Application of absorbing boundary condition to few-body cluster dynamics

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We show the formulation of the absorbing boundary condition (ABC) and demonstrate its applicability to resonant phenomena induced by reactions of few-body cluster systems. The resonance parameter and the strength function, which are important quantities in astrophysics, are calculated by the ABC method, and the results are compared with the complex scaling method, which is another tool to handle the resonant phenomena. We will show the realistic applications of ABC to the $3/2^+$ resonance in $^{19}$Ne and discuss the prescription of ABC in the three-body problem.

KEYWORDS: non-Hermite systems, few-body cluster systems, resonance parameters

1. Introduction

Dynamics induced by reactions of few-body nuclear systems in the unbound energy region gives an important impact on the research field about nuclear astrophysics. For example, a resonance formation induced by the binary collision and dissociation of a nucleus into two- or three-body fragments in continua are typical examples of the microscopic dynamical process, which are essential in macroscopic astrophysical phenomena. From the viewpoint of the nuclear physics, it is important to evaluate the resonance parameters, such as the resonant energy and the decay width, and the so-called strength function in the few-body dynamical reaction.

Since the resonant phenomena occur at the particle unbound and continuum energy region, in a naive treatment, a scattering boundary condition should be imposed among the interacting particles. However, imposing the scattering boundary condition is complicate if three particles participate in the considered reaction process. In order to avoid the complexity of the three-body scattering boundary condition, the scattering problem is often reduced to the bound-state-like problem by transforming the Hamiltonian of a total system into a non-Hermite form. There are two representative methods of the non-Hermitian transformations: the complex scaling method (CSM) [1] and the method of the absorbing boundary condition (ABC), or the method of the complex absorbing potential (CAP) [2–6].

In CSM, the radial coordinates and the respective momenta in the Hamiltonian of the total system are simply rotated with the angle of $\theta$ in the complex plane, such as $r \rightarrow re^{i\theta}$ and $k \rightarrow ke^{i\theta}$, while, in ABC, the negative imaginary potential is placed at the outer region of the system. These two procedures commonly give rise to the damping of the wave function in the asymptotic region. Therefore, the scattering problem can be transformed into the bound-state-like problem, in which the variational calculation using the basis expansion technique is available.

There are many sophisticated applications of CSM to the unbound continuum states [1]. However, the application of CSM is difficult in some special problems, for example, the microscopic cluster model called the generator coordinate method (GCM) [4]. Therefore, it is instructive to develop the ABC method as another tool to handle the unbound resonant phenomena. We have advanced the application of the ABC method to various few-body cluster systems. In the present report, we will...
explain the basic aspects of the ABC method and show the several applications to the dynamical reaction in the two- or three-body cluster systems: a binary cluster system and a three-body problem composed of identical three-bosons. All of the results in this article are compressed from Refs. [4–8].

2. Framework of absorbing boundary condition

2.1 Calculation of energy eigenvalues

In the ABC calculation, we solve the eigenvalue problem of the total Hamiltonian $H$ with the negative imaginary potential $-i\eta W$, such as
\[
(H - i\eta W) \Psi(\eta) = E(\eta) \cdot \Psi(\eta).
\]
Here $\eta$ means the strength of the imaginary potential and hence, the wave function $\Psi(\eta)$ and the energy eigenvalues $E(\eta)$ depend on the strength of $\eta$. Eq. (1) is possible to be solved by the basis expansion method because the solution with the absorber, $\Psi(\eta)$, has a damping behavior in the asymptotic region. In Eq. (1), no transformations are imposed on $H$ itself and hence, the computational technique of the Hamiltonian matrix is unchanged in introducing absorber. This simple implementation of ABC especially matches the microscopic cluster model, such as the generator coordinate method (GCM) [4,12]. This is a great advantage in ABC and marked contrast to the complex scaling method (CSM), where $H$ must be transformed by the complex rotation [4].

The functional form of $W$ is not arbitrary and various conditions are required as discussed in Ref. [2]. In a simple two-body problem, for instance, we introduce the shifted polynomial function in the radial coordinate of $r$ such as
\[
W \rightarrow W(r - r_0) = \theta(r - r_0) \cdot (r - r_0)^p.
\]

The polynomial absorber is standard and has been usually employed in previous studies [2, 3]. A starting point of the absorber $r_0$ should be taken to the outside of the physical interaction region. The power of the polynomial is set to $p = 4$ in the present calculation although the power should be carefully chosen by considering the computational situation [4].

Since the energy eigenvalues and the wave function depend on the absorber strength, $\eta$, we should optimize $\eta$ to determine the resonance parameters such as resonance energy and decay width. If the basis set is complete, the correct resonance parameters can be obtained as a limit of $\eta \rightarrow 0$. In the finite basis set calculations, however, a finite $\eta$ gives approximate resonance parameters.

