An importance sampling algorithm for generating exact eigenstates of the nuclear Hamiltonian

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(November 26, 2018)

Abstract

We endow a recently devised algorithm for generating exact eigensolutions of large matrices with an importance sampling, which is in control of the extent and accuracy of the truncation of their dimensions. We made several tests on typical nuclei using a correlated basis obtained from partitioning the shell model space. The sampling so implemented allows not only for a substantial reduction of the shell model space but also for an extrapolation to exact eigenvalues and E2 strengths.

02.70.-c 21.60.Cs
I. INTRODUCTION

New effective methods for solving exactly the shell model (SM) eigenvalue problem in complex nuclei have been developed in recent years. A notable one is the Monte Carlo technique [1] for generating exact SM ground states [2–4]. Its application, however, has been rather restricted because of the well known minus-sign problem.

Alternative methods face directly the diagonalization of the SM Hamiltonian by resorting to algorithms like Lanczos [5] and Davidson [6]. The critical points of direct diagonalization methods are the amount of memory needed and the time spent in the diagonalization process.

In order to overcome these limitations there have been attempts to combine the stochastic methodology with the standard diagonalization approach [7–12]. In [7] the use of Gaussian-like single-particle basis states with random oscillator frequencies was suggested. The authors of [8–10] proposed a stochastic truncation of the SM matrices and suggested for the energies so obtained an exponential extrapolation law to the exact eigenvalues. In the so call quantum Monte Carlo diagonalization method (QMCD) [11,12] the reduction of the dimension of the SM space is achieved by using the auxiliary field Monte Carlo technique to select the relevant basis states. Though quite successful, the latter method is not free from problems. Indeed, one has to deal with the redundancy of the basis states, which may slow considerably the convergence of the procedure, as well as with the problem of restoring the symmetries generally broken in stochastic approaches.

In a recent paper [13], we have developed an iterative algorithm for determining a selected set of eigenvectors of a large matrix which is faster than the other, currently adopted, algorithms, including Lanczos, and extremely simple to be implemented. It is, moreover, robust, yielding always ghost-free stable solutions.

Like the other methods, however, it requires the storage of at least one eigenvector, which exceeds the limits of modern computers in many complex systems. The present paper deals with the problem of overcoming this limitation. To this purpose, we endowed the algorithm with an importance sampling for reducing the sizes of the matrix. The sampling is closely linked to the iterative algorithm and is in full control of the accuracy of the eigensolutions. This will emerge clearly from the results of the exhaustive tests presented and discussed in this paper. In fact, we adopted the importance sampling to solve the shell model problem for three typical nuclei, the semi-magic $^{108}$Sn, the $N = Z$ doubly even $^{48}$Cr, and the $N \neq Z$ odd $^{133}$Xe. In order to enhance its efficiency we used a correlated basis obtained from partitioning the shell model space according to a method developed in Ref. [14]. We will show that the method not only allows for a drastic truncation of the SM space but yields naturally extrapolation laws to exact eigenvalues and eigenvectors as well as to the occupation numbers and the $E2$ transition probabilities.

II. THE ALGORITHM

Let us first give a brief outline of the algorithm [13]. For the sake of simplicity, we consider here a symmetric matrix

$$A = \{a_{ij}\} = \{\langle i | \hat{A} | j \rangle\}$$  (2.1)
representing a self-adjoint operator $\hat{A}$ in an orthonormal basis $\{|1\rangle, |2\rangle, \ldots, |N\rangle\}$. The algorithm goes through several iteration loops. The first loop consists of the following steps:

1a) Diagonalize the two-dimensional matrix $(a_{ij})$ (i,j=1,2),
1b) select the lowest eigenvalue $\lambda_2$ and the corresponding eigenvector

$$| \phi_2 \rangle = c_1^{(2)} | 1 \rangle + c_2^{(2)} | 2 \rangle,$$  \hfill (2.2)

