Resonances and continuum states in the complex scaling method

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Abstract. Resonances and continuum states in the complex scaling method construct an extended completeness relation, which is one of useful instruments to investigate drip-line nuclei. Because an appropriate $L^2$ basis set is used in the complex scaling method to describe resonant and continuum states, we can discretize the continuum states naturally. We apply this method to calculation of continuum level density and the scattering phase shifts.

1. Introduction

Recently, much interest has been concentrated on the structure of short-lived drip-line nuclei. In the extremely weak binding nuclei, the exotic structure such as halo has been revealed [1]. To understand those properties, it is necessary to develop a new tool for describing the weak binding systems. For the new approach, it is demanded to describe the weak binding states together with resonant and continuum states.

In this report, we show that the complex scaling method (CSM) [2] provides us useful tools for describing bound and unbound states on the same footing. A key of the useful tools is the extended completeness relation. The idea about separation of the continuum states into resonances and remaining continuum was proposed by Berggren [3]. He introduced a deformed contour to reveal the resonances hidden in the second Riemann sheet. The complex scaling method provides the deformed contour that is a rotation of the branch cut in the natural way. We call the completeness relation (the resolution of the identity) in the complex scaling method as the extended completeness relation (ECR) [4], and the proof of the completeness is easily performed [5].

The advantage of ECR in CSM is not only to separate the unbound states into resonances and rotated continuum states but also to distinguish the continuum states starting from different threshold energies. Based on this property of ECR, we can investigate the structure of the continuum states. As the useful methods to study continuum structure, we here show two physical quantities presented using ECR. One They are the strength function $S_\lambda(E)$ for a $\lambda$-pole transition and the continuum level density $\Delta(E)$ [6]. The electric-dipole transition strength function $S_{E1}(E)$ is directly related with the Coulomb dissociation cross section of unstable nuclei. We can calculate the three-body breakup cross sections within CSM using a basis function method. Diagonalization of the complex scaled Hamiltonian $H(\theta)$ in the basis function method gives discrete eigenvalues of the complex energy. Applying these discrete complex-eigenvalues to calculation of the Green function, we can calculate the continuum level density.
2. Complex scaling method (CSM)
In CSM [2], coordinate $r$ and wave number $k$ are transformed as
\[ U(\theta) : r \rightarrow r \exp(i\theta), \quad k \rightarrow k \exp(-i\theta), \]
where $U(\theta)$ is a scaling operator and $\theta$ is a real number called as a scaling parameter. Under this transformation, the asymptotic divergent behavior $\exp(ik_r r)$ of a resonant state with a complex wave number $k_r = \kappa - i\gamma$ is changed into a dumping form $\exp\{i(\kappa - i\gamma)(r \cos \theta + ir \sin \theta)\} = \exp\{(\gamma \cos \theta - \kappa \sin \theta)r\} \cdot \exp\{i(\kappa \cos \theta + \gamma \sin \theta)r\}$ for $\theta > \tan^{-1}\gamma/\kappa$. Therefore, resonance states and bound states are obtained as discrete solutions of the following complex scaled Schrödinger equation:

\[ H(\theta)\Phi^\theta = E\Phi^\theta, \]

where $H(\theta) = U(\theta)HU^{-1}(\theta)$. Because of request to the complex scaled Hamiltonian for no singularity, the scaling parameter $\theta$ has an upper limit $\theta_C$. For the Gaussian potential, $\theta_C$ is $\pi/4$. For $\theta < \theta_C$, the solutions of bound states and resonances with $\gamma/\kappa < \tan \theta$ are squared-integrable because of their dumping forms at the asymptotic region. Therefore, taking appropriate scaling parameter $\theta$, in addition to bound states, we can solve resonant states by using squared-integrable basis expansion such as Harmonic oscillator or Gaussian functions $\{\phi_n\}$:

\[ \Phi^\theta = \sum_{n=1}^{N} c_n(\theta)\phi_n. \]

3. Extended completeness relation
Bound and scattering (continuum) states form a complete set that is represented by the completeness relation (resolution of the identity)

\[ 1 = \sum_b |\chi_b\rangle\langle\chi_b| + \int_{0}^{\infty} dE |\chi_E\rangle\langle\chi_E|, \]

\[ = \sum_b |\chi_b\rangle\langle\chi_b| + \int_{-\infty}^{\infty} dk |\chi_k\rangle\langle\chi_k|, \]

where $\chi_b$ and $\chi_E$ are the bound (the discrete negative part of the energy spectrum) and continuum (the continuous positive part) states, respectively, on the first Riemann sheet of the energy plane. The continuum states ($\chi_k$, $\chi_{-k}$) in the momentum representation belong to the states on the real $k$ axis. Therefore, integration over the $k$ axis corresponds to that along the rims of the cut of the first Riemann sheet of the energy plane, as shown in Fig. 1(a). In the case of a potential problem, the mathematical proof of the completeness relation (Eq. (4)) was given by Newton[7] using the Cauchy theorem.

