

Three-potential formalism for the three-body Coulomb scattering problem

Z. Papp

Institute of Nuclear Research of the Hungarian Academy of Sciences, P.O. Box 51, H-4001 Debrecen, Hungary

(Received 8 October 1996)

We propose a three-potential formalism for the three-body Coulomb scattering problem. The corresponding integral equations are mathematically well behaved and can successfully be solved by the Coulomb-Sturmian separable expansion method. The results show perfect agreements with existing low-energy n - d and p - d scattering calculations. [S0556-2813(97)01103-5]

PACS number(s): 21.45.+v, 03.65.Nk, 02.30.Rz, 02.60.Nm

I. INTRODUCTION

Since the Faddeev equations are the fundamental equations of the three-body problems their solutions are of central interest in many branches of physics. This is especially true in nuclear physics because three-body calculations serve as a distinguished tool for studying the fundamental nucleon-nucleon interactions. A general interaction may have a local or nonlocal short-range part and a long-range Coulomb part. The solution of the Faddeev equations with such type of potentials is not an easy job, especially the Coulomb interaction and the scattering dynamics make the procedure very complicated. There exists extensive literature on the subject (see, e.g., Refs. [1–3] and references therein) so we restrict ourselves only to practical approaches.

There are two genuinely different approaches in the practical Faddeev calculations that in some extent can handle Coulomb-like interactions in scattering-state problems. One of them is based on the solution of the configuration-space differential equations using the asymptotic boundary conditions [4]. In the other approach, in order that the standard techniques could be applied, the long-range Coulomb potential is screened, and then, as the screened Coulomb potential goes to the unscreened one, a renormalization procedure is applied [5]. However, in spite of the rapid development we have witnessed in the past few years, only limited solutions below or above the breakup threshold are available yet (see, e.g., Refs. [6–8]).

Another approach to the nuclear three-body problem with Coulomb interaction were derived along the two-potential formalism. The first, and formally exact, approach was proposed by Noble [9]. In this formulation all the Coulomb interactions were included in “free” Green’s operator. Thus the corresponding Faddeev-Noble equations are mathematically well behaved and in the absence of Coulomb interaction they fall back to the standard equations. However, the associated Green’s operator is not known, so this formalism is not suitable for practical calculations.

The aim of this paper is to treat the three-body Coulomb scattering problem via the solution of the Faddeev-Noble integral equations. In Sec. I below we shall derive a “three-potential” formalism. We will arrive at a set of Lippmann-Schwinger and Faddeev equations which form a mathematically well-behaved set of integral equations. In Sec. II below we shall describe how the solution can be reached. In Sec. III below we shall compare our calculations with existing

benchmark n - d and p - d below-breakup scattering results. It is found that in all cases excellent agreement is achieved. The method therefore appear as a promising and efficient tool for solving the Coulomb three-body scattering problem, as it can be adapted to more general cases and can be extended to above-breakup Coulomb scattering calculations.

II. THREE-POTENTIAL FORMALISM FOR THE THREE-BODY COULOMB SCATTERING PROBLEM

The Noble’s approach, which is, in fact, a two-potential formalism, requires the knowledge of the complete solution of the three-body Coulomb problem. Bencze has suggested to replace the incalculable three-body Coulomb Green’s operator by the channel-distorted Coulomb Green’s operator [10]. In this section below we will follow the derivation of Ref. [10], but instead of neglecting the intermediate range polarization potential, we will link the three-body Coulomb Green’s operator to the channel-distorted Coulomb Green’s operator via a Lippmann-Schwinger equation. Thus we will arrive at a set of Faddeev-Noble and Lippmann-Schwinger integral equations which are mathematically well behaved because all the long-range interactions are kept in the Green’s operator.

The Hamiltonian of a three-body system with short-range plus Coulomb two-body interactions reads

$$H = H^0 + v_\alpha^s + v_\beta^s + v_\gamma^s + v_\alpha^C + v_\beta^C + v_\gamma^C, \quad (1)$$

where H^0 is the three-body kinetic energy operator, v_α denotes the interaction in subsystem α , and the superscript s and C stand for short range and Coulomb, respectively. We introduce here the usual configuration-space Jacobi coordinates ξ_α and η_α ; ξ_α is the coordinate between the pair (β, γ) and η_α is the coordinate between the particle α and the center of mass of the pair (β, γ) . Thus the potential v_α , the interaction between the pair (β, γ) , appears as $v_\alpha(\xi_\alpha)$.

