A theoretical treatment of four-body resonances by using the complex scaling method

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A theoretical treatment of four-body resonances by using the complex scaling method is discussed. In order to reduce the dimension of the Hamiltonian matrix, the stochastic variational method is applied for the subsystems of the four-body system. Furthermore, to investigate the resonant solutions embedded in the continuum states we employ the complex-range Gaussian basis function, and two comments in applying the complex-range basis function to the complex scaling method are given. We also introduce the additional four-body pseudo potential to clarify whether the obtained solution is a true resonance or not. As a numerical example, we investigate the applicability of the present method to the 0± states of 4He, which is a four-nucleon resonant system.

Subject Index D11, D21

1. Introduction

Recently, few-body resonances in atomic nuclei such as the triple α [1,2], the tetraneutron 4n (n+n+n+n) [3,4], the super-heavy hydrogen 7H (t+n+n+n+n) [5,6], etc. have attracted much attention. One useful method for analyzing such few-body resonances is the complex scaling method (CSM) [7,8]. In Ref. [9], the application of the CSM to many-body systems was discussed, and examples of three-body systems with the Gaussian expansion method (GEM) [10] were reviewed. The application of the CSM for systems with more than three bodies is straightforward. However, the actual calculations are limited even now [11], mainly because of the rapid increase of the necessary basis functions in the GEM.

For bound states, the stochastic variational method (SVM) has been employed to reduce the dimension of the Hamiltonian matrix [12,13]. Although the SVM is very useful and gives equivalent solutions to those obtained by other major methods [14], it cannot be directly applied to resonances. Since a minimum energy state is sought based on the variational principle in the SVM, the algorithm gives the lowest continuum (bound) state solution. Varga et al. proposed the complex scaling method combined with the stochastic variational method (CSM–SVM) to avoid such a problem, where the stationary solution on the complex energy plane is sought [15]. This method is very useful when looking for a resonant solution which is not far from the real energy axis. However, in many cases for the nuclear few-body resonances, since the decay width is the same order as the resonance energy, or even larger, step (2) in Ref. [15] would not give a candidate resonant solution for the next step because we cannot distinguish the resonant solution from the continuum solutions. Therefore, in the present paper, another approach of the complex scaling method combined with
the stochastic variational method (CSM+SVM) is proposed, in which the SVM is applied to the subsystems.

As mentioned above, many of the nuclear few-body resonances have large decay widths, and the separation of the resonant solutions from the continuum solutions is not easy. In the standard GEM, tempered (real-range) Gaussian basis functions are used, but using the basis function in the CSM creates a large numerical instability, especially for the continuum solutions. Recently, the application of the complex-range Gaussian (CG) basis function to the CSM was proposed to describe the oscillation properties of a complex scaled wavefunction [16]. By using the CG basis function, the separation of the resonant solution from the continuum solutions becomes easy. In the present study, the CG basis functions are employed to analyze the resonances embedded in the continuum states.

Although it seems to be very successful numerically [16], the complex basis functions such as the CG basis function are not theoretically applicable for the conventional CSM. Therefore, in this paper, an improvement of the CSM framework is explained in order to apply theoretically the CG basis function to the CSM. Also, the naive extension of the application of the CG basis function by using bound-state-type discussions may break the Hilbert space limit, which is the essence of the standard resonant theory. This point is also discussed in the next section in order to safely apply the CG basis function to the CSM.

In a previous paper [17,18], the author proposed changing the strength of the additional pseudo potential and performing the extrapolation of the resonant solution by using the CSM solution, called ACCT+C-SVM, in order to search for resonance embedded in the continuum states. In the present study, as an additional useful technique in the study of the four-body resonance, a pseudo four-body potential is introduced in order to separate the resonant solution from the continuum solutions.

In the present paper, we use CSM+SVM with the CG basis function. The second 0^+ state and the first 0^- state of 4He are studied with the Minnesota potential [19] as a practical application example. More quantitative results for 4He (including other spin states) with realistic interactions will be given elsewhere, because the present paper is a basic description of the proposed treatment for the four-body system. These two states are considered to have 3N+N (t+p, h+n) structures [20]. This is a typical example of cluster formation in the excited energy region and an example of the so-called inversion doublet partner [21]. Furthermore, these resonances exist in the energy region of the astrophysical S-function of d(d,p)t and d(d,n)h reactions, which are important reactions for making t and 3He in Big Bang nucleosynthesis [22,23]. Thus, the underlying physics itself is very interesting. The ratios of the experimental decay width to the resonance energies are \( \frac{\Gamma}{E_{\text{c}}}=1.27 \) for 0^+_2 and \( \frac{\Gamma}{E_{\text{c}}}=1.71 \) for 0^-, respectively [24]. The determination of a resonant solution having such a large decay width is one of the challenging problems for the resonant theory of the four-body problem. Actually, the resonant solutions for 0^\pm have not been obtained with the standard CSM technique. This is one of the motivations for the present work. By using the procedure (CSM+SVM) proposed in the present paper, 0^\pm resonant solutions are analyzed.

The purpose of the present paper is to explain the CSM+SVM technique and to give the theoretical framework for the application of the CG to the CSM. Two important comments for the application of the CG to the CSM are also given, which were not given in the original paper [16]. Further, we show the usefulness of using CSM+SVM with the CG by applying it to the 0^\pm states of 4He. The methods are described in Sect. 2. The calculated results and discussions are given in Sect. 3. A summary and list of future problems are given in the last section.
2. Method

2.1. Hamiltonian

The Hamiltonian employed is

\[ \hat{H} = \sum_{i=1}^{4} \hat{T}_i - \hat{T}_{\text{cm}} + \sum_{i<j}^{4} \hat{V}_{ij} + \sum_{i<j}^{4} \hat{V}_{ij}^C, \]

(1)

where \( \hat{T}_i \) is the kinetic energy of the \( i \)th nucleon, \( \hat{V}_{ij} \) is the two-nucleon potential, and \( \hat{V}_{ij}^C \) is the Coulomb potential. The center-of-mass kinetic energy, \( \hat{T}_{\text{cm}} \), is subtracted. We use the Minnesota (MN) potential [19] for \( \hat{V}_{ij} \). The \( u \) parameter in the MN potential is set to be \( u = 1 \). No spin–orbit force is included. The MN potential has been applied to many nuclei as a typical effective interaction by many authors. The three-nucleon binding energy is also reproduced in addition to the reproduction of properties of two-nucleon systems, not introducing the three-nucleon force. Thus, it is a reasonable interaction to calculate four-nucleon systems as the present purpose of exploratory calculations.

