Complex nuclear spectra in a large scale shell model approach

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Abstract. We report on a shell model implementation of an iterative matrix
diagonalization algorithm in the spin uncoupled scheme. A new importance sampling
is adopted which brings the eigenvalues to convergence with about 10% of the basis
states. The method is shown to be able to provide an exhaustive description of the
low-energy spectroscopic properties of $^{132-134}$Xe isotopes and of the spectrum of $^{130}$Xe.

1. Introduction

Large scale shell model (SM) calculations require the diagonalization of the nuclear
Hamiltonian in spaces whose dimensions may exceed the capability of the most
powerful computers. Hence, the necessity of developing more and more efficient matrix
diagonalization codes.

Practically all of them are implementations of the Lanczos [1] algorithm. Some
codes, like Nathan [2, 3] and Nushell [4], exploit a spin-coupled SM basis, others, like
Antoine [3], adopt an uncoupled $m$-scheme. The SM Hamiltonian matrices obtained in
the coupled spin have relatively small dimensions. They, however, are highly dense and
composed of quite involved matrix elements. The matrices constructed in the $m$-scheme,
though of much larger dimensions, are sparse and easy to compute.

The performance of these codes may be enhanced by resorting to sampling
techniques which effectively reduce the dimensions of the Hamiltonian matrices. A
successful importance sampling is the quantum Monte Carlo diagonalization (QMCD)
method [5] which generates stochastically a truncated basis by exploiting the Monte
Carlo technique, first adopted for studying the nuclear ground state properties [6]. The
wavefunctions so generated do not have well defined spin, isospin and parity. Specific
projection techniques are to be adopted in order to extract the good quantum numbers.

A new iterative algorithm, endowed with an importance sampling, was proposed few
years ago [7, 8]. We have now implemented the algorithm in the $m$-scheme and proposed
a new importance sampling [9, 10]. The upgraded method yields a large number of levels

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for each angular momentum and, therefore, offers a complete description of the low-lying nuclear spectroscopic properties. An illustrative example is provided by the study of the spectra of some heavy Xe isotopes, discussed in [10]. After review briefly the algorithm, we will discuss its convergence properties and present the most meaningful results of the study performed on \(^{130-134}\)Xe.

2. The algorithm

Let us consider a symmetric matrix \(A = \{a_{ij}\}\) representing a self-adjoint operator \(\hat{A}\) in an orthonormal basis \(\{|1\rangle, |2\rangle, \ldots, |i\rangle, \ldots, |N\rangle\}\). The diagonalization algorithm prescribes a sequence of iteration loops. The first loop consists of:

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

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

1c) Construct and diagonalize the matrix

\[
A_k^{(1)} = \begin{pmatrix}
\Lambda_k^{(1)} & B_k^{(1)} \\
B_k^{(1)T} & A_k^{(1)v}
\end{pmatrix},
\]

where \(\Lambda_k^{(1)} \equiv \{\lambda_1, \ldots, \lambda_i, \ldots, \lambda_v\}\) is a \(v\)-dimensional diagonal matrix and \(A_k^{(1)v} = \{a_{ij}\}\) \((i, j = (k-1)p+1, \ldots, k p)\) is a \(p\)-dimensional submatrix. The off diagonal block \(B_k^{(1)}\) is composed of the matrix elements \(b_{ij}^{(k)} = \langle \Lambda_k^{(1)}(i) | \hat{A} | j \rangle (i = 1, \ldots, v; j = (k-1)p+1, \ldots, k p)\), \(B_k^{(1)T}\) is its transpose.

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 \(|\varphi_1^{(1)}\rangle, \ldots, |\varphi_v^{(1)}\rangle\) plus the basis states \(|j\rangle \approx |n_1 + 1 \rangle, \ldots, |n_2\rangle\), 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

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

The basis composed of the eigenvectors \(|\psi_k^{(1)}\rangle\) plus the original basis states \(\{|j\rangle\}\) are the new entries for a new iteration loop. The loops are iterated until a sequence of \(v\) vectors \(|\psi_1^{(i)}\rangle, \ldots, |\psi_v^{(i)}\rangle\) converges to the exact eigenstates [7].

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

We add to the nuclear Hamiltonian \(H\) a spin term multiplied by a positive constant \(c\)

\[
H_J = H + c[J^2 - J(J + 1)]^2.
\]
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 \( M = m_1 + \ldots + m_i + \ldots + m_p \).

Let us decompose the full space as a direct sum of subspaces \( \sum_k \oplus H_k \), each composed of a set of partitions \( \{n_i\}_k = \{a_{n_i}^1, \ldots, a_{n_i}^{n_i}, \ldots\}_k \), where \( \sum_i n_i = p \). The partitions in \( H_k \) differ from those in \( H_{k-1} \) by at most two single particle shells \( a_i \). Let us also fix a sequence of positive small numbers of decreasing values \( \epsilon_1 > \ldots > \epsilon_k > \ldots > \epsilon_F \).

We first diagonalize the Hamiltonian \( H_J \) in \( H_0 \) obtaining \( v \) lowest eigenvalues \( E^{(0)}_1, \ldots, E^{(0)}_v \) and eigenvectors \( \psi^{(0)}_1, \ldots, \psi^{(0)}_v \) spanning a subspace \( \mathcal{E}_0 \). These eigenstates 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 \( H_1 \) only. We pick up only the basis states \( |j\rangle \) of \( H_1 \) that fulfill the condition

\[
|\langle j | H_J | \phi^{(k-1)}_i \rangle|^2 > \epsilon_k
\]

with \( k = 1 \). The eigenvalue problem is thus solved in \( \mathcal{E}_0 \oplus H_1(\epsilon_1) \) yielding new \( v \) eigensolutions \( E^{(1)}_1(\epsilon_1), \psi^{(1)}_1(\epsilon_1) \) defining the subspace \( \mathcal{E}_1^{(\epsilon_1)} \). We now explore the full subspace complementary to \( H_0 \oplus H_1(\epsilon_1) \) and select all the states \( |j\rangle > \) that fulfill the condition (4) with \( k = 2 \). The states so selected span a subspace \( H_2^{(\epsilon_2)} \in H_0 \oplus H_1 \oplus H_2 \). The above procedure is iterated with updated eigensolutions and decreasing sampling values \( \epsilon_k \) until the full space is covered. The states obtained by such a sampling process are orthonormal and have a good \( J \) for a sufficiently small \( \epsilon \).

