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Testing convergence of the solution of the continuum discretized coupled channels method for deuteron-induced reactions

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Abstract: We briefly introduced the formalism of the CDCC method in which reactions involving weakly bound nuclei are treated as a three-body system and took into account the contribution of breakup states. Numerically examined results were done for the elastic scattering of two typical d + ^{12}C and d + ^{58}Ni systems. Truncations of E_{max}, $l_{max,}$ and R_{match} for model spaces in CDCC calculations were established. A description of realistic elastic d + ^{12}C and d + ^{58}Ni scattering data at 80 MeV was made to see the valuable CDCC method and the vital role of deuteron breakup effects.

Keywords: *scattering of weakly bound nuclei, breakup effects, CDCC method*.

I. INTRODUCTION

Deuteron is well known to be a weakly bound **nucleus** with binding energy being 2.25 MeV. It is easily distinguished into neutron and proton, thus elastic cross sections for deuteron-induced reactions could not be described by standard optical potentials. An alternative method is commonly used to be the continuum discretized coupled channels (CDCC) which was developed to take into account explicitly the breakup of the projectile and/or target. CDCC method was first developed in the 1970s [1]. The base idea of the CDCC method is that d + nucleus scattering is treated as a three-body system involving n + p + target nuclei. Significant progress was made possible by introducing breakup states of the deuteron which are continuous and positive energies. This leads to the idea of a discretized continuum which was subsequently used by many authors (see, for example, Refs. [2–4] for reviews). For more than 20 years, the three-body CDCC method was successfully applied to reactions involving weakly bound nuclei, such as ^{6}Li and ^{11}Be which can be seen as ^{4}He + d and ^{10}Be + n systems, respectively. The CDCC theory represents a natural framework for reactions involving exotic nuclei. The main property of exotic nuclei is the low breakup threshold, and couplings to the continuum are quite important.

Although we benefit from the CDCC method in describing exactly elastic scattering involving weakly bound nuclei, we cost computation time and computer resources. Therefore determining a model space truncation which reduces computation time, is very vital. In this work, we test a model space truncation of continuously positive energy (E_{max}), proton-neutron relative angular momentum (l_{max}), and radius matching (R_{match}) in CDCC calculations of d+^{12}C and d+^{58}Ni systems. The established model space is used to describe the realistic data at 80 MeV [6, 7].

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II. CDCC FORMALISM

Because deuteron is well known to be a weakly bound nucleus consisting of proton (*p*) and neutron (*n*), deuteron-nucleus nuclear reaction processes are often treated as a $p + n + A$ three-body system. The CDCC method [2,3] was introduced as an approximate solution to the three-particle Schrodinger equation. Figure 1 is schematics of a three-body system of deuteron-nucleus scattering. Where $\vec{R}$ is the projectile-target coordinate, $\vec{R}_p = \vec{R} + \frac{1}{2}\vec{r}$ is the proton-target coordinate, $\vec{R}_n = \vec{R} - \frac{1}{2}\vec{r}$ is the neutron-target coordinate, and $\vec{r}$ is the internal coordinate of the deuteron.

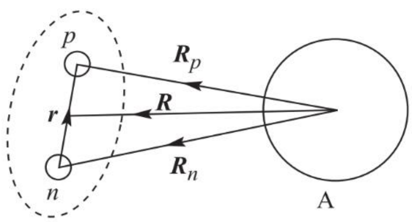

Fig. 1. Schematics of deuteron-nucleus scattering.

In the CDCC method, the total wave function describing the neutron and proton in the presence of the target nucleus is denoted by $\Psi(\vec{R},\vec{r})$ and included relative wave function $\chi(\vec{R})$ and relative proton-neutron motion in deuteron, $\phi(\vec{r})$. The internal coordinates of the nucleons in the target nucleus and the antisymmetrization of the wave function for the interchange of the incident nucleons in the deuteron with the nucleons in the target are ignored. The total wave function is given explicitly as form [1]

$$\Psi(\vec{R},\vec{r}) = \chi_b(\vec{R})\phi_b(\vec{r}) + \sum_l^{\infty}\sum_L^{\infty}[Y_l(\Omega_r) \otimes Y_L(\Omega_R)]_{JM} \times \frac{1}{R}\int_0^{\infty} \phi_l(k,r)\chi_{lLJ}(P,R)dk \quad (1)$$