Since many nuclear resonances have a large decay width, the resonant solutions are embedded in the continuum solutions. This makes it difficult to find the resonant solution in practical calculations. In order to search for a resonant solution with a very large decay width, such as the soft dipole resonance of \(^6\text{He}\), the so-called ACCC+CSM is proposed [17,18]. In the ACCC+CSM, by magnifying the strength \( \lambda \) of the additional pseudo potential, \(-\lambda V\), the trajectory of the resonant solution is investigated in the sharp decay width region and/or the bound state region. And the resonant pole position of \( \lambda = 0 \) is extrapolated with the Padé approximation [25,26] even when a resonant solution with very large decay width is not directly obtained by the CSM. As will be shown later in the practical calculations, the trajectory of the complex energy as a function of the coupling constant \( \lambda \) is very useful even for a solution with decay width \( E_r \sim \Gamma/2 \), where the resonant solution is barely embedded in the continuum states. This type of technique has been employed as a useful form of CSM [1,4,16]. In this paper, since we investigate resonances of relatively large decay width \( E_r \sim \Gamma/2 \), we introduce an additional pseudo four-body potential,

\[ \hat{H}(\lambda) = \hat{H} - \lambda V^{4N}, \]

(2)

\[ V^{4N} = \exp \left( -\frac{(r_1 - r_2)^2 + (r_2 - r_3)^2 + (r_3 - r_4)^2 + (r_4 - r_1)^2}{b^2} \right), \quad b = 4 \text{ fm}, \]

(3)

where \( \lambda \) is a coupling constant. In the present study, the four-body potential would be suitable because it does not change the wavefunctions of the subsystems much.

2.2. Improvement of the complex scaling method for the complex basis function

Here, we describe the improvement of the CSM framework when we use a complex basis function such as the CG instead of the \( L^2 \) real basis function. In Ref. [16], the application of the CG was proposed, but it is not applicable for the conventional framework of the CSM as explained below. However, the numerical results are very promising. Therefore, theoretical explanations should be given. The purpose of this subsection is to recall the limitation of the CSM, why the complex basis function is not applicable, and how to improve the framework of the CSM in order to use the CG.

In the CSM, the coordinate \( r \) and its conjugate momentum \( p \) are transformed as \( U(\theta)r = re^{i\theta} \) and \( U(\theta)p = pe^{-i\theta} \). The Hamiltonian \( H \) is transformed as

\[ H(\theta) = U(\theta)HU^{-1}(\theta), \]

(4)
where $U^{-1}(\theta) = U(-\theta)$. The Schrödinger equation, $H\Psi = E\Psi$, is rewritten as

$$H(\theta)\Psi(\theta) = E(\theta)\Psi(\theta),$$

$$\Psi(\theta) = U(\theta)\Psi.$$  \hspace{1cm} (5)

For the resonance, $E(\theta) = E_r - i\Gamma/2$ does not have $\theta$ dependence; its real part corresponds to the resonance energy $E_r$ and its imaginary part corresponds to half of the decay width $\Gamma$ \[7, 8\].

Since the eigenvalues of the complex scaled Hamiltonian $H(\theta)$ are complex, $H(\theta)$ is not Hermitian, $H^\dagger(\theta) \neq H(\theta)$. Therefore, we cannot use the Hermite conjugate state in order to define the norm of the resonance by using the (Hermitian) inner product. Alternately, we use the so-called adjoint state $\tilde{\Psi}$ \[27\], which is the solution of the adjoint Schrödinger equation

$$H^\dagger(\theta)\tilde{\Psi}(\theta) = E^\ast(\theta)\tilde{\Psi}(\theta).$$

By using the adjoint state, the norm is defined as \[27\]

$$\mathcal{N} = \int_\Omega \tilde{\Psi}^\ast(\theta)\Psi(\theta)d\tau,$$

whose integration is carried out for the whole space $\Omega$. The problem is how to get $\tilde{\Psi}$ with the framework of the CSM. More general explanations for the adjoint states and the norm in Gamow (non-Hermitian) quantum mechanics are given in the appendix.

The complex scaled wavefunction is obtained by the diagonalization of the Hamiltonian matrix, which is made by the basis expansion as

$$|\Psi(\theta)\rangle = \sum_j C_j(E, \theta)|\psi_j\rangle,$$

where $C_j$ are complex coefficients and $|\psi_j\rangle$ are real basis functions. We can choose $|\psi_j\rangle$ satisfying the orthogonal condition $\langle \psi_i | \psi_j \rangle = \delta_{ij}$. For example, although the tempered Gaussian basis functions $|\phi_i\rangle$ are non-orthogonal basis functions, we can make the orthogonal basis function, $|\psi_j\rangle = \sum c_i |\phi_i\rangle$, through the diagonalization of the overlap matrix $N_{ij} = \langle \phi_i | \phi_j \rangle$.