1c) for $j = 3, \ldots, N$, diagonalize the matrix

$$\begin{pmatrix} \lambda_{j-1} & b_j \\ b_j & a_{jj} \end{pmatrix}$$  \hfill (2.3)

where $b_j = \langle \phi_{j-1} | \hat{A} | j \rangle$ and select the lowest eigenvalue $\lambda_j$ together with the corresponding eigenvector $| \phi_j \rangle$. This zero approximation loop yields the approximate eigenvalue and eigenvector

$$E^{(1)} \equiv \lambda_N, \quad | \psi^{(1)} \rangle \equiv | \phi_N \rangle = \sum_{i=1}^{N} c_i^{(N)} | i \rangle.$$  \hfill (2.4)

With these new entries we start an iterative procedure which goes through $n = 2, 3, \ldots$ refinement loops, consisting of the same steps with the following modification. At each step $j = 1, 2, \ldots, N$ of the $n$-th loop ($n > 1$) we have to solve an eigenvalue problem of general form, since the states $| \phi_{j-1} \rangle$ and $| j \rangle$ are no longer orthogonal. The eigenvalue $E^{(n)} \equiv \lambda_N$ and eigenvector $| \psi^{(n)} \rangle \equiv | \phi_N \rangle$ obtained after the $n$-th loop are proven to converge to the exact eigenvalue $E$ and eigenvector $| \psi \rangle$ respectively [13].

The algorithm has been shown to be completely equivalent to the method of optimal relaxation [15] and has therefore a variational foundation.

Because of its matrix formulation, however, it can be generalized with minimal changes so as to generate at once an arbitrary number $v$ of eigensolutions. Indeed, the first loop goes through the following steps:

1a) Start with $m (\geq v)$ basis vectors and diagonalize the $m$-dimensional principal submatrix $\{a_{ij}\} (i,j = 1, m)$,
1b) select the $v$ lowest eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_v$ and the corresponding eigenvectors $| \phi_1 \rangle, | \phi_2 \rangle, \ldots, | \phi_v \rangle$.

For $k = 2, 3, \ldots, k_N$, where $k_N$ are the steps necessary to exhaust the whole $N$-dimensional matrix,
1c) diagonalize the matrix

$$\begin{pmatrix} \Lambda_k & B_k \\ B_k^T & A_k \end{pmatrix}$$  \hfill (2.5)

where $\Lambda_k$ is a $v$-dimensional diagonal matrix whose non-zero entries are the eigenvalues $\lambda_1^{(k-1)}, \lambda_2^{(k-1)}, \ldots, \lambda_v^{(k-1)}$, $A_k = \{a_{ij}\} (i,j = (k-1)p+1, \ldots, kp)$ is a $p$-dimensional submatrix, $B_k$ and its transpose are matrices composed of the matrix elements $b_{ij}^{(k)} = \langle \phi_i^{(k-1)} | \hat{A} | j \rangle$ (i = 1, ..., $v$; j = $(k-1)p + 1, \ldots, kp)$.

1d) Select the $v$ lowest eigenvalues $\lambda_1^{(k)}, \lambda_2^{(k)}, \ldots, \lambda_v^{(k)}$ and the corresponding eigenvectors $| \phi_1^{(k)} \rangle, | \phi_2^{(k)} \rangle, \ldots, | \phi_v^{(k)} \rangle$. 


Once the basis is exhausted, the process yields \( v \) approximate eigenvalues and eigenvectors, which are the new entries for a new iteration. This goes through the same steps with one essential modification. Each loop, in fact, can be viewed as the solution of the eigenproblem for the restriction \( \hat{A}|_S \) of the operator \( \hat{A} \) to a subspace defined by the span of the set of vectors \( |i_p\rangle \equiv \{\phi^{(k)}_1, \ldots, \phi^{(k)}_v, |(k-1)p+1, \ldots, kp\rangle\} \). Since the vectors \( \phi^{(k)}_i \) are linear superpositions of all the basis vectors \( |j\rangle \) we started with, the basis obtained after the first approximation loop is no longer orthonormal, just as in the one-dimensional eigenspace, and may be even redundant. We have therefore to solve an eigenvalue problem of general form. This is done most effectively through a pivotal Choleski decomposition of the overlap matrix \( \langle i_p | i_p' \rangle \) [16]. As outlined in a forthcoming paper, this procedure is very easy to be implemented and extremely fast, specially in view of the very limited dimensions of the matrices coming into play. With this modifications, the subsequent iteration loops proceed as the first one. In this way we generate a sequence of \( v \) vectors \( \psi^{(k)}_1, \ldots, \psi^{(k)}_v \). The restriction of the operator \( \hat{A} \) to these sets defines a sequence of diagonal matrices, whose non zero elements are the current eigenvalues \( \lambda^{(k)}_1, \ldots, \lambda^{(k)}_v \), with decreasing norms. This monotonic sequence is certainly bounded from below and therefore convergent.

