IMPORTANCE TRUNCATION IN THE SU(3) SYMMETRY-ADAPTED NO-CORE SHELL MODEL*

František Knapp

Faculty of Mathematics and Physics, Charles University
V Holešovičkách 2, 18000 Praha, Czech Republic

Tomáš Dytrych

Czech Academy of Sciences, Nuclear Physics Institute
Řež 130, 25068 Řež, Czech Republic

Daniel Langr

Czech Technical University in Prague, Faculty of Information Technology
Thákurova 9, 16000 Praha, Czech Republic
and
Výzkumný a zkušební letecký ústav, a.s.
Beranových 130, 199 05 Praha, Czech Republic

Tomáš Oberhuber

Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering
Břehová 7, 11519 Praha, Czech Republic

(Received December 28, 2017)

We apply, for the first time, the importance-truncation (IT) procedure based on the many-body perturbation theory for the multi-shell SU(3) scheme basis of the *ab initio* symmetry-adapted no-core shell model (SA-NCSM). It is shown that the IT method can yield a quantitative justification for the symmetry-based truncation of the SA-NCSM approach. Furthermore, we demonstrate that the IT algorithm can be applied in a symmetry-truncated model space and it leads to even more dramatic reduction in dimensionality of the nuclear eigenvalue problem.

DOI:10.5506/APhysPolBSupp.11.65

* Presented at the XXIV Nuclear Physics Workshop "Marie and Pierre Curie", Kazimierz Dolny, Poland, September 20–24, 2017.

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]. This accomplishment was propelled by a major progress in the development of realistic nuclear potential models [4, 5] along with the emergence of massively parallel supercomputers. Extending reach of first-principle 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 multi-shell SU(3) scheme basis that underpins the SA-NCSM approach [6].

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

The SA-NCSM is a many-body configuration-interaction method founded on techniques of the no-core shell model (NCSM). It solves the Schrödinger equation for A nucleons

$$\hat{H}\psi(\vec{r}_1,\ldots,\vec{r}_A) = E\psi(\vec{r}_1,\ldots,\vec{r}_A) \tag{1}$$

by computing eigenstates and eigenvalues of the nuclear Hamiltonian matrix in a basis representation. The intrinsic non-relativistic nuclear Hamiltonian is defined as

$$\hat{H} = \hat{T}_{\rm rel} + \hat{V}_{NN} + \hat{V}_{3N} + \ldots + \hat{V}_{\rm Coulomb}\,, \tag{2}$$

where $\hat{T}_{\rm rel}$ is the relative kinetic energy $\hat{T}_{\rm rel} = \frac{1}{A}\sum_{i<j}\frac{(\vec{p}_i-\vec{p}_j)^2}{2m}$ (m is the nucleon mass), the $\hat{V}_{NN}$ is the nucleon–nucleon interaction included along with the Coulomb interaction $\hat{V}_{\rm Coulomb}$ between the protons and possibly higher rank $\hat{V}_{3N}$, $\hat{V}_{4N}$, ... interactions.

Both NCSM and SA-NCSM approaches retain many-nucleon basis states of a fixed parity, consistent with the Pauli principle, and limited by a many-body basis cutoff $N_{\rm max}$. The $N_{\rm max}$ cutoff is defined as the maximum number of harmonic oscillator (HO) quanta allowed in a many-nucleon basis state above the minimum for a given nucleus. While the NCSM calculations are typically performed in an M-scheme basis, where the many-nucleon basis states are constructed with a good total magnetic projection M that is the same for all basis states, the SA-NCSM framework adapts multi-shell SU(3) scheme basis.