If we multiply $\langle \psi_i |$ from the left in the complex scaled Schrödinger equation of Eq. (5), it is described as

$$\sum_j C_j(E, \theta)\langle \psi_i | H(\theta) | \psi_j \rangle = E(\theta) \sum_j C_j(E, \theta)\langle \psi_j | \psi_j \rangle,$$

$$\sum_j H_{ij}(\theta)C_j(E, \theta) = E(\theta) \sum_j N_{ij}C_j(E, \theta),$$

where

$$H_{ij}(\theta) = \langle \psi_i | H(\theta) | \psi_j \rangle,$$

$$N_{ij} = \langle \psi_i | \psi_j \rangle = \delta_{ij}.$$  \hspace{1cm} (12)

We replace the suffix $i$ and the suffix $j$ and use the symmetric property of the complex scaled Hamiltonian $H(\theta)$, $H_{ij}(\theta) = H_{ji}(\theta)$, to rewrite Eq. (11) as

$$\sum_i C_i(E, \theta)H_{ij}(\theta) = E(\theta) \sum_i C_i(E, \theta)N_{ij}.$$  \hspace{1cm} (13)
This can be read as a left-hand expression of the eigenvalue problem, and the bra-state is written as

\[ (\Psi(\theta)| = \sum_i C_i(E, \theta)\langle \psi_i| \] \tag{14} \]

As discussed for Eq. (A7) in the appendix, since the bra-state is only a transpose of the ket-state, \( \langle \psi_i| \) must be equal to \( \langle \psi^*_i| \). In other words, \( \psi \) should be a real basis function to assure the symmetric property of \( H_{ij}(\theta) \).

In the general case with the complex basis function, the Hamiltonian matrix is not symmetric as \( H_{ij}(\theta) \neq H_{ji}(\theta) \). Therefore, we cannot use the bra wavefunction as Eq. (14). However, for the complex basis function, we also know the bra-state which can define the norm with the c-product \[ \text{[32]} \] by considering the right-hand eigenvector matrix,

\[ (\Psi_k(\theta)| = \sum_i \langle \Psi_k(\theta)| \Psi_i| \] \tag{15} \]

whereas

\[ |\Psi_j(\theta)) = \sum_j C(\theta)_{ij}|\Psi_j| \] \tag{16} \]

Then, the norm is defined as

\[ N_k = (\Psi_k(\theta)|\Psi_k(\theta)) = \sum_{ij} C^{-1}(\theta)_{ik}C(\theta)_{jk}\langle \psi_i|\psi_j| = 1, \] \tag{17} \]

where the orthogonal condition \( \langle \psi_i|\psi_j| = \delta_{ij} \) is used.

Equations (14) and (15) might seem similar at a glance, but the meaning would be very different because we have to know all the right-hand (ket) solutions (see also the appendix) to define the bra-state through the inverse matrix \( C^{-1} \). This and its properties are very interesting in the further study of the CSM, but thus is outside the scope of the present paper, whose main purpose is the realistic treatment of four-body resonances.

2.3. Complex-range Gaussian basis functions and the CSM

In this subsection, a brief explanation of the complex-range Gaussian basis function (CG) is given and two comments on the application of the CG to the CSM are discussed. Recently, Ohtsubo et al. proposed using the CG on the framework of the CSM and applied it to the triple-\( \alpha \) problem \[ \text{[16]} \]. The numerical results were impressive, not only reproducing the previous calculations but also succeeding in determining the resonance energy with a large decay width, such as \( 0^+ \) in \( ^{12}\text{C} \). However, the theoretical explanation of the CG basis function was carried out for the harmonic oscillator potential, not for the resonant states.

Here, we explain the CG basis function for the one-dimensional case for simplicity. The real-range Gaussian (RG) is written as \( u_l(a_i, r) = r^l \exp(-a_ir^2) \). In the CG, the range parameter \( a_i \) is replaced by \( a_i(1 \pm \omega) \):

\[ u_l(a_i, r) = r^l \exp(-(1 + i\omega)a_ir^2), \] \tag{18} \]

\[ u_l^*(a_i, r) = r^l \exp(-(1 - i\omega)a_ir^2). \] \tag{19} \]
Another equivalent set of the CG, which we call the oscillating Gaussian basis function (OG), is deduced by a unitary transformation,

\[
\begin{pmatrix}
    u_i^{(\sin)}(a_i, r) \\
    u_i^{(\cos)}(a_i, r)
\end{pmatrix}
= U
\begin{pmatrix}
    u_i(a_i, r) \\
    u_i^*(a_i, r)
\end{pmatrix},
\]

where \( U \) is a unitary matrix satisfying \( U^\dagger U = U^{-1}U = 1 \). From this OG expression, we can easily see that it is an extension of the tempered Gaussian basis function: \( \sin(\omega a_i r^2) \) and \( \cos(\omega a_i r^2) \) describe the oscillation of the wavefunction. By using these basis functions, the relative wavefunction is described as

\[
\chi_i(r) = \sum_{i=1}^{N} (c_i u_i(a_i, r) + c_i^* u_i^*(a_i, r))
\]

\[
= \sum_{i=1}^{N} \left( c_i^{(\cos)} u_i^{(\cos)}(a_i, r) + c_i^{(\sin)} u_i^{(\sin)}(a_i, r) \right).
\]

Thus, the CG basis function related with the OG is a unitary basis function.

The first comment is related to the discussion in the previous subsection, in which the CG is not applicable to the conventional framework of the CSM. The simplest way to define the bra wavefunction is using the OG rather than the CG. Because the OG is a real function as the RG, the complex scaled matrix becomes a complex symmetric matrix. Therefore, the bra wavefunction is easily obtained as Eq. (14) in the same way as the standard CSM formalism. Also, we can use the CG because the complex eigenvalue should be the same both in the CG and OG, taking note that the definition of the wavefunction is changed considerably, as described in Eq. (15).

