Calculation of three-body reactions with Coulomb interaction

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Three-body nuclear reactions with Coulomb interaction are treated using the formalism of Alt, Sandhas, and Ziegelmann when two of the three particles are charged. Aspects of the numerical calculation are discussed and its difficulties are pointed out. Calculations are presented by considering the total energy of the system under breakup threshold and increasing values of the target atomic number.

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I. INTRODUCTION

Inclusion of the Coulomb interaction in the nuclear three-body problem is by no means simple due to the long-range character of the interaction. Although a variety of methods [1–6] have been proposed to treat the Coulomb interaction adequately, the calculations are rather complex. Among these methods, the formalism of Alt, Sandhas, and Ziegelmann (ASZ) [4–6] has been widely utilized for cross-section calculations of reactions in which only three nucleons (p,n,p) take place. Starting from equations [7] like Faddeev equations, the two-body transition operators, which are present, are put in such a form that the contribution of the Coulomb interaction is isolated. The Coulomb singularities are avoided by considering the screened Coulomb potential, which leads to screened scattering amplitudes. The transition to unscreened scattering amplitudes is made by following the renormalization procedure of Gorshkov [8] and others [9,10]. The ASZ equations are actually effective two-body equations that are solved by means of their momentum representation.

Our aim in this work is to analyze aspects of the numerical calculation of the ASZ equations when two of the three particles are charged and for increasing values of the product of their atomic numbers. Basically, the assumptions made about the system we consider are that the target is structureless and infinitely heavy and that the short-range interactions are of the separable s-wave Yamaguchi potential [11]. Although one has to solve two-body equations, their kernels have a complex singularity structure: the effective free Green function presents singularities of the fixed-point type; for total energies above the breakup threshold the kernels develop the well-known moving singularities [12]; and finally, the kernels have a quasisingular character due to the screened Coulomb potential [13,14]. Here we restrict ourselves to total energies under the breakup threshold.

In solving the ASZ equations numerically some difficulties arise and to overcome them one may proceed as follows: the Born approximation is done for the two-body Coulomb transition operator, in order to reduce the solution of the ASZ equations to manageable size; a detailed numerical representation should be taken for the quasisingular behavior of the screened Coulomb potential present in the kernels. Besides these points, in the elastic case one has to make subtractions to get the scattering amplitude; this is a possible source of errors. In this paper we will discuss these questions and show our calculations by exhibiting the cross sections of the reactions—elastic scattering of deuteron, deuteron induced stripping reactions (d,p) and (d,n), and the (p,n) reaction, considering increasing values of the target atomic number.

This paper is organized as follows. In Sec. II we introduce the two-body interactions and give a brief description of the ASZ method. In Sec. III we present the method for the numerical calculation of the transition amplitudes. Finally, Sec. IV is devoted to the presentation of the numerical results and comments.

II. THE THREE-BODY SYSTEM AND THE ASZ EQUATIONS

We consider a system composed of a target, a proton, and a neutron, which are denoted by 1, 2, and 3, respectively. The masses of the proton and the neutron are taken to be equal and that of the target, infinite. In the c.m. frame of the three-particle system, $\mathbf{q}_\alpha$ is the momentum of the particle α, where α is either 1, 2, or 3, relative to the c.m. of the pair α, defined by the two other particles, and $\mathbf{p}_\alpha$ is the relative momentum in the pair α. The corresponding reduced masses are denoted by M_α and μ_α. The two-body nuclear potentials are treated as separable, rank-one, s wave. In pair 3, target-proton, there is the addition of the Coulomb interaction, described by the screened potential

$$\mathcal{V}_R(r)=Z_T e^2\frac{\exp(-r/R)}{r}\ , \tag{1}$$

which in the momentum representation is written as

$$\mathcal{V}_R(\mathbf{p}'-\mathbf{p})=Z_T\frac{e^2\hbar^2}{2\pi^2}\frac{1}{|\mathbf{p}'-\mathbf{p}|^2+\hbar^2/R^2}\ , \tag{2}$$