In the optimization of $\eta$, we impose the following condition on the energy eigenvalue of $E(\eta)$:
\[
\left| \eta \frac{dE(\eta)}{d\eta} \right|_{\eta = \eta_o} = \min.
\]

This condition means that the energy eigenvalue becomes stationary at the optimal strength of $\eta = \eta_o$. In the pragmatic calculation, the derivatives $\eta \cdot dE(\eta)/d\eta$ are obtained simply by employing the generalized Hellmann-Feynman theorem [9] like
\[
\left| \eta \frac{dE(\eta)}{d\eta} \right| = \eta \left| \langle \chi^2 \vert W \vert \chi^2 \rangle \right| \equiv \langle W(\eta) \rangle.
\]

An argument to justify the condition of Eq. (3) was presented in Refs. [2,4,5].

2.2 Strength function

We also calculate the strength function of the breakup into the continuum. A general definition of the strength function is given by
\[
S(E) = \sum_{\Psi} \left| \langle \Psi \vert \mathcal{O} \vert \Psi \rangle \right|^2 \delta(E - E_\gamma),
\]
where $\Psi_i$ and $\Psi_f$ are the initial bound state and the $\nu$-th final state having the energy eigenvalue $E_\nu$ in the continuum, respectively. In Eq. (5), $\hat{O}_\lambda$ denotes the operator of an external field with the rank $\lambda$.

The calculation of the strength function in Eq. (5) can be achieved by assuming the extended completeness relation (ECR) for the discrete solutions under the absorbing boundary,

$$\hat{1} = \sum_{n} |\Psi_n^\eta\rangle <\Psi_n^\eta| = \sum_{n \in B} |\Psi_n^\eta\rangle <\Psi_n^\eta| + \sum_{n \in R} |\Psi_n^\eta\rangle <\Psi_n^\eta| + \sum_{n \in C} |\Psi_n^\eta\rangle <\Psi_n^\eta| \ .$$

(6)

Here $\Psi_n^\eta$ denotes the $n$-th solution of Eq. (1), which is obtained by the basis expansion method. In the last equation, the summation is decomposed into three parts: the bound states ($B$), the resonant states ($R$), and the non-resonant continuum states ($C$). The final expression of the strength function, on which the ECR is implemented, is given by

$$S^\eta_\lambda(E) = -\frac{1}{\pi} \Im \{ R^\eta_\lambda(E) \}$$

(7)

$$R^\eta_\lambda(E) = \sum_{n} <\Psi_i^{\eta}|\delta|\Psi_n^\eta\rangle <\Psi_n^\eta|\hat{O}_\lambda|\Psi_i^{\eta}> \big/ (E - E_{n\eta}) = R^\eta_{\lambda B}(E) + R^\eta_{\lambda R}(E) + R^\eta_{\lambda C}(E) \ .$$

(8)

In Eqs. (7) and (8), $R^\eta_\lambda(E)$ is called the response function, which is decomposed into three parts in accordance with Eq. (6). This decomposition is very useful in the analysis of the reaction mechanism [1,6]. For example, we can understand the dominant breakup process, such as the resonance decay or the direct breakup, in which the ground state directly goes into the continuum states. In this response function, the denominator contains a complex number of $E_{n\eta}$, which is the $n$-th eigenvalue in the ABC solution for Eq. (1). Thus, this function is converged to a finite value even if the excitation energy $E$ is close to the real part of $E_{n\eta}$.

3. Results

3.1 Simple two-body system

We demonstrate the ABC calculation by showing the simple application to the two-body problem. A model Hamiltonian with a schematic potential [1] of

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(r) \ ,$$

(9)

$$V(r) = -V_1 e^{-\mu_1 r^2} + V_2 e^{-\mu_2 r^2} \ .$$

(10)

is used in the present demonstration. Here the parameters of the potential $V(r)$ is chosen to $V_{1,2} = 8.0$ (MeV), 4.0 (MeV) and $\mu_{1,2} = 0.16$ (fm$^{-2}$), 0.04 (fm$^{-2}$). In the kinetic energy part, we set $\mu = 1$ for simplicity. Thus, the dimension of the energy equals the (length)$^{-2}$. The complex scaling method (CSM) was applied to the resonance problem in this potential, and the resonant energies are deeply analyzed in Ref. [1].