The second comment is that we had better not use large \( \omega \) values, as discussed in Ref. [29], because the divergent behavior of the complex scaled matrix elements is increased by the \( \omega \) parameter. Here, we discuss the parameter \( \omega \) in the CG with the so-called back-rotation formalism of the CSM. The explanation using the back-rotation formalism may be better than that given in Ref. [29] to show directly the divergent property of the complex scaled matrix elements. Equation (11) is rewritten as

\[
\sum_j \langle \phi_j^{-\theta} | H - E(\theta) | \phi_j^{-\theta} \rangle C_j(E, \theta) = 0,
\]

\[
| \phi_j^{-\theta} \rangle = U^{-1}(\theta) | \phi_j \rangle,
\]

\[
\langle \phi_i | H(\theta) | \phi_j \rangle = \langle \phi_i^{-\theta} | H | \phi_j^{-\theta} \rangle, \quad \langle \phi_i | \phi_j \rangle = \langle \phi_i^{-\theta} | \phi_j^{-\theta} \rangle.
\]

The matrix element should be the same in both expressions, \( \langle \phi_i | O(\theta) | \phi_j \rangle = \langle \phi_i^{-\theta} | O(\phi_j^{-\theta}) \). We choose a CG basis function having an outgoing wave property as \( | \psi_j \rangle = \exp(-a(1 - i\omega)r^2) \), and perform the back rotation as

\[
|r|\psi_j^{-\theta} \rangle = \exp(-a(1 - i\omega)r^2 e^{-2i\theta}),
\]

\[
= \exp(-ar^2(\cos 2\theta - \omega \sin 2\theta)) \times \exp(iar^2(\sin 2\theta + \omega \cos 2\theta)).
\]

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The first part is a dumping part when \(\cos 2\theta - \omega \sin 2\theta > 0\) and the second part is an outgoing oscillating part. When \(\cos 2\theta - \omega \sin 2\theta \leq 0\), the convergence of the matrix element \(\langle \phi_i^{\pm \theta} | O | \phi_j^{\pm \theta} \rangle / \langle \phi_i^{\pm \theta} | \phi_j^{\pm \theta} \rangle\) is not self-evident because of the divergent property of the basis function. In other words, it exceeds the square integrable Hilbert space limit. If the operator \(O\) is a divergent operator at \(r \to \infty\) such as the E1 operator, \(rY_{10}(\hat{r})\), this matrix element has a divergent property. If the operator \(O\) is a quickly dumping operator at \(r \to \infty\) such as the Gaussian potential, \(\exp(-\alpha r^2)\), the matrix element might converge.

In the case of the conventional CSM (\(\omega = 0\)), the maximum scaling angle which satisfies the condition is \(\theta_{\text{max}} = \pi / 4\). In the case of \(\omega = 1\), it becomes a half value, \(\theta_{\text{max}} = \pi / 8\). This angle, \(2\theta = 45^\circ\), corresponds to the condition of \(\text{Re}(E) = \text{Im}(E)\). In this paper, since we calculate \(0^+\) and \(0^-\) states of \(^4\text{He}\) which are \(\text{Re}(E) \simeq \text{Im}(E)\), \(\omega = 0.6\) is employed, with \(\theta_{\text{max}} = 0.515\) rad. Although this is smaller than standard values of \(\omega\) (e.g., \(\pi / 2 = 1.57\) [16]), the divergent property and/or the long-range property of the complex scaled matrix element would be reduced.

### 2.4. Basis functions for the four-nucleon system

The basis function of \(^4\text{He}\) is written as

\[
\Psi_{JM} = \sum_{\alpha} c_{\alpha} \Phi_{\alpha JM}(K) + \sum_{\beta} d_{\beta} \Phi_{\beta JM}(H),
\]

where \(K\) and \(H\) mean the type of Jacobi coordinates. The \(K\)-type coordinate is defined as \(x_1 = r_2 - r_1, \ x_2 = r_3 - (r_1 + r_2)/2, \ x_3 = r_4 - (r_1 + r_2 + r_3)/3\), which is suitable for representing 3N+1N correlations. \(r_i\) is the position coordinate of the \(i\)th nucleon. The other coordinate, called \(H\)-type, is defined as \(y_1 = r_2 - r_1, \ y_2 = r_4 - r_3, \ y_3 = (r_3 + r_4)/2 - (r_1 + r_2)/2\), which is suitable for representing 2N+2N correlations.

The parts of basis function are

\[
\Phi_{JM}(K) = A \left[ \left[ \chi^{(1)} \chi^{(2)} \chi^{(3)} \chi^{(4)} \right]_{1234} \right]_{JM}
\]

\[
\times \left[ \tau^{(1)} \tau^{(2)} \tau^{(3)} \tau^{(4)} \right]_{1234},
\]

\[
\Phi_{JM}(H) = A \left[ \left[ \chi^{(1)} \chi^{(2)} \chi^{(3)} \chi^{(4)} \right]_{1234} \right]_{JM}
\]

\[
\times \left[ \tau^{(1)} \tau^{(2)} \tau^{(3)} \tau^{(4)} \right]_{1234},
\]

where \(\psi\) is the space part, \(\chi\) is the spin part, and \(\tau\) is the isospin part of the basis functions.

For the isospin part, we employ the particle representation, which describes well the isospin part of asymptotic wavefunctions \((t+p, h+n, d+d)\). For example, when \(T_{123} = 1/2\), \(M_{123} = 1/2(-1/2)\), and \(S_{123} = 1/2\), it corresponds to \(t(h)\), and when \(T_{12} = M_{12} = 0\) and \(S_{12} = 1\), it corresponds to \(d\). The space part is assumed to be expressed by the superposition of the Gaussian-type function as

\[
\psi_{LM}^{(i)}(x_i) = N_L x_i^{l_f} \exp \left(-\frac{x_i^2}{b_k^2} (1 \pm i\omega)\right) Y_{LM}^{(i)}(\hat{x}_i),
\]

where \(N_L\) is a normalization factor. \((b_{k_1}, b_{k_2}, b_{k_3})\) is a parameter to characterize the spatial extending property of the basis function, and \(\omega\) is a parameter for the complex-range Gaussian.
Thus, the basis functions are superposed for suffixes
\[ \alpha = \{ L_1, L_2, L_{12}, L_3, L_4, S_{12}, S_{123}, S, T_{123}, M_{123}, M_4; b_{k1}, b_{k2}, b_{k3} \} \]  
for $K$-type, and
\[ \beta = \{ L_1, L_2, L_{12}, L_3, L_4, S_{12}, S_{34}, S, T_{12}, M_{12}, T_{34}, M_{34}; b_{k1}, b_{k2}, b_{k3} \} \]
for $H$-type. Since we have to prepare many sets of basis functions by $\alpha$ and $\beta$ to get the converged solutions, this makes the dimension of the Hamiltonian (overlap) matrix much larger. The problem is how to reduce the dimension of the matrix in order to compute it within the CPU power and the memory size of available supercomputers.

