the s.p. shell \( a_i \). Under the action of \( J^2 \), the states \( | i \rangle \) of a given configuration \( \{ a_i^{n_i} \} \) transform among themselves in virtue of the commutation relations \([J_i, J_j^2] = 0\).

For fixed \( J \), we diagonalize the Hamiltonian matrix \( H_J \) in \( M_0 \) by using, for instance, the algorithm outlined in Sect. 2. If the constant \( c \) is chosen so as to push up in energy the eigenvalues with total spin \( J' \neq J \), the algorithm generates \( v \) lowest eigenvalues \( E_1^{(0)}, \ldots, E_v^{(0)} \) and eigenvectors \( \psi_1^{(0)}, \ldots, \psi_v^{(0)} \). These have a good \( J \) in virtue of the rotational invariant Hamiltonian and the mentioned invariance of each configuration \( \{ a_i^{n_i} \} \) with respect to \( J^2 \).

The eigenvectors \( \psi_1^{(0)}, \ldots, \psi_v^{(0)} \) are coupled by \( H \) only to those basis states of the complementary subspace \( M_0^{(C)} \) that differ from the ones in \( M_0 \) by at most two s.p. states or, in the second quantization language, two particle-two holes \((2p - 2h)\). Let us denote them by \( | j > 2 \). We now consider the subspace spanned by the eigenvectors \( \psi_1^{(0)}, \ldots, \psi_v^{(0)} \) plus the basis states \( | j > 2 \) and adopt the algorithm to diagonalize \( H_J \) in this subspace. A new set of lowest eigenvalues \( E_1^{(1)}, \ldots, E_v^{(1)} \) and eigenvectors \( \psi_1^{(1)}, \ldots, \psi_v^{(1)} \) is generated.

These new eigenvectors are coupled only to the basis states, to be denoted by \( | j > 4 \), differing from the original \( | j > 0 \) by at most \( 4p - 4h \). The diagonalization of \( H_J \) in the new subspace, spanned by \( \psi_1^{(1)}, \ldots, \psi_v^{(1)} \) plus \( \{ | j > 4 \} \), generates a new set of \( v \) lowest eigenvectors 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. The importance sampling revisited

Even after having exploited the sparsity of the Hamiltonian matrix, the diagonalization procedure might become prohibitively lengthy as the dimensions of the space increase. It is therefore useful, if not necessary, to resort to the sampling procedure. This has been simplified as follows.

Let us fix a sequence of positive small numbers \( \epsilon_i \) of decreasing values \( \epsilon_0 > \epsilon_1 > \ldots > \epsilon_i > \ldots > \epsilon_l \). Once the diagonalization of \( H_J \) in the initial subspace \( M_0 \) yields the lowest \( v \) eigenvalues \( E_1^{(0)}, \ldots, E_v^{(0)} \) with the corresponding eigenvectors \( \psi_1^{(0)}, \ldots, \psi_v^{(0)} \), we pick only the \((2p - 2h)\) basis states \( |j\rangle \) that fulfill the condition

\[
\frac{b_0^2(kj)}{a_{jj} - E_k^{(0)}} > \epsilon_0
\]

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 \( b_0(kj) = \langle j|H_J|\psi_k^{(0)} \rangle \).

We then adopt the diagonalization algorithm to diagonalize \( H_J \) in the subspace spanned by the \( v \) states \( \{\psi_k^{(0)}\} \) plus the basis states \( \{|j\rangle\} \) selected according to the sampling condition (5). New eigenvalues \( E_1^{(1)}, \ldots, E_v^{(1)} \) and eigenvectors \( \psi_1^{(1)}, \ldots, \psi_v^{(1)} \) are generated. These eigenfunctions are now 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 explore again the subspace complementary to \( M_0 \) and select all the states \( |j\rangle \) that fulfill the condition (5) with the following replacements \( E_k^{(0)} \rightarrow E_k^{(1)}, b_0(kj) \rightarrow b_1(kj) = \langle j|H_J|\psi_k^{(1)} \rangle \), \( \epsilon_0 \rightarrow \epsilon_1 \). 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 eigenvalues \( E_1^{(2)}, \ldots, E_v^{(2)} \) 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 applying at the \( i_{th} \) iteration the sampling condition

\[
\frac{b_i^2(kj)}{a_{jj} - E_k^{(i)}} > \epsilon_i
\]

where \( b_i(kj) = \langle j|H_J|\psi_k^{(i)} \rangle \). Once the full space is covered, the process yields a set of eigenvalues and eigenfunctions that approach the exact values in the limit \( \epsilon_l \rightarrow 0 \). In practice, as we shall see, the exact eigensolutions are reached for a sufficiently small \( \epsilon_l \neq 0 \).

4. Numerical implementation

The sampling algorithm was applied to \(^{116}\text{Sn}\). The model space is defined by the neutron shells \( \{2d_{5/2}, 1g_{7/2}, 2d_{3/2}, 3s_{1/2}, 1h_{11/2}\} \). The single particle energies were borrowed from Ref. [17], while a renormalized G matrix [18] derived from the CD-Bonn potential [19] was taken as a two-body interaction. The \( E2 \) transition strengths were computed using the proton and neutron effective charges \( e_p = 1.5 \) and \( e_n = 1 \).

An initial subspace \( M_0 \) of dimensions \( n_0 \simeq 50 \) was sufficient to generate ten lowest eigenstates with good \( J \). Once chosen \( M_0 \), we applied the iterative sampling procedure using a set of decreasing values of \( \epsilon_i \). At each iteration, the sampling condition picks up new states that differ from the \(0p - 0h\) states of the original subspace \( M_0 \) by an increasing number of \( p - h \) states.

Fig. 1 plots the lowest ten \( J^\pi = 0^+ \) eigenvalues of \(^{116}\text{Sn}\) versus the dimensions \( n \) of the sampled matrix, normalized to the full matrix dimensions \( N \). The value \( n/N \) is uniquely
determined by the running sampling parameter $\epsilon$. As shown in the plots, all eigenvalues approach closely the exact values for less than 10% of the basis states. This can be seen also in Figs 2 and 3 for the $J^\pi = 2^+$ and $J^\pi = 4^+$ lowest levels, respectively. 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 make an extrapolation to the exact quantities.
5. Concluding remarks

The case of $^{116}$Sn, illustrated here, shows that the algorithm, implemented in the $m$-scheme, enables us to generate quite a large number of low-lying eigenstates for each $J$ value.

The importance sampling described above allows to achieve a rapid convergence of the iterative procedure for both energies and wavefunctions, as illustrated for the levels of few $J$ values and for some $E2$ transition strengths.

This rapid convergence induces effectively a cut of the dimensions of the matrix Hamiltonian by at least an order of magnitude. In virtue of this property, the method should be able to treat Hamiltonian matrices of very large dimensions. Very recent calculations [16] confirm this expectation.

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