The multi-shell 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 significance of the SU(3) group for a microscopic description of the nuclear collective 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 dominant symmetries of nuclear collective motion. The SA-NCSM basis states are labeled schematically as

$$|\vec{\gamma}; N(\lambda\,\mu)\kappa L; (S_p S_n)S; JM\rangle\,, \tag{3}$$

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) irreducible representation, or "irrep". The SU(3) irrep labels $(\lambda\,\mu)$ bring forward important information about nuclear shapes and deformation, according to an established mapping [9]. For example, (00), $(\lambda\,0)$ and $(0\,\mu)$ describe spherical, prolate and oblate deformation, respectively. 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. Specifically, in each major HO shell η with degeneracy Ω_η, protons (or neutrons) are arranged into antisymmetric $\mathrm{U}(\Omega_\eta) \times \mathrm{SU}(2)_{S_\eta}$ irreps [10], with $\mathrm{U}(\Omega_\eta)$ further reduced with respect to SU(3), providing the single-shell labels $\left[f_1,\ldots,f_{\Omega_\eta}\right]\alpha_\eta(\lambda_\eta\,\mu_\eta)S_\eta$. Note that a spatial symmetry associated with a Young tableau $\left[f_1,\ldots,f_{\Omega_\eta}\right]$ is uniquely determined by the imposed antisymmetrization and the associated intrinsic spin S_η [10]. A multiplicity index α_η is required to distinguish multiple occurrences of SU(3) irrep $(\lambda_\eta\,\mu_\eta)$ in a given $\mathrm{U}(\Omega_\eta)$ irrep. Coupling of these single-shell configurations further yield inter-shell $\mathrm{SU}(3)\times\mathrm{SU}(2)_S$ quantum numbers for protons and for neutrons; the proton and neutron configurations are finally coupled to good $(\lambda\,\mu)\kappa LS; JM$. All of these labels uniquely determine the SA-NCSM basis states (3).

There are two major advantages of the SA-NCSM that follow from the use of the SU(3) scheme basis:

1. The SU(3)-based organization of the model space allows the complete $N_{\max}$ space to be down-selected to the physically relevant subspace that tracks with an inherent preference of a system towards low-spin and high-deformation dominance. The SA-NCSM approach enables to refine the definition of the model space, which for the NCSM is

fixed by simply specifying the $N_{\max}$ cutoff. In particular, SA-NCSM model spaces can be characterized by a pair of numbers $\langle N^{\perp}_{\max}\rangle N_{\max}$, which implies inclusion of the complete space up through $N^{\perp}_{\max}$, and a subspace spanned by complete sets of equivalent irreps $N(\lambda\,\mu)S_pS_nS$ for $N^{\perp}_{\max} < N \leq N_{\max}$. This makes calculations in larger $N_{\max}$ spaces feasible with current computational resources.

2. Within the space down-selected to a subset of $N(\lambda\,\mu)$ irreps and intrinsic spins S_p, S_n, and S, the spurious center-of-mass (CM) motion can be factored out exactly. This ensures the translational invariance of the SA-NCSM wave functions.

3. Importance truncation

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 $N_{\max}$ model space. Our aim is to couple the IT method with the unique ability of the SA-NCSM approach to restrict model space to physically relevant subsets of irreps and study properties of this combined method.

Let us suppose that $\mathcal{H}$ is a large model space spanned by many-body states $|i\rangle$. We assume that the size of this model space prohibits direct diagonalization of the Hamiltonian matrix. It is important to note that while in the traditional IT-NCSM approach a model space is fixed by the $N_{\max}$ cutoff, in our new method, one can also define the model space to include only a subset of states that span dominant $N(\lambda\,\mu)S_pS_nS$ irreps. Let us define a subspace $\mathcal{H}' \subset \mathcal{H}$, characterized by the cutoff $N'_{\max}$, $N'_{\max} < N_{\max}$, to be a starting point of the calculation. We assume that within this subspace, one can perform exact diagonalization of the Hamiltonian, and compute corresponding eigenvalues and eigenvectors. This decomposition defines Hamiltonian $\hat{H}_0$ and a set of reference states

$$|\Psi^{\nu}_{\rm ref}\rangle = \sum_{i\in\mathcal{H}'} C^{\nu}_i |i\rangle\,, \tag{4}$$

which satisfy

$$\hat{H}_0|\Psi^{\nu}_{\rm ref}\rangle = E^{\nu}_{\rm ref}|\Psi^{\nu}_{\rm ref}\rangle\,. \tag{5}$$

