Absorbing Boundary Condition Approach for Breakup Reactions of Halo Nuclei

Kazuhiro YABANA, Manabu UEDA and Takashi NAKATSUKASA*

Institute of Physics, University of Tsukuba, Tsukuba 305-8571
* Physics Department, Tohoku University, Sendai 980-8578

Application of the absorbing boundary condition is discussed to analyse breakup reactions of weakly bound nuclei. The key ingredient is an introduction of the absorbing potential outside the physical area which simulates the outgoing boundary condition approximately. The scattering problem is then recasted into the Schrödinger like equation with a source term in the interaction region and with the vanishing boundary condition at the boundary. We demonstrate usefulness of the method taking a few examples. Deuteron breakup reactions are examined comparing present results with those by the continuum-discretized coupled-channel method. We next discuss the breakup reactions of single-neutron halo nucleus, $^{11}$Be.

§1. Introduction

Nuclei around drip line are characterized by their small separation energy for breakup (fragmentation). Measurements of the breakup processes have been major sources of information on their structural properties. Developments of reaction theories which are capable of describing breakup processes have thus been urged.

The eikonal approximation can take account of breakup processes and provides the most powerful scheme to describe reactions of weakly bound projectile at high incident energies. In fact, the eikonal approximation was employed to investigate the halo structure quantitatively through analyses of the anomalously large interaction and fragmentation cross sections. As the precise measurements at lower incident energy have come to be available, demands for developments of reaction theories beyond eikonal approximation have been increasing. There have been several attempts in this direction. Among them, the coupled channel approach incorporating breakup processes into continuum states, which is known as the continuum-discretized coupled-channel (CDCC) method, is expected to be useful for this purpose. The CDCC method has been successful to describe direct reactions of nuclei with small separation energy for fragmentation, such as deuteron and $^{6,7}$Li. The method has recently been applied to the reactions of halo nuclei, as is reported by Tostevin in this symposium. Although the CDCC approach has been well-tested and widely applied, it includes construction of artificial discretized continuum states and requires delicate examination for the convergence of the results.

In this report, we would like to show that the absorbing boundary condition (ABC) approach, which was originally developed in the field of chemical reactions, provides a convenient and flexible descriptions of breakup reactions. In this approach, we can directly obtain real-space scattering wave function in the interaction region without introducing any discretized continuum channels and scattering bound-
ary condition. The trade-off for its conceptual simplicity is a heavy computational cost to calculate wave function in real-space. Since the problem can be recasted into a linear algebraic equation with a sparse, large-size matrix, we can make the best use of the state-of-the-art techniques to treat these problems.

The organization of this report is as follows. We first explain what the ABC is, by taking a simple potential scattering problem as an example. We then apply it to breakup reactions of deuteron for which detailed CDCC analyses are available. We can examine validity and usefulness of our approach in this example. We then apply the method to reaction of single-neutron halo nuclei, $^{11}$Be, and discuss some characteristic features in the breakup reaction.

§2. Absorbing Boundary Condition: Potential Scattering

We first explain a basic idea of the ABC for scattering problem, taking the simplest example, a point particle scattered by a potential $V(r)$.

The wave function with outgoing boundary condition is expressed, as usual, as a sum of the incident plane wave and the scattered outgoing wave as

$$\psi^{(+)}(r) = e^{ikz} + \psi_{\text{scat}}(r).$$

The scattered wave $\psi_{\text{scat}}(r)$ is expressed employing the Green’s function as

$$\psi_{\text{scat}} = \frac{1}{E + i\epsilon - T - V} e^{ikz},$$

where $\epsilon$ is a positive infinitesimal and specifies the outgoing boundary condition.

The basic trick of the ABC is a replacement of the infinitesimal positive number $\epsilon$ with a finite, space-dependent function $\epsilon(r)$. If the function is regarded as a part of the Hamiltonian, $T + V - i\epsilon(r)$, the replacement is equivalent to adding absorbing potential $-i\epsilon(r)$ to the Hamiltonian. To simulate outgoing boundary condition, one introduces sufficiently smooth and strong enough positive function $\epsilon(r)$ outside a certain radius $R$ beyond which the potential $V(r)$ can be ignored. Placing the absorbing potential in radial region $R < r < R + \Delta R$, we put a vanishing boundary condition at $r = R + \Delta R$. If the absorbing potential works ideally, only outgoing wave can exist just inside the radius $R$. Since the scattering amplitude can be calculated from the exact wave function in the interaction region, it is sufficient that the ABC provides accurate wave functions in the spatial region $r < R$.