with Z_T the atomic number of the target and R the screening radius. The three subsystems of two particles each possess a bound state. According to our assumptions the two-body potentials can be expressed as

$$V_\alpha=|\chi_\alpha\rangle\lambda_\alpha\langle\chi_\alpha|+\mathcal{V}_R\delta_{\alpha 3},\quad \alpha=1,2,3 \tag{3}$$

where χ_α is of the Yamaguchi form [11]

$$\chi_\alpha(\mathbf{p}_\alpha)=\frac{N_\alpha}{p_\alpha^2+b_\alpha^2} . \tag{4}$$

To get the exact transition amplitudes we utilize the ASZ method [4–6] which, starting from the quasiparticle equations [7], provides effective two-body equations for the transition operators

$$T_{\beta\alpha}^{(R)}=V_{\beta\alpha}^{(R)}+\sum_\gamma V_{\beta\gamma}^{(R)}G_{0,\gamma}T_{\gamma\alpha}^{(R)} , \tag{5}$$

where R indicates the dependence on the screening radius. In Eq. (5) $G_{0,\gamma}$ is an effective free Green function [15] and $V_{\beta\alpha}^{(R)}$ is the effective two-body potential [15]

$$\begin{aligned}V_{\beta\alpha}^{(R)}=&\bar{\delta}_{\beta\alpha}\langle\chi_\beta|G_0(E)+(\delta_{\alpha3}+\delta_{\beta3}+\bar{\delta}_{\beta3}\bar{\delta}_{\alpha3})\\&\times G_0(E)\mathcal{T}_R(E)G_0(E)|\chi_\alpha\rangle\\&+\delta_{\beta\alpha}\bar{\delta}_{\alpha3}\langle\chi_\beta|G_0(E)\mathcal{T}_R(E)G_0(E)|\chi_\alpha\rangle ,\end{aligned} \tag{6}$$

with E the three-body energy, $G_0(E)$ the three-body free Green function, and $\bar{\delta}_{\beta\alpha}=1-\delta_{\beta\alpha}$. In Eq. (6), $\mathcal{T}_R$ is the two-body transition operator, related to the screened Coulomb potential $\mathcal{V}_R$, Eq. (1), and satisfying a Lippmann-Schwinger equation.

The ASZ method decomposes the potential $V_{\beta\alpha}^{(R)}$ into a short-range contribution, and into a long-range one proportional to the screened Coulomb potential $\mathcal{V}_R$. With this decomposition the on-shell screened transition amplitudes become

$$T_{\beta\alpha}^{(R)}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)=\delta_{\beta\alpha}\bar{\delta}_{\alpha3}\mathcal{T}_R(\mathbf{q}'_\alpha,\mathbf{q}_\alpha)+T_{sR,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha) , \tag{7}$$

where $T_{sR,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ is the screened Coulomb modified nuclear transition amplitude and with $\mathbf{q}'_\beta$ and $\mathbf{q}_\alpha$ on the energy shell.

In order to get the unscreened transition operator $T_{\beta\alpha}$, the ASZ method renormalizes Eq. (7) and then takes the zero screening limit, $R\to\infty$. Following this procedure one gets from Eq. (7)

$$\begin{aligned}&\lim_{R\to\infty} Z_{\beta,R}^{-1/2}(q'_\beta)T_{\beta\alpha}^{(R)}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)Z_{\alpha,R}^{-1/2}(q_\alpha)\\&\quad=T_{\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\\&\quad=\delta_{\beta\alpha}\bar{\delta}_{\alpha3}\mathcal{T}_C(\mathbf{q}'_\alpha,\mathbf{q}_\alpha)+T_{sC,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha) ,\end{aligned} \tag{8}$$

where

$$\begin{aligned}&Z_{\gamma,R}(q_\gamma)=e^{(i2\phi_{\gamma,R}(q_\gamma))},\quad \gamma=1,2\\&Z_{3,R}(q_3)=1 ,\end{aligned} \tag{9}$$

and

$$\phi_{\gamma,R}(q_\gamma)=-\frac{M_\gamma}{\hbar q_\gamma}\int_{\hbar/2q_\gamma}^{\infty}\mathcal{V}_R(r)dr . \tag{10}$$