III. IMPORTANCE SAMPLING

The just 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 which allows for a truncation of the space by selecting only the basis states relevant to the exact eigen solutions. A notable example is the stochastic diagonalization method [6], which samples the basis states relevant to the ground state through a combination of plane (Jacobi) rotations and matrix inflation.

A similar, but more efficient, strategy 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 can devise a sampling which makes use of the first loop only. This is to be accordingly modified and goes through the following steps:

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

\[
A = \begin{pmatrix}
\Lambda_v & \vec{b}_j \\
\vec{b}_j^T & a_{jj}
\end{pmatrix},
\]

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 \( j \).

We can avoid such a time consuming sampling procedure by resorting to an alternative, though completely equivalent, route based on the method developed for deriving an exact non perturbative shell model Hamiltonian [17]. We carry the similarity transformation
\[ A' = \Omega^{-1} A \Omega \]  \hspace{1cm} (3.3)

where

\[ \Omega = \begin{pmatrix} I_v & 0 \\ \vec{\omega} & I_Q \end{pmatrix}. \]  \hspace{1cm} (3.4)

Here, \( I_v \) is the \( v \)-dimensional unit matrix and \( \omega \) a \( v \)-dimensional vector.

The transformed matrix has the following structure

\[ A' = \begin{pmatrix} \Lambda_v + \vec{b}_j \otimes \vec{\omega} & \vec{b}_j \\ \vec{b}_j' & a_{jj} - \vec{\omega} \cdot \vec{b}_j \end{pmatrix} \]  \hspace{1cm} (3.5)

where

\[ \vec{b}_j' = -(\vec{\omega} \cdot \vec{b}_j)\vec{\omega} - \vec{\omega} \Lambda_v + a_{jj} \vec{\omega} + \vec{b}_j^T. \]  \hspace{1cm} (3.6)

We now impose the decoupling condition

\[ \vec{b}_j' = -(\vec{\omega} \cdot \vec{b}_j)\vec{\omega} - \vec{\omega} \Lambda_v + a_{jj} \vec{\omega} + \vec{b}_j^T = 0. \]  \hspace{1cm} (3.7)

Once we find the solution \( \omega \), the matrix element \( a_{jj} - \vec{\omega} \cdot \vec{b}_j \) becomes an eigenvalue of the matrix \( A' \) and, therefore, of matrix \( A \). Right multiplying Eq. (3.7) by \( \vec{b}_j \), we obtain the dispersion relation

\[ \vec{\omega} \cdot \vec{b}_j = -\sum_{i=1,v} b_{ij}^2 a_{jj} - \lambda_i - \vec{\omega} \cdot \vec{b}_j. \]  \hspace{1cm} (3.8)

This admits \( v + 1 \) solutions, corresponding to the \( v + 1 \) eigenvalues of \( A \). In correspondence of the lowest solution \( (\vec{\omega} \cdot \vec{b}_j)_{\min} \), we get the maximum eigenvalue

\[ \lambda'_{\max} = a_{jj} - (\vec{\omega} \cdot \vec{b}_j)_{\min}. \]  \hspace{1cm} (3.9)

The eigenvalues \( \lambda_i, i = 1, \ldots, v \) separate at least in weak sense the new eigenvalues \( \lambda'_i, i = 1, \ldots, v + 1 \) [18], namely

\[ \lambda'_1 \leq \lambda_1 \leq \lambda'_2 \leq \ldots \leq \lambda'_v \leq \lambda_v \leq \lambda'_{\max}. \]  \hspace{1cm} (3.10)