Here, as an example, we explain how to employ the parameters of the basis function in the present proposed procedure for the $t+p$ channel. $[\psi_L^{(1)}(x_1)\psi_L^{(2)}(x_2)]_{L_{12}}$, $[[x^{(1)} X^{(2)}]_{S_{12}} X^{(3)}]_{S_{123}}$, and $[[\tau^{(1)} \tau^{(2)}]_{T_{12}} \tau^{(3)}]_{T_{123} M_{123}}$ in Eq. (31) correspond to the $t$ cluster in the four-body system. When we assume the triton cluster, there are two channels, $\{ L_1, L_2, L_{12}, S_{12}, S_{123} = 1/2, T_{12} = 0, T_{123} = 1/2, M_{123} = 1/2 \}$ and $\{ L_1, L_2, L_{12}, S_{12}, S_{123} = 1/2, T_{12} = 1, T_{123} = 1/2, M_{123} = 1/2 \}$, which are a part of suffix $\alpha$ for the four-body basis function. The spatial part, $[\psi_0^{(1)}(x_1)\psi_0^{(2)}(x_2)]_{T_0}$, has two width parameters of $b_1$ and $b_2$ in Eq. (33). These two parameters, $b_1$ and $b_2$, are randomly generated in addition to the undetermined channel suffix ($T_{12} = 0$ or $T_{12} = 1$). We search the energy minimum state, changing the set of $\{ b_1, b_2, T_{12} \}$ with the fixed number of basis functions by using the SVM (see the textbook [13] for the practical algorithm).

In the standard GEM [10] with the geometric progression, a typical number of basis functions for the two-body system is around $N_b = 10 \times 10 = 100$ channels. In the present paper, we employ the number of basis functions $N_b = 200$ for $t$ and $h$, $N_b = 5$ for $d$. This number for the SVM is reduced a lot (200 $\rightarrow$ 15). As described in Table 1, although the number of basis functions is very limited, the known values are reproduced. The number of matrix elements is the square of $N_b$, which is less than the standard GEM calculation at least. Further, the computational time of the diagonalization is known to be proportional to $N_b$, which exceeds $N_b^2$ (matrix elements) around $N_b = 10^3 \sim 10^4$. This is the reason why reducing $N_b$ by using the SVM technique has been employed in many studies. In particular, for the resonant state, $N_b$ for the two-body system increases to 20 $\sim$ 40 from $N_b = 10$ for the bound state due to the oscillating property of the resonant wavefunction. The reduction of the basis function becomes more serious as the present purpose of the realistic treatments of the four-body resonance.

In Table 2, we describe the ground state energy of $t$ by using CSM+SVM with the CG (OG) to show the efficiency. The calculational energy of the CG is the same as that of OG except for a very small difference.

**Table 1.** The ground-state energies ($E$) and root-mean-square radii ($R_{rms}$) of $t$, $h$, and $d$ clusters calculated with the Minnesota potential [19]. $N_b$ is the number of Gaussian basis functions employed.

<table>
<thead>
<tr>
<th>Cluster</th>
<th>Present</th>
<th>Suzuki et al. [28]</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N_b$</td>
<td>$E$(MeV) $R_{rms}$(fm)</td>
<td>$E$(MeV) $R_{rms}$(fm)</td>
</tr>
<tr>
<td>$t(\frac{1}{2}^+)$</td>
<td>15</td>
<td>-8.38 1.70</td>
<td>-8.38 1.71</td>
</tr>
<tr>
<td>$h(\frac{1}{2}^+)$</td>
<td>15</td>
<td>-7.70 1.72</td>
<td>-7.71 1.74</td>
</tr>
<tr>
<td>$d(1^+)$</td>
<td>5</td>
<td>-2.20 1.94</td>
<td>-2.20 1.95</td>
</tr>
</tbody>
</table>
Table 2. The calculated ground-state energies of $t$ with changing complex scaling angle. $N_b$ is the number of Gaussian basis functions employed. The second column is the calculated energy for the RG, the third column is that for the CG (OG) with $\omega = 0.6$, the fourth column is that for the CG (OG) with $\omega = 1.57$, and the fifth column is that for the tempered Gaussian with the geometric progression (GP).

<table>
<thead>
<tr>
<th>$N_b$</th>
<th>RG</th>
<th>CG (OG)</th>
<th>CG (OG)</th>
<th>GP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\omega$</td>
<td>15</td>
<td>30</td>
<td>30</td>
<td>800</td>
</tr>
<tr>
<td>$E(\theta = 0.0)(\text{MeV})$</td>
<td>$-8.38$</td>
<td>$-8.30$</td>
<td>$-4.77$</td>
<td>$-8.385$</td>
</tr>
<tr>
<td>$E(\theta = 0.2)(\text{MeV})$</td>
<td>$-8.51-0.04$</td>
<td>$-8.34-0.03$</td>
<td>$-5.23-1.10$</td>
<td>$-8.385-0.872\times10^{-4}$</td>
</tr>
<tr>
<td>$E(\theta = 0.4)(\text{MeV})$</td>
<td>$-8.89-0.48$</td>
<td>$-8.47+i0.02$</td>
<td>$-6.35-1.85$</td>
<td>$-8.388-0.006$</td>
</tr>
</tbody>
</table>

