An upgraded version of an importance sampling algorithm for large scale shell model calculations

Bianco D, Andreozzi F, Lo Iudice N, Porrino A, Dimitrova S

1Universita di Napoli Federico II, Dipartimento Scienze Fisiche, Monte S. Angelo, via Cintia, 80126 Napoli, Italy
2Institute of Nuclear Research and Nuclear Energy, Sofia, Bulgaria

E-mail: loiudice@na.infn.it

Abstract. An importance sampling iterative algorithm, developed few years ago, for generating exact eigensolutions of large matrices is upgraded so as to allow large scale shell model calculations in the uncoupled \( m \)-scheme. By exploiting the sparsity properties of the Hamiltonian matrix and projecting out effectively the good angular momentum, the new importance sampling allows to reduce drastically the sizes of the matrices while keeping full control of the accuracy of the eigensolutions. Illustrative numerical examples are presented.

1. Introduction

Even after the advent of powerful computing facilities, standard diagonalization methods are not suitable for large scale shell model(SM) calculations. They require in fact \( N^3 \) operations, \( N \) denoting the dimensions of the matrix [1]. On the other hand, if one is interested in few nuclear eigenstates, as it is often the case, one may resort to alternative methods.

Most of them are based on the Lanczos [2] algorithm and are especially efficient for determining the low lying eigenvalues [3]. Its numerical implementation, however, deserves special care. In fact, the generated states are mathematically but not numerically orthogonal. The error so induced propagates rapidly with the number of iterations and may yield ”ghost” or spurious states, like the multiple appearance of the same state or the intrusion of states of unwanted angular momenta. Several codes based on Lanczos are now available. Among them, widely adopted is Antoine [4], which takes full advantage of the sparse nature of the nuclear Hamiltonian when used in the \( m \)-scheme.

An alternative approach, that circumvents the direct diagonalization of \( H \), is the shell model Monte Carlo (SMMC) method [5, 6, 7]. This has to deal with the famous sign problem which has not found yet a clear-cut solution. Even with this limitation, SMMC has proved to be a powerful and efficient tool for studying ground-state and thermal properties of medium-mass nuclei as well as electroweak nuclear properties. SMMC evaluates expectation values and strength functions, but does not give explicit eigenvectors.

The quantum Monte Carlo diagonalization (QMCD) method combines the two approaches [8, 9]. It is basically an importance sampling method which generates stochastically by a MC technique a truncated basis for the direct diagonalization of the many-body Hamiltonian. On the other hand, the basis states so generated are not orthogonal and form in general a redundant set. Moreover, they do not have the spin as good quantum number. Specific procedures have
been developed to obviate these shortcomings. QMCD has been adopted extensively and with success for systematics in the \((s, d)\) and \((f, p)\) nuclear regions.

An approximate method, based on the density matrix renormalization group (DMRG) [10], was adopted to achieve a drastic truncation of the shell model space in nuclear systems [11]. The method came out to work more effectively in the coupled scheme and, in this form, was used to compute the low energy spectra of nuclei in the \((f, p)\) shell, like \(^{48}\text{Cr}\) [12, 13].

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 asymptotic values.

The method was implemented in the coupled \(j\)-scheme only, which is too time consuming in the construction of the Hamiltonian matrix. On the other hand, in the \(m\)-scheme one has to deal with matrices whose sizes become prohibitively large as the number of shells increases. In order to circumvent this problem, we have modified the sampling procedure [16] according to some prescriptions, inherent the method, that allow a drastic cut of the dimensions of the Hamiltonian matrix. How this is done will be illustrated shortly here.

2. The algorithm

Let us consider a symmetric matrix \(A = \{a_{ij}\}\) representing a self-adjoint operator \(\hat{A}\) in an orthonormal basis \(|1\rangle, |2\rangle, \ldots, |N\rangle\). Let us suppose, for simplicity, that the basis states are ordered according to some criterion, for instance increasing unperturbed energies, when the operator \(\hat{A}\) is the nuclear shell model Hamiltonian.