Since

\[ \sum_{i=1,v+1} \lambda'_i = \sum_{i=1,v} \lambda'_i + a_{jj} - (\vec{\omega} \cdot \vec{b}_j)_{\min} = a_{jj} + \sum_{i=1,v} \lambda_i \]  \hspace{1cm} (3.11)

we have

\[ \sum_{i=1,v} (\lambda'_i - \lambda_i) = (\vec{\omega} \cdot \vec{b}_j)_{\min}. \]  \hspace{1cm} (3.12)

Condition (3.2) is therefore equivalent to
\[(\vec{\omega} \cdot \vec{b}_j)_{min} > \epsilon.\]  
\(3.13\)

The just outlined sampling procedure requires only the solution of the dispersion equation (3.8), which is of the type

\[f(z) = z\]  
\(3.14\)

and fulfils the condition

\[1 - df(z)/dz > 0.\]  
\(3.15\)

We can therefore easily solve it by using the Newton method of derivative. This alternative sampling procedure is not only rigorous but also more economical. It avoids, in fact, the \((N - v)\)-fold iterated diagonalization of \(v + 1\) dimensional matrices.

**IV. MULTIPARTITIONING METHOD**

The extent of truncation induced by the sampling is maximal when the eigenvectors are highly localized. This condition is fulfilled in most physical problems. Even when this is not the case, we can approach the above condition by using a correlated basis obtained by a multipartitioning method [14]. This goes through the following prescriptions:

i) Partition the shell model space for \(N\) valence nucleons into orthogonal subspaces, \(P_1\) and \(P_2\) according to

\[P = P_1 + P_2,\]  
\(4.1\)

ii) distribute \(N_1\) and \(N_2\) nucleons \((N_1 + N_2 = N)\) among these subspaces in all possible ways.

iii) decompose the Hamiltonian \(H\) into

\[H = H_1 + H_2 + H_{12},\]  
\(4.2\)

iv) solve the eigenvalue equations

\[H_i | \alpha_i N_i \rangle = E_{\alpha_i} | \alpha_i N_i \rangle\]  
\(4.3\)

obtaining the eigenstates \(| \alpha_1 N_1 \rangle\) and \(| \alpha_2 N_2 \rangle\) of \(H_1\) and \(H_2\) respectively in \(P_1\) and \(P_2\). Once this is done, it is possible to replace the standard shell model basis with one composed of the states

\[| \alpha N \rangle = | \alpha_1 N_1 \alpha_2 N_2 \rangle.\]  
\(4.4\)

We use the above basis to diagonalize the residual term \(H_{12}\) of the SM Hamiltonian. The new basis is in general highly correlated and, therefore, highly localized in the Fock space, a feature which enhances considerably the efficiency of the method.
V. SELECTIVE NUMERICAL TESTS

We applied the sampling algorithm to the semi-magic $^{108}$Sn, the N=Z even-even $^{48}$Cr and the N > Z odd-even $^{133}$Xe. The model spaces are:

1) \( P \equiv \{2d5/2, 1g7/2, 2d3/2, 3s1/2, 1h11/2\} \) for the 8 valence neutrons of $^{108}$Sn and for the 4 valence protons and 3 valence neutron holes of $^{133}$Xe,
2) \( P \equiv \{1f7/2, 1f5/2, 2p3/2, 2p1/2\} \) for the 4 valence protons and neutrons of $^{48}$Cr.

We adopted a realistic effective interaction deduced from the Bonn-A potential [19] for $^{108}$Sn and $^{133}$Xe, and used the KB3 interaction [20] for $^{48}$Cr. For $^{108}$Sn we used the single particle (s.p.) energies (in MeV) \( \epsilon_{2d5/2} = 0, \epsilon_{1g7/2} = 0.2, \epsilon_{3s1/2} = 2.2, \epsilon_{2d3/2} = 2.3, \epsilon_{1h11/2} = 2.9 \). Apart from the first two currently in use, the other energies were deduced from a fit on $^{111}$Sn for \( \{2d3/2, 3s1/2\} \) and from the level 9\(^{-} \) in $^{106}$Sn for 1h11/2. We used the same set of energies for protons in $^{133}$Xe, while for neutron-holes we used the slightly different values \( \epsilon_{2d5/2} = 0, \epsilon_{1g7/2} = 0.2, \epsilon_{3s1/2} = 1.72, \epsilon_{2d3/2} = 1.88, \epsilon_{1h11/2} = 2.7 \). The different set accounts effectively, at least in part, for the significant asymmetry between proton and neutron numbers which yield different contributions from the three- and more-body forces, not included in the effective interaction. As for $^{48}$Cr, we used the same energies adopted in Ref. [20], namely \( \epsilon_{1f7/2} = 0, \epsilon_{2p3/2} = 2.0, \epsilon_{2p1/2} = 4.0, \epsilon_{1f5/2} = 6.5 \).