small numerical error. Since this numerical equivalence is essentially checked for all calculations of this paper, hereafter we will only describe the CG except when the basis functions need to be distinguished. The second row is the calculated energy with the RG. The energy of $E = -8.38$ MeV for $\theta = 0.0$ rad is the same as the known precise energy. If we change the scaling angle $\theta$, the energy should not be changed from $E = -8.38 - i0.00$ MeV because of the so-called ABC theorem [7–9]. However, there is a large numerical deviation at $E = -8.89 - i0.48$ MeV for $\theta = 0.4$ rad. In the standard GEM [10] with the geometric progression (GP), $E = -8.38 - i0.00$ MeV for $\theta = 0.4$ rad, as described in the fifth column. In other words, the restricted number of basis functions is not sufficient to describe the complex scaled triton wavefunction. Even if we employ these basis functions for the four-body system, it is expected to cause a large numerical error. Thus, the CSM+SVM does not work when the RG is employed as the basis function.

In the third row of Table 2, the energies calculated by using the CSM+SVM with the CG are given. The $\omega$ parameter is 0.6, which is smaller than the standard value ($\omega = 1 \sim 2$), but it is almost an application limit of the CG to the CSM as discussed in the previous subsection. In many nuclear resonances, and in the application examples of this paper, the broad resonant states of $E_r \sim \Gamma/2$ are discussed. In that case, the typical scaling angle is $\theta \sim 0.5$ rad at least. When we employ $\omega = 0.6$, $\theta_{\text{max}}$ is 0.515 rad because of the Hilbert space condition discussed in the previous section. As seen from the Table 2, the deviation of the imaginary part of the energy from the precise value 0 is much smaller than that of the RG. This is naturally expected as the oscillating property of the CG is appropriate to describe the complex scaled triton wavefunction. We also show the case of a large $\omega = 1.57$, whose $\theta_{\text{max}}$ is 0.283 rad. In this case, the calculated energy $E$ is $-4.77$ MeV, which is largely different from $E = -8.38$ MeV. This is naively understood in that the CG basis function is not an economical basis function for a simply dumping S-wave wavefunction of $t$. Even when we perform the complex scaling, the accurate solutions are not obtained as $E = -5.23 - i1.10$ MeV for $\theta = 0.2$ rad and $E = -6.35 - i1.85$ MeV for $\theta = 0.4$ rad. In other words, the standard value of $\omega$ is not employed in the CSM+SVM, where the basis number is much reduced. Thus, the choice of $\omega$ based on the Hilbert space condition would be a reasonable choice in the CSM+SVM.

The $\psi_{L_j}^{(3)}(x_3)$ part of Eq. (31) represents the $t+p$ relative wavefunction. For the $b_3$ parameter, the geometric progression is employed: $b_3 = b_3^{\text{min}} \gamma^{i-1}$ ($i = 1, \ldots, N$), $b_3^{\text{max}} = b_3^{\text{min}} \gamma^{N-1}$. For the $t+p$ channel in the calculations of the next section, we employ a typical basis number of the CSM, $N = 30$ ($N = 20$ is not enough to converge the calculated energies in the next section). Therefore, the total number of basis functions for $t+p$ in the four-body calculation with CSM+SVM+CG is $N_b = 900$ ($= 30 \times 30$), whereas that for the standard CSM is $N_b = 24000$ ($= 800 \times 30$). The computational
Fig. 1. Phase shifts of $^3P_0$ in $^4$He with the MN interaction by using the MRM. The solid, dotted, and dashed lines are phase shifts of the $t+p$, $h+n$, and $d+d$ channels, respectively. The vertical solid line at $E = -6.64$ MeV and the shaded area are the estimated energy and width.

3. Results

3.1. $0^-$ state

We investigate the $0^-$ state of $^4$He as a typical resonance embedded in the continuum states, which has a large decay width in comparison with the resonance energy measured from the nearest $h+n$ decay threshold. Experimentally, $0^-$ is observed as a resonance, $E = -7.29$ MeV ($E^{p+p}_{r} = 1.20$ MeV, $E^{p+n}_{r} = 0.53$ MeV) and $\Gamma = 0.84$ MeV [24].

Before investigating the four-body complex energy eigenvalues with the complex scaling method (CSM), in Fig. 1 we exhibit the phase shifts for $^3P_0$ using the microscopic R-matrix method (MRM) [31] in order to clarify the circumstances of the $0^-$ resonance (the details are described in Ref. [30]). In the MRM, the wavefunctions are obtained so as to connect to two-body asymptotic wavefunctions (e.g. Coulomb function) [31].

The solid, dotted, and dashed lines are phase shifts of the $t+p$, $h+n$, and $d+d$ channels, respectively. The $t+p$ ($h+n$) phase shift shows attractive behavior but it is not crossing $\pi/2$, which means a resonance with a broad decay width. The energy and the decay width for $0^-$ are estimated as $E \sim -6.64$ MeV [30] and $\Gamma \sim 2$ MeV (shaded area in Fig. 1). The resonance energy is a little higher and the decay width is a little broader than experiment, which is not consistent with a naive expectation due to the lack of tensor and spin–orbit interactions for the MN [30]. Since the phase shift for the $d+d$ channel (dashed line) shows a repulsive behavior, the $0^-$ resonance of the $d+d$ structure is not expected to be observed. Thus, a resonance with a broad width is expected to exist a little above the $h+n$ threshold.