The energy distribution of these states plotted in the complex energy plane is shown in the left panel of Fig. 1 [6]. In this energy calculation, the strength of the absorber is set to be $\eta = 10^{-5}$. In the energy distribution of the left panel, the bound state (open square), first resonance (solid circle) and second resonance (solid diamond) are clearly separated from the non-resonant continuum (asterisks). The negative energy state around $\Re(E) = E_R \sim -0.7$ fm$^{-2}$ is a bound state, while the positive energy state around $E_R \sim 1.17$ fm$^{-2}$ is the first resonant state. The width of this resonance is quite small ($\Gamma_R / E_R \sim 10^{-2}$) and hence, it appears quite close to the real axis. The second resonance appears at $E_R \sim$
2 fm$^{-2}$ and $\Gamma_R/2 \sim 0.5$ fm$^{-2}$ with a broad width ($\Gamma_R/E_R \sim 0.5$). These two resonances are clearly separated from the continuum states (solid circles) because the imaginary part of the continuum states is systematically larger than that of the separated resonant states. Here all the resonance parameters are calculated at the optimal strength of $\eta = \eta_0$, and resultant parameters are consistent to the results obtained by CSM [1].

In the right panel of Fig. 1, the strength function is shown by the solid curve. According to the energy distribution in the left panel, the strength function is decomposed, and the results are also shown in the same figure. The individual contributions in the decomposed strength function (right panel) are plotted by the respective symbols shown in the energy eigenvalues (left panel). In the right panel, the contributions from the first resonance (dashed curve with the solid circle) and the second resonance (dotted curve with the diamond) are predominant, but the continuum states (two-dotted-dashed curve with the asterisk) provide a considerable contribution in the total strength function (the solid curve).

### 3.2 $J^\pi = 3/2^+$ resonances in $^{19}$Ne

We have applied the ABC method to the coupled-channel problem for the binary system of He + O in $^{19}$Ne [8]. There is an important reason why we focus on the $^{19}$Ne nucleus. The $^{15}$O($\alpha$,γ)$^{19}$Ne reaction is known to play a crucial role in the advanced stages of astrophysical hydrogen burning, and the most crucial resonance is known to arise through the $J^\pi = 3/2^+$ resonant level at 504 keV with respect to the $\alpha + ^{15}$O threshold ($E_x = 4.03$ MeV). Unfortunately, no theoretical calculation was successful in reproducing this resonant state. The experimental analyses in Ref. [13] have pointed out that the intrinsic structure of the resonance at 504 keV in $^{19}$Ne is not the $\alpha + ^{15}$O cluster structure, but the five particle–two hole ($5p-2h$) shell-model configuration with the $^{14}$O$_{g.s.}$ core. The $5p-2h$ configuration has a large overlap with the shell model limit of the $^5$He $+ ^{14}$O configuration. Therefore, the coupling of $^5$He + $^{14}$O on the $J^\pi = 3/2^+$ state is important in the cluster model approach.
In fact, it is well known that $^3\text{He} + ^{16}\text{O}$ and $\alpha + ^{15}\text{O}$ cluster configurations are insufficient to reproduce the $3/2^+$ resonance [14]. Therefore, in the present analysis, we have performed the microscopic calculation of $(^3\text{He}+^{16}\text{O}) + (\alpha+^{15}\text{O}) + (^3\text{He}+^{16}\text{O})$ in $J^\pi = 3/2^+$. In this calculation, the internal wave function of the individual clusters are described by the microscopic shell model configuration, and the anti-symmetrization effect among the nucleons is completely taken into account. The total Hamiltonian is composed of the kinetic energy and the two-body nucleon-nucleon interaction. The calculation is performed by applying the generator coordinate method (GCM) [11] plus ABC [8]. The details of the computational procedure is explained in Refs. [4, 12].

In the strict treatment, the threshold energies, which means the dissociation energy of $^{19}\text{Ne}$ into individual $\text{He} + \text{O}$, partitions, should be simultaneously reproduced. However, this reproduction is difficult in the GCM treatment. This problem always arises in the full microscopic treatment. In order to avoid this threshold problem, we replace the theoretical thresholds in the $^3\text{He} + ^{16}\text{O}$ and $^5\text{He} + ^{14}\text{O}$ to the experimental ones (8.4 and 14 MeV, respectively). In this modified GCM calculation, we have found that the $3/2^+$ resonance appears around $E - 2$ MeV with respect to the $\alpha$ threshold [8]. Therefore, we can conclude that the $^5\text{He} + ^{14}\text{O}$ partition plays an important role for the formation of $3/2^+$ resonance just above the $\alpha$ threshold.

### 3.3 Application to three-body system

In this section, we present the formulation of ABC in the three-body system. In the variational treatment of the three-body systems, the coordinate rearrangement among the three particles is important to obtain the fast conversion in binding energy [16]. The variational calculation with the coordinate rearrangement is called the coupled-rearrangement-channel variational method (CRCVM). The formulation of the ABC method in CRCVM was unclear although the CSM + CRCVM calculation has already been established in the three-body problem [1].

