Nuclear spectra in a large scale shell model approach

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Abstract. An iterative matrix diagonalization algorithm is briefly outlined. Its implementation in the spin uncoupled scheme for large scale shell model calculations is discussed with special attention at the convergence properties of the iterative process which establish the domain of applicability of the method. Within this domain, the method is able to generate a large number of eigenstates and, therefore, to provide an exhaustive description of low-lying nuclear spectra. The performance of the method is illustrated by its application to $^{130-134}$Xe isotopes.

1. Introduction
The advent of increasingly powerful computer facilities has stimulated the development of highly sophisticated and efficient matrix diagonalization codes for facing large scale shell model (SM) calculations.

Practically all successful SM codes are implementations of the Lanczos [1] algorithm. Some of them, like Nathan [2, 3] and Nushell [4], use a spin-coupled scheme, others, like Antoine [3], adopt the uncoupled $m$-scheme.

The coupled scheme yields SM Hamiltonian matrices of relatively small dimensions. These matrices, however, are highly dense and quite involved. Those obtained in the $m$-scheme, though of much larger dimensions, are sparse and easy to compute.

Sampling techniques for truncating effectively the SM space have also been developed. The quantum Monte Carlo diagonalization (QMCD) method [5], for instance, adopts the Monte Carlo technique, first introduced for studying the nuclear ground state properties [6], to generate stochastically a truncated basis for the diagonalization of the many-body Hamiltonian. Total spin and other symmetries, broken by the stochastic sampling procedure, are restored by specific techniques.

Another method for truncating the basis is based on the density matrix renormalization group (DMRG) [7] and applied recently to medium nuclei [8].

Few years ago, a new iterative algorithm for diagonalizing large matrices was proposed [9, 10]. The method is simple to implement and is endowed with an importance sampling. Its first application was made in the coupled $j-\bar{j}$ scheme, which came out to be too much time consuming in the construction of the Hamiltonian matrix at each iterative step.

We have now implemented the algorithm in the the $m$-scheme and proposed a new importance sampling. The method was presented and discussed in [11, 12]. The attention was focused on the

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convergence properties of the iterative process which allow to establish the extent of applicability of the method [12].

In the nuclei where it can be applied, the method yields a large number of levels for each angular momentum and, therefore, offers a complete description of low-lying nuclear spectroscopy. An example was offered by the study of the spectroscopic properties of $^{132-134}$Xe and, partly, of $^{130}$Xe [12].

Here, we will review briefly the iterative algorithm and its convergence properties. We will also show how it is applied to $^{130-134}$Xe and discuss some important properties of these nuclei.

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 $|i\rangle (n_0 << N)$, construct and diagonalize the $n_0 \times n_0$ submatrix $A_0 = (a_{ij})$.

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

1c) construct and diagonalize the matrix

$$A_k^{(1)} = \begin{pmatrix} \Lambda_{k-1}^{(1)} & B_k^{(1)}(T) \\ B_k^{(1)} & A_k^{(1)}(C) \end{pmatrix},$$

where $\Lambda_k^{(1)}$ is a $v$-dimensional diagonal matrix

$$\Lambda_{k-1}^{(1)} = \begin{pmatrix} \lambda_{k-1}^{(1)}(1) & 0 & \ldots & 0 \\ 0 & \lambda_{k-1}^{(1)}(2) & \ldots & 0 \\ 0 & \ldots & \ldots & 0 \\ 0 & \ldots & \ldots & \lambda_{k-1}^{(1)}(v) \end{pmatrix},$$

and

$$A_k^{(1)}(C) = \{a_{ij}\} \quad (i, j = (k-1)p + 1, \ldots, kp)$$

is a $p$-dimensional submatrix. The two submatrices are coupled by $B_k^{(1)}$ and its transpose, whose matrix elements are

$$b_{ij}^{(k)} = \langle \lambda_{(k-1)}^{(1)}(i) | \hat{A} | j \rangle, \quad (i = 1, \ldots, v; j = (k-1)p + 1, \ldots, kp),$$

