Letter

A new approach for many-body resonance spectroscopy with the complex scaling method

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We present a new approach to carry out the complex scaling calculations for resonance spectroscopy of nuclear quantum many-body systems. By combining the recently proposed Sakurai–Sugiura (SS) method with the complex scaling method (CSM), we can easily calculate the candidates of resonance energies and wave functions and can identify a resonance energy that does not move against the scaling angle. This new approach is especially useful to extend the feasibility of large-scale complex scaling calculations needed in analyzing many-body resonance states.

Subject Index D10, D13

Introduction  Resonance spectroscopy has been of particularly interest for weakly bound and unbound nuclei far from the stability line [1]. Moreover, studies of many-body resonance spectroscopy have recently been in progress, for instance, four-body resonances [2,3] and five-body resonances [4,5]. In investigating resonance and continuum state of nuclear systems, the complex scaling method (CSM) [6] is a well established approach, in particular in combination with the cluster model and the shell model [6–8]. The Gamow shell model (GSM) [9,10] is also known to obtain the resonances. With the CSM, such states are often studied through diagonalization of a complex symmetric (non-Hermitian) Hamiltonian matrix of which eigenvalues are generally complex.

Up to now, a direct diagonalization method1 for complex scaling calculations has been in use because of the complex symmetric nature of the Hamiltonian matrix. In the direct diagonalization method, there is, however, a severe restriction on the dimension of a diagonalizable matrix. Considering many-body resonance spectroscopy, the dimension of the Hamiltonian matrix inevitably increases according to the number of degrees of freedom to be treated. A breakthrough is needed to overcome such a dimensional difficulty. In the present letter, we propose a new approach, combining the recently proposed Sakurai–Sugiura (SS) method [11,12] with the CSM, and extend the feasibility of large-scale complex scaling calculations.

1 For example, a solver Zgeev in the LAPACK, which is a famous software package of numerical computation for linear algebra, is a direct diagonalization method and is designed to solve complete or partial eigenvalues and eigenvectors for a general complex matrix.
The SS method is a new diagonalization method based on Cauchy’s contour integral on a complex plane, which is regarded to be an iteration method based on the Krylov subspace, i.e., \( \{ v, Hv, H^2v, H^3v, \ldots \} \) \( (H \) is a matrix and \( v \) is a vector). As a typical iteration method, energy eigenvalues can be obtained by increasing the dimension of the Krylov subspace. The necessary iteration number (dimension of the Krylov subspace) to obtain a well converged energy is, in general, extremely small compared to the dimension of the original Hamiltonian matrix, \( H \). This iteration number is, however, crucially important to efficiently calculate energies and wave functions. For instance, for nuclear-shell-model calculations with the Lanczos method, which is a typical iteration method based on the Krylov subspace, low-lying states are known to be calculated within a small number of iterations but, for higher excited states, the necessary iteration number rapidly increases. Recently, the SS method has also been successfully applied to nuclear-shell-model calculations \([14]\) where energy eigenvalues are real, and its convergence property is found to be quite similar to that of the Lanczos method.

In this letter, we consider how to combine the SS method with the CSM where the complex symmetric (non-Hermitian) matrix plays a central role. Examining a convergence property for complex energies in detail, we find that resonance energies and wave functions can be easily calculated within a small number of iterations. Moreover, we find that energies and wave functions of resonance states at a given scaling angle can be efficiently calculated by using resonant wave functions at a nearby scaling angle. Based on these features, we propose a new approach to efficiently calculate resonance energies and wave functions in complex scaling calculations.

**COSM and complex energies** First briefly introduce the cluster orbital shell model (COSM) with complex scaling (CS-COSM) because it is employed throughout this paper (for a detailed explanation, see Ref. \([6]\)).

In the COSM, a nucleus is handled as a many-body system consisting of valence nucleons, protons and neutrons, around a core nucleus such as an \( \alpha \)-particle. For example, the proton-rich unbound nucleus \(^8\)C is handled as the five-body system of \( \alpha + p + p + p + p \). Hereafter we take this example as a touchstone for the present method because the resonance state of \(^8\)C has a genuine many-body (not two-body) resonance nature, in addition to the fact that it needs a huge number of basis states. Moreover, the first resonance is the ground state and is interesting from an experimental point of view because its energy and decay width have recently been measured \([13]\).