With the replacement $\epsilon \rightarrow \epsilon(r)$, we can rewrite the equation for $\psi_{\text{scat}}$ as the following linear inhomogeneous equation,

$$(E + i\epsilon(r) - T - V) \psi_{\text{scat}} = Ve^{ikz}. \quad (2.3)$$

After the partial wave expansion and discretization in radial coordinate, this is a linear algebraic problem with a complex symmetric coefficient matrix. We can then calculate scattered solution just by solving this linear algebraic problem.

The outgoing boundary condition imposed in this approach is not exact, since any imaginary potential can never absorb incoming waves completely. One should
choose the function \( \epsilon(r) \) so that the reflection wave becomes as small as possible. The following linear absorbing potential

\[
\begin{align*}
i\epsilon(r) &= \begin{cases} 
0 & (r < R) \\
 iW_{\text{abs}} \frac{r-R}{\Delta R} & (R < r < R + \Delta R)
\end{cases}
\end{align*}
\tag{2.4}
\]

has been often used and well tested.\(^{13),14)}\) Here the absorbing potential works in the region \( R < r < R + \Delta R \). \( W_{\text{abs}} \) is a positive constant and specifies the strength of the absorbing potential. In practical applications, the parameters should satisfy following conditions for a good absorber,\(^{13),14)}\)

\[
20 \frac{E^{1/2}}{\Delta R \sqrt{8m}} < W_{\text{abs}} < \frac{1}{10} \Delta R \sqrt{8m} E^{3/2},
\tag{2.5}
\]

where \( E \) represents the incident energy and \( m \) is the relevant mass. The left inequality originates from the condition that the absorption is strong enough to suppress any reflection at \( r = R + \Delta R \), while the right inequality from the condition that the reflection at \( r = R \) is sufficiently small. As the incident energy \( E \) becomes lower, the wider absorbing area \( \Delta R \) is required to find appropriate value of \( W_{\text{abs}} \) satisfying condition (2.5), because of the increase of the wave length.

As a demonstration, we show in Fig. 1 the scattering of \(^{10}\)Be-\(^{12}\)C described with the optical potential. The radial wave function is shown for a partial wave of \( L = 20 \) in the left hand panel, and the absolute value of the scattering matrix in the right hand panel. The Woods-Saxon shape is used for the potential with parameters, \( V = 123 \text{ MeV} \), \( r_V = 0.75 \text{ fm} \), \( a_V = 0.80 \text{ fm} \), \( W = 65 \text{ MeV} \), \( r_W = 0.78 \text{ fm} \), and \( a_W = 0.80 \text{ fm} \). The incident energy is set at \( E_{\text{lab}} = 300 \text{ MeV} \). In solving Equation (2.3) in the partial wave expansion, the plane wave \( e^{ikz} \) in the right hand side is replaced by the regular Coulomb wave function and \( V \) in the right hand side represents the potential in which the point Coulomb potential is subtracted. The radial equation is discretized with \( \Delta r = 0.2 \text{ fm} \) grid, and the discrete variables representation is

![Fig. 1. The potential scattering calculated with the ABC. \(^{10}\)Be-\(^{12}\)C scattering with the optical potential at incident energy \( E = 300 \text{ MeV} \). [Left] The radial wave function for \( L = 20 \) with three different choices of absorbing potential strength. [Right] Absolute value of scattering matrix calculated with the ABC (curves), in comparison with accurate values (dots).](image-url)
We put an absorber outside $R = 20$ fm with $\Delta R = 10$ fm thick. Results with several choices for $W_{abs}$ are compared in the figure, $W_{abs} = 20, 100, 2500$ MeV. The choice of $W_{abs} = 100$ MeV satisfies the criterion given by Eq. (2.5), while others do not. As seen from the right hand panel of Fig. 1, the scattering matrix is rather insensitive to the choice of the absorbing potential. One may thus obtain accurate scattering matrix with a rather wide window of $W_{abs}$.