The algorithm consists of several iteration loops. The first loop goes through the following steps:

1a) Consider the lowest \(n_0\) basis states \(|i\rangle > (n_0 << N)\), construct and diagonalize the \(n_0 \times n_0\) submatrix \(A_0 = (a_{ij})\),

1b) select the lowest \(v\) eigenvalues \(\lambda_1^{(0)}, \lambda_2^{(0)}, \ldots, \lambda_v^{(0)}\) and the corresponding eigenvectors \(|\varphi_k^{(0)}\rangle = \sum_{i=1}^{n_0} \varphi_i^{(0)} |i\rangle\), \(k = 1, v\) (1)

1c) consider now the subspace spanned by the \(v\) eigenvectors \(|\varphi_k^{(0)}\rangle\) plus the basis states \(|i\rangle > (i = n_0 + 1, n_0')\), and construct the new submatrix \(A_1 = \left( \begin{array}{cc} A_0 & B_0 \\ B_0^T & A_0' \end{array} \right)\), \(2\)

where \(A_0\) is the \(v\)-dimensional diagonal matrix, composed of the eigenvalues \(\lambda_k^{(0)}\) \((k = 1, v)\), \(A_0' = \{a_{ij}\} (i, j = n_0 + 1, n_0')\) is a submatrix of dimensions \(n_1 = n_0' - n_0\), \(B_0\) and its transpose are off-diagonal blocks composed of the matrix elements \(b_{kj}^{(0)} = \langle\varphi_k^{(0)} | \hat{A} | j\rangle\) \((k = 1, v, j = n_0 + 1, n_0')\),

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

1e) consider now the new subspace spanned by the new lowest \(v\) eigenvectors \(|\varphi_k^{(1)}\rangle\) plus the basis states \(|i\rangle > (i = n_0' + 1, n_0'')\), 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 \(\lambda_k^{(2)}\) \((k = 1, v)\) and the corresponding eigenvectors \(|\varphi_k^{(2)}\rangle\).
The just outlined procedure is iterated until the full basis is exhausted. This zero approximation loop yields the approximate $v$ eigenvalues and eigenvectors

$$E^{(1)}_k \equiv \lambda^{(N)}_k, \quad |\psi^{(1)}_k\rangle \equiv |\varphi^{(N)}_k\rangle = \sum_{i=1}^{N} c^{(N)}_k(i) |i\rangle.$$  

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

3. Importance sampling

The outlined algorithm, though of simple implementation, requires the storage of at least one eigenvector. Since for many complex systems the dimensions of the Hamiltonian matrix become prohibitively large, one must rely on some importance sampling that allows to truncate the space by selecting only the basis states relevant to the exact eigensolutions. A notable example is the stochastic diagonalization method [17], which samples the basis states relevant to the ground state through a combination of plane (Jacobi) rotations and matrix inflation.

A similar sampling procedure can be implemented in the framework of our diagonalization process. Exploiting the fact that the algorithm yields quite accurate solutions already in the first approximation loop, we have devised a sampling which makes use of the first loop only, accordingly modified:

1a) Turn the $v$-dimensional principal submatrix $\{a_{ij}\}$ $(i,j = 1,v)$ into the diagonal form $\Lambda_v$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_v$.

1b) For $j = v+1, \ldots, N$, diagonalize the $v+1$-dimensional matrix

$$A = \begin{pmatrix} \Lambda_v & \vec{b}_j \\ \vec{b}_j & a_{jj} \end{pmatrix},$$  

where $\vec{b}_j = \{b_{1j}, b_{2j}, \ldots, b_{vj}\}$.

1c) Select the lowest $v$ eigenvalues $\lambda'_i, (i = 1,v)$ and accept the new state only if

$$\sum_{i=1,v} |\lambda'_i - \lambda_i| > \epsilon$$  

Otherwise restart from point 1b) with a new $j$. The outcome of this procedure is that the selected states span a $n_s(<N)$ dimensional space, so that the subsequent refinement loops iterate only on the smaller set of $n_s$ basis vectors. The number of operations is thereby reduced by a factor $n_s/N$.

4. Importance sampling algorithm (ISA) in the $m$-scheme

The model space under consideration is spanned by the states $|j\rangle = |\alpha_1, \alpha_2, \ldots, \alpha_v, M\rangle$, where $M = m_1 + \ldots + m_i + \ldots + m_v$ is the total magnetic quantum number of a system of $v$ valence nucleons and $\alpha_i = \{a_i m_i\}, (a_i = \{n_i l_i j_i\})$ denote the single particle quantum numbers.

Let us consider the modified Hamiltonian

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

where $H$
where $H$ is a two-body Hamiltonian of general form, $J$ the total spin operator, and $\epsilon$ a positive constant.