We partitioned the shell model space for $^{108}$Sn according the following prescriptions:

\[
P \equiv \{2d5/2, 1g7/2, 2d3/2, 3s1/2, 1h11/2\} \quad \xrightarrow{P_1} \{2d5/2, 1g7/2\} \quad \xrightarrow{P_2} \{2d3/2, 3s1/2, 1h11/2\}. \tag{5.1}
\]

This partition is dictated by the large energy gap (\( \sim 2 \) MeV) between the two corresponding sets of single particle energies.

For $^{48}$Cr and $^{133}$Xe, we simply decompose the space into a proton and neutron subspace

\[
P = P_p + P_n. \tag{5.2}
\]

We adopted then the multipartitioning method [14] to generate a new correlated basis

\[
| j \rangle = | \alpha N \rangle \tag{5.3}
\]

and used this new basis to implement the importance sampling.

A. Eigenvalues

For illustrative purposes we discuss only few of the lowest states of the nuclei under investigation. As shown in the plot of Fig. 1, the sampling parameter \( \epsilon \) varies very smoothly with the dimensions \( n \) of the reduced matrices. In these, as in all other states considered, it scales according to

\[
\epsilon = b \frac{N}{n^2} \exp \left[ -c \frac{N}{n} \right] \tag{5.4}
\]

In virtue of this law, the increment of the dimensions of the matrix is modest for large values of \( \epsilon \), but grows dramatically as \( \epsilon \) gets smaller and smaller. This behavior reflects
the density of the unperturbed levels which is very low at low energy and raises steeply around a centroid at high energy. This is shown in the upper panel of Fig. 2. It follows that the running sum of the unperturbed basis states grows very slowly at low energy, then raises steeply toward its saturating full $N$ value in a relatively small energy interval (middle panel of Fig. 2). It is important to point out that this is the distribution of our unperturbed correlated states defined by Eq. (4.4). The partitioning of the shell model space is responsible for the squeezing of their energies around a centroid. Had we adopted the standard SM basis, the state distribution would have resulted more spread out and the running sum would have grown discontinuously through several steps in correspondence of each sub-shell (lower panel of Fig. 2).

Figs. 3-5 plot the eigenvalues versus the dimensions $n$ of the matrices resulting from decreasing values of the sampling parameter $\epsilon$ for some low-lying states of $^{108}$Sn, $^{48}$Cr, and $^{133}$Xe, respectively.

In all nuclei and for all states, the eigenvalues decrease monotonically and smoothly with $n$. The only meaningful exceptions are represented by the curves of the first excited $J^\pi = 0^+$ and $J^\pi = 2^+$ and few other, similarly behaving, high-lying states of $^{48}$Cr. These undergo a jump from an upper to a lower curve at some small value of the sampling parameter $\epsilon$, a signal of energy crossing. Even in these cases, however, the subsequent behavior of the energies is smooth as for the other states. It follows that, in all cases, starting from a sufficiently small $\epsilon$, the energies scale with the dimensions $n$ according to the law

$$E = E_0 + b \frac{N}{n} \exp \left[ -c \frac{N}{n} \right]$$

(5.5)

where $b$, $c$, and $E_0$ are constants specific of each state and the full dimension $N$ provides the scale. This fit allows for an extrapolation to asymptotic eigenvalues which differ from the exact ones in the second or third decimal digit. This is explicitly proven for $^{108}$Sn and $^{48}$Cr (Table I). The reliability of the extrapolation in the case of $^{133}$Xe is inferred from the rapid convergence of the iterative procedure, as clearly illustrated in Fig. 5. Indeed, the curves reach a plateau of practically constant energies starting from an $n$ value which is smaller than the full dimension $N$ by more than one order of magnitude in $^{108}$Sn, $^{48}$Cr, and by more than two in $^{133}$Xe.