The screening approach consists in calculating the amplitudes $T_{\beta\alpha}^{(R)}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ and $\mathcal{T}_R(\mathbf{q}'_\alpha,\mathbf{q}_\alpha)$ for finite R. Their difference provides the screened Coulomb modified nuclear amplitude $T_{sR,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$, which is renormalized in the way discussed above. Repeating the calculations for increasing values of R one gets the unscreened transition amplitude $T_{sC,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$,

$$\begin{aligned}&\lim_{R\to\infty} Z_{\beta,R}^{-1/2}(q'_\beta)[T_{\beta\alpha}^{(R)}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)\\&\qquad-\delta_{\beta\alpha}\bar{\delta}_{\alpha3}\mathcal{T}_R(\mathbf{q}'_\alpha,\mathbf{q}_\alpha)]Z_{\alpha,R}^{-1/2}(q_\alpha)\\&\quad=\lim_{R\to\infty} Z_{\beta,R}^{-1/2}(q'_\beta)T_{sR,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)Z_{\alpha,R}^{-1/2}(q_\alpha)\\&\quad=T_{sC,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha) .\end{aligned} \tag{11}$$

To obtain the transition amplitude $T_{\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ one analytically adds to the calculated amplitude $T_{sC,\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ the Coulomb transition amplitude $\mathcal{T}_C(\mathbf{q}'_\alpha,\mathbf{q}_\alpha)$ according to Eq. (8). It is worth noting that $\mathcal{T}_C$ is added only in the elastic-scattering case $\beta=\alpha\neq3$.

III. METHOD FOR THE CALCULATION OF THE TRANSITION AMPLITUDES

To calculate numerically the screened transition amplitudes $T_{\beta\alpha}^{(R)}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)$ we solve the ASZ equations (5), by first considering their momentum representation and then performing the following partial-wave decomposition:

$${}^lT_{\beta\alpha}^{(R)}(q'_\beta,q_\alpha)={}^lV_{\beta\alpha}^{(R)}(q'_\beta,q_\alpha)+\frac{4\pi}{2l+1}\sum_\gamma\int dq''_\gamma q''^2_\gamma\frac{1}{E^+-q''^2_\gamma/2M_\gamma-\epsilon_\gamma}{}^lV_{\beta\gamma}^{(R)}(q'_\beta,q''_\gamma)\,{}^lT_{\gamma\alpha}^{(R)}(q''_\gamma,q_\alpha) , \tag{12}$$

where the quantities ${}^lT_{\beta\alpha}^{(R)}$ and ${}^lV_{\beta\alpha}^{(R)}$ are obtained from equations of the form

$${}^lX_{\beta\alpha}(q'_\beta,q_\alpha)=\frac{2l+1}{2}\int_{-1}^{1}d\cos\theta X_{\beta\alpha}(\mathbf{q}'_\beta,\mathbf{q}_\alpha)P_l(\cos\theta) , \tag{13}$$

with P_l the Legendre polynomial and θ the angle between the momenta $\mathbf{q}'_\beta$ and $\mathbf{q}_\alpha$.

The singularities of the kernels are generated by the Green function and the effective potential. To determine them we must fix the total energy of the system E. Here, we work with energies under the breakup threshold $E<0$. The Green function has fixed-point singularities $\pm\sqrt{2\mu_\gamma(|\epsilon_\gamma|-|E|)}\pm i\rho$ at an infinitesimal distance ρ from the real axis of integration, and the effective potential as well as the screened Coulomb potential have no singularities on this axis.