In order to establish the formulation of ABC in the three-body system, we have considered the identical three-bosons, which interact by the Gaussian potential in Eq. (10) with the condition of $\hbar^2/m = 1$ [15]. In this boson system, we consider the S wave state for simplicity, and the symmetrization among three bosons is explicitly considered by performing the coordinate rearrangement. As for the ABC treatment, we consider two ways of introducing the absorbing potential. In a naive treatment, the absorber should be included in accordance with the Jacobi coordinate in each of the rearrangement channel, such as

$$ W \rightarrow \sum_{c=1,2,3} \left( W(r_c - r_a) + W(R_c - R_a) \right). \quad (11) $$

Here $r_c$ and $R_c$ represent the absolute values of the Jacobi vectors in the rearrangement channel of $c$, while $r_a$ and $R_a$ show the respective starting points of the absorber. In Eq. (11), the absorbing potentials are introduced along the Jacobi coordinate in the $c$-th rearrangement channels, and they are symmetrized on the channel suffix $c$. Another possible way of introducing the absorber is the imaginary potentials among the pair of two particles,

$$ W \rightarrow \sum_{i>j} W(s_{ij} - r_a), \quad (12) $$

where $s_{ij}$ denotes the magnitude of the relative coordinate of the $i$-th and $j$-th particles. In Eqs. (11) and (12), the function form of $W$ is given by Eq. (2) with a setting of $p = 4$ and $r_a = R_a = 14$ fm.

In the ABC + CRCVM calculation, we have confirmed one bound state and two resonant states. The resonance parameters for the first resonance are summarized in Table I. In the second row from the top, the resonance parameters calculated from the Jacobi absorber (Eq. (11)) are shown, while the parameters obtained from the pair absorber (Eq. (12)) are shown in the third row. The result of the Jacobi absorber is the case as those of the pair absorber. These two results of ABC are consistent with the CSM calculation, shown in the bottom row. As for the second resonance, the results are also consistent to CSM. Thus, our formulation is considered to be successful in the three-body system.
Table I. Resonance parameters for the first resonance calculated at the optimal strength \( \eta_0 \). The resonance energy \( E_R \) and the resonance width \( \Gamma_R \) are shown in the unit of MeV. \( < W(\eta_0) > \) represent the expectation value of the absorber at \( \eta_0 \). In the second row, the result of the ABC method is shown, while the results of CSM is shown in the lowest row. This table is taken from Ref. [7].

<table>
<thead>
<tr>
<th>Method</th>
<th>( E_R )</th>
<th>( \Gamma_R/2 \times 10^{-3} )</th>
<th>( &lt; W(\eta_0) &gt; )</th>
<th>( \eta_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABC (Jacobi)</td>
<td>0.424</td>
<td>5.239\times 10^{-3}</td>
<td>6.942\times 10^{-7}</td>
<td>1.78\times 10^{-6}</td>
</tr>
<tr>
<td>ABC (pair)</td>
<td>0.424</td>
<td>5.239\times 10^{-3}</td>
<td>7.118\times 10^{-7}</td>
<td>X</td>
</tr>
<tr>
<td>CSM</td>
<td>0.424</td>
<td>5.260\times 10^{-3}</td>
<td>X</td>
<td>X</td>
</tr>
</tbody>
</table>

4. Summary

In summary, we have shown the basic formulation and application of the absorbing boundary condition (ABC) to the resonant phenomena in the few-body cluster systems. Here we have handled three problems: simple two-body system, microscopic two-body system, and identical three-boson system. As for the simple two-body problem, we have obtained the numerical results the same as the complex scaling method (CSM), which is an alternative method to handle the resonant phenomena. This result means that ABC is basically a powerful tool in handling resonant phenomena as well as the CSM treatment. Since the application of CSM becomes difficult in the microscopic cluster model, such as the generator coordinate method (GCM), the successful application of ABC to GCM is quite meaningful as we have shown in the \(^{19}\text{Ne} \) problem.

Furthermore, we have tried to formulate the ABC method in the three-body problem with the coordinate rearrangement. Two possible ways in the absorbing potential have been checked, such as the Jacobi absorber and the relative absorber, and both of the calculations give the same results as that obtained by the CSM calculation. Thus, we believe that our prescription to introduce the absorber is successful in handling general three-body problems. The important subject of ABC is the application to full microscopic three-body problem, such as the GCM calculation of \(^{12}\text{C} = 3\alpha \). The application of ABC to the \( 3\alpha \) GCM is now being prepared.

References