Where index *b* indicates the bound state of the deuteron, and *k* denotes the continuum state in which relative energies of the proton-neutron system in the deuteron are positive. The spherical harmonics, $Y_l(\Omega_r)$, and $Y_L(\Omega_R)$, are angular components of the deuteron wave function and relative wave function between the deuteron and target, respectively. The $\phi_l(k,r)$ and $\chi_{lLJ}(P,R)$ are radial components of the deuteron wave function and relative wave function of deuteron and target as vector $\vec{r}$ and $\vec{R}$, respectively. *P* and *L* are linear and orbital angular momenta of the motion between the deuteron and target, respectively. *J* is given by vector coupling of angular momenta *l* and *L*. The deuteron wave function $\phi_l(k,\vec{r}) = \phi_l(k,r)Y_l(\Omega_r)$ is a complete set of eigenstate Hamilton operator

$$H_{np}(r)\phi_l(k,\vec{r}) = [T_{np} + V_{np}(r)]\phi_l(k,\vec{r}) = \epsilon_k\phi_l(k,\vec{r}) \quad (2)$$

Here T_{np}, is the kinetic-energy operator of relative neutron-proton motion, $V_{np}(r)$ is a neutron-proton potential, *k* and *l* are the neutron-proton relative linear and angular momenta, respectively, and *m* is the projection of *l* along the *z-axis*. Energies are $\epsilon_b = 2.225$ MeV for the bound state case and $\epsilon_k = k^2/\mu$ for the continuum states. The total wave function satisfies the Schrodinger equation

$$(H - E)\Psi(\vec{R},\vec{r}) = 0, \quad (3)$$

where the total Hamilton

$$H = T_R + V_N(\vec{R},\vec{r}) + H_{np}(r). \quad (4)$$

Where T_R is the relative kinetic operator of the deuteron and target nucleus, the potential $V_N(\vec{R},\vec{r})$ is given by the sum of nucleon-nucleus optical potentials as [1]

$$V_N(\vec{R},\vec{r}) = V_{p-A}\left(\left|\vec{R} + \tfrac{1}{2}\vec{r}\right|\right) + V_{n-A}\left(\left|\vec{R} - \tfrac{1}{2}\vec{r}\right|\right). \quad (5)$$

In the CDCC method, the wave function of continuous breakup states is discretized into a finite number N of bins, each with a width $\Delta = k_i - k_{i-1}$ as

$$\phi_{il}(r) = \frac{1}{\sqrt{\Delta}}\int_{k_{i-1}}^{k_i} \phi_{il}(k,r)dk. \quad (6)$$

The discretized wave function satisfies an orthogonal condition

$$\int \phi_{ilm}^*(\vec{r})\phi_{i'l'm'}(\vec{r})d\vec{r} = \delta_{ii'}\delta_{ll'}\delta_{mm'}. \quad (7)$$

Thus, the total wave function (1) is rewritten as form

$$\Psi(\vec{R},\vec{r}) = \chi_b(\vec{R})\phi_b(\vec{r}) + \frac{1}{R}\sum_l^\infty \sum_L^\infty \sum_i^N [Y_l(\Omega_r) \otimes Y_L(\Omega_R)]_{JM}\phi_{il}(r)\chi_{ilJ}(P,R). \quad (8)$$

In principle, summation (8) to infinity is unavailable, in place three sums must be truncated at the values of l_{max}, L_{max}, k_{max} (E_{max}), and N which are large enough to converge the total wave function.