Formally, one can decompose full Hamiltonian to

$$\hat{H} = \sum_{\nu} E^{\nu}_{\rm ref}|\Psi^{\nu}_{\rm ref}\rangle\langle\Psi^{\nu}_{\rm ref}| + \sum_{\mu\notin\mathcal{H}'} E^{\mu}|\mu\rangle\langle\mu|\,, \tag{6}$$

and define perturbation $\hat{W} = \hat{H} - \hat{H}_0$. The perturbation part $\hat{W}$ can be approximately taken into account via the Rayleigh–Schrödinger perturbation

theory. The set of reference states (4) represents zeroth-order approximation of the wave function. The first-order correction is given by

$$|\Psi_1^\nu\rangle = -\sum_{j\notin\mathcal{H}'} \frac{\left\langle j|\hat{W}|\Psi_{\rm ref}^\nu\right\rangle}{E_j - E_{\rm ref}^\nu}|j\rangle = -\sum_{j\notin\mathcal{H}'} \frac{\left\langle j|\hat{H}|\Psi_{\rm ref}^\nu\right\rangle}{E_j - E_{\rm ref}^\nu}|j\rangle\,. \tag{7}$$

It is, therefore, natural to define an importance-measure parameter of the basis state $|i\rangle \notin \mathcal{H}'$ as follows:

$$\kappa_i^\nu = -\frac{\left\langle i|\hat{H}|\Psi_{\rm ref}^\nu\right\rangle}{E_i - E_{\rm ref}^\nu}\,. \tag{8}$$

Note that the IT approach is based on the assumption that κ_i^ν 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 $\kappa_{\rm min} \geq 0$ defines the limit for the acceptance of a basis state $|i\rangle \notin \mathcal{H}'$. For a set of reference states, the basis state $|i\rangle \notin \mathcal{H}'$ is accepted if it satisfies $|\kappa_i^\nu| \geq \kappa_{\rm min}$ for at least one reference state. The model space $\mathcal{H}'$ can be augmented by a set of accepted basis states for a given threshold $\kappa_{\rm min}$, and one can diagonalize Hamiltonian in this new model space. Resulting eigenvectors can, in turn, establish a new set of reference states (4), and the procedure can be repeated with a smaller value of $\kappa_{\rm min}$. In the limit $\kappa_{\rm min} \to 0$, one obtains eigenvalues and eigenvectors of Hamiltonian in the complete model space $\mathcal{H}$.

4. Numerical results

We augmented the SA-NCSM framework as implemented by the state-of-art code LSU3shell [12] by the IT algorithm. As the proof-of-concept study, we investigated the lowest lying states of ^{6}Li using realistic JISP16 nucleon–nucleon interaction [5] and HO energy $\hbar\Omega = 20\,$MeV.

The initial set of reference states was generated by diagonalizing Hamiltonian in the complete $N'_{\rm max} = 2$ space. A starting value of the numerical threshold was set to $\kappa_{\rm min} = 0.1$, and exponentially decreased at each step of the algorithm. The number of accepted states for a given $\kappa_{\rm min}$ threshold depends on the total number of reference states. Obviously, a greater number of reference states entails higher probability that a given basis state will be accepted. In the current study, we utilized three reference states as our aim was to investigate several lowest lying states.

The relation between the importance-measure value κ_i^ν and corresponding coefficient in the wave function expansion C_i for the ground state in ^{6}Li is shown in Fig. 1 for several values of numerical threshold $\kappa_{\rm min}$. Fractions

of selected basis states η are displayed in each panel. One can observe clear correlation between the two quantities, which demonstrates the fact that the importance-measure parameter κ_i^ν can be used as a reasonable estimate of the relevance of the basis state in the wave function.

