Eigenvector continuation in nuclear shell-model calculations

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1. Introduction

The nuclear shell-model calculation is one of the most powerful tools to discuss various nuclear structures microscopically. In a traditional shell-model framework such as [1, 2], the parameters of the shell-model Hamiltonian are obtained employing the effective-interaction theory and these values are corrected phenomenologically so that the shell-model results well reproduce the experimental binding and excitation energies. For the analysis of the uncertainty caused by this correction [3, 4], we have to perform many shell-model calculations repeatedly by changing these parameters slightly. In such a situation, the eigenvector-continuation (EC) technique [5] is expected to shorten the computation time of these calculations. In this report, we introduce the EC to nuclear shell-model calculations and discuss its performance. This report is condensed from Ref. [6].

2. Theoretical Framework

The nuclear shell-model Hamiltonian is defined as

$$H(c) = \sum_i e_i c_i^\dagger c_i + \sum_{i<j,k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \quad (1)$$

where $c_i^\dagger$ is a creation operator of the single-particle state i in the model space. The e_i and v_{ijkl} are parameters, which are determined so that the eigenvalue agrees with the experimental value keeping rotational and isospin symmetries. c denotes a set of the parameters to define e_i and v_{ijkl}. The eigenenergy $E(c)$ and the eigenvector $|\phi(c)\rangle$ are given by solving the eigenvalue problem

$$H(c)|\phi(c)\rangle = E(c)|\phi(c)\rangle, \quad (2)$$

by means of the Lanczos method. However, the dimension of the Hamiltonian matrix is often huge [7], which would prevent us from solving the eigenvalue problem many times by changing the parameters.

Here, we introduce the EC technique to the shell-model calculations to estimate the eigenenergies and related physical observables without performing the diagonalization for each different interaction. In the preparation stage of the EC method, we prepare a set of sample interactions, $H(s)$, which are given randomly. We solve the eigenvalue problems of these sample interactions and obtain the sample eigenvectors $|\phi_s\rangle$ as

$$H(s)|\phi_s\rangle = E_s|\phi_s\rangle. \quad (3)$$

By using these prepared eigenvectors, the eigenvalue of a target Hamiltonian $H(t)$ is estimated without solving its eigenvalue problem as follows. The eigenvector of $H(t)$ is approximated by solving the generalized eigenvalue problem in the subspace spanned by the sample vectors. It is obtained by

$$\sum_{s'=1}^{N_s} \tilde{H}_{ss'} \tilde{v}_{s'} = \tilde{E}_t \sum_{s'=1}^{N_s} \tilde{N}_{ss'} \tilde{v}_{s'}, \quad (4)$$

with

$$\begin{aligned} \tilde{H}_{ss'} &= \langle \phi_s | H(\mathbf{t}) | \phi_{\mathbf{s}'} \rangle \\ \tilde{N}_{ss'} &= \langle \phi_s | \phi_{s'} \rangle, \end{aligned} \quad (5)$$

where $\tilde{E}_t$ is the estimated value of the exact eigenvalue of $H(\mathbf{t})$. The dimension of this generalized eigenvalue problem, namely the number of samples N_s, is far smaller than the original eigenvalue problem in Eq. (3). The eigenvector of $H(t)$ is also approximated by a linear combination of the sample eigenvectors with the coefficients $\tilde{v}_s$ as

$$|\phi_t\rangle \sim |\tilde{\phi}_t\rangle = \sum_s \tilde{v}_s |\phi_s\rangle, \quad (6)$$

which is used to estimate other physical quantities.

To perform shell-model calculations and the EC estimation efficiently, one of the authors developed a new shell model code "ShellModel.jl", which is written in the Julia language and is publicly available [8].

3. Benchmark Results

Here we present a benchmark result of the EC estimation in shell-model calculations. We take two sd-shell nuclei, ^{28}Si and ^{25}Mg, with the sd-shell model space as examples. In this case, the number of parameters for the shell-model Hamiltonian is 66. The M-scheme dimension is 93,710 for ^{28}Si and 44,133 for ^{25}Mg.

As a first example, we take the yrast 0^+, 1^+, 2^+, and 3^+ energies of ^{28}Si. We prepare 250 sample interactions generated by the sum of the USDB interaction [1] and random numbers with the 1-MeV standard deviation. For validation, we prepare 100 target interactions in the same way and estimate the energies by the EC method employing the sampling results. Figure 1 shows the EC estimated energies against the exact ones of the yrast $J = 0^+, 1^+, 2^+, 3^+$, and 4^+ states of ^{28}Si. They agree quite well and its typical error is less than 1%. Note again that the EC estimate requires little additional computations.

As an example of odd nuclei, the energies of $J = 1/2^+, 3/2^+, 5/2^+, 7/2^+$, and $9/2^+$ states of ^{25}Mg are estimated by the EC method with the same 100 target interactions. Figure 2 shows the EC estimated energies agree quite well with the exact one similarly to Fig. 1.

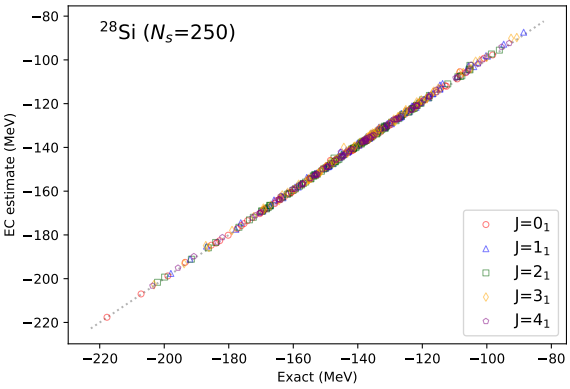

Figure 1. EC estimated energies of the $J = 0^+, 1^+, 2^+, 3^+$, and 4^+ states of ^{28}Si against the exact ones. The EC estimation is performed for the 100 different interactions with employing 250 samples. The dotted line shows the ideal agreement. Taken from Ref. [6].

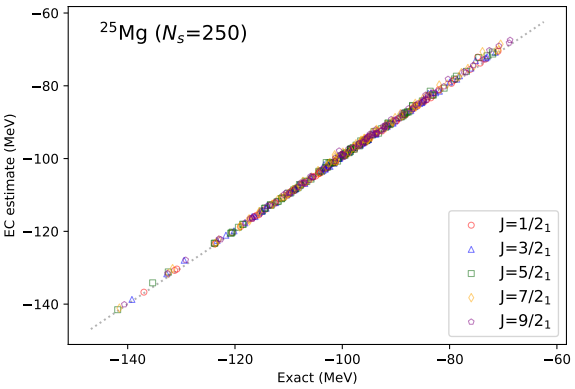

Figure 2. EC estimated energies of the $J = 1/2^+, 3/2^+, 5/2^+, 7/2^+$, and $9/2^+$ states of ^{25}Mg against the exact ones. See the caption of Fig. 1 for details. Taken from Ref. [6].

4. Summary

We introduce the EC method to nuclear shell-model calculations and investigate its performance. We demonstrated that the EC estimated energies well reproduce the exact eigenenergies for sd-shell nuclei.

The accuracy of the EC estimation concerning quadrupole and magnetic moments and excitation energies is further discussed in Ref. [6]. Moreover, the approximated wave function given by the EC method can be used as an initial vector of the Lanczos iterations, which shortens the number of the iterations [6].

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