The method [16] used to treat this kind of singularity introduces an auxiliary equation

$$\begin{aligned}{}^l\Gamma_{\beta\alpha}(q'_\beta,q_\alpha)=&{}^lV_{\beta\alpha}^{(R)}(q'_\beta,q_\alpha,E)\\&+\sum_\gamma 2M_\gamma\frac{4\pi}{2l+1}\int dq''_\gamma q''^2_\gamma\,{}^lA_{\beta\gamma}(q'_\beta,q''_\gamma)\\&\times{}^l\Gamma_{\gamma\alpha}(q''_\gamma,q_\alpha) ,\end{aligned} \tag{14}$$

with a nonsingular kernel on the real axis

$$ {}^{l}A_{\beta\gamma}(q'_\beta,q''_\gamma)=\frac{{}^{l}V^{(R)}_{\beta\gamma}(q'_\beta,q''_\gamma)-{}^{l}V^{(R)}_{\beta\gamma}(q'_\beta,q_\gamma)}{q^2_\gamma-q''^2_\gamma} \tag{15} $$

being the on-shell transition amplitudes written as

$$ {}^{l}T^{(R)}_{\beta\alpha}(q_\beta,q_\alpha)={}^{l}\Gamma_{\beta\alpha}(q_\beta,q_\alpha) + \sum_\gamma {}^{l}\Gamma_{\beta\gamma}(q_\beta,q_\gamma)\,{}^{l}I_{\gamma\alpha}(q_\gamma,q_\alpha)\ . \tag{16} $$

The quantity ${}^{l}I$ is a solution of the equation

$$ {}^{l}I_{\beta\alpha}(q_\beta,q_\alpha)={}^{l}d_{\beta\alpha}(q_\beta,q_\alpha)+\sum_\gamma {}^{l}d_{\beta\gamma}(q_\beta,q_\gamma)\,{}^{l}I_{\gamma\alpha}(q_\gamma,q_\alpha)\ , \tag{17} $$

where

$$ {}^{l}d_{\beta\alpha}(q_\beta,q_\alpha)=2M_\beta\frac{4\pi}{2l+1}\int dq'_\beta\, q'^2_\beta\frac{{}^{l}\Gamma_{\beta\alpha}(q'_\beta,q_\alpha)}{q^2_\beta-q'^2_\beta-i\rho}\ . \tag{18} $$

The integrand of ${}^{l}d$ has singularities on the real axis for $\rho\to 0$; to circumvent them one adds to, and subtracts from, the integrand the quantity $q^2_\beta\,{}^{l}\Gamma_{\beta\alpha}(q_\beta,q_\alpha)/(q^2_\beta-q'^2_\beta-i\rho)$ and gets the following equation with a nonsingular integrand:

$$ {}^{l}d_{\beta\alpha}(q_\beta,q_\alpha)=2M_\beta\frac{4\pi}{2l+1} \times\int dq'_\beta\frac{q'^2_\beta\,{}^{l}\Gamma_{\beta\alpha}(q'_\beta,q_\alpha)-q^2_\beta\,{}^{l}\Gamma_{\beta\alpha}(q_\beta,q_\alpha)}{q^2_\beta-q'^2_\beta} -iM_\beta\frac{4\pi^2}{2l+1}q_\beta\,{}^{l}\Gamma_{\beta\alpha}(q_\beta,q_\alpha)\ . \tag{19} $$

In Eqs. (16) and (19) one needs the knowledge of ${}^{l}\Gamma$ both on shell and off shell. To do this, first one solves Eq. (14), which gives the off-shell quantities ${}^{l}\Gamma$ and then, using this same equation, one calculates ${}^{l}\Gamma$ on shell.

In the case of elastic scattering, $\beta=\alpha\neq 3$, one also needs to solve the Lippmann-Schwinger equation for the two-body transition operator ${}^{l}\mathcal{T}_R$; one proceeds in the same way as above, since its kernel has the same kind of singularities as Eq. (12). Then one subtracts ${}^{l}\mathcal{T}_R$ from ${}^{l}T^{(R)}_{\beta\alpha}$ to get ${}^{l}T_{sR,\beta\alpha}$.