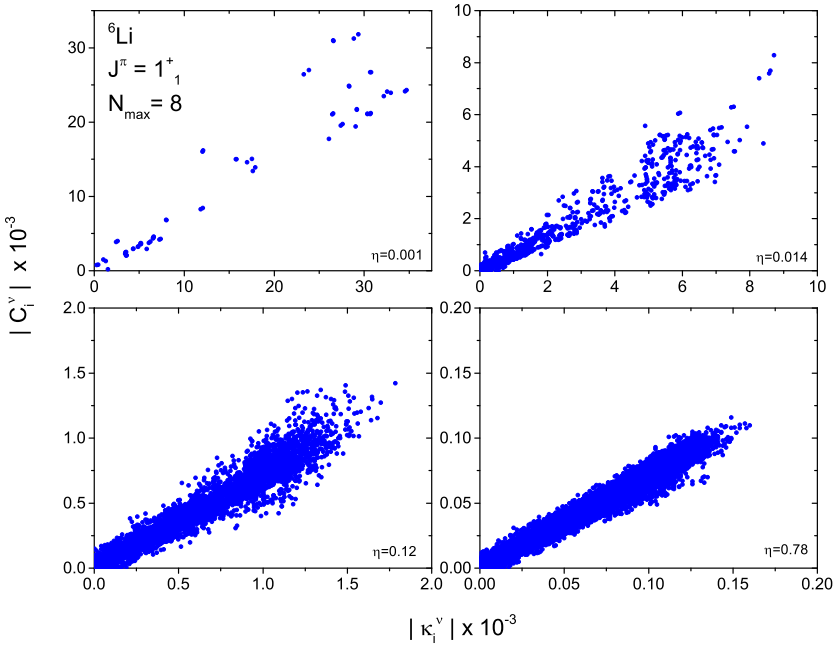

Fig. 1. Correlation between the importance-measure value κ_i^ν and corresponding coefficient C_i in the ground state of ^{6}Li is depicted for different fractions η of the complete $N_{\max} = 8$ model space.

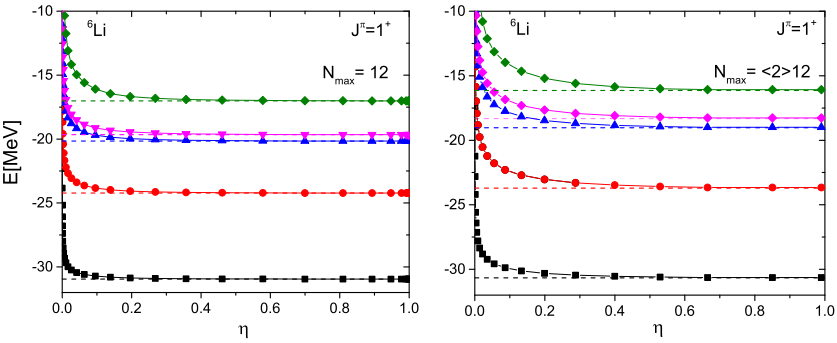

Fig. 2. Binding energies of the five lowest 1^+ states in ^{6}Li as a function of the fraction η of states selected in the complete $N_{\max} = 12$ model space (left) and $\langle 2 \rangle 12$ symmetry-adapted model space (right). Data points represent IT calculations for different values of numerical threshold $\kappa_{\min}$ ranging from 0.1 to 0.

The convergence rate for the lowest $J^\pi = 1^+$ states is demonstrated in the left panel of Fig. 2, where the convergence of energies in the complete $N_{\max} = 12$ model space is shown. Less than 10% of basis states, corresponding to $\kappa_{\min} \approx 1.19^{-4}$, accounts for 99% of the $N_{\max} = 12$ ground state binding energy. The total probability amplitudes of the most dominant SU(3)×SU(2)$_S$ subspaces in the ground state wave function are listed in Table I. A striking pattern can be recognized from this decomposition. Namely, a dominance of states with high deformation $(\lambda\, 0), (\lambda-2\, 1), (\lambda-4\, 2)$ and low spins $S_p = 1/2, S_n = 1/2, S = 1$. This familiar picture known from the SA-NCSM calculations [6] is confirmed here quantitatively by the IT algorithm. Comparison of the probability amplitudes between truncated and complete $N_{\max} = 12$ model space shows large similarity.

TABLE I

Total probability amplitudes of the most dominant SU(3) × SU(2)$_S$ subspaces in the ^{6}Li ground state wave function obtained for $\kappa_{\min} \approx 1.19^{-4}$ truncated model space and the complete $N_{\max} = 12$ model space ($\kappa_{\min} = 0$).