1d) diagonalize $A_1$ and 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) consider now the new subspace spanned by $|\varphi_1^{(1)}\rangle, \ldots, |\varphi_v^{(1)}\rangle$ plus the basis states $|j\rangle = |n_1 + 1\rangle, \ldots, |n_2\rangle$, 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

\[
E_{k}^{(1)} \equiv \lambda_{k}^{(N)}; \quad |\psi_{k}^{(1)} \rangle \equiv |\psi_{k}^{(N)} \rangle = \sum_{i=1}^{N} \xi_{k}^{(N)}(i) |i\rangle.
\]

These eigensolutions are the new entries for a new iteration. 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 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 [9].

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

We start with the modified Hamiltonian

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

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 \( |i >= |\alpha_1, \alpha_2, \ldots, \alpha_p> \), 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 \( |i> \) have a good magnetic quantum number \( M = m_1 + \ldots + m_i + \ldots + m_p \).

The full space can be thought to be decomposed into several subspaces

\[
\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \ldots \oplus \mathcal{H}_k \ldots \oplus \mathcal{H}_F.
\]

Each subspace \( \mathcal{H}_k \) is composed of a set of partitions \( \{n_i\}_k = \{a_1^{n_1}, \ldots, a_i^{n_i}, \ldots\}_k \), where \( \sum_i n_i = p \). It is, therefore, invariant with respect to \( J \). The partitions in \( \mathcal{H}_k \) differ from those in \( \mathcal{H}_{k-1} \) by at most two single particle shells \( a_i \).

We first diagonalize the Hamiltonian \( H_{J} \) in \( \mathcal{H}_0 \) obtaining \( v \) lowest eigenvalues \( E_1^{(0)}, \ldots, E_v^{(0)} \) and eigenvectors \( \psi_1^{(0)}, \ldots, \psi_v^{(0)} \) spanning a subspace \( \mathcal{E}_0 \). These eigensolutions are exact in this subspace and have all the same spin \( J \) if the constant \( c \) is chosen so as to push the states with \( J' \neq J \) up in energy.

Because of its two-body nature, the Hamiltonian couples the subspace \( \mathcal{E}_0 \) to \( \mathcal{H}_1 \) only. It is, therefore, sufficient to diagonalize \( H_{J} \) in the subspace \( \mathcal{E}_0 \oplus \mathcal{H}_1 \) to generate new updated eigenvalues \( E_1^{(1)}, \ldots, E_v^{(1)} \) and eigenvectors \( \psi_1^{(1)}, \ldots, \psi_v^{(1)} \), defining the subspace \( \mathcal{E}_1 \). We proceed iteratively. Once the updated eigensolutions defining the subspace \( \mathcal{E}_k \) are obtained, we diagonalize the Hamiltonian in the upgraded subspace \( \mathcal{E}_k \oplus \mathcal{H}_{k+1} \). We cover eventually the full space obtaining the exact \( v \) eigensolutions \( \{E_i, \psi_i\} \).

Even after having exploited the sparsity of the Hamiltonian matrix, the diagonalization procedure might become prohibitively lengthy as the dimensions of the space increase. In order to cut effectively the basis we adopted the follow sampling procedure.

Let us fix a sequence of positive small numbers of decreasing values \( \epsilon_1 > \ldots \epsilon_k > \ldots > \epsilon_F \).