Finally, following the basic idea of Fredholm's method [17], one transforms the integral equations (14) in algebraic linear equations, approximating the integrals by sums.

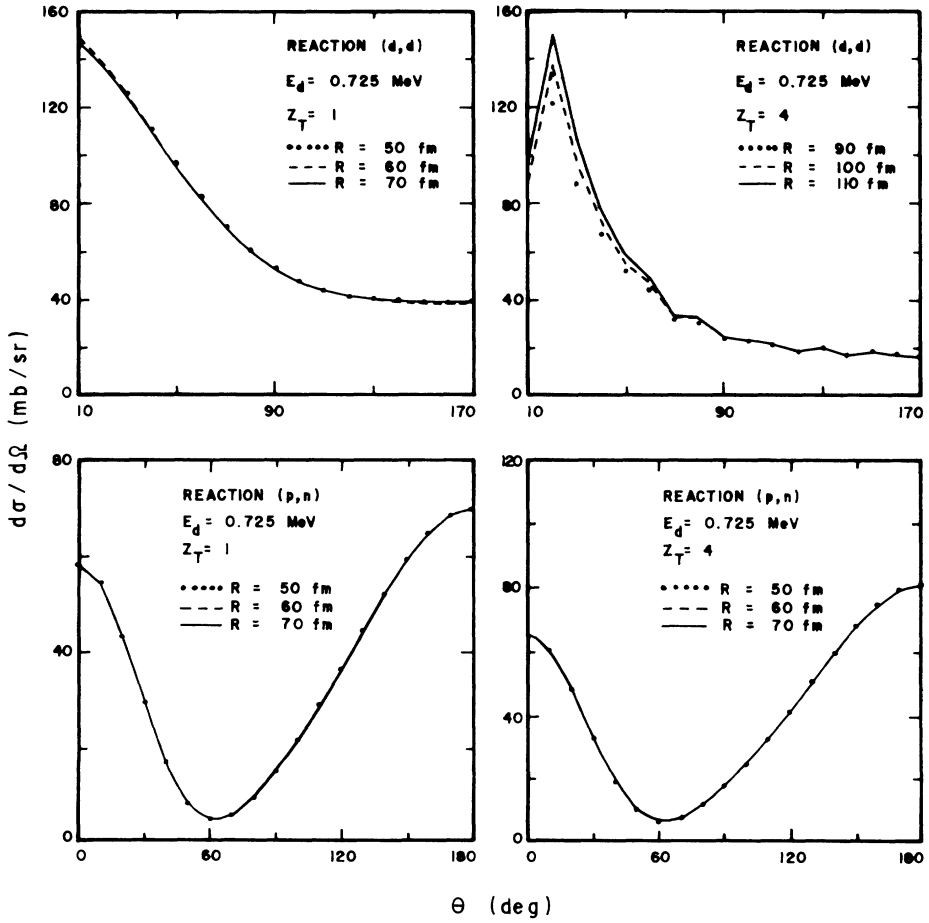

FIG. 1. Convergence of the differential cross section with the screening radius R as a function of the scattering angle, for the (d,d) and (p,n) reactions.

IV. NUMERICAL RESULTS AND COMMENTS

In Sec. III we outlined the method for the calculation of the screened transition amplitudes and here we describe some of the problems encountered in performing these calculations.

A. Two-body input

First we introduce the two-body input used in our calculations. In order to determine the potentials V_α, Eq. (3), we fix the range parameters b_α and the binding energies $|\epsilon_\alpha|$ of the two-body bound states. Table I summarizes our choice for the quantities concerning the pairs 2, neutron-target, and 3, proton-target. For pair 1, proton-neutron, we use the values $|\epsilon_1|=2.225$ MeV and $b_1=285.8$ MeV, corresponding to the binding energy of the deuteron and the triplet scattering length $a_t=5.38$ fm. We consider energies of the three-body system under breakup, specifically $E<-1.0$ MeV, and values of the target atomic number Z_T up to 4.