Inserting total wave function (8) and total Hamilton (4) into Schrodinger equation (3), we get the coupled channel equations as form [2-4]

$$[T_R + V_{\alpha\alpha}(\vec{R},\vec{r}) - E_\alpha]\chi_\alpha(\vec{R}) = -\sum_{\alpha' \neq \alpha} V_{\alpha'\alpha}(\vec{R},\vec{r})\chi_{\alpha'}(\vec{R}), \quad (9)$$

with $\alpha = (i, l, L, J, M)$. The coupled channel equation includes the elastic channel which corresponds to $\alpha = (0,0,J,J,M)$.

$$V_{\alpha'\alpha}(\vec{R},\vec{r}) = \left\langle \phi_{\alpha'}(\vec{r}) \middle| V_{p-A}\left(\left|\vec{R} + \frac{1}{2}\vec{r}\right|\right) + V_{n-A}\left(\left|\vec{R} - \frac{1}{2}\vec{r}\right|\right) \middle| \phi_\alpha(\vec{r}) \right\rangle \quad (10)$$

The equation (9) is called the coupled channel equation, coupling the projectile ground state to continuum states. The solution of the coupled channel equations provides the wave functions $\chi_k(\vec{R})$. The observed scattering is extracted from the asymptotic form of $\chi_k(\vec{R})$.

III. NUMERICAL RESULTS

To test the convergence of the total wave function, we perform CDCC calculation for typical d+^{12}C and d+^{58}Ni systems with three types of truncations; i) truncation of neutron-proton relative linear momenta k_{max} (here we used relative energy as $E_{max} = \frac{\hbar^2}{2\mu}k_{max}^2$), ii) truncation of neutron-proton relative angular momenta l_{max}, and setting the asymptotic boundary condition at a finite value R_{match}. The potential ingredients used in the CDCC calculations were fixed, where the proton-neutron potential V_{np} which describes the deuteron wave function at the ground state, and proton-neutron relative wave function in continuum states is taken as a single Gaussian interaction [5]

$$V = -V_0 e^{-(r/\alpha)^2}, \quad (11)$$

with V_0 = 72.15 MeV and $\alpha = 1.484$ fm. The potential reproduces the deuteron binding energy of 2.225 MeV and low energy p-n scattering phase shifts [5]. The interaction between proton-target and neutron-target are optical potentials that fit the elastic scattering at half the deuteron laboratory energy and are given as Woods-Saxon form potentials. The parameters are taken from the global fit by Varner *et al.* [8] (CH89). The CDCC calculations were done by FRESCO code [9].

Firstly, we test the truncation of the relative energy E_{max} and ΔE in the elastic scattering of d+^{58}Ni system. To evaluate the influence of E_{max} on the convergence of the total wave function, the neutron-proton relative angular momenta is fixed at l_{max}=2, while the asymptotic boundary condition is given as R_{match} = 60 fm. Figure 1 illustrates the influence of truncation E_{max} and ΔE on the convergence of the total wave function which is expressed through the angular distribution of the elastic scattering cross section. The upper panel is the calculated CDCC results using differently truncated energy values of E_{max}=10, 20, 40, and 60 MeV. The convergence was determined at E_{max} = 40 MeV which the obtained CDCC result of elastic scattering cross section differs insignificantly from the result given by truncation at E_{max}=60 MeV, while those results with truncated at E_{max} = 10 and 20 MeV are different, especially the cross section at angles in the range from 40° to 80°. The lower panel presents the convergent test in CDCC calculations with various values of energy width ΔE=3, 5, 10, and 20 MeV which correspond to bin numbers N to 14, 8, 4, and 2. The calculated CDCC results showed that the convergence occurred with ΔE = 5 MeV.