Having generated the lowest \( v \) eigenvectors \( \psi_1^{(0)}, \ldots, \psi_v^{(0)} \) in \( \mathcal{H}_0 \), we proceed as in the exact case with one constraint: In going from \( \mathcal{H}_{k-1} \) to \( \mathcal{H}_k \), we pick up only the basis states \( |j> \) that fulfill the condition

\[
\frac{|<j|H_J|\psi_{i}^{(k-1)}>|^2}{a_{jj} - E_{i}^{(k-1)}} > \epsilon_k.
\]
More specifically, in the first step \((k = 1)\), the above condition selects a set of states \(\{|j>\}\) forming a subspace \(\mathcal{H}_1^{(\epsilon_1)} \subseteq \mathcal{H}_1\). The eigenvalue problem is thus solved in \(\mathcal{E}_0 \oplus \mathcal{H}_1(\epsilon_1)\) yielding new \(\nu\) eigensolutions \(E^{(1)}_k(\epsilon_1), \psi^{(1)}_k(\epsilon_1)\) defining the subspace \(\mathcal{E}_1^{(\epsilon_1)}\). We now explore the full subspace complementary to \(\mathcal{H}_0 \oplus \mathcal{H}_1(\epsilon_1)\) and select all the states \(|j>\) that fulfill the condition (9) with \(\epsilon_2\) replacing \(\epsilon_1\). The states so selected span a subspace \(\mathcal{H}_2^{(\epsilon_2)} \subseteq \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2\). The above procedure is iterated with updated eigensolutions and decreasing sampling values \(\epsilon_k\) until the full space is covered.

The sampling procedure is stable and yields orthonormal eigenfunctions. These are obtained, at each step, by the diagonalization of a symmetric submatrix. The subspaces selected by the sampling are not strictly invariant with respect to \(J\). The invariance, however, is restored as the sampling value \(\epsilon\) becomes sufficiently small. We will show, in fact, that all sampled eigenstates reach soon a good \(J\).

**Figure 1.** (Color online) Convergence rate of the eigenvalues in \(^{130}\text{Xe}\) and \(^{132}\text{Xe}\).

**Figure 2.** (Color online) Convergence rate of the \(B(E2; 2^+_1 \rightarrow 0^+_1)\) strengths in \(^{130}\text{Xe}\) and \(^{132}\text{Xe}\).
4. Application to Xe isotopes
The sampling algorithm was applied to the even isotopes $^{134-130}$Xe using a configuration space determined by the shells $\{2d_{5/2}, 1g_{7/2}, 2d_{3/2}, 3s_{1/2}, 1h_{11/2}\}$. The valence protons are particles...
external to the Z=50 core, while the valence neutrons are described as holes referred to the N=82 core. An effective two-body interaction based on a G matrix [13] derived from the CD-Bonn potential [14] has been employed. This includes the core polarization contributions appropriate for the model space under consideration. We used the proton and neutron effective charges $e_p = 1.6$ and $e_n = 0.7$, respectively, for the $E(2)$ strengths and a spin gyromagnetic quenching factor $g_s = 0.5$ for the $M1$ transition probabilities.

Having chosen an initial subspace $H_0$ of dimensions $n_0 \simeq 100$ to generate ten lowest eigenstates with good $J$, we started the iterative sampling procedure using a set of decreasing values of $\epsilon_k$. Each $\epsilon_k$ determines uniquely the dimension $n_k$ of the Hamiltonian matrix to be diagonalized.

The dimensions of the Hamiltonian matrices in $^{132}$Xe are of the order $N \sim 3.7 \times 10^7$. Although the full space could be covered easily, it was largely sufficient to carry the iterative procedure up to $\sim 70\%$ of the basis states.

In the case of $^{130}$Xe, the dimensions of the Hamiltonian matrices are $N \sim 0.8 \times 10^9$. In this case, we were forced to stop the sampling at $\sim 10\%$ of the basis states. Proceeding further is possible but too time consuming on a desktop. Thus, the sampling will produce reliable results only in case of fast convergence.

This is the case for the energy eigenvalues and the $B(E2; 2^+_1 \rightarrow 0^+_1)$ [11]. As shown in figure 1, about 10\% of the states are enough to reach the convergence of the two quantities.

On the other hand, the convergence of the strengths of the transitions between excited states was not sufficiently fast to allow to reach the asymptotic values with only $\sim 10\%$ of the sampled states [12].