B. Numerical calculation

The solution of the coupled equations (14) needs the knowledge of the two-body screened Coulomb transition operator $\langle q_3' |{}^l\mathcal{T}_R(E-q_3''^2/2M_3)|q_3''\rangle$ for q_3' and q_3'' off shell, via the effective potential (6). Then to reduce the numerical solution of Eq. (14) to manageable size, one takes the approximation ${}^l\mathcal{T}_R \approx {}^l\mathcal{V}_R$. One can wonder about the quality of this approximation. As it was pointed out by Kok and Haeringen [18] the ensuing errors in the measurable quantities will depend on the relative importance of the nuclear and Coulomb potentials. This is a hard task to be carried out, however, in the cases in which

$$\langle q_3' |{}^l\mathcal{T}_R(E-q_3''^2/2M_3)|q_3''\rangle / \langle q_3' |{}^l\mathcal{V}_R|q_3''\rangle \equiv {}^l\mathcal{R} \approx 1$$

one can certainly assure the above approximation is well justified. Still from Ref. [18] and for the repulsive Coulomb potential one can have the following: (1) ${}^1\mathcal{R}\approx 1$ for $\xi=E-q_3''^2/2M_3<0$ and for small values of the modulus of the Sommerfeld parameter, η $[\eta=Z_T e^2(\mu_3/2\xi)^{1/2}]$; (2) $|{}^l\mathcal{R}|\approx 1$ for $\xi>0$ and for small

TABLE I. Binding energies $|\epsilon_\alpha|$ and the parameters b_α of the nuclear interaction for pairs 2 and 3, for different atomic numbers Z_T of the target.

Z_T	$\lvert\epsilon_2\rvert$ (MeV)	$\lvert\epsilon_3\rvert$ (MeV)	b_2 (MeV)	b_3 (MeV)
1	10.0	8.75	200.0	200.0
4	8.9	8.00	172.6	172.6