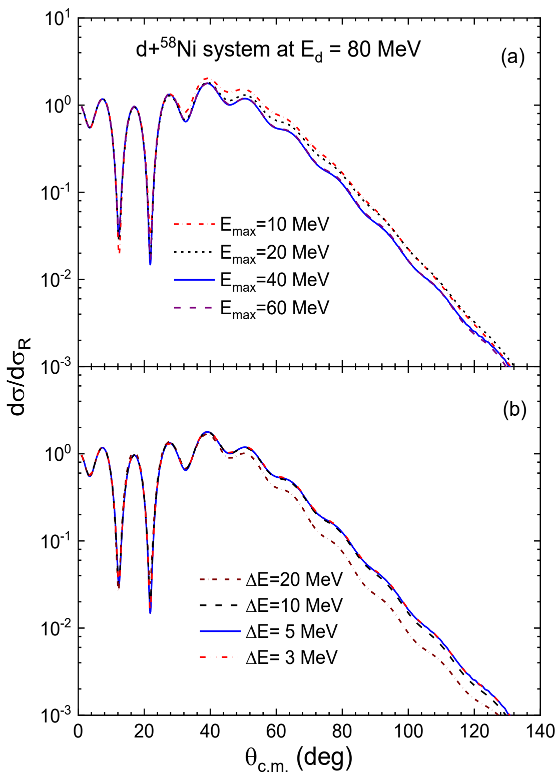

Fig. 1. Test convergence of the total wave function in CDCC calculation for the elastic d+^{58}Ni scattering with truncation of E_{max} and ΔE. Upper panel illustrates the CDCC results with variation of E_{max} from 10 to 60 MeV. Lower panel is those with energy width ΔE = 3, 5, 10, and 20 MeV.

Next, we tested the truncation of proton-neutron relative angular momentum l_{max}. A series of CDCC calculations were done with different l_{max} to find out the best value. The calculated results with various l_{max} are illustrated in Fig. 2. There is a significant difference between the computed results with l_{max}=2 and l_{max}=0. In contrast, a slight difference exists between the results with l_{max} = 1 and l_{max}=0 (see clearly in Fig. 2b). There is also a negligibly small discrepancy between the calculated results for l_{max}=3 and l_{max}=2. This demonstrates that angular momenta l = 0, 2 gives significant contributions, whereas angular momenta l=1,3 gives small ones. The difference between the computed results with l_{max}=3 and l_{max}=6 is insignificant, hence using l_{max}=3 is sufficient for the CDCC calculations to be stable.

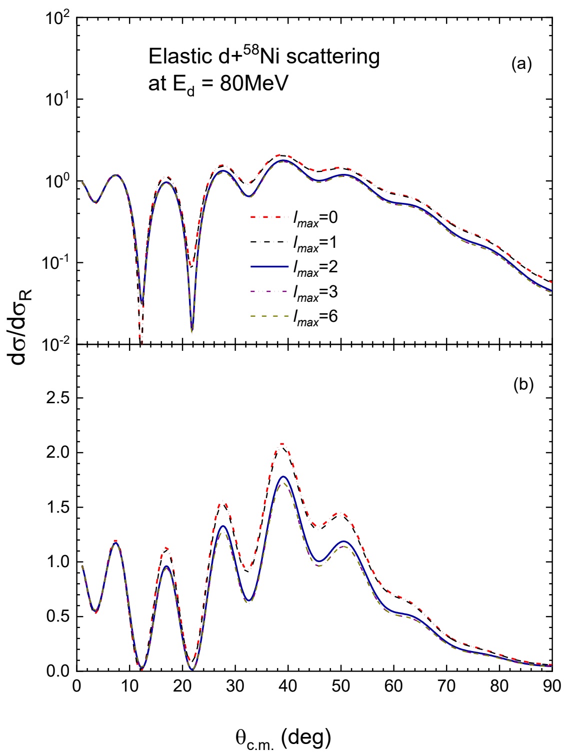

Fig. 2. Test convergence of the total wave function in CDCC calculation for the elastic d+^{58}Ni scattering with various truncations of l_{max}.

Lastly, truncation of matching radius (R_{match}) at which relative wave function matches the asymptotic form has been tested. While the matching radius is minimal to reduce computation time, it must be large enough to guarantee the convergence of the discretized wave function. Our CDCC computations with E_{max} = 40 MeV and l_{max}=3 determined the convergent point at R_{match}=30 fm. Thus, combining with two above truncations, we established a model space truncation for the d+^{58}Ni system. The term "CDCC" means the calculations in model space truncation R_{match} = 30 fm coupling to continuum states having energy E_{max} = 40 MeV with step ΔE = 5 MeV and relative angular momentum l_{max} = 3. The term "one-channel" refers to three-body computations of the p+n+^{58}Ni system without coupling to the continuum states of the deuteron. Fig. 3 illustrates the one-channel and CDCC calculated results of the elastic d+^{58}Ni scattering in comparison with experiment data at E_d = 80 MeV [6]. Influences of continuum states on the elastic scattering are expressed clearly by reducing the cross section in range angles 30°-60° and enhancing those at angles larger than 90° to match measured data.