Our exponential extrapolation law is somewhat different from the one proposed in Refs. [9,10]. On the other hand, it is valid for all states and nuclei examined and follows directly from the sampling, as it can be inferred from the following heuristic argument.

Let us consider the simplest case of one-dimensional eigenspace ($v = 1$). From Eqs. (3.8) and (3.12), we can write the corresponding sampling prescription as

$$\Delta \lambda = \sum_j \Delta \lambda_j = \sum_j (\lambda'_j - \lambda_j) = -\sum_j \frac{b^2_{1j}}{a_{jj} - \lambda_j - \Delta \lambda_j}.$$

(5.6)

Expanding $\Delta \lambda_j$, we get a solution whose leading term is

$$\Delta \lambda_j = \frac{b^2_{1j}}{a_{jj} - \lambda}.$$

(5.7)

From the plots it is clear that the extrapolation law holds for an energy range of 1-2 MeV in proximity of the exact eigenvalue. It accounts therefore for small contributions coming from
a small fraction of the basis states in the $\sum_j$ in the high density region around the peak, as shown in Fig. 2. Since, in this range, the energies $E_j$ of our correlated basis states are closely packed and approach the $E_n$ value, we can put $(a_{jj} - \lambda) \propto n$ in first approximation. It remains to analyze the matrix elements $b^2_{ij}$. These are given by

$$\langle \phi_j \mid v \mid j \rangle^2$$

(5.8)

where

$$| \phi_j \rangle = \sum_{i=1}^j c_i^j | i \rangle.$$  

(5.9)

For the lowest eigenvalue, the dominant $c_i$ components of $| \phi_j \rangle$ are the low-energy ones with small $i$ values. It follows that the probability, $b^2_{ij}$, that the interaction couples $| \phi_j \rangle$ to $| j \rangle$ is small and random for $j \leq n$ and vanishes for $j > n$, as prescribed by the sampling criterion. This implies that the dimension $n$ represents the range of the allowed events. We can therefore put $b^2_{ij} \propto \exp(-j/n)$, where $j$ is a label representative of the small fraction of $j$ terms of the sum $\sum_j$. We used the factor $N$ to fix the scale. The scaling law (5.4) for $\epsilon$ follows from the one for the energy $E$ since $\epsilon$ is essentially the derivative of $E$ with respect to $n$.

We have also compared the sampling with the energy truncation of the Hamiltonian matrix. As shown in Fig. 6, the sampling is obviously more effective and accurate. The two procedures, however, tend to become equivalent for a value of $n$ which, though large, is still much smaller than the full dimension $N$. It is to be pointed out, however, that, in our case, the effectiveness of the energy truncation is due to a great extent to the use of the correlated basis obtained through the multi-partitioning method.

B. Eigenvectors and E2 transitions

An accuracy of the same quality is reached for the eigenstates of the $n$-dimensional truncated Hamiltonian matrix

$$\psi_n = \sum_{i=1}^n c_i^{(n)} | i \rangle,$$  

(5.10)

where $| i \rangle$ are the correlated basis states obtained by the partitioning method.

In Fig. 7 we give the the overlap of $\psi_n$ with the exact eigenvector $\psi$ for the first five $J^{\pi} = 2^+$ states of $^{108}$Sn and $J^{\pi} = 0^+$ of $^{48}$Cr. The convergence to unity is fast for all five states, even if, for some of them, the overlap is very small at small $n$. Small fluctuations are noticeable at small $n$ values. They reflect the interference between the components of different wave functions in correspondence of partial energy crossings. The above two features represent a further proof of the robustness of the iterative algorithm.