§3. Absorbing Boundary Condition: Breakup Reactions

The advantage of the ABC manifests itself in the three-body scattering problems. Let us consider reaction of a projectile (P) composed of core (C) plus neutron (n), $P = C + n$, on a target nucleus (T). Expressing projectile-target relative coordinate by $R$ and neutron-core relative coordinate by $r$, the Hamiltonian of this three-body system is expressed as

$$H = -\frac{\hbar^2}{2\mu} \nabla_R^2 - \frac{\hbar^2}{2m} \nabla_r^2 + V_{NC}(r) + V_{nT}(r_{nT}) + V_{CT}(R_{CT})$$

where $\mu$ and $m$ are reduced masses of projectile-target relative motion and neutron-core relative motion, respectively. $V_{NC}$, $V_{nT}$, $V_{CT}$ are the interaction potentials of constituent particles. $V_{CT}$ includes the Coulomb potential. $V_{nT}$ and $V_{CT}$ may include imaginary potentials which represent loss of flux from the model space, while $V_{NC}$ is taken to be real.

We introduce redundant ‘distorted’ wave with outgoing boundary condition by the following equation,

$$\left\{ -\frac{\hbar^2}{2\mu} \nabla_R^2 + V_{PT}(R) \right\} \psi^{(+)}(R) = E\psi^{(+)}(R),$$

where $V_{PT}$ may be chosen arbitrary but should include the Coulomb potential. The total wave function may be expressed as a sum of the distorted wave in the incident channel and the scattered wave.

$$\psi^{(+)}(R, r) = \psi^{(+)}(R) \phi_0(r) + \Psi_{scat}(R, r)$$

where $\phi_0(r)$ is the initial bound orbital of neutron-core relative motion. The scattered wave $\Psi_{scat}$ satisfies the following inhomogeneous equation in the ABC,

$$\{ E + e_0 + i\epsilon_{nC}(r) + i\epsilon_{PT}(R) - H \} \Psi_{scat}(R, r) = \{ V_{nT}(r_{nT}) + V_{CT}(R_{CT}) - V_{PT} \} \psi^{(+)}(R) \phi_0(r),$$

where $E$ is the energy of projectile-target relative motion in the incident channel and $e_0$ is the binding energy in the projectile. One should note that the right hand side $\{ V_{nT} + V_{CT} - V_{PT} \} \psi^{(+)}(R) \phi_0(r)$ is a localized function in space. Namely, this function vanishes if either $R$ or $r$ is large enough. The absorbing potentials, $\epsilon_{nC} + \epsilon_{PT}$, assure the outgoing boundary condition to be satisfied approximately at spatial region where either $R$ or $r$ is large.
In practice, Equation (3.4) is solved in the partial wave expansion, expressing the wave function $\Psi^+(R, r)$ as

$$\Psi^+(R, r) = \sum_{Ll} \frac{u_J^{Ll}(R, r)}{Rr} Y_L(R) Y_l(r) J^L.$$  \hspace{1cm} (3.5)

Denoting the angular momentum channels specified by $L$ and $l$ as $a$, and assuming $s$-wave state for $\phi_0(r)$, the equation for $u_J^{Ll}(R, r)$ reads

$$\begin{cases}
E + e_0 + i\epsilon_{nC}(r) + i\epsilon_{PT}(R) \\
- \left( \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial R^2} + \frac{h^2}{2m} \frac{\partial^2}{\partial r^2} + \frac{\hbar^2 l_a(l_a + 1)}{2mr^2} + V_{nC}(r) \right) u_a^J(R, r) \\
- \sum_{a'} V_{aa'}^J(R, r) u_{a'}^J(R, r)
\end{cases}
= \begin{cases}
V_{aa_0}^J(R, r) - \delta_{a_0} V_{PT}(R), \quad w_J(R) v_0(r) \end{cases}$$

where $a_0$ is the angular momentum channel of incident wave, $v_0$ is the radial wave function of $\phi_0(r)$, $w_J(R)$ is the radial wave function of $\psi^+(R)$ for partial wave $J$, $V_{aa'}^J(R, r)$ is a multipole expansion of the potential $V_{nC} + V_{PT}$.