For the solutions of the complex scaled Hamiltonian $H(\theta)$, it is also interesting to consider the completeness relation. Recently, a mathematical proof for the completeness relation in CSM was given by Giraud et al. [5] for the single- and coupled-channel cases. In the case of the complex scaling, the momentum (real $k$) axis is rotated by $\theta$, and the resonant poles enter the semicircle used in the Cauchy integration (Fig. 1(b)). Therefore, the resonances appear in the completeness relation for the complex scaled Hamiltonian $H(\theta)$,

\[ 1 = \sum_b |\chi^\theta_b\rangle(\chi^\theta_b| + \sum_r^{n_r} |\chi^\theta_r\rangle(\chi^\theta_r| + \int_{L^E} dE |\chi^\theta_E\rangle(\chi^\theta_E|, \]

\[ = \sum_b |\chi^\theta_b\rangle(\chi^\theta_b| + \sum_r^{n_r} |\chi^\theta_r\rangle(\chi^\theta_r| + \int_{L^k} dk |\chi^\theta_k\rangle(\chi^\theta_k|, \]

(5)
Figure 1. The Cauchy integral contours in the momentum and energy planes for the completeness relation (a) without and (b) with CSM. \( b_1, b_2, \ldots \) and \( s_1, s_2, \ldots \) are the bound and resonant poles, respectively.

where \( \chi^\theta_b \) and \( \chi^\theta_r \) are the complex scaled bound states and complex scaled resonant states, respectively. Only those complex scaled resonant states that enter the semicircle rotated by \( \theta \) are taken into consideration, and their number is expressed by \( n^\theta_r \). Furthermore, continuum states \( \chi^\theta_E \) and \( \chi^\theta_k \) are located on the rotated cut \( L^\theta_E \) of the Riemann plane and on the rotated momentum axis \( L^\theta_k \), respectively. We call this completeness relation in CSM as the extended completeness relation (ECR).

Here, we note that the definition of the complex scaled bra- and ket-states for the non-Hermitian \( H(\theta) \) are different from the usual one for the Hermitian \( H \). In the latter case, the bra-state is the complex conjugate of the ket-state. On the other hand, in the case of \( H(\theta) \), bi-orthogonal states must be defined: The momentum of the bi-orthogonal bra-state, which is conjugate to the ket-state with momentum \( k \), is denoted as \( \tilde{k} \). For discrete states (bound and resonance), we have \( \tilde{k} = -k^* \), whereas for continuum states, we have \( \tilde{k} = k^* \). For the wave function of discrete states, we can use the same wave function for the bra- and ket-states, and for continuum states, the wave function of a bra-state is given by that of the ket-states divided by the \( S \)-matrix.

4. Strength function

Applying ECR to calculations of physical quantities enables us to see the contributions from bound, resonant and continuum states. The strength function \( S(E) \) is expressed in terms of response function \( R(E) \) as

\[
S_\lambda(E) = \sum_\nu \langle \chi_i | \tilde{O}_\lambda | \chi_\nu \rangle \langle \chi_\nu | \tilde{O}_\lambda | \chi_i \rangle \delta(E - E_\nu) = -\frac{1}{\pi} \text{Im} R_\lambda(E),
\]

\[
R_\lambda(E) = \int dr dr' \chi_i^*(r) \tilde{O}_\lambda^\dagger G(E, r, r') \tilde{O}_\lambda \chi_i(r'),
\]

where \( E \) is the energy on the real axis, and \( |\chi_i\rangle, |\chi_\nu\rangle \) and \( \tilde{O}_\lambda \) are the initial states, final states and an arbitrary transition operator of rank \( \lambda \), respectively. The quantities \( E_\nu \) are the energies of the final state. In this expression, we assume that the bound (initial) and final states form a complete set of the Hamiltonian \( H \):

\[
1 = \sum_{\nu(i)} |\psi_\nu\rangle \langle \psi_\nu|,
\]

where the summation includes the initial state \((i)\) as an element of the complete set.
using the complex scaled initial wave functions $\chi^\theta_i$, the Hamiltonian $H(\theta)$ and the transition operator $\hat{O}^\theta_\lambda$, the response function is expressed as

$$ R_\lambda(E) = \int d\mathbf{r} d\mathbf{r}' \chi^\theta_i(\mathbf{r}) (\hat{O}^\lambda_\lambda)^\theta (\mathbf{r}, \mathbf{r}') \hat{O}^\theta_\lambda \chi^\theta_i(\mathbf{r}'), $$