Next we proceed to the basis functions, which are given, for cluster orbits of a valence proton with an angular momentum \( l \), by \( r^l e^{-\sqrt{r}^2} Y_{lm}(\hat{r}) \), where \( r_n \) takes a geometrical progression \([6]\). The many-body basis wave functions are expressed by the Slater determinants \( |\phi_k(J)\rangle \) coupled with the total angular momentum \( J \), and are non-orthogonal to each other. The energy of the state \( |\Psi_J^\theta\rangle = \sum x_k^\theta |\phi_k(J)\rangle \) is obtained by solving the following generalized eigenvalue problem:

\[
H^{\theta,J}_{k',k} x_k^\theta = \epsilon_k^\theta N_k^{\theta,J} x_k^\theta,
\]

where \( \theta \) is the scaling angle, being a real value, \( \epsilon_k^\theta = \langle \phi_k(J) | H^\theta | \phi_k(J) \rangle \), and \( N_k^{\theta,J} = \langle \phi_k(J) | \phi_k(J) \rangle \). The bases \( |\phi_k(J)\rangle \) are non-orthogonal. In a later analysis, these non-orthogonal bases \( |\phi_k(J)\rangle \) are orthogonalized and then we solve the eigenvalue equation as

\[
\tilde{H}^{\theta,J}_{k',k} x_k^\theta = \tilde{\epsilon}_k^\theta x_k^\theta,
\]

where the Hamiltonian matrix \( \tilde{H}^{\theta,J}_{k',k} \) in the orthogonal bases \( |\tilde{\phi}_k(J)\rangle \) is also complex symmetric.
Fig. 1. Distribution of complex energies for $^8$C as a typical example of the CS-COSM [5]. The scaling angle is $20^\circ$ and the dimension of the Hamiltonian matrix is 22 582. The complex energies are shown by filled circles on the complex $z$-plane. The resonance energy is enclosed by the (blue) open square. The iteration number of the COCG method at each point is shown by the contour lines, the iteration numbers of which are 200, 500, 700, 2000, and 3000, respectively. The (red) open circles designate complex energies obtained using the SS method.

In Fig. 1, we show a typical energy distribution on a complex plane for $^8$C as an example [5]. The scaling angle is taken as $20^\circ$. The energies for continuum states align along several straight lines and the resonance energy is located near the real axis, which is rather isolated from the energies of continuum states. This isolation of the resonance energy on the complex plane plays an important role in calculating resonance energies.

**SS method and its convergence property**

Next we consider the SS method, the central quantity of which is the following moment $\mu_p (p = 0, 1, 2, \ldots)$, defined on the complex $z$-plane as

$$\mu_p = \frac{1}{2\pi i} \int_{\Gamma} \frac{\langle \tilde{\phi} | (z - \varepsilon_0)^p | \tilde{\phi} \rangle}{z - \tilde{H}} dz,$$

where $|\tilde{\phi}\rangle$ is a wave function and $\tilde{H}$ is a Hamiltonian matrix concerning the orthogonalized basis, which is complex-symmetric (non-Hermitian). For the sake of brevity, we omit the scaling angle $\theta$. Cauchy’s integration contour $\Gamma$ is taken so as to enclose energy eigenvalues of interest, and $\varepsilon_0$ is a point located inside $\Gamma$. With this moment, we construct the following Hankel matrices $M$ and $N$ as

$$M = \begin{pmatrix} \mu_1 & \mu_2 & \cdots & \mu_n \\ \mu_2 & \mu_3 & \cdots & \mu_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n-1} \end{pmatrix},$$

(4)

and

$$N = \begin{pmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{pmatrix}.$$  

(5)
where $n$ is the number of eigenvalues within the integral contour $\Gamma$ and is less than about 20 in the present calculations. Then, the original eigenvalue problem reduces to the following small-scale generalized eigenvalue problem with these Hankel matrices as

$$Mx = \lambda Nx,$$  \hspace{1cm} (6)

where the eigenvalue $\lambda$ corresponds to one of the original eigenvalues $\varepsilon_k$ ($k = 1, 2, \ldots$) of Eq. (2) as $\lambda = \varepsilon - \varepsilon_0$ ($\varepsilon_0$ is defined in Eq. (3)) and $x$ gives us the corresponding wave function of Eq. (2). The proof is shown in Refs. [11,12,14].

