IMPORTANCE BASIS TRUNCATION IN THE SYMMETRY-ADAPTED NO-CORE SHELL MODEL*

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We apply the importance-truncation procedure in the framework of the *ab initio* symmetry-adapted no-core shell model. We study efficacy of this new method for the description of energies and E2 transitions of the ground-state rotational band in ^{12}C. We demonstrate that the coupling SU(3)-scheme basis with the perturbative relevance estimate leads to a dramatic reduction in dimensionality of the nuclear eigenvalue problem.

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1. Introduction

Over the last decade, *ab initio* approaches to nuclear structure and reactions succeeded in achieving first-principles descriptions of light p-shell nuclei [1–3]. Extending reach of first-principles nuclear structure studies towards heavier open-shell nuclei places serious demands on computational resources and represents a great challenge even for the emerging exascale computing facilities. This points to the need of further major advances in many-body methods to access a wider range of nuclei and experimental observables, while retaining the *ab initio* predictive power. These considerations motivate us to develop and investigate the importance-truncation method for the SU(3) scheme basis that underpins the symmetry-adapted no-core shell model (SA-NCSM) approach [6]. The significance of the SU(3) group for a microscopic description of low-energy nuclear dynamics can be seen from the fact that it is the symmetry group of the successful Elliott model [7], and a subgroup of the physically relevant $\mathrm{Sp}(3,\mathbb{R})$ symplectic model [8], which provides a comprehensive theoretical foundation for understanding the symmetries of nuclear collective motion. The organization of basis according to symmetries enables to restrict model space to a small subspace spanned by physically relevant sets of equivalent irreducible representations (irreps). The aim of this paper is to study the effectivness of the importance-truncation (IT) algorithm for selecting dominant SU(3) scheme configurations and study properties of this combined method.

2. Ab initio SA-NCSM and SU(3) scheme basis

The SA-NCSM is a many-body configuration-interaction method that solves the Schrödinger equation by finding eigensolution of the nuclear Hamiltonian matrix expressed in the SU(3) scheme basis of a physically relevant model space. The model space is given by a fixed parity and limited by cutoff $N_{\max}$. The $N_{\max}$ cutoff is defined as the maximum number of harmonic oscillator (HO) excitation quanta that an allowed SU(3) basis state can carry. The SU(3) scheme basis states are decomposed into spatial and intrinsic spin parts, where the spatial part is further classified according to the SU(3)⊃SO(3) group chain. The SA-NCSM basis states are labeled schematically as

$$|\vec{\gamma}; N(\lambda\,\mu)\kappa L; (S_p S_n)S; JM\rangle \ , \tag{1}$$

where S_p, S_n, and S denote proton, neutron, and total intrinsic spins, respectively, N is the total number of HO excitation quanta, and $(\lambda\,\mu)$ represent a set of quantum numbers that labels an SU(3) irrep. The SU(3) irrep labels $(\lambda\,\mu)$ bring forward important information about nuclear shapes and deformation [9]. The label κ distinguishes multiple occurrences of the same

orbital momentum L in the parent irrep $(\lambda\,\mu)$. The L is coupled with S to the total angular momentum J and its projection M. The symbol $\vec{\gamma}$ schematically denotes the additional quantum numbers needed to specify a distribution of nucleons over the major HO shells and their single-shell and inter-shell quantum numbers.

3. Selection of relevant states

The importance-truncation (IT) algorithm [11] has emerged as a successful method capable of selecting a relevant basis states that are essential for a close reproduction of a target wave function in a large model space. Let us suppose that $\mathcal{H}$ is spanned by many-body states $|i\rangle$ with cuttof $N_{\max}$ for which diagonalization of the Hamiltonian is impracticable but one can carry out diagonalization in a subspace $\mathcal{H}' \subset \mathcal{H}$, with a cutoff $N'_{\max}$, $N'_{\max} < N_{\max}$. Eigenvectors of this "unperturbed" Hamiltonian $\hat{H}_0$ define a set of reference states $|\Psi^{\nu}_{\rm ref}\rangle$ which satisfy

$$\hat{H}_0\,|\Psi^{\nu}_{\rm ref}\rangle = E^{\nu}_{\rm ref}\,|\Psi^{\nu}_{\rm ref}\rangle\ . \tag{2}$$

The rest of the model space can be taken into account as a perturbation $\hat{W} = \hat{H} - \hat{H}_0$ by using the Rayleigh–Schrödinger perturbation theory. The set of reference states (2) represents zeroth-order approximation of the target wave functions. The first-order correction is given by

$$|\Psi^{\nu}_1\rangle = -\sum_{i\notin\mathcal{H}'} \frac{\langle i|\hat{W}\,|\Psi^{\nu}_{\rm ref}\rangle}{E_i - E^{\nu}_{\rm ref}}|i\rangle = -\sum_{i\notin\mathcal{H}'} \kappa^{\nu}_i|i\rangle\,, \qquad \kappa^{\nu}_i \equiv -\frac{\langle i|\hat{H}\,|\Psi^{\nu}_{\rm ref}\rangle}{E_i - E^{\nu}_{\rm ref}}\,, \tag{3}$$

where we defined an importance-measure parameter $\kappa^{\nu}_i$of the basis state $|i\rangle$. The value $|\kappa^{\nu}_i|$ is correlated with the probability amplitude of the basis state $|i\rangle$ in the eigenvector obtained in the full model space $\mathcal{H}$.

