# FILTER DIAGONALIZATION: A NEW METHOD FOR LARGE-SCALE SHELL-MODEL CALCULATIONS*

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A new method, which is called filter diagonalization, is presented for large-scale shell-model calculations. This method is alternative to the widely used Lanczos method to evaluate shell-model energy and electromagnetic properties. In this contribution, we especially focus on its application to the mirror energy differences (MED) due to small isospin breaking.

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## 1. Introduction

The Lanczos method [1] has been widely used for exact solutions of shell-model calculations. By combining it with the $M$-scheme representation, the Lanczos method is quite useful for large-scale shell-model calculations. It needs, however, a dedicated treatment for conservation of angular momentum and it is difficult to evaluate highly excited states.

Recently a completely different algorithm for diagonalization has been proposed by Sakurai and Sugiura [2, 3]. This method is called Sakurai–Sugiura (SS) method and it uses the Cauchy's integral formula to obtain eigenvalues and eigenvectors. For large-scale shell-model calculations, we use "shift" algorithms [4] in addition to the SS method. The application of this method in the shell-model calculation has been shown in Ref. [5]. In this contribution, we especially focus on its application in the mirror energy differences (MED).

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## 2. Method

Central quantities of the SS method in the shell-model calculations are the following moments $\mu_p (p = 0, 1, 2, \ldots)$ defined by Cauchy's integral as

$$\mu_p = \frac{1}{2\pi i} \int_{\Gamma} \left\langle \psi \left| \frac{(z-\epsilon)^p}{z-H} \right| \phi \right\rangle dz \,, \tag{1}$$

where $|\psi\rangle$ and $|\phi\rangle$ are arbitrary wave functions, and $H$ is a shell-model Hamiltonian. The $\epsilon$ denotes a target energy and the $\Gamma$ is an integral contour.

By the theorem of residue, Cauchy's integral is formally performed as

$$\mu_p = \sum_{k \in \Gamma} (e_k - \varepsilon)^p c_k d_k \,, \tag{2}$$

where $c$s and $d$s are expansion coefficients with $\sum |c_i|^2 = 1$ and $\sum |d_i|^2 = 1$, that is, $|\psi\rangle = \sum c_i |\varphi_i\rangle$ and $|\phi\rangle = \sum d_i |\varphi_i\rangle$. The $e_i$s and $|\varphi_i\rangle$s are eigen-energies and eigen-functions of the $H$. The summation over $k$ in Eq. (2) is carried out if energy eigenvalues are inside the $\Gamma$.

To extract the energy eigenvalues $e_k$ located inside the $\Gamma$ from these moments, we solve the following generalized eigenvalue problem as

$$Mx = \lambda N x \,, \tag{3}$$

where $M$ and $N$ are the $n \times n$ Hankel matrices defined by $M_{ij} \equiv \mu_{i+j-1}$ and $N_{ij} \equiv \mu_{i+j-2}$. The eigenvalues $\lambda_k$ in the Eq. (3) can be shown to be equal to $e_k - \varepsilon$. Its proof needs a fact that the Hankel matrices can be always factorized with the Vandermonde matrix [2]. The associated eigenvectors can be also obtained in the same way as [2].

To evaluate the moments numerically, $\frac{1}{z-H}$ is an obstacle. To remove it, we define a new wave function $|\chi\rangle \equiv \frac{1}{z-H}|\phi\rangle$ and can numerically solve a linear equation as

$$(z - H)|\chi\rangle = |\phi\rangle \,, \tag{4}$$

by the complex orthogonal conjugate gradient (COCG) method [6].

The Cauchy's integration in the moments can be also carried out by numerical integration by taking circle as the integration contour $\Gamma$, that is

$$z = \varepsilon + re^{i\theta} \qquad (\varepsilon, r : \text{real}, \qquad \theta = [0, 2\pi]) \,. \tag{5}$$

For this numerical integration, we need a lot of integral points. For each point, the above linear equation should be solved. However, thanks to the "shift" algorithms [4], the computation becomes remarkably faster. Its details in the case of the shell-model calculations are presented in Ref. [5].