Thus, the convergence analysis states clearly the domain of applicability of the algorithm. In our specific case, we can carry out an exhaustive study of the spectroscopic properties of $^{132,134}$Xe, while, for $^{130}$Xe, we can provide a reliable description of the energy levels and the $B(E2; 2^+_1 \rightarrow 0^+_1)$ strengths.

$^{134}$Xe isotopes have been recently under intensive experimental investigations [15, 16, 17]. Their attention was focused mainly on the evolution of the MS states [18]. These are states non symmetric with respect to the exchange of valence proton and neutron pairs and describe quadrupole vibrations of protons versus neutrons. They were observed unambiguously and copiously in $^{94}$Mo [19] and, since then in several other nuclei in the vicinity of the N=50 and N=82 shell closures.

A review which includes also the theoretical studies may be found in [20]. Mixed Symmetry (MS) states in the vicinity of N=82 were investigated recently within the QPM [21, 22] and in a large scale shell model calculation [23].

The $E2$ and $M1$ transitions between excited states were studied extensively in [12]. Here we report some meaningful results.

The strengths of the $E2$ transitions to the ground state in $^{130-134}$Xe are shown in figures 3. The SM peaks are close to the experimental ones. The SM $2^+_1$ collects by far the largest strength of the $E2$ transitions to the ground state. This is shown to be isoscalar indicating that the SM $2^+_1$ corresponds to the IBM symmetric one-boson $2^+$ or, in microscopic terms, to the QPM isoscalar one-phonon quadrupole vibrational mode. The residual $2^+_1 \rightarrow 0^+_1$ $E2$ strength is collected by the $2^+_3$ state. This corresponds to the IBM MS state. Indeed, the $2^+_3 \rightarrow 0^+_1$ $E2$ transition was shown to be isovector.

The strengths of the $E2$ and $M1$ transitions between excited $2^+$ states in $^{132}$Xe are shown in figure 4. The agreement between SM and experimental strengths of the $2^+_1 \rightarrow 2^+_1$ transitions is generally good. Only the $2^+_2$ is strongly coupled to the $2^+_1$ by the isoscalar $E2$ operator. It is therefore strongly collective and corresponds to a proton-neutron symmetric two-boson state.

The measured $M1$ strength is concentrated mostly, if not solely, on a single $2^+$ state, while the SM strength is distributed among few $2^+$ states, all clustered around a pronounced peak,
lying close to the experimental one.

It is interesting to notice that all transitions are almost purely orbital except for the highest in energy which is due to spin. If we exclude this transition, the total SM strength coincides with the experimental value within the errors.

5. Concluding remarks

When it is implemented in the $m$-scheme, the importance sampling algorithm becomes certainly more efficient. It requires, in fact, an execution time which grows linearly with the dimensions $N$ of the Hamiltonian matrix.

It becomes, nonetheless, too slow, at least on a desktop, as the dimensions of the Hamiltonian matrix approach $N \approx 10^9$. It follows that, in nuclei like $^{130}$Xe, the method is able to sample up to 10% of the basis states. This fraction of states is sufficient to bring to convergence the energy levels and the $B(E2; 2^+_1 \rightarrow 0^+_1)$ but not the strengths of the $E2$ and, especially, the $M1$ transitions among excited states.

In order to improve the performance we may try to find out a sampling criterion which exploits more efficiently the sparsity of the Hamiltonian matrix and/or to develop a parallel version of the code. Such a parallelization should, hopefully, reduce drastically the execution time.

In its present status, the algorithm can be applied to space of dimensions of several hundred millions. Within these limits, the method yields at once an arbitrary number of orthogonal eigenstates with a given $J$. It provides therefore an exhaustive description of the low-lying spectroscopic properties in the nuclei at reach.

The calculations on $^{132-134}$Xe isotopes offer a meaningful example. We get complete spectra and a full scheme of electromagnetic transitions. The spectra as well as the $E2$ and $M1$ transitions are generally consistent with the experiments. Their analysis allows to determine the collectivity and the proton-neutron symmetry of the low-lying states.

References