Large-scale shell-model studies of exotic nuclei and nuclear level densities

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Abstract

An applicability of large-scale shell-model calculations grows rapidly owing to the developments of both the methodology and high-performance computing. We briefly describe two methods to go beyond the standard Lanczos method in the large-scale shell model calculations: the Monte Carlo shell model and the stochastic estimation of nuclear level density. For the latter one, we adopt an eigenvalue-density estimation based on a shifted Krylov-subspace method. It enables us to describe both a low-lying spectroscopy and the nuclear level density microscopically in a unified manner.

Keywords: *Nuclear shell model, Monte Carlo shell model, nuclear level density*

1 Introduction

Large-scale shell-model calculations is one of the powerful methods to study exotic structure of neutron-rich nuclei, which has been intensively investigated due to a recent growth of the high-performance computing enhancing a feasibility of the large-scale shell-model calculations in medium-heavy nuclei. The recent limit of the large-scale shell-model calculation with the conventional Lanczos diagonalization reaches $O(10^{11})$ M-scheme dimension [1, 2].

Tokyo nuclear theory group in the University of Tokyo has been continuing to promote the utilization of the high performance computing for the large-scale shell model calculations under the HPCI Strategic Program field 5 and priority issue 9 to be tackled by using post-K computer [3]. Conventionally the large-scale shell-model calculations are performed by solving an eigenvalue problem for a huge Hamiltonian matrix utilizing the Lanczos algorithm [1]. We developed a shell-model code "KSHELL" for the Lanczos calculations on a massively parallel computer and showed its capability up to $O(10^{11})$ M-scheme dimensions [4].

2 Monte Carlo shell model

In order to overcome the limitation of the standard Lanczos method, M. Honma, T. Mizusaki and T. Otsuka have suggested the Monte Carlo shell model (MCSM) [5],

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and the Tokyo group extended it by introducing a sophisticated variational method [6] and an extrapolation utilizing an expectation value of the energy variance [7]. The MCSM framework with these new features is called an "advanced MCSM". It enables us to obtain the low-lying spectra with large model spaces. It is applied to no-core shell-model calculations in p-shell nuclei and large-scale shell-model calculations in medium-heavy nuclei.

In the application of the MCSM to the no-core shell-model calculations called no-core MCSM, we adopted the JISP16 interaction [8] and demonstrated that a cluster structure emerges in the intrinsic states of Be isotopes [9]. It also enables us to extrapolate the binding energies of the p-shell nuclei to those corresponding to the infinite size of the model space [10].

In the applications of the MCSM to medium-heavy nuclei, we investigated an exotic structure of neutron-rich nuclei such as neutron-rich Ni isotopes [11]. Recently we successfully reproduced a sudden drop of the 2^+ excitation energies in Zr isotopes around $N = 60$, and revealed that it is caused by the first-order quantum phase transition from spherical shape to prolate deformation [12, 13].

3 Stochastic estimation of level density

For understanding a neutron-capture process, a nuclear level density is an important input in the Hauser–Feshbach theory. Nuclear shell-model calculations are considered to be one of ideal methods to evaluate the level density. In the shell-model calculations, the level density is obtained as an eigenvalue density of the Hamiltonian matrix. However, there is a difficulty in numerical computation: the conventional Lanczos method shows a slow convergence and a lot of memory usages.

Although the MCSM provides a good description of the ground states and a few low-lying excited states, it cannot provide the nuclear level density. It is difficult to compute the nuclear level density by a direct counting of the eigenvalues obtained by the Lanczos method, since the number of eigenvalues to be obtained reaches a few thousands and the convergence of highly-excited states is slow in the Lanczos method. Several methods to obtain the nuclear level density were proposed based on shell-model calculations [14–16]. In Ref. [17], we adopted a stochastic estimation of eigenvalue count based on a shifted Krylov-subspace method [18] and applied it to the nuclear shell-model calculations. This estimation works efficiently especially for sparse matrices.

Here we describe the framework of this estimation method. The shell-model wave function is written as a linear combination of many-body configurations which are called the M-scheme basis states [1]. Since the eigenenergy of the shell-model Hamiltonian is obtained as an eigenvalue of the M-scheme shell-model Hamiltonian matrix, H, the nuclear level density corresponds to the number of the eigenvalues in a certain eigenvalue region. We count the number of eigenvalues μ_k in the range $E^{(k-1)} < E < E^{(k)}$ by evaluating the residue of the contour integral Γ_k in Fig. 1.