The boundary condition is given as, for arbitrary $R$ and $r$, $u_J^{Ll}(R, 0) = u_J^{Ll}(0, r) = 0$ at origin and $u_J^{Ll}(R, r_{\text{max}}) = u_J^{Ll}(R_{\text{max}}, r) = 0$ at the boundaries, $R_{\text{max}}$ and $r_{\text{max}}$.

§4. Deuteron Reaction

In this section we apply the ABC approach to breakup reactions of deuteron. Since the deuteron reaction has been investigated in detail with the CDCC method, \cite{9,15}, we can assess reliability of the ABC by comparing results of both methods.

We consider $d + ^{58}\text{Ni}$ reaction at incident deuteron energy $E_d = 80$ MeV. The wave function is expanded in partial waves, as given in Eq. (3.5). The spatial parameters of the wave function are set as follows: The relative angular momenta between proton and neutron of $l=0$ and 2 are included. The radial wave function $u_J^{Ll}(R, r)$ is discretized with grid spacing of 0.2 fm for $R$ and 0.5 fm for $r$. The radial region up to 50 fm are treated, and each absorbing potential is placed in the regions larger than 25 fm. The absorbing potentials are thus characterized by $\Delta r = \Delta R = 25$ fm. Their strengths of $W_R = 50$ MeV and $W_r = 20$ MeV are employed. The potential parameters of $p, n - ^{58}\text{Ni}$ are taken to be the same as those adopted in Ref. 15). The proton-neutron potential is a central force, and $s$-wave is assumed in the ground state.

We first discuss computational aspects of our method. Denote the number of radial grid points for $R$ as $N_R$ and that for $r$ as $N_r$, and the number of angular momentum channels specified by $Ll$ as $N_{Ll}$. The wave function is then expressed as a column vector of dimension $N_{\text{dim}} = N_R N_r N_{Ll}$. The Hamiltonian operator is a sparse, complex symmetric matrix. The scattering problem of Eq.(3.6) thus results in the linear algebraic problem of this dimension. For the present deuteron reaction,
For such problem of large size, iterative methods are useful. We employ Bi-CG (Conjugate Gradient) method which is useful for problems with complex non-hermite coefficient matrix. A preconditioning utilizing diagonal elements of the coefficient matrix makes the convergence faster, since it gets rid of huge diagonal elements at small $R$ and $r$ region due to the centrifugal barrier.

We show in Fig. 2 the wave function in the partial wave expansion, $\text{Re}[u_{Ll}^J(R, r)]$ for $J = 17$, $L = 17$, and $l = 0$. This includes both the incident and breakup waves. In the small $r$ region, the wave function is dominated by the incident wave, and shows oscillation as a function of $R$ reflecting the incident relative wave function. The amplitude of the wave function decreases at large $R$ due to the absorption by $\epsilon_{PT}(R)$. The wave function at large $r$ shows breakup components of deuteron into $p + n$ continuum state. The amplitude of the wave function also decreases at large $r$ due to the absorption by $\epsilon_{nC}(r)$.

In Fig. 3, we show comparison of elastic scattering S-matrix and cross section between the CDCC\textsuperscript{15} and the ABC calculations. These figures shows that the ABC calculation accurately reproduces the CDCC results. We thus confirm that the ABC approach has the same physical contents as those of the CDCC method, although the discretized continuum channels are never introduced in the ABC calculation. We also calculated the scattering matrices into deuteron breakup channels specified by the relative momentum between proton and neutron. We again confirmed that the ABC gives the same scattering matrices as those by the CDCC.
§5. **Application to $^{11}\text{Be} + ^{12}\text{C}$ reaction**

We here report analysis of reactions of single-neutron halo nucleus $^{11}\text{Be}$ on $^{12}\text{C}$ target. The $s$-wave bound state of $^{10}\text{Be} + n$ relative motion is assumed for $^{11}\text{Be}$ ground state. The $^{10}\text{Be}-n$ potential is taken as Woods-Saxon shape whose depth is set to give the $2s$ orbital binding energy at 0.504 MeV. Optical potential for $^{10}\text{Be}$-$^{12}\text{C}$ is the same as that in Sect.2 (without energy dependence), and the Bechetti-Greenlees potential is used for $n^{-}\text{^{12}C}$. The radial grid is chosen as 0.2 fm for $R$ and 0.5 fm for $r$. The radial region up to 30 fm and 50 fm are used for $R$ and $r$, respectively. The absorbing potential is placed in the region $20$ fm $< R < 30$ fm and $25$ fm $< r < 50$ fm. The neutron-$^{12}\text{C}$ relative angular momenta up to $l=3$ are included. The matrix size for the wave function is thus about 240,000.