Next we go inside this formulation to show how the SS method is regarded as an iteration method of diagonalization. To evaluate the moment $\mu_p$, we introduce a numerical integration for Cauchy’s contour integral. By choosing a circle with its center at $z = \varepsilon_0$ as the integration contour $\Gamma$, complex variable $z$ is represented by $\varepsilon_0 + re^{i\theta}$ where $r$ is real and $\theta$ takes 0 to $2\pi$. The numerical expression of the moment by the trapezoidal rule with respect to angle $\theta$ is given as

$$\mu_p \sim \frac{1}{N_0} \sum_{k=0}^{N_0-1} \frac{\langle \tilde{\phi} | (z_k - \varepsilon_0)^{p+1} \phi \rangle}{z_k - \tilde{H}} = \frac{1}{N_0} \sum_{k=0}^{N_0-1} (z_k - \varepsilon_0)^{p+1} \langle \phi | \chi_k \rangle,$$ \hspace{1cm} (7)

where $N_0$ is a number of mesh points and $z_k = \varepsilon_0 + re^{i\frac{2\pi}{N_0}(k+\frac{1}{2})}$. A new vector $|\chi_k\rangle$ is introduced by solving

$$\tilde{\phi} = (z_k - \tilde{H})|\chi_k\rangle.$$ \hspace{1cm} (8)

To solve the above equations for all $k$, we use the complex orthogonal conjugate gradient (COCG) method [16] and the shift algorithm [17]. The COCG method is an iteration method based on the Krylov subspace. For each mesh point $k$, with $\sigma_k^{(0)} = 1$, $p_k^{(0)} = 0$, $|\chi_k^{(0)}\rangle = 0$, and $|r_k^{(0)}\rangle = |p_k^{(0)}\rangle = |\tilde{\phi}\rangle$, we repeat the following recursion equations as

$$|\chi_k^{(m+1)}\rangle = |\chi_k^{(m)}\rangle + \alpha_k^{(m)} |p_k^{(m)}\rangle,$$ \hspace{1cm} (9)

$$|r_k^{(m+1)}\rangle = |r_k^{(m)}\rangle - \alpha_k^{(m)} (z_k - \tilde{H}) |p_k^{(m)}\rangle,$$ \hspace{1cm} (10)

$$|p_k^{(m+1)}\rangle = |r_k^{(m+1)}\rangle + \beta_k^{(m)} |p_k^{(m)}\rangle,$$ \hspace{1cm} (11)

where $\alpha_k^{(m)} = \langle r_k^{(m)} | p_k^{(m)} \rangle / \langle p_k^{(m)} | (z_k - \tilde{H}) p_k^{(m)} \rangle$ and $\beta_k^{(m)} = \langle r_k^{(m+1)} | r_k^{(m+1)} \rangle / \langle r_k^{(m)} | r_k^{(m)} \rangle$. Note that $\langle y_k^{(m)} | \neq \langle y_k^{(m)} \rangle$ for $y = \chi, r, p$. By this procedure, the Krylov subspaces are generated as $|\tilde{\phi}\rangle, (z_k - \tilde{H})|\tilde{\phi}\rangle, (z_k - \tilde{H})^2|\tilde{\phi}\rangle, (z_k - \tilde{H})^3|\tilde{\phi}\rangle, \ldots$. By increasing the dimension of this Krylov subspace, we can obtain the convergent vector $|\chi_k\rangle$ of Eq. (8). These Krylov subspaces are, however, identical to that of $|\tilde{\phi}\rangle, (z - \tilde{H})|\tilde{\phi}\rangle, (z - \tilde{H})^2|\tilde{\phi}\rangle, (z - \tilde{H})^3|\tilde{\phi}\rangle, \ldots$ ($z$ is a certain point on the complex plane) because $z$ is a constant diagonal matrix element. Matrix-vector multiplications to generate such Krylov subspaces can, therefore, become common for all the mesh points. Then the principal part of the COCG calculations can be performed only at single point $z$, independent of $z_k$. This is called the shift algorithm [17] and the diagonalization calculation with the SS method becomes quite efficient [11,14].

Next we consider a convergence property of the COCG calculation. In Fig. 6 of Ref. [14], the convergence property of the COCG method has been discussed in the case of shell-model calculations where real energy eigenvalues are considered, while the COCG calculations are needed for a complex number $z$. The convergence of the COCG calculation becomes, in general, faster as the calculation point $z$ goes away from energy poles and is faster for $z$ in a low level density region, i.e., for the ground state and low-lying states. On the other hand, the convergence becomes worse for $z$...
in a high level density region. Now we apply this convergence property to the present problem. In the complex scaling calculations, continuum energies are roughly aligned as shown in Fig. 1. The level density tends to become very high for the continuum energies, which form a narrow region inclined to the bottom right. Hereafter we call it the continuum energy region. For several continuum energies located near the boundary of the continuum energy region, the level density is rather low. The resonance energy is almost isolated from the continuum energy region, especially for a large scaling angle. Therefore, their convergences are expected to be very fast.