(10)

where the complex scaled Green function is written

$$ G^\theta(E, \mathbf{r}, \mathbf{r}') = \left( \frac{1}{E - H(\theta)} \right) |_{\mathbf{r}'} \right). $$

(11)

Here, it is worth noting that $R_\lambda(E)$ does not depend on the scaling. Substituting Eq. (5) into Eq. (11), we can separate the Green function into three terms, as

$$ G^\theta(E, \mathbf{r}, \mathbf{r}') = \sum_b \frac{\chi^\theta(b, \mathbf{k}) \bar{\chi}^\theta(b', \mathbf{k})}{E - E_B^b} + \sum_r \frac{\chi^\theta(r, k_R) \bar{\chi}^\theta(r', k_R)}{E - E_R^r} $$

$$ + \int_{L_k} dk \frac{\chi^\theta(r, k) \bar{\chi}^\theta(r', k)}{E - E_\theta}, $$

(12)

where $E_B^b$ and $E_R^r (= E_r - \frac{i}{2} \Gamma)$ are the energy eigenvalues of the bound states and resonances, respectively. From Eq. (10), we obtain the following relations for the response function:

$$ R_\lambda(E) = R_{\lambda,B}(E) + R_{\lambda,R}(E) + R_{\lambda,k}(E), $$

(13)

$$ R_{\lambda,B}(E) = \sum_b \frac{\chi^\theta(b, \mathbf{k}) \bar{\chi}^\theta(b', \mathbf{k})}{E - E_B^b}, $$

(14)

$$ R_{\lambda,R}(E) = \sum_r \frac{\chi^\theta(r, k_R) \bar{\chi}^\theta(r', k_R)}{E - E_R^r}, $$

(15)

$$ R_{\lambda,k}(E) = \int_{L_k} dk \frac{\chi^\theta(r, k) \bar{\chi}^\theta(r', k)}{E - E_\theta}. $$

(16)

The strength function given in Eq. (6) is similarly separated as

$$ S_\lambda(E) = S_{\lambda,B}(E) + S_{\lambda,R}(E) + S_{\lambda,k}(E). $$

(17)

The matrix elements of the scaled operator are independent of $\theta$. [8] The $\theta$ dependence of $R_{\lambda,R}(E)$ and $R_{\lambda,k}(E)$ comes only from $n^\theta_l$, $L^k_\theta$ and $E_\theta$, respectively. The strength function $S_\lambda(E)$ is an observable, and it is positive definite for any energy and independent of $\theta$.

CSM allows us to calculate each term of Eq. (17) easily, because bound states and resonant states are obtained under the same boundary conditions, and continuum states are obtained on the rotated contour determined by $\theta$ uniquely. In particular, due to such a decomposition of the unbound final states, we can unambiguously determine which state forms the structure of the strength function. These are prominent points of CSM. This framework is also applicable to three-body cases, including Borromean systems.

5. Continuum level density

The level density $\rho(E)$ of Hamiltonian $H$ is defined as

$$ \rho(E) = \delta(E - E_i), $$

(18)
where $E_i$ are eigenvalues of $H$, and summation and integration are taken for discrete and continuum eigenvalues, respectively. This definition of the level density is also expressed by using Green’s function:

$$\rho(E) = -\frac{1}{\pi} \text{Im} \int dr \frac{1}{E - H} \left| r \right> \left< r \right|$$.  

(19)

Here we apply the CSM and ECR to the expression of Green’s function, we can obtain

$$\rho(E) = -\frac{1}{\pi} \text{Im} \int dr \frac{1}{E - H(\theta)} \left| r \right> \left< r \right| = -\frac{1}{\pi} \text{Im} \int dr \left[ \sum_B \frac{\Phi_B^\theta(r)\Phi_B^{\theta\ast}(r)}{E - E_B} + \sum_R \frac{\Phi_R^\theta(r)\Phi_R^{\theta\ast}(r)}{E - E_R} + \int_{L_a} dk_0 \frac{\Phi_{k_0}^\theta(r)\Phi_{k_0}^{\theta\ast}(r)}{E - E_{k_0}} \right]$$,  

(20)

where $N_B$ and $N_R^\theta$ are numbers of bound states and resonances in the wedge region between the real energy axis and the $2\theta$-lines, respectively. The detailed explanation of the extended completeness relation is given in Ref. [4].