A numerical threshold $\kappa_{\min} \geq 0$ defines a limit for the acceptance of a basis state $|i\rangle \notin \mathcal{H}'$. The state is accepted if $|\kappa^{\nu}_i| \geq \kappa_{\min}$ for at least one reference state $|\Psi^{\nu}_{\rm ref}\rangle$. The model space $\mathcal{H}'$ can be augmented by a set of accepted basis states for a given threshold $\kappa_{\min}$, and one can diagonalize Hamiltonian in this enlarged model space. Resulting eigenvectors can, in turn, establish a new set of reference states (2), and the procedure can be repeated with a smaller value of $\kappa_{\min}$. In the limit $\kappa_{\min} \to 0$, one obtains eigenvalues and eigenvectors of Hamiltonian in the complete model space $\mathcal{H}$.

4. Numerical example: ^{12}C

We augmented the SA-NCSM framework as implemented by the state-of-art code LSU3shell [12] by the IT algorithm. Here, we investigate performance of IT procedure for low-lying $0^+_1, 2^+_1, 4^+_1$ states of ^{12}C using realistic

chiral $\mathrm{NNLO_{opt}}$ nucleon–nucleon interaction [5] in the configuration space up to $N_{\max} = 6$. Such a model space is not capable of providing results independent of the basis parameter $\hbar\omega$. However, the purpose of the present study is to demonstrate the effectiveness of the IT procedure rather than a presentation of fully converged NCSM results.

The initial set of reference states was generated by diagonalizing Hamiltonian in the complete $N'_{\max} = 2$ space. A starting value of the threshold was set to $\kappa_{\min} = 0.005$, and linearly decreased at each step of the calculation. In the limit $\kappa_{\min} \to 0$, we exhausted complete $N_{\max} = 6$ model space. A condition $|\kappa_i^\nu| \geq \kappa_{\min}$ leads to a selection of N_{IT} states (for a given $\kappa_{\min}$). We denote the fraction of accepted states $\eta = N_{\mathrm{IT}}/N_{\mathrm{tot}}$, where N_{tot} denotes the number of $J = 0$ basis states spanning the complete $N_{\max} = 6$ model space. This value is generally larger if more than one reference state is used in the IT procedure. In the current study, we utilized three lowest reference states with the corresponding J as our aim was to investigate convergence of several lowest levels.

First, we examined how convergence is influenced by the basis parameter $\hbar\omega$ for different values of $\kappa_{\min}$. This is demonstrated in Fig. 1 for the ground-state energy. For example, the ground-state binding energy obtained in a model space truncated with $\kappa_{\min} \approx 1.2 \times 10^{-3}$ importance threshold represents 91–96% of the binding energy obtained in the complete space. At the same time, selected basis states span just $\approx$ 2.2–2.9% of the complete $N_{\max} = 6$ basis, in particular, corresponding dimensions are $\approx 3 \times 10^4$ and 1.2×10^6, respectively.

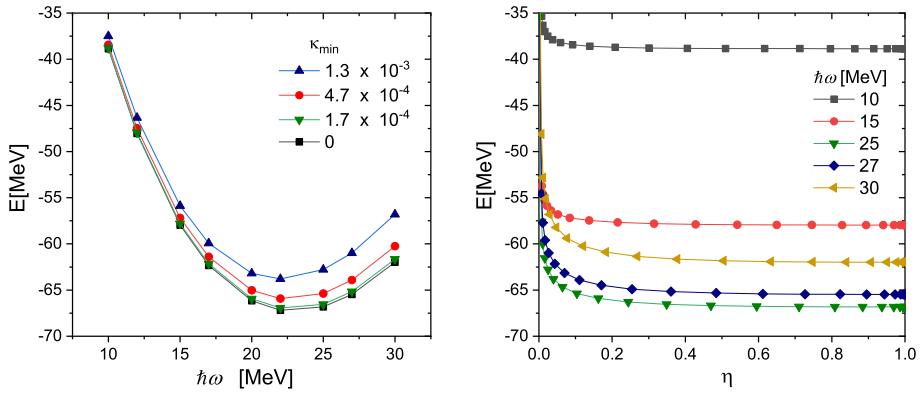

Fig. 1. The ground-state energy of ^{12}C as a function of HO strength $\hbar\omega$ in the interval 10–30 MeV and different threshold $\kappa_{\min}$ parameters (left). The convergence of the ground-state energy with respect to the fraction of accepted states η shown for different $\hbar\omega$ (rigth).