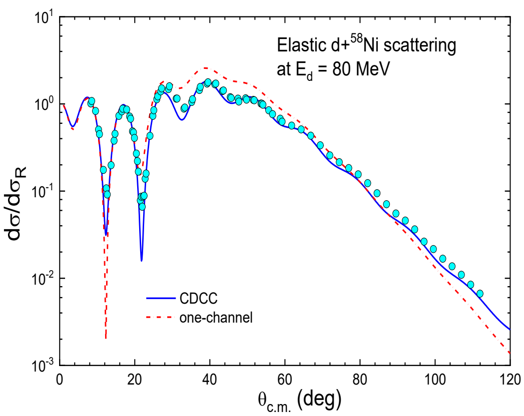

Fig. 3. One-channel and CDCC calculations of the elastic d+^{58}Ni scattering in comparison with data measured at E_d=80 MeV [6].

For the d + ^{12}C at 80 MeV case, our calculations indicated that the CDCC computation truncated at E_{max}= 30 MeV with energy width ΔE=3.0 MeV, and radius matching at 20 fm. The proton-neutron relative angular momentum was truncated at l_{max}=3 as above d + ^{58}Ni case. Figure 4a shows truncated E_{max} dependence of the calculated CDCC results d + ^{12}C system. Thus, the model space truncation for the d+^{12}C system was established completely. Our calculations for elastic d+^{12}C scattering at E_d= 80 MeV were done using one-channel and CDCC methods. Figure 4b illustrates the computed results in comparison with the experimental data [7]. Again, one can see that the CDCC results agree with data points in whole angles, while the one-channel results overestimate the data at small angles and underestimate those at large angles.

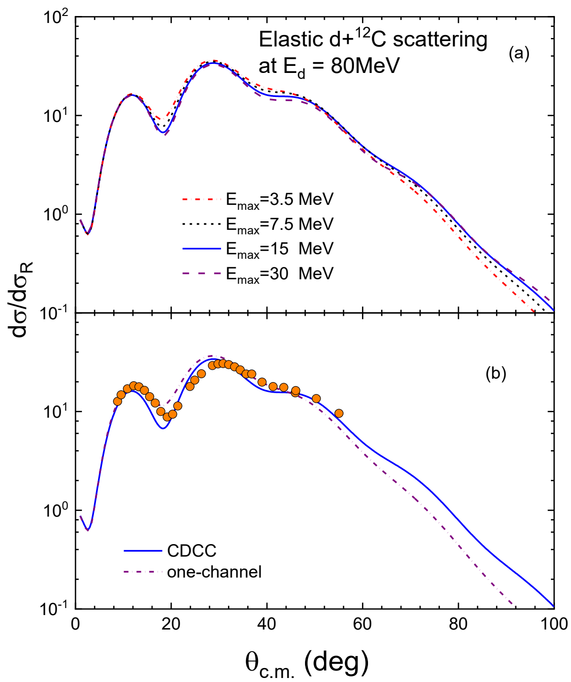

Fig. 4. Upper panel illustrates the CDCC results with the variation of E_{max} from 10 to 60 MeV. Lower panel presents one-channel and CDCC results of the elastic d+^{12}C scattering in comparison with data measured at E_d=80 MeV [7].

IV. SUMMARY

We have numerically examined the CDCC method in various model space truncations. As the model space, the discretization of the continuum energies *E*, the angular momentum of the *p-n* pair, and the relative wave function matching the asymptotic form are truncated at E_{max}, l_{max}, and R_{match}. The values of E_{max}, $l_{max,}$, and R_{match} in the CDCC practices are established for d + ^{12}C and d + ^{58}Ni cases. We have kept these model truncations to test elastic d + ^{12}C and d + ^{58}Ni scattering at E_d = 80 MeV as typical realistic examples. CH89 nucleon-nucleus optical potentials at 40 MeV which is half the incident deuteron energy have been used in the present work. A good description of angular distribution data of elastic scattering cross section has demonstrated the success of the CDCC method and the vital role of breakup effects in the reaction involving weakly bound nuclei.

V. ACKNOWLEDGEMENT

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