$N\hbar\omega$	$(\lambda\mu)$	S_p	S_n	S	Prob. [%] $\kappa_{\min} \approx 1.19^{-4}$	Prob. [%] $\kappa_{\min} = 0$
0	(0 1)	1/2	1/2	0	1.234	1.187
	(2 0)	1/2	1/2	1	60.802	59.587
2	(4 0)	1/2	1/2	1	12.861	13.065
	(0 2)	1/2	1/2	1	2.662	2.604
	(2 1)	1/2	1/2	1	2.001	1.992
4	(6 0)	1/2	1/2	1	7.334	7.618
	(2 2)	1/2	1/2	1	1.079	1.106
	(4 1)	1/2	1/2	1	0.554	0.570
6	(8 0)	1/2	1/2	1	2.871	3.101
	(4 2)	1/2	1/2	1	0.458	0.492
	(6 1)	1/2	1/2	1	0.374	0.392
8	(10 0)	1/2	1/2	1	1.050	1.172
	(6 2)	1/2	1/2	1	0.183	0.210
	(8 1)	1/2	1/2	1	0.124	0.135
10	(12 0)	1/2	1/2	1	0.343	0.385
	(8 2)	1/2	1/2	1	0.070	0.082
	(10 1)	1/2	1/2	1	0.044	0.048
12	(14 0)	1/2	1/2	1	0.072	0.080
	(10 2)	1/2	1/2	1	0.015	0.024
	(12 1)	1/2	1/2	1	0.011	0.014

We also investigated the efficiency of the IT algorithm when applied to symmetry-truncated $\langle 2\rangle 12$ model space, which is spanned by the most relevant SU(3)×SU(2)$_S$ subspaces (for details, see [6]). The convergence of

the binding energies is shown in the right panel of Fig. 2. We conclude that $\approx 30\%$ of selected basis states are responsible for 99% of $\langle 2 \rangle 12$ model space binding energies.

5. Conclusion

Importance-truncation procedure was, for the first time, applied to multi-shell SU(3) scheme basis of the *ab initio* SA-NCSM. We have shown that it can provide a quantitative prescription for the selection of relevant basis states thus enabling a significant reduction of matrix dimensions used in SA-NCSM calculations. The combination of symmetry-guided selection of relevant subspaces with IT selection criteria can be used for even more dramatic reduction of model spaces, which is a necessary step towards advancing applicability of *ab initio* studies towards medium-heavy nuclei.

This work was supported by the Czech Science Foundation under grant No. 16-16772S. This work is also a part of the "PRAC Collaborative Research: Advancing first-principle symmetry-guided nuclear modeling for studies of nucleosynthesis and fundamental symmetries in nature" PRAC allocation support by NSF (award number OAC-1713690), and is a part of the Blue Waters sustained-petascale computing project, which is supported by NSF (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.

REFERENCES

[1] P. Navrátil, J.P. Vary, B.R. Barrett, *Phys. Rev. Lett.* **84**, 5728 (2000).
[2] S. Quaglioni, P. Navrátil, *Phys. Rev. Lett.* **101**, 092501 (2008).
[3] G. Hagen, T. Papenbrock, M. Hjorth-Jensen, *Phys. Rev. Lett.* **104**, 182501 (2010).
[4] D.R. Entem, R. Machleidt, *Phys. Rev. C* **68**, 041001)(R) (2003).
[5] A.M. Shirokov, J.P. Vary, A.I. Mazur, T.A. Weber, *Phys. Lett. B* **644**, 33 (2007).
[6] T. Dytrych *et al.*, *Phys. Rev. Lett.* **111**, 252501 (2013).
[7] J.P. Elliott, *Proc. R. Soc. Lond. A* **245**, 128 (1958); **245**, 562 (1958).
[8] G. Rosensteel, D.J. Rowe, *Phys. Rev. Lett.* **38**, 10 (1977).
[9] O. Castaños, J.P. Draayer, Y. Leschber, *Z. Phys. A* **329**, 33 (1988).
[10] J.P. Draayer, Y. Leschber, S.C. Park, R. Lopez, *Comput. Phys. Commun.* **56**, 279 (1989).
[11] R. Roth, P. Navrátil, *Phys. Rev. Lett.* **99**, 092501 (2007).
[12] T. Dytrych *et al.*, *Comput. Phys. Commun.* **207**, 202 (2016).