We select a set of configurations $\{a_1^{n_1}, a_2^{n_2}, \ldots, a_i^{n_i} \ldots, a_v^{n_v}\}$, where $n_i$ is the occupation number of the s.p. configurations $a_i$. They define a subspace $M_0$. Under the action of $J^2$, the states $|j,N\rangle = |a_1^{n_1}, a_2^{n_2}, \ldots, a_i^{n_i} \ldots, a_v^{n_v}\rangle$, belonging to a given configuration, transform among themselves in virtue of the commutation relations $[J,j^2] = 0$.

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 $\epsilon$ is chosen so as to push up in energy the eigenvalues with total spin $J' \neq J$, the diagonalization algorithm generates $v$ lowest eigenvalues $\lambda_1^{(0)}, \ldots, \lambda_v^{(0)}$ and eigenvectors $\varphi_1^{(0)}, \ldots, \varphi_v^{(0)}$. These have a good $J$ in virtue of the rotational invariant Hamiltonian and the mentioned invariance of each configuration $\{a_1^{n_1}, a_2^{n_2}, \ldots, a_i^{n_i} \ldots, a_v^{n_v}\}$ with respect to $J^2$.

The eigenvectors $\varphi_1^{(0)}, \ldots, \varphi_v^{(0)}$ 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 single particle states or, in the second quantization language, two particle-two hole $(2p−2h)$ states. Let us denote them by $|j\rangle$. We now consider the subspace spanned by the eigenvectors $\varphi_1^{(0)}, \ldots, \varphi_v^{(0)}$ plus the basis states $|j\rangle$ and adopt the algorithm to diagonalize $H_J$ in this subspace. A new set of lowest eigenvalues $\lambda_1^{(1)}, \ldots, \lambda_v^{(1)}$ and eigenvectors $\varphi_1^{(1)}, \ldots, \varphi_v^{(1)}$ is generated.

These new eigenvectors are coupled only to the basis states, to be denoted by $|j\rangle > \epsilon_4$, differing from the original $|j\rangle > \epsilon_0$ by at most $4p−4h$. The diagonalization of $H_J$ in the new subspace, spanned by $\varphi_1^{(1)}, \ldots, \varphi_v^{(1)}\rangle \rangle$ plus $|j\rangle > \epsilon_4$, generates a new set of $v$ lowest eigensolutions 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.

4.1. Upgraded importance sampling

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 $\epsilon_0 > \epsilon_1 > \ldots > \epsilon_i > \ldots > \epsilon_n$. Once the diagonalization of $H_J$ in the initial subspace $M_0$ yields the lowest $v$ eigenvalues $\lambda_1^{(0)}, \ldots, \lambda_v^{(0)}$ with the corresponding eigenvectors $\varphi_1^{(0)}, \ldots, \varphi_v^{(0)}$, we pick only the $(2p,2h)$ basis states $|j\rangle > \epsilon_0$ that fulfill the condition

$$\frac{b_0^2(kj)}{a_{jj} - \lambda^{(0)}_k} > \epsilon_0$$

(7)

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 $\varphi_k^{(0)}$ through the matrix element $b_0(kj) = < j | H_J | \varphi_k^{(0)} >$.

We then adopt the diagonalization algorithm to diagonalize $H_J$ in the subspace spanned by the $v$ states $\{\varphi_k^{(0)}\}$ plus the basis states $\{|j\rangle\}$ selected according to the sampling condition (7). New eigenvalues $\lambda_1^{(1)}, \ldots, \lambda_v^{(1)}$ and eigenvectors $\varphi_1^{(1)}, \ldots, \varphi_v^{(1)}$ 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 (7). We now explore again the subspace complementary to $M_0$ and select all the states $|j\rangle > \epsilon_1$ that fulfill the updated condition

$$\frac{b_0^2(kj)}{a_{jj} - \lambda^{(1)}_k} > \epsilon_1$$

(8)

where $k = 1, v$ and $b_1(kj) = < j | H_J | \varphi_k^{(1)} > (j = n_0 + 1, N)$.
The diagonalization algorithm applied to the new subspace spanned by the $v$ states $\{\phi_k^{(1)}\}$ plus the set of states $\{|j>\}$ yields new eigensolutions $\lambda_1^{(2)}, \ldots, \lambda_v^{(2)}$ and eigenvectors $\varphi_1^{(2)}, \ldots, \varphi_v^{(2)}$. These updated eigenvectors include $2p-2h$ states not admitted in the first run (since $\epsilon_0 > \epsilon_1$) 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 properties of the lowest $J^\pi = 0^+$ eigenvalues in $^{48}$Cr