To complete the analysis we study the behavior versus $1/\epsilon$ of the strengths of the $E2$ transitions between some low-lying states in $^{108}$Sn and $^{48}$Cr (Fig. 8), as well as in $^{133}$Xe (Fig. 9). In all cases, the strengths reach soon a plateau and, then, undergo very small variations, appreciable only on a very small scale (see inset). This fine tuning analysis
shows that each strength grows slowly with $1/\epsilon$, apart from the transition $1/2^+_1 \rightarrow 3/2^+_1$, whose strength decreases at an even slower rate. In all cases, their smooth behavior allows for an extrapolation to asymptotic values through a formula having the same structure as the scaling law adopted for the energies (Eq. 5.5). Table II shows that the strengths computed at a relatively large $\epsilon$ differ very little from the extrapolated ones, which in turn practically coincide with the exact values. This rapid convergence is quite significant in view of the extreme sensitivity of the transition strengths to even very small components of the wave function.

VI. CONCLUDING REMARKS

We have shown that the importance sampling is inherent in the iterative algorithm for diagonalizing large matrices. The truncation of the dimensions of the matrices it promotes is not only kept under strict control, but is also quite severe when the eigenvectors are highly localized. For shell model nuclear Hamiltonians, we achieved this localization by adopting a correlated basis obtained by partitioning the shell model space into two or more subspaces. As clearly illustrated by the calculations carried out on some typical nuclei, the sampling so implemented allows to reduce the sizes of the Hamiltonian matrix by at least an order of magnitude with no detriment of the accuracy. We get in fact very accurate energies, wave functions and $E2$ reduced strengths. Moreover, it generates extrapolation laws to asymptotic eigenvalues and $E2$ transition probabilities which coincide practically with the exact corresponding quantities, whenever these are available.

It is important to point out that the method is specially effective when applied to $^{133}$Xe, having a neutron excess. On the ground of this result, we feel confident that the sampling, combined with the use of the correlated basis, will enable us to face successfully the eigenvalue problem in heavier nuclei, all having a neutron excess. We also like to stress that the partition method is specially suitable for enlarging the standard shell model valence space through the inclusion of n-particle n-hole correlated configurations. We plan to make such an implementation in order to study the intruder states in light as well as heavy nuclei.

ACKNOWLEDGMENTS

The work was partly supported by the Prin 01 of the Italian MURST
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FIGURES

FIG. 1. Importance sampling parameters versus the dimensions $n$ of the truncated matrices resulting from the sampling.

FIG. 2. Energy distribution of the $J^\pi = 0^+$ basis states in $^{48}$Cr obtained by the multipartition method (MP) and corresponding running sum. This is compared with the running sum of the standard shell model (SM) basis states.

FIG. 3. low-lying $J^\pi = 2^+$ eigenvalues of $^{108}$Sn versus the dimensions $n$ of the truncated matrices resulting from the sampling.

FIG. 4. The same as Fig. 3 for $^{48}$Cr.

FIG. 5. The same as Fig. 3 for $^{133}$Xe.

FIG. 6. Eigenvalues obtained by the sampling and by energy truncation versus the truncated dimensions $n$.

FIG. 7. Overlap of the lowest five $J^\pi = 2^+$ and $J^\pi = 0^+$ sampled eigenfunctions with the corresponding exact ones in $^{108}$Sn and $^{48}$Cr, respectively.

FIG. 8. Sampling of the strengths of $J^\pi = 2^+ \rightarrow J^\pi = 0^+$ $E2$ transitions in $^{108}$Sn and $^{48}$Cr.

FIG. 9. Sampling of the strengths of some $E2$ transitions in $^{133}$Xe.
TABLE I. Approximate, extrapolated and exact (when available) energies (in MeV). The extrapolation parameters are also given.