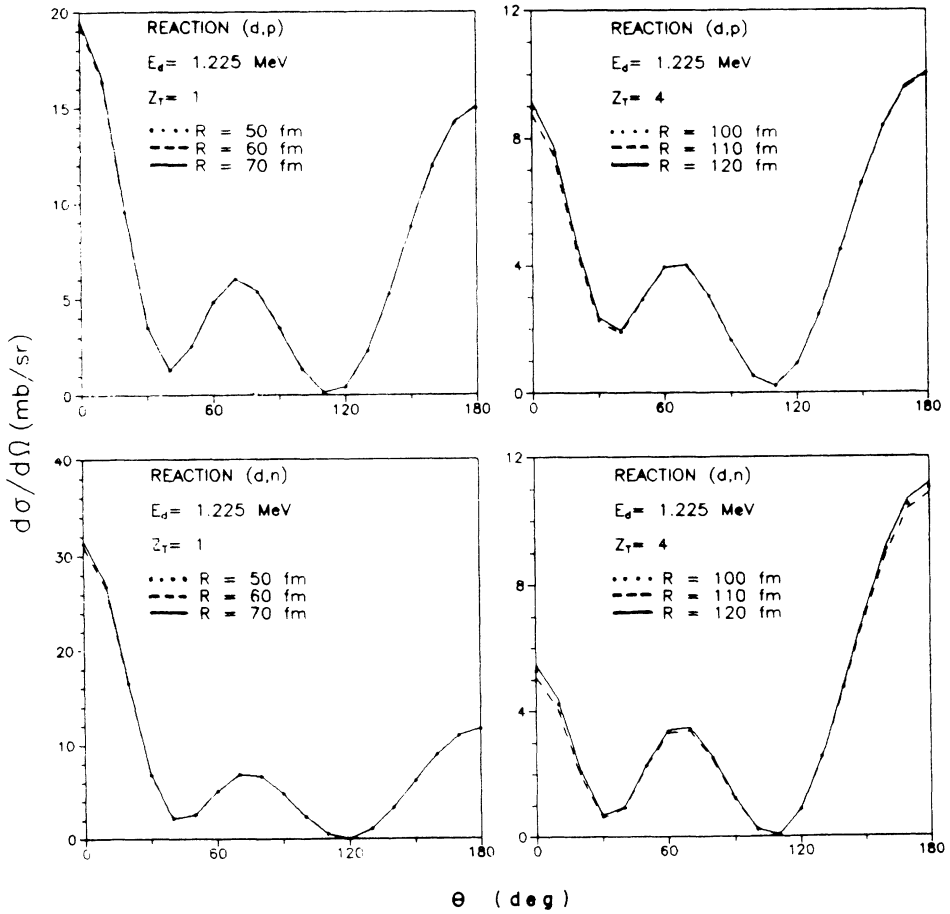

FIG. 2. Same as Fig. 1 for the (d,p) and (d,n) reactions.

values of $|\eta|$. The first case can be achieved if the total energy of the system is negative, $E<0$, for q_3'' is a variable of integration in Eq. (14) and hence one can get small values for $|\eta|$. The second case can be achieved if $E>0$; however, as q_3'' varies ξ assumes decreasing values, leading to large values of $|\eta|$, and so η no longer fulfills the condition corresponding to the second case. Thus in this case the Born approximation for ${}^l\mathcal{T}_R$ should be investigated with care. Regarding our system, we have $|\eta|<1$ for the energies considered, $E<-1$ MeV.

Concerning the partial-wave decomposition, one should mention that the partial effective potential ${}^lV_{\beta\alpha}^{(R)}$ is written as a sum of four contributions [4]; two of them have an analytical form and the other two are calculated from Eq. (13) by using the Gaussian quadrature method [19] (GQM). In order to get a good convergence of the differential cross sections with l we need up to 14 partial waves, for the energies and target atomic numbers considered.

The crucial point in solving Eq. (14) numerically is the quasisingular character of the screened Coulomb potential present in its kernel. This behavior can be seen by considering the momentum representation of this potential $\mathcal{V}_R(\mathbf{p}'-\mathbf{p})$, Eq. (2). When $\mathbf{p}'\to\mathbf{p}$ and R is large, $\mathcal{V}_R$ tends toward a sharp peak, becoming more singular with increasing Z_T. In addition, the localization of this quasisingular behavior of the kernel on the axis of the variable of integration depends on the value of the momentum q'_β in ${}^l\Gamma_{\beta\alpha}^{(R)}(q'_\beta,q_\alpha)$. Since each value of q'_β generates one equation for ${}^l\Gamma_{\beta\alpha}^{(R)}$, this quasisingular behavior is not localized; therefore, the numerical representation of the kernel cannot be made suitable simultaneously, unless a very large number of points of the integration axis is used. In our calculations we consider up to 120 points of the GQM.

Figures 1 and 2 show the convergence of the differential cross sections with the screening radius R. The cross section is proportional to the square modulus of the amplitude $T_{sC,\beta\alpha}$, Eq. (7), except for the elastic-scattering case; however, even in this case we did not add to $T_{sC,11}$ the Coulomb transition amplitude $\mathcal{T}_C$, since the resulting sum would mask the question of convergence [13].

From Figs. 1 and 2 one notes that for $Z_T=1$ the convergence with R is quite good irrespective of the type of reaction considered. Concerning the questions mentioned above, 64 points of the GQM were used both for the calculation of the partial-wave decomposition of the effective potential and for the numerical representation of the kernel. For $Z_T=4$ the convergence with R is good but for the elastic scattering of the deuteron. In order to achieve this, 120 points of the GQM were used. We think the unsatisfactory result obtained in the elastic case comes from the subtractions performed to get $T_{sR,11}$, these being needed only in the elastic scattering case.

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