We compute the contour integral along Γ_k by discretizing the contour line with mesh points $z_j^{(k)}$ (blue crosses in Fig. 1) and their weights w_j as

$$\mu_k = \frac{1}{2\pi i} \oint_{\Gamma_k} dz \ \mathrm{Tr}\left(\frac{1}{z-H}\right) = \sum_j w_j \ \mathrm{Tr}\left(\frac{1}{z_j^{(k)}-H}\right). \tag{1}$$

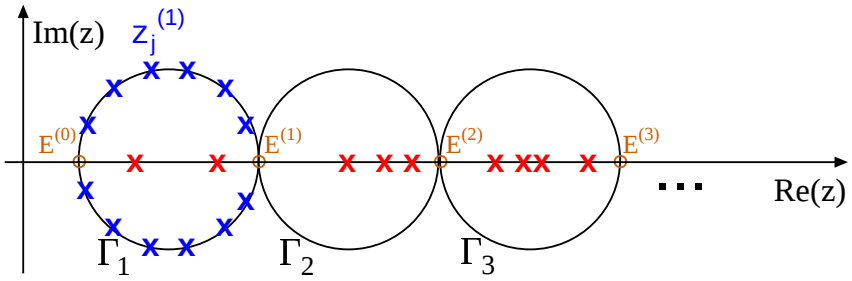

Figure 1: Schematic drawing of the contour line to count the eigenvalues between $E^{(k-1)}$ and $E^{(k)}$ in the complex plane of z. The red and blue crosses denote the eigenvalues and the discretized mesh points $z_j^{(1)}$ along the Γ_1. The figure is taken from Ref. [17].

Since the trace of the inverse of matrix in Eq. (1) cannot be directly calculated, it is stochastically estimated by Hutchinson's estimator [19] as

$$\mathrm{Tr}\left(\frac{1}{z-H}\right) \simeq \frac{1}{N_s}\sum_{s}^{N_s} \boldsymbol{v}_s^T \frac{1}{z-H}\boldsymbol{v}_s, \tag{2}$$

where $\boldsymbol{v}_s$ are vectors whose components take values of 1 or -1 randomly with equal probability. N_s denotes the number of these random vectors. Typically, N_s is taken as 32 and its stochastic error is small enough.

In order to estimate the trace in Eq. (2), we have to compute $\boldsymbol{v}_s^T(z_j^{(k)}-H)^{-1}\boldsymbol{v}_s$. In the case of shell-model Hamiltonian matrix which is quite sparse, it is inefficient to compute the inverse matrix directly. Since the matrix H is quite sparse, we solve the linear equations $\boldsymbol{v}_s = (z-H)\boldsymbol{x}$ utilizing a Krylov-subspace method and obtain the $(z-H)^{-1}\boldsymbol{v}_s$. Among the Krylov-subspace methods, we adopt the block bilinear form of the blocked complex orthogonal conjugate gradient (BCOCG) method [20] for efficient computation. On top of that, we need to solve the equations $\boldsymbol{v}_s = (z-H)\boldsymbol{x}$ for any $z = z_j^{(k)}$. These equations are solved simultaneously based on the shifted algorithm [21].

As a benchmark for the validity of the estimation, Fig. 2 shows the level density obtained by the present estimation in comparison with the exact shell-model level density obtained by the Lanczos method. The model space is taken to be the *sd* shell and the USD interaction [22] is used. The result of the stochastic estimation shows a good agreement with the exact one with a certain stochastic error. The present method allows us to estimate the level density of a large system with the M-scheme dimension of up to 2×10^{10} [17]. This dimension is almost the current limit of the Lanczos method to obtain a few low-lying states.

This method enables us to estimate the level density in medium-heavy nuclei utilizing a realistic effective interaction successfully describing low-lying excited states and their spectroscopic information. In Ref. [17], using such a realistic effective interaction, we successfully reproduced an experimentally observed equilibration of $J^\pi = 2^+$ and 2^- states in ^{58}Ni.

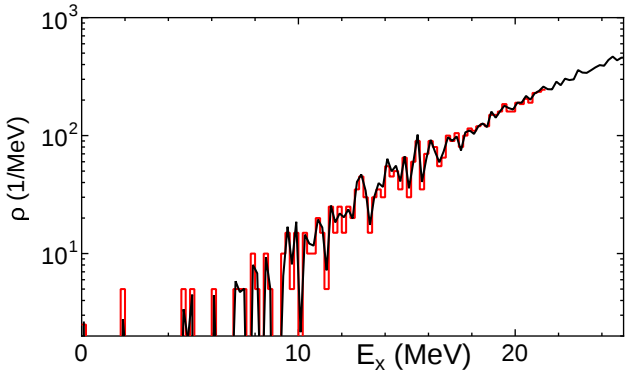

Figure 2: Benchmark test of the level density in ^{28}Si vs the excitation energy E_x. Red solid histogram — exact shell-model calculation by Lanczos method, black line — stochastic estimation. The figure is taken from Ref. [17].

4 Summary

In order to extend the limit of large-scale shell-model calculations, we developed the advanced MCSM for obtaining low-lying states and for the stochastic estimation of the nuclear level density. Further details and a review of the advanced MCSM can be found in Refs. [23,24]. A recent achievement of the MCSM calculations of Zr isotopes is available in Ref. [12]. Concerning the stochastic estimation of the level density, Refs. [17,25] are referred.

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