| $^A X$ | $J^\pi$ | N   | $E_0$   | b      | c      | n  | $E_i^{(n)}$ | $E_i^{(extr)}$ | $E_i^{(ex)}$ |
|--------|----------|------|---------|--------|--------|----|------------|----------------|-------------|
| $^{108}$Sn | $2^+_1$   | 17467 | -3.145  | 0.0028 | 0.0032 | 1867 | -3.120  | -3.143(001) | -3.151    |
|         | $2^-_1$   |       | -2.466  | 0.0029 | 0.0034 | -2.439 | -2.463(001) | -2.469    |
|         | $2^+_3$   |       | -2.244  | 0.0030 | 0.0021 | -2.216 | -2.244(001) | -2.266    |
| $^{48}$Cr | $0^+_1$   | 41355 | -32.972 | 0.01721| 0.00456| 5739  | -32.851 | -32.955(019) | -32.954    |
|         | $0^+_2$   |       | -28.638 | 0.03450| 0.01486| -28.414 | -28.604(011) | -28.565    |
|         | $0^+_3$   |       | -27.166 | 0.06038| 0.01280| -26.819 | -27.166(042) | -27.158    |
|         | $2^-_1$   | 182421 | -32.164 | 0.019  | 0.008  | 14642 | -31.952 | -32.145(020) | -32.148$^a$|
|         | $2^+_2$   |       | -29.133 | 0.0114 | 0.0009 | -29.012 | -29.122(016)    |
|         | $2^+_3$   |       | -28.745 | 0.0238 | 0.0037 | -28.552 | -28.721(053)    |
| $^{133}$Xe | $1/2^+_1$ | 125756| -11.280 | 0.0014 | 0.0018 | 6763  | -11.256 | -11.279(002)    |
|          | $1/2^+_2$ |       | -10.319 | 0.0019 | 0.0019 | -10.285 | -10.317(001)    |
|          | $1/2^+_3$ |       | -9.498  | 0.0021 | 0.0019 | -9.464  | -9.496(007)      |
|          | $3/2^+_1$ | 242308| -11.491 | 0.0009 | 0.0012 | 7417   | -11.466 | -11.490(002)    |
|          | $3/2^+_2$ |       | -10.491 | 0.0012 | 0.0012 | -10.455 | -10.490(003)    |
|          | $3/2^+_3$ |       | -10.292 | 0.0013 | 0.0013 | -10.255 | -10.292(002)    |
|          | $11/2^+_1$ | 497666| -11.222 | 0.0004 | 0.0005 | 6742   | -11.192 | -11.222(003)    |
|          | $11/2^+_2$ |       | -10.013 | 0.0006 | 0.0005 | -9.971  | -10.012(003)    |
|          | $11/2^+_3$ |       | -9.439  | 0.0008 | 0.0002 | -9.386  | -9.438(008)      |

$^a$from Ref. [21].

TABLE II. Approximate, extrapolated and exact (when available) $B(E2)$ (in $e^2fm^4$).

| $^A X$ | $J^\pi_i \rightarrow J^\pi_f$ | $\epsilon$ | $n_i$ | $n_f$ | $B(E2)_i^{(ex)}$ | $B(E2)_i^{(extr)}$ | $B(E2)_i^{(ex)}$ |
|--------|-------------------------------|------------|------|-------|-----------------|-------------------|-----------------|
| $^{108}$Sn | $2^+_1 \rightarrow 0^+_1$   | 1.x10$^{-4}$ | 1867 | 1034  | 42.45          | 42.68(02)         | 42.71           |
| $^{48}$Cr | $2^+_1 \rightarrow 0^+_1$   | 4.x10$^{-5}$ | 14642 | 8144  | 226.5          | 227.8(8)          | 228             |
| $^{133}$Xe | $1/2^+_1 \rightarrow 3/2^+_1$ | 7.x 10$^{-5}$ | 6763 | 7417  | 110.1          | 109.3(7)          |                 |
|          | $1/2^+_2 \rightarrow 3/2^+_1$ |            |      |       | 230.9          | 233.0(3)          |                 |
Fig. 1
Fig. 2
Fig. 3
Fig. 4
Fig. 5
Fig. 6

\[ ^{133}\text{Xe} \]
\[ J^\pi = 1/2^+ \]

Samp

E cut
Fig. 7

$^{48}\text{Cr}$

$J\pi = 0^+$

$^{108}\text{Sn}$

$J\pi = 2^+$
Fig. 8
Fig. 9

$B(E2) (e^2 \text{fm}^4)$

$1/2^+_2 \Rightarrow 3/2^+_1$

$1/2^+_1 \Rightarrow 3/2^+_1$