The merits of this method are following:

1. Highly excited state can be directly solved without obtaining yrast and lower excited states.

2. The conservation of angular momentum and other quantum numbers are stably realized during the computations.

In Fig. 1, we show an example of the filter diagonalization by taking 6th and 7th, $J = 0$ and $T = 0$ states of $^{48}$Cr with full $pf$ shell.

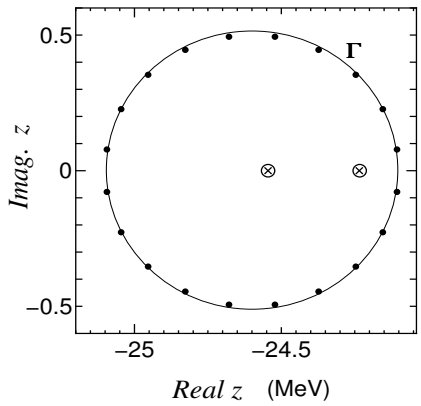


Fig. 1. (Color online) Demonstration of the filter diagonalization for the 6th and 7th, $J = 0$ and $T = 0$ states of $^{48}$Cr on the complex $z$-plane. The crosses and small circles show energies obtained by the filter diagonalization and the Lanczos method, respectively. The solid circles show the integral points.

## 3. MED calculations

In the usual shell-model calculation, we assume isospin symmetry, while there exists, in principle, isospin symmetry breaking due to the Coulomb force and the strong nucleon–nucleon ($NN$) interaction. Such an effect can be seen in $N \sim Z$ nuclei.

For such an investigation, mirror pair nuclei, that is a pair of nuclei with exchanged proton and neutron numbers, plays a principal role. The MED are a measure of isospin symmetry breaking and are defined by

$$\mathrm{MED}_J = E_x(J, T, T_z = -T) - E_x(J, T, T_z = T)\,, \tag{6}$$

where $E_x(J, T, T_z)$ are the excitation energies of analogue states with spin $J$ and isospin $T$, $T_z$. For instance, the mirror nuclei $^{67}$Se and $^{67}$As have recently been measured and have been discussed [7, 8]. The shell model calculations

in this mirror pair can be performed well with the Lanczos method, while for a mirror pair with $N = Z =$ odd and $N = Z + 2$, $M$-scheme Lanczos shell model calculations may become difficult for some $J$s. For instance, to solve state ($|\psi^{T\sim 1}_{J=4}\rangle$) with $T \sim 1$ and $J = 4$ for $^{66}$As and $^{66}$Ge, this state becomes highly excited states in $M = 4$, $N = Z$ space due to the existence of $T \sim 0$ states. By the Lanczos method, it is quite difficult to solve, while, if we ignore the isospin breaking, we can solve state ($|\psi^{T=1}_{J=4}\rangle$) with $T = 1$ and $J = 4$ in $N = Z + 2$ space because this space does not contain $T = 0$ states.

The $|\psi^{T=1}_{J=4}\rangle$ state is a good approximation to the $|\psi^{T\sim 1}_{J=4}\rangle$ state as isospin breaking is small. To use the same shell model space (*i.e.,* $N = Z$ space), we consider $T_-|\psi^{T=1}_{J=4}\rangle$ state where $T_-$ is a ladder operator of isospin. Here, we can perform the filter diagonalization by taking this state as the $|\psi\rangle$ and $|\phi\rangle$ in Eq. (1). The target energy $\varepsilon$ can be estimated by $|\psi^{T=1}_{J=4}\rangle$ state. By taking small circle around this target energy $\varepsilon$ as an integral contour, we can stably and efficiently evaluate a correct shell model energy by the filter diagonalization.

## 4. Conclusion

We have presented a new shell model diagonalization method, called filter diagonalization. The advantage of this method is to solve highly excited states directly. Especially in the MED calculations, this advantage is shown to be quite useful. We are now pursuing other applications on which the filter diagonalization plays a significant role.

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