In Fig. 2, we plot complex energy eigenvalues of $0^-$ by using the CSM. The RG basis function is employed in the left panel and the CG basis function is employed in the right panel. The $\omega$ parameter for the CG basis functions is 0.6. We do not show the OG case because the calculated energy is the same, except for a very small numerical error. The scaling angle $\theta$ is 0.44 rad. The $b_1$ and $b_2$ parameters in the basis functions in Eq. (33) are determined by the SVM for the subsystem, as explained in the previous section. For the $b_3$ parameter, corresponding to the relative coordinate $x_3$, the geometric progression is employed: $b_3 = b_{3 \min} \gamma^{i-1} \{i = 1, \ldots, N\}$. The parameters of the
Fig. 2. Complex energy eigenvalues of $0^-$ in $^4$He for the RG basis function (left) and the TG basis function (right). The scaling angle $\theta$ is 0.44 rad. $\omega$ is 0.6 for the CG.

Basis functions are $b_{min}^3 = 0.2$ fm, $b_{max}^3 = 50$ fm, and $N = 30$ for the $t+p$ and $h+n$ channels, and $b_{min}^3 = 0.2$ fm, $b_{max}^3 = 40$ fm, and $N = 20$ for the $d+d$ channel.

In the right panel (CG), two-body continuum solutions are clearly seen on the so-called $2\theta$ lines, which are starting from $t+p$, $h+n$, and $d+d$ thresholds. On the other hand, in the left panel (RG), the starting points of the two-body continuum solutions deviate greatly from the real energy axis ($\text{Im}(E) = 0$). The large deviation is expected from the discussion for the triton in Table 2, where the bound state solution of the triton having $\text{Im}(E) \sim 0$ is not obtained for the RG basis function (second column in Table 2), whereas it is obtained for the CG basis function (third column in Table 2).

Further, we cannot see any candidate for the resonance for the RG (left) as the estimated energy region with the phase shift in Fig. 1. It would be a bad description of the asymptotic wavefunctions $t+p$ and $h+n$. For the case of the CG, there is a candidate solution, $E = -6.86 - i1.00$ MeV, which deviates from the $h+n$ continuum line. This is not consistent with the $0^-$ resonance inferred by the phase shift with the MRM. However, it is difficult to judge from this figure whether it is a resonance or not, because the solution is very near to the $h+n$ continuum solutions.

In order to confirm that the solution corresponds to a true resonance, we include an additional potential acting at the interaction region [17,18]. The four-body potential would be the best for this purpose. For example, for the $h+n$ continuum states, the four-body potential does not give a direct contribution between $h$ and $n$ clusters in the asymptotic region ($\lim x_3 \to \infty V_{4N} = 0$).

In Fig. 3, changing the strength $\lambda$ of Eq. (3), the complex energy eigenvalues are plotted. The saltire, the cross, the asterisk, and the square are $\lambda = 0, 10, 20,$ and $30$, respectively. The candidate for the $0^-$ resonant solution ($E = -6.86 - i1.00$ MeV) moves to the binding region. On the other hand, other solutions stay at almost the same positions. Although several solutions near to the resonance move slightly, it is natural to consider that the coupling between resonance and two-body continuum states are slightly modified by changing the strength of the additional potential.

In Fig. 4, we plot the complex energy eigenvalues with the so-called $\theta$ trajectory [9]. In the CSM, when we change the scaling angle $\theta$, the continuum solutions depend on $\theta$ ($2\theta$ line) but the resonant solutions should stay at the resonance energy. In the practical calculation, it has a stationary point because the number of basis functions is limited. As seen from Fig. 4, two-body continuum lines are rotated, whereas the resonance solution stays at almost the same energy. The stationary angle

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Fig. 3. Complex energy eigenvalues of $0^-$ in $^4$He. The scaling angle $\theta$ is 0.44 rad. The strength of the additional four-body potential is changed from $\lambda = 0$ to $\lambda = 30$.

Fig. 4. Complex energy eigenvalues of $0^-$ in $^4$He. The scaling angle is changed from $\theta = 0.43$ rad to 0.46 rad.

of the present calculation is $\theta = 0.44$ rad. Thus, we conclude that the solution of $0^-$ is obtained as $E = -6.86 - i1.00$ MeV. Using the CG (OG) basis function instead of the RG basis function is one of the keys for the proposed method: CSM+SVM. Although introducing the imaginary part ($\omega$) in the Gaussian basis function is essential, it is noted that the convergence of the solution becomes bad or completely breaks down when we employ large $\omega$ values. This is expected from the discussion for the fourth column in Table 2.

3.2. $0^+$ state

Experimentally, a $0^+$ resonant state is observed a little above the $t+p$ threshold, $E = -8.086$ MeV ($E_{t+p}^{t+p} = 0.395$ MeV) and $\Gamma = 0.50$ MeV [24]. Although the ratio of the experimental decay width ($\frac{\Gamma}{E_{t+p}^{t+p}} = 1.27$) is smaller than that of $0^-$ ($\frac{\Gamma}{E_{t+p}^{t+p}} = 1.71$), the determination of the resonance energy in the GEM is difficult because of the singular property of the near threshold state ($k \rightarrow 0, \lambda = \frac{2\pi}{k} \rightarrow \infty$). In other words, we have to solve the spatially extending wavefunction for the near threshold state. For example, the de Broglie wave length for the $t+p$ system at 0.1 MeV is $\lambda = \frac{2\pi}{k} \sim 100$ fm. Therefore, we would be better to increase the maximum range of the basis function $b_{3}^{\text{max}}$ from that of the $0^-$ state ($b_{3}^{\text{max}} = 50$ fm).

In Fig. 5, we plot complex energy eigenvalues of $0^+$ in $^4$He. The scaling angle $\theta$ is 0.3 rad. The oscillation parameters for the $3N + N$ channel and the $2N + 2N$ channel are $b_{3}^{\text{min}} = 0.2$ fm,
Fig. 5. Complex energy eigenvalues of $0^+$ in $^4$He. The scaling angle $\theta$ is 0.30 rad.

Fig. 6. Complex energy eigenvalues of $0^+$ in $^4$He. The scaling angle $\theta$ is 0.30 rad. The strength of the additional four-body potential is changed from $\lambda = 0$ to $\lambda = 8$.