We also studied the efficacy of the IT-based selection procedure for the description of the 2_1^+ and 4_1^+ states of the ground-state rotational band. To be consistent, we used the same numerical thresholds $\kappa_{\min}$ to determine $0_{\rm gs}^+$, 2_1^+ and 4_1^+ states. The evolution of energies is shown in Fig. 2. The spectrum obtained for $\kappa_{\min} \approx 3 \times 10^{-4}$ is reasonably close to the "exact" one, while the dimensions are reduced typically to $\approx 9\%$ of the complete model space. The convergence pattern is similar for all studied values of the total angular momenta J.

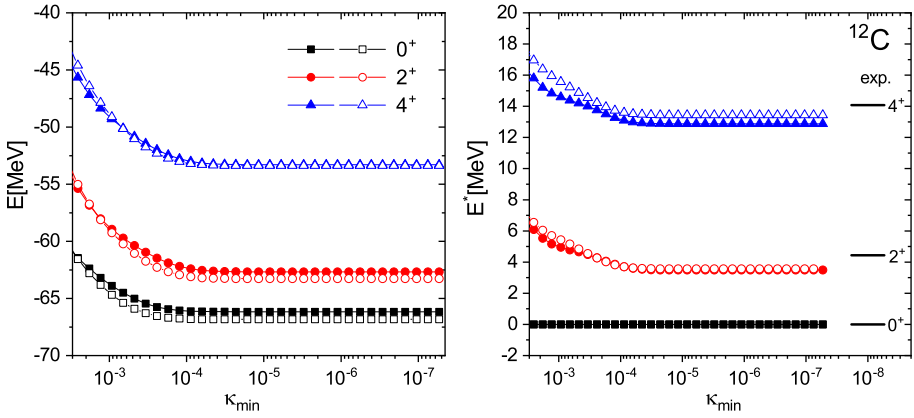

Fig. 2. Dependence of absolute (left) and excitation (right) energies for a sequence of $0_1^+, 2_1^+, 4_1^+$ ground-state band on numerical threshold $\kappa_{\min}$ calculated for $\hbar\omega = 20$ MeV (filled symbols) and $\hbar\omega = 25$ MeV (open symbols).

An overlap between truncated and full eigenfunction and transition matrix elements are essential quantities indicating a quality of the wavefunctions obtained in spaces selected by the IT procedure. In particular, we utilize wavefunctions obtained for a given threshold $\kappa_{\min}$ to study the efficacy of the IT selected model space for the description of the reduced electromagnetic B(E2) transition strengths.

Figure 3 shows the dependence of $B(\mathrm{E2}, J_i \to J_f)$ on the fraction of accepted basis states with the total angular momenta J_i for two values of $\hbar\omega$. Apparently, convergence is very fast for transitions from the ground as well as excited state. A closer look unveils that major contribution to the transition strength originates from a small fraction of basis states.

5. Conclusion

We have applied the importance-truncation procedure in the framework of multi-shell SU(3) scheme basis of the *ab initio* SA-NCSM. In particular, we studied the efficacy of the IT based selection procedure for the descrip-

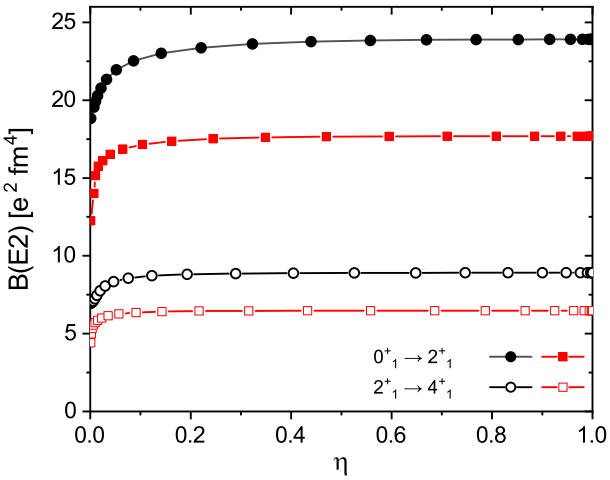

Fig. 3. Reduced transition probability for E2 transitions $0^+_1 \rightarrow 2^+_1$ (filled symbols) and $2^+_1 \rightarrow 4^+_1$ (open symbols) calculated for $\hbar\omega = 20$ MeV (black) and $\hbar\omega = 25$ MeV (gray/red). Each point represent a calculation for a specific value $\kappa_{\min}$ resulting to a fraction of selected states η in the model space of initial state.

tion of the ground state and its rotational band in ^{12}C. The calculations of energies and E2 transitions demonstrate that the IT procedure provides a recipe for the selection of relevant basis states which leads to a significant reduction of matrix dimensions used in SA-NCSM. The symmetry-guided selection with quantitative criteria rooted in many-body perturbation theory can be used for even more dramatic reduction of model spaces, which is an important step towards advancing applicability of *ab initio* SA-NCSM studies towards medium-heavy nuclei.

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