In the integration over $r$ in Eq. (20), bound state and resonance parts can be calculated to be unity because of normalized wave functions, but the continuum part can not be calculated due to the singular integration. This singular integration of the continuum part becomes a normal integration, when we discretized the continuum spectra using the basis function method with a finite number $N$ of basis functions. Then, the approximated density of states $\rho_0^N(E)$ for the basis number $N$ is expressed as

$$\rho_0^N(E) = \sum_B \delta(E - E_B) - \frac{1}{\pi} \text{Im} \sum_R \frac{1}{E - E_R} - \frac{1}{\pi} \text{Im} \sum_k \frac{1}{E - \varepsilon_k(\theta)}$$  

(21)

As explained in the previous subsection, the energy of resonance is obtained as $E_R = E_r - i\Gamma_r/2$, then each resonance term has a Breit-Wigner form

$$\text{Im} \frac{1}{E - E_R} = \frac{-\Gamma_r/2}{(E - E_r)^2 + \Gamma_r^2/4}$$.  

(22)

For the continuum part, each discretized continuum state is obtained on the $2\theta$-line in the complex energy plane, $\varepsilon_k(\theta) = \varepsilon_k^R - i\varepsilon_k^I$, where $\varepsilon_k^I/\varepsilon_k^R = \tan 2\theta$. Therefore, the continuum part in the level density is also expressed by the Lorentzian function similar as the Breit-Wigner form:

$$\text{Im} \frac{1}{E - \varepsilon_k(\theta)} = \frac{-\varepsilon_k^I}{(E - \varepsilon_k^R)^2 + \varepsilon_k^I^2}$$.  

(23)

Inserting Eqs. (22) and (23) into Eq. (21), we obtain the level density in the basis function method as

$$\rho_0^N(E) = \sum_B \delta(E - E_B) + \frac{1}{\pi} \sum_R \frac{\Gamma_r/2}{(E - E_r)^2 + \Gamma_r^2/4} + \frac{1}{\pi} \sum_k \frac{\varepsilon_k^I}{(E - \varepsilon_k^R)^2 + \varepsilon_k^I^2}$$ .

(24)

The continuum level density (CLD) $\Delta(E)$ is expressed as a difference between the density of state $\rho(E)$ obtained by the Hamiltonian $H$ and the density of continuum states, $\rho_0(E)$, obtained by the asymptotic Hamiltonian $H_0$ as

$$\Delta(E) = \bar{\rho}(E) - \rho_0(E)$$.  

(25)
where $\bar{\rho}(E)$ is defined by subtraction of the bound state term from $\rho(E)$. The physical meaning of this $\triangle(E)$ is the density of levels which are provided by the interaction of a finite range. Furthermore, $\triangle(E)$ is related with a phase shift $\delta(E)$ of the state from the phase of the free state due to the interaction as [9]

$$\triangle(E) = \frac{1}{\pi} \frac{d\delta}{dE}. \quad (26)$$

In the basis function method with the number $N$ of basis states,

$$\triangle^N_\theta(E) = \rho^N_\theta(E) - \rho^N_0(\theta)(E). \quad (27)$$

Although the first term of the right hand side is given by the level density in which the bound state term is subtracted from Eq. (21), the second term is expressed by eigenvalues $\varepsilon^0_k(\theta) = \varepsilon^0_k^R - i\varepsilon^0_k^I$ of the asymptotic Hamiltonian $H_0(\theta)$ which has the only continuum spectra on $2\theta$-lines:

$$\rho^N_0(\theta)(E) = \frac{1}{\pi} \sum_k \frac{\varepsilon^0_k^I}{(E - \varepsilon^0_k^R)^2 + \varepsilon^0_k^I^2}. \quad (28)$$

Thus, we have

$$\pi\triangle^N_\theta(E) = \sum_R^{N_R} \frac{\Gamma_r^2/2}{(E - E_r)^2 + \Gamma_r^2/4} + \sum_k^{N-N_R-N_R^\theta} \frac{\varepsilon_k^I}{(E - \varepsilon_k^R)^2 + \varepsilon_k^I^2} - \sum_k^N \frac{\varepsilon_k^0^I}{(E - \varepsilon_k^0^R)^2 + \varepsilon_k^0^I^2}. \quad (29)$$

The $\theta$ dependence in $\triangle^N_\theta(E)$ disappears by cancellation of the $\theta$ dependence in the second and third terms of Eq. (29). When we take a small value of $\theta$ and then no resonance are obtained in the wedge region, the CLD is expressed by the second and third terms.

6. Conclusion

We have shown that CSM provides us useful tools for describing bound and unbound states on the same footing. The key of these tools is the extended completeness relation (ECR). Applying ECR to calculation of the Green function, we obtain the strength function distinguishing resonances and different continuum states. Furthermore, the continuum level density can be calculated in CSM with square integrable basis functions. From the continuum level density, the scattering phase shifts are obtained without solving the scattering problems.

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