The numbers of basis functions for the $3N + N$ channel and the $2N + 2N$ channel are $N = 30$ and $N = 20$, respectively. The $\omega$ parameter for the complex Gaussian basis functions is chosen as $\omega = 0.6$.

Two-body continuum lines starting from the $t+p$ threshold and the $h+n$ threshold are clearly seen. Furthermore, there is a candidate for the $0^+$ resonant solution which deviates from the $t+p$ continuum line, $E = -8.31 - i0.06$ MeV. Since the threshold energy of $t+p$ is $-8.38$ MeV, the resonance energy measured from the $t+p$ decay threshold is $E_r = 0.07$ MeV.

In order to confirm whether the obtained solution is a resonance or not, in Fig. 6 we plot the resonance energy, changing the strength $\lambda$ of the additional four-body potential. The employed values are $\lambda = 0$ (saltire), 4 (cross), and 8 (asterisk). The resonant solution moves to the binding region as expected, whereas two-body continuum solutions stay at the same points. Thus, we conclude the solution of $0^+$ is obtained as $E = -8.31 - i0.06$ MeV. We should mention that the convergence of the solution for the $\theta$ trajectory (the stationary angle is around 0.3 rad) is not good for this calculation. One reason is that the complex energy solution near the threshold energy does not move much, and another reason is that the spatially extending wave functions are not described well by the limited number of basis functions. The estimated numerical error is around several tens of keV.
4. Summary
In the present paper, a theoretical treatment of four-body resonances using the CSM was discussed. For the four-body system, since the dimension of the Hamiltonian matrix is too large to solve it, we introduce the CSM+SVM to reduce the dimension, in which the basis function corresponding to the subsystem is determined by the SVM. In order to investigate the resonant solutions embedded in the continuum states, we employ the CG basis function instead of the RG basis function. Two comments in applying the CG to the CSM were given in Sect. 2. The first one is for the bra-state whose definition should be changed from the standard definition for the real basis function. The second is for the divergent property of the matrix element (Hilbert space limit) when we employ a large \( \omega \) value. Furthermore, we introduce the additional four-body potential to clarify whether the obtained solution is a true resonant solution.

As a numerical example, we apply the present method to the \( 0^\pm \) resonant states of \(^4\)He, which are four-nucleon resonance states. The \( 0^+ \) state is obtained a little above the \( t+p \) threshold as \( E = -8.31 - i0.06 \) MeV, and the \( 0^- \) state is obtained above the \( h+n \) threshold as \( E = -6.86 - i1.00 \) MeV. These two states correspond well to the experimental ones. But, quantitatively, the energies obtained deviate slightly from the experimental values, mainly because of the lack of tensor interaction and the spin–orbit interaction in the MN. This should be improved by using a realistic interaction which has a tensor part and a spin–orbit part, although this makes the dimension of the matrix increase. However, it comes within the computational power of standard massively parallel computers using the proposed method, CSM+SVM. In the near future, we will investigate the resonances in \(^4\)n, \(^4\)H, \(^4\)He, and \(^4\)Li with realistic interactions by using the present treatment of the four-body resonances.

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Appendix. The adjoint state and the norm of the resonances

One of the typical ways to define the adjoint state is using the c-product. The c-product is defined as \( (f|g) = \int_{\Omega} f g d\tau \) instead of the (Hermitian) inner product \( (f|g) = \int_{\Omega} f^* g d\tau \) [32]. In order to see the generalized definition of the norm, we use the matrix form of the Schrödinger equation [32]

\[
H \Psi_j^R = E_j \Psi_j^R,
\]

where \( H \) is the complex Hamiltonian matrix, \( E_j \) is the \( j \)th energy eigenvalue, and \( \Psi_j^R \) is the eigenvector corresponding to the ket-state. We use the suffix \( R \) in order to clarify the right-hand solution of the eigenvalue problem. The bra-state should be calculated as the left-hand eigenvector with the same Hamiltonian:

\[
\langle \Psi_i^L | H \rangle = E_i^L \langle \Psi_i^L |,
\]

\[
\langle \Psi_i^L | H \rangle = E_i^L \langle \Psi_i^L |,
\]

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where the left-upper suffix $^t$ means a transpose. Since the eigenvalues of the transposed matrix $^tH$ are the same as those of the original matrix $H$,

$$^tH\Psi_i^L = E_i \Psi_i^L.$$  \hspace{1cm} (A4)

Therefore, when the Hamiltonian matrix is Hermitian, $^tH=H^*$,

$$\Psi_i^L = (\Psi_i^R)^*.$$  \hspace{1cm} (A5)

Thus, the norm is defined as

$$N_i = (\Psi_i^L | \Psi_i^R) = \int_\Omega ^t(\Psi_i^L)\Psi_i^R d\tau = \int_\Omega ^t(\Psi_i^R)^*\Psi_i^R d\tau.$$  \hspace{1cm} (A6)

This is nothing but the standard definition of the inner product.

If the Hamiltonian matrix is complex symmetric, $^tH=H$, which is the case of the standard CSM with the real basis function,

$$\Psi_i^L = \Psi_i^R.$$  \hspace{1cm} (A7)

This means the left (column) eigenvector and the right (column) eigenvector are identical, and the bra-state is a transpose of the ket-state. The adjoint state $\tilde{\Psi}$ by Hokkyo in Eq. (7) is written as the right eigenvector as $^t(\Psi_i^R)^*$. Then, the norm is defined as

$$N_i = (\Psi_i^L | \Psi_i^R) = \int_\Omega ^t(\Psi_i^L)\Psi_i^R d\tau = \int_\Omega ^t(\Psi_i^R)^*\Psi_i^R d\tau.$$  \hspace{1cm} (A8)

It is noted that $^tH=H$, which means that the complex basis function is not applicable to the standard resonant theories with the above definition of the norm or the wavefunction.

References