The asymptotic Hamiltonian is defined as

$$H_\alpha = H^0 + v_\alpha^s + v_\alpha^C, \quad (2)$$

and the asymptotic states are the eigenstates of H_α

$$H_\alpha |\Phi_\alpha\rangle = E |\Phi_\alpha\rangle, \quad (3)$$

where $\langle \xi_\alpha \eta_\alpha | \Phi_\alpha \rangle = \langle \eta_\alpha | \chi_\alpha \rangle \langle \xi_\alpha | \phi_\alpha \rangle$, a product of a free motion in coordinate η_α and a bound-state in the two-body subsystem ξ_α .

We define two asymptotic Coulomb Hamiltonians as

$$H_\alpha^C = H^0 + v_\alpha^s + v_\alpha^C + v_\beta^C + v_\gamma^C \quad (4)$$

and

$$\tilde{H}_\alpha = H^0 + v_\alpha^s + v_\alpha^C + u_\alpha^C, \quad (5)$$

where u_α^C is an auxiliary potential in coordinate η_α , which is required to have the asymptotic form

$$u_\alpha^C \sim \frac{Z_\alpha(Z_\beta + Z_\gamma)}{\eta_\alpha} \quad (6)$$

as $\eta_\alpha \rightarrow \infty$. In fact u_α^C is an effective Coulomb interaction between the center of mass of the subsystem α (with charge $Z_\beta + Z_\gamma$) and the third particle (with charge Z_α).

Let us introduce the resolvent operators,

$$G(z) = (z - H)^{-1}, \quad (7)$$

$$G_\alpha^C(z) = (z - H_\alpha^C)^{-1}, \quad (8)$$

$$\tilde{G}_\alpha(z) = (z - \tilde{H}_\alpha)^{-1}. \quad (9)$$

The operator G_α^C is Noble's channel Coulomb Green's operator and \tilde{G}_α is the channel distorted Coulomb Green's operator introduced by Bencze [10]. These operators are connected via the following resolvent relations:

$$G(z) = G_\alpha^C(z) + G_\alpha^C(z) V^\alpha G(z), \quad (10)$$

$$G_\alpha^C(z) = \tilde{G}_\alpha(z) + \tilde{G}_\alpha(z) U^\alpha G_\alpha^C(z), \quad (11)$$

where $V^\alpha = v_\beta^s + v_\gamma^s$ and $U^\alpha = v_\beta^C + v_\gamma^C - u_\alpha^C$.

In the potential U^α the Coulomb tail of $v_\beta^C + v_\gamma^C$ is compensated by u_α^C . As concerning the asymptotic motion U^α is of short-range type, so Eq. (11) is mathematically well behaved. The scattering states

$$|\Phi_\alpha^{C(\pm)}\rangle = \lim_{\varepsilon \rightarrow 0} i\varepsilon G_\alpha^C(E \pm i\varepsilon) |\Phi_\alpha\rangle \quad (12)$$

satisfy the Lippmann-Schwinger equations

$$|\Phi_\alpha^{C(\pm)}\rangle = |\tilde{\Phi}_\alpha^{(\pm)}\rangle + \tilde{G}_\alpha(E \pm i0) U_\alpha |\Phi_\alpha^{C(\pm)}\rangle, \quad (13)$$

where

$$|\tilde{\Phi}_\alpha^{(\pm)}\rangle = \lim_{\varepsilon \rightarrow 0} i\varepsilon \tilde{G}_\alpha(E \pm i\varepsilon) |\Phi_\alpha\rangle. \quad (14)$$

In configuration-space representation the states $|\tilde{\Phi}_\alpha^{(\pm)}\rangle$ are given as

$$\langle \xi_\alpha \eta_\alpha | \tilde{\Phi}_\alpha^{(\pm)} \rangle = \langle \eta_\alpha | \tilde{\chi}_\alpha^{(\pm)} \rangle \langle \xi_\alpha | \phi_\alpha \rangle, \quad (15)$$

where $\langle \eta_\alpha | \tilde{\chi}_\alpha^{(\pm)} \rangle$ are scattering functions in the Coulomb-like potential u_α^C .

In Eq. (10) the potential V^α is of short-range type and G_α^C contains all the Coulomb interactions. Now, all the formulas which exist in the conventional short-range three-body theory can analogously be derived, only the channel Green's operator G_α has to be replaced, à la Noble, by G_α^C throughout. One can analogously perform the Faddeev decomposition and for the Faddeev components $|\psi_\alpha^{(\pm)}\rangle$ of the scattering function

$$|\Psi_\alpha^{(\pm)}\rangle = \lim_{\varepsilon \rightarrow 0} i\varepsilon G(E_\alpha \pm i\varepsilon) |\Phi_\alpha\rangle \quad (16)$$

one arrives at the Faddeev-Noble integral equations

$$|\psi_\alpha^{(\pm)}\rangle = \delta_{\beta\alpha} |\Phi_{\alpha m}^{C(\pm)}\rangle + G_\alpha^C(E \pm i0) [v_\alpha^s |\psi_\beta^{(\pm)}\rangle + v_\alpha^s |\psi_\gamma^{(\pm)}\rangle] \quad (17)$$

with a cyclic permutation in α, β, γ .