In Fig. 1, the iteration numbers of the COCG calculations at all the points on the complex $z$ plane are shown by contour lines. We can see that the iteration number becomes very large in the continuum energy region while, at a resonance energy and at the boundary of the continuum energy region, the iteration number becomes small. In fact, we can calculate such resonance and continuum energies with small iteration numbers, which are designated by open square and open circles, respectively. Here we confirm the resonance energy, comparing it with the result of direct diagonalization. Next we consider how to efficiently identify the resonance energy with the SS method in a self-contained manner.

**Complex scaling and SS method** Next we consider how to examine whether calculated energies are of resonances or not within the present method. For this purpose, we change the scaling angle. Note that, in a direct diagonalization method, all the energies should be calculated from scratch at each scaling angle.

In the SS method, we can use the wave function $|\tilde{\phi}\rangle$ explicitly in the moment expression, Eq. (3). For the calculations of Fig. 1, this wave function is randomly given. Here let us consider setting this wave function by one of those calculated at a certain scaling angle. The SS method can be considered to resolve the wave function $|\tilde{\phi}\rangle$ by eigenfunctions, the eigenenergies of which are within Cauchy’s integral contour $\Gamma$, and then convergence becomes faster if we take a better wave function in the moment expression. Moreover, a variation of the wave function is expected not to be so large if we change the scaling angle slightly. Therefore, if we solve the eigenvalue problem, setting a wave function in the moment expression by that calculated at a certain nearby scaling angle, convergence is expected to become fast. By repeating this procedure concerning the scaling angle, we can easily calculate a series of energies and wave functions as a function of the scaling angle. If we start this procedure from a continuum wave function, we can obtain a series of the continuum wave functions, the energies of which move according to the scaling angle. On the other hand, if we start it from a resonance wave function, the energies obtained are expected not to move.

In Fig. 2, we show several typical trajectories of energy eigenvalues obtained by the above procedure. As a numerical demonstration, we solve an $^{8}\text{C}$ five-body problem, the Hamiltonian matrix dimension of which is 203,545, by adopting different Gaussian expansion parameters from those of Ref. [5]. Note that this problem with such a huge matrix has never been solved before. In Fig. 2, first we solve this problem at the scaling angle $21^\circ$ and obtain several candidates for the resonance state. Next we solve the eigenvalue problem at $18^\circ$, starting from these candidate wave functions at $21^\circ$. We repeat this procedure up to $3^\circ$. As shown in Fig. 2, as the scaling angle decreases, the energies labeled by B, C, D, and E continuously move as an arc, which shows that these states are continuum ones. On the other hand, the energies labeled by A do not substantially move, which shows that they stand for resonance states. This example shows that the calculated energies can be efficiently classified as resonance or continuum ones because the calculation at each scaling angle is not necessarily carried out from scratch, unlike a direct diagonalization method.
Summary

Diagonalization of a complex symmetric (non-Hermitian) matrix has been a key tool to study the resonance spectroscopy with the complex scaling method. Moreover, recently diagonalization of complex symmetric matrices with larger dimensions has been demanded for a study of many-body resonance spectroscopy with the CS-COSM [8], e.g., four-body and five-body resonances [2–5]. There exists, however, a clear limitation in diagonalizing such large matrices by a direct diagonalization method (see footnote 1).

In the present letter, we have presented a new approach for the many-body resonance spectroscopy, combining the recently proposed SS method [11,12] with the complex scaling method. By studying the convergence property of the COCG method utilized in the SS method, we found that resonance energies and wave functions can be calculated with a small iteration number, especially at a large scaling angle, thanks to the isolation of the resonance energy on the complex plane. In addition, we have presented a way to track resonance and continuum states as a function of the scaling angle by utilizing the moment expression of the SS method, and we can identify resonance states among them. In the numerical demonstration of the present approach, we successfully presented large-scale complex scaling calculations with the COSM, the matrix dimensions of which exceed $2 \times 10^5$. These huge CS-COSM calculations have never been carried out before.

The present approach makes use of eigenvalue distribution on the complex energy plane in the complex scaling calculations and it is applicable not only to narrow but also rather broad resonances with $(\Gamma/E_r) < \tan(\pi/4)$. Moreover, it is also applicable to the coupled rearrangement channel calculations of few-body systems and the GSM, as similar eigenvalue distributions are expected. Thus, the present approach will be able to extend the frontier of many-body resonance spectroscopy by enabling large-scale complex scaling calculations.

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