4. Application to Xe isotopes

The method was applied to \(^{134-130}\text{Xe}\). A series of experiments \([11, 12, 13]\) have produced a large variety of data for these isotopes, which allowed to perform a thorough investigation of their low-energy states, and, especially, of those having a
mixed symmetry (MS) with respect to the exchange of valence proton and neutron pairs [14]. These MS states were observed unambiguously in $^{94}$Mo [15] and, since then, in several other nuclei in the vicinity of the N=50 and N=82 shell closures. Theoretical studies for nuclei in the vicinity of N=82 were carried out within the QPM [16, 17] and in a large scale shell model calculation [18].

The configuration space was determined by the shells $\{2d_{5/2}, 1g_{7/2}, 2d_{3/2}, 3s_{1/2}, 1h_{11/2}\}$. A G matrix [19] derived from the CD-Bonn potential [20] was taken as a two-body interaction. The dimensions of the Hamiltonian matrices range from $N \sim 3.7 \times 10^7$ for $^{132}$Xe to $N \sim 0.8 \times 10^9$ for $^{130}$Xe.

As shown in Figure 1, a good convergence for the energies is obtained by sampling $\sim 10\%$ of the basis states. The same is true for the strengths $B(E2; 2^+_i \rightarrow 2^+_1)$ of the transitions to the ground state [9]. The computed spectra are in remarkable agreement with the experimental levels [10].

A larger fraction of sampled states is needed in order to reach convergence for the strengths of the transitions between excited states [10]. Since this would be too time consuming for $^{130}$Xe, we have considered only the transitions of $^{132,134}$Xe [10]. Here, we report some meaningful results.

The strengths of the $E2$ transitions to the ground state are in good agreement with the experiments [10]. The SM $2^+_1$ collects by far the largest strength and is shown to correspond to the IBM symmetric one-boson $2^+$ or, in microscopic terms, to the QPM isoscalar one-phonon quadrupole vibrational mode. The residual strength goes to the isovector $2^+_3 \rightarrow 0^+_1$ which qualifies the $2^+_3$ state as MS one-boson state.

Figure 2 (left panel) shows that a very good agreement with experiments was obtained also for the $2^+_1 \rightarrow 2^+_1$ transitions. 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 same Figure 2 (right panel) shows that 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. 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

We have seen that the iterative sampling procedure brings the energy eigenvalues to convergence with about 10% of the basis states. A larger fraction of states is necessary for the convergence of the strengths of the $E2$ and, especially, the $M1$ transitions among excited states. It is, therefore, desirable to explore the possibility of developing a parallel version of the code in order to reduce 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 $J$ and provides an exhaustive description of the low-lying spectroscopic properties of nuclei.

Indeed, when applied to $^{132-134}$Xe isotopes, the method yielded complete spectra and a full scheme of electromagnetic transitions in good agreement with the experiments. It allowed also to determine the collectivity and the proton-neutron symmetry of the low-lying states.

References

[1] Lanczos C 1950 J. Res. Natl. Bur. Stand. 45 252
[2] Caurier E and Nowacki F 1999 Acta Phys. Pol. B 30 705
[3] Caurier E et al 2005 Rev. Mod. Phys. 77 427
[4] Brown B A and Raen W D M 2007 NUSHELL@MSU, MSUNSCL Report (unpublished)
[5] Otsuka T et al 2001 Prog. Part. Nucl. Phys. 47 319
[6] Koonin S E, Dean D J and Langanke K 1997 Phys. Rep. 278 1
[7] Andreozzi F, Porrino A and Lo Iudice N 2002 J. Phys. A 35 L61
[8] Andreozzi F, Lo Iudice N and Porrino A 2003 J. Phys. G: Nucl. Part. Phys. 29 2319
[9] Bianco D, Andreozzi F, Lo Iudice N, Porrino A and Knapp F 2011 J. Phys. G: Nucl. Part. Phys. 38 025103
[10] Bianco D, Andreozzi F, Lo Iudice N, Porrino A and Knapp F 2011 Phys. Rev. C 84 (2011) 024310
[11] von Garrel H et al. 2006 Phys. Rev. C 73 054315
[12] Ahn T et al. 2009 Phys. Lett. B 679 19
[13] Coquard L et al. 2010 Phys. Rev. C 82 024317
[14] Arima A, Otsuka T, Iachello F and Talmi I 1977 Phys. Lett. B 66 205
[15] Pietralla N et al. 1999 Phys. Rev. Lett. 83 1303
[16] Lo Iudice N, Stoyanov Ch and Tarpanov D 2008 Phys. Rev. C 77 044310
[17] Lo Iudice N, Stoyanov Ch and Pietralla N 2009 Phys. Rev. C 80 024311
[18] Sieja K, Martínez-Pinedo G, Coquard L and Pietralla N 2009 Phys. Rev. C 80 054311
[19] Hjorth-Jensen M et al. 1995 Physics Reports 261 125
[20] Machleidt R 1989 Adv. Nucl. Phys. 19 189