**Figure 2.** Convergence properties of the lowest $J^\pi = 0^+$ eigenvalues in $^{110}$Sn

### 5. Numerical implementation

We applied the sampling algorithm to the semi-magic $^{110}$Sn and the N=Z even-even $^{48}$Cr. The model spaces are:

1) $P = \{2d5/2, 1g7/2, 2d3/2, 3s1/2, 1h11/2\}$ for the valence neutrons of $^{110}$Sn,

2) $P = \{1f7/2, 1f5/2, 2p3/2, 2p1/2\}$ for the 4 valence protons and neutrons of $^{48}$Cr.

For $^{110}$Sn we used the single particle energies (in MeV) [20] $\epsilon_{2d5/2} = 0$, $\epsilon_{1g7/2} = 0.08$, $\epsilon_{3s1/2} = 2.45$, $\epsilon_{2d3/2} = 2.55$, $\epsilon_{1h11/2} = 3.20$. As for $^{48}$Cr, we used the same energies adopted in Ref.[19], namely $\epsilon_{1f7/2} = 0$, $\epsilon_{2p3/2} = 2.0$, $\epsilon_{2p1/2} = 4.0$, $\epsilon_{1f5/2} = 6.5$.

We adopted a realistic effective interaction deduced from the CD-Bonn potential [18] for $^{110}$Sn, and used the KB3 interaction [19] for $^{48}$Cr.

The first task consisted in choosing the initial subspace $M_0$. Its dimensions $n_0$ increase with the number of eigenstates of good $J$ we intend to generate. To yield six eigenstates, as in our case, the space dimensions came out to be of the order $n_0 \sim 100$. Having chosen $M_0$, we applied the iterative sampling procedure (7) for a given $\epsilon$. At each iteration, the sampling condition (7) 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. We applied the sampling procedure with decreasing values of
\( \epsilon \). Each value of \( \epsilon \) determines uniquely the dimension \( n_i \) of the Hamiltonian matrix to be the diagonalized.

Figs. 1 and 2 plot the lowest six \( J = 0 \) eigenvalues of \( ^{48}\text{Cr} \) and \( ^{110}\text{Sn} \) versus the dimensions \( n \) of the matrices resulting from the corresponding decreasing values of the sampling parameter \( \epsilon \).
As shown in the plots, all six eigenvalues approach closely the exact values for relatively small $n$-dimensional subspaces, especially in $^{110}$Sn (Fig. 2).

The convergence is more rapid than in other approaches like the DMRG. This is illustrated for the lowest $J = 0$ and $J = 2$ levels of $^{48}$Cr in Figs. 3 and 4. It is to be pointed out, however, that the DMRG seems to be more effective in the $j$-coupled scheme [12, 13]. Figs. 5 ad 6 show that a fast convergence is achieved also for the the $E2$ transitions strengths.

The smooth behavior of energies and $E2$ strengths versus $n$ is to be noticed. This allows to extrapolate the computed data to asymptotic values. These are shown to practically coincide with the exact quantities.

6. Concluding remarks

According to the present results, the $m$-scheme implementation of the importance sampling iterative algorithm for diagonalizing large matrices looks very promising. The $m$-scheme combined with an effective $J$-projection of the states allow to take advantage of the sparsity of the Hamiltonian matrix thereby reducing drastically the sizes of the matrix. The $J$-projection allows also to generate a number of low-lying eigenstates for each $J$ value that is appreciably larger than in other approaches.

A further crucial reduction is achieved by the importance sampling properly upgraded with respect to the original formulation. The importance sampling enhances greatly the convergence of the iterative process and makes possible an extrapolation to asymptotic values for energies and transition strengths that practically coincide with the exact values.

A high accuracy of the results is achieved also for the wavefunctions, as illustrated by the convergence properties of the $E2$ transition strengths. Some illustrative examples show that the convergence rate is appreciably faster than in other approaches. In virtue of these features, we are confident that the method can be applied to Hamiltonian matrices of very large dimensions. This hope is supported by preliminary calculations.

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