The total reaction and the elastic breakup cross sections are expected to be well described with the eikonal approximation at medium and high incident energies. Below a certain incident energy, treatment beyond the eikonal approximation would be required. One may expect that the validity of the eikonal approximation at low incident energy can be examined by investigating separately the two-body scatterings of constituent particles in the eikonal approximation. In the right-hand panel of Fig. 4, the elastic scattering cross section of neutron-$^{12}\text{C}$ scattering is shown. This cross section is expected to be related to the elastic breakup cross section of $^{11}\text{Be}$ into $^{10}\text{Be}+n$ fragments, because the elastic breakup process is considered to be dominated by the elastic scattering of halo neutron by the target nucleus. The eikonal approximation comes to lose accuracy below incident energy of 50 MeV and underestimates the cross section. The energy dependence of the cross section also looks different between the exact and eikonal calculations. The eikonal approximation is expected to be more accurate for $^{10}\text{Be}$-$^{12}\text{C}$ reaction cross section because of the shorter wave length at the same incident energy per nucleon for this system.

We now move to the three-body reaction problem. In the left-hand panel of Fig. 4, we show the elastic breakup cross sections of $^{11}\text{Be}$-$^{12}\text{C}$ reaction. The filled circles are the calculation with the ABC and the open circles by the eikonal ap-
proximation. The elastic breakup cross section is substantially larger than that in the eikonal approximation at lower incident energy. This clearly shows the necessity to solve the problem beyond eikonal approximation below the incident energy less than 50 MeV per nucleon. Comparing left and right panels, qualitative features in the cross sections are similar between the elastic breakup cross section of $^{11}\text{Be}-^{12}\text{C}$ and the neutron-$^{12}\text{C}$ elastic cross sections. This confirms the above argument that the elastic breakup process is dominated by the elastic scattering of neutron-target. However, looking at quantitatively, the discrepancy between the exact and eikonal approximation is much larger for the neutron breakup reactions. We think it necessary to examine further the convergence of the calculations with respect to, for example, the relative angular momentum of neutron-core.

§6. Summary

We have presented the ABC approach to describe breakup reactions of weakly bound projectile. With the ABC, a general scattering problem with outgoing boundary condition is recasted into an linear inhomogeneous differential equation with vanishing boundary condition. Thus the scattering problem may be treated without introducing any asymptotic form for the wave function. In the partial wave expansion and radial discretization, the linear inhomogeneous equation results in the linear algebraic problem with sparse, complex symmetric coefficient matrix. Efficient iterative solvers are useful to solve this linear problem.

We show application of our method to deuteron reaction for which detailed analyses with the CDCC method is available. We have confirmed that the ABC cal-
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calculation accurately reproduce the CDCC results. Thus the ABC approach provides an alternative approach to describe reactions where breakup processes into continuum channels are important. Comparing two approaches, the ABC is advantageous in that the scattering wave function is obtained directly in real-space, avoiding introduction of virtual continuum channels. The convergence of the calculation can be examined with a few, intuitive, parameters related to the shape of absorbing potential. The trade-off for its simplicity is a heavy computational task to solve the large linear problem.

We have applied the ABC approach for breakup reaction of single neutron-halo nucleus $^{11}$Be on $^{12}$C target. It is found that the eikonal approximation becomes inaccurate at incident energy below 50 MeV/A. The eikonal approximation substantially underestimates the breakup cross section.

Although we here discuss only reaction problems, the ABC will be useful for any circumstances where the scattering boundary condition comes into play. Responses in the continuum is one of the other problems where the ABC is extremely useful, as discussed in another report in this symposium.\textsuperscript{10,14}

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