The S -matrix elements of scattering processes can be obtained from the resolvent of the total Hamiltonian by the reduction technique [11]

$$S_{\beta n, \alpha m} = \lim_{t \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} i\varepsilon e^{i(E_{\beta n} - E_{\alpha m})t} \langle \Phi_{\beta n} | G(E_{\alpha m} + i\varepsilon) | \Phi_{\alpha m} \rangle. \quad (18)$$

The subscript m and n denote the m th and n th eigenstates of the corresponding subsystems, respectively. If we substitute now Eq. (10) into Eq. (18) we can get, like in [10], the following two terms:

$$S_{\beta n, \alpha m}^{(1,2)} = \lim_{t \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} i\varepsilon e^{i(E_{\beta n} - E_{\alpha m})t} \langle \Phi_{\beta n} | G_\alpha^C(E_{\alpha m} + i\varepsilon) | \Phi_{\alpha m} \rangle, \quad (19)$$

$$S_{\beta n, \alpha m}^{(3)} = \lim_{t \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} i\varepsilon e^{i(E_{\beta n} - E_{\alpha m})t} \langle \Phi_{\beta n} | G_\alpha^C(E_{\alpha m} + i\varepsilon) \times V^\beta G(E_{\alpha m} + i\varepsilon) | \Phi_{\alpha m} \rangle. \quad (20)$$

We substitute again Eq. (11) into Eq. (19) and the first term yields again two further terms

$$S_{\beta n, \alpha m}^{(1)} = \lim_{t \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} i\varepsilon e^{i(E_{\beta n} - E_{\alpha m})t} \langle \Phi_{\beta n} | \tilde{G}_\alpha(E_{\alpha m} + i\varepsilon) | \Phi_{\alpha m} \rangle, \quad (21)$$

$$S_{\beta n, \alpha m}^{(2)} = \lim_{t \rightarrow \infty} \lim_{\varepsilon \rightarrow 0} i\varepsilon e^{i(E_{\beta n} - E_{\alpha m})t} \langle \Phi_{\beta n} | \tilde{G}_\alpha(E_{\alpha m} + i\varepsilon) \times U^\alpha G_\alpha^C(E_{\alpha m} + i\varepsilon) | \Phi_{\alpha m} \rangle. \quad (22)$$

Making use of the properties of the resolvent operators the limits can be performed and we arrive at the following, physically very plausible, result. The first term, $S_{\beta n, \alpha m}^{(1)}$, is the S matrix of a two-body single channel scattering on the potential u_α^C

$$S_{\beta n, \alpha m}^{(1)} = \delta_{\beta\alpha} \delta_{nm} S(u_\alpha^C). \quad (23)$$

If u_α^C is a pure Coulomb interaction $S(u_\alpha^C)$ falls back to the S matrix of the Rutherford scattering. The second term, $S_{\beta n, \alpha m}^{(2)}$, describes a two-body multichannel scattering on the potential U^α

$$S_{\beta n, \alpha m}^{(2)} = -2\pi i \delta_{\beta\alpha} \delta(E_{\beta n} - E_{\alpha m}) \langle \tilde{\Phi}_{\beta n}^{(-)} | U^\alpha | \Phi_{\alpha m}^{C(+)} \rangle. \quad (24)$$

The third term gives an account of the complete three-body dynamics

$$S_{\beta n, \alpha m}^{(3)} = -2\pi i \delta(E_{\beta n} - E_{\alpha m}) \langle \Phi_{\beta n}^{C(-)} | V^\beta | \Psi_{\alpha m}^{(+)} \rangle. \quad (25)$$

Utilizing the properties of the Faddeev components [12] the matrix elements in Eq. (25) can be rewritten in a form which is better suited for numerical calculations

$$\langle \Phi_{\beta n}^{C(-)} | V^\beta | \Psi_{\alpha m}^{(+)} \rangle = \sum_{\gamma \neq \beta} \langle \Phi_{\beta n}^{C(-)} | v_\beta^s | \psi_{\gamma m}^{(+)} \rangle. \quad (26)$$

We note, that if the Coulomb interactions are absent the whole ‘‘three-potential’’ formalism falls back to the conventional short-range formalism.

III. SOLUTION OF THE THREE-BODY INTEGRAL EQUATIONS

To solve operator equations in quantum mechanics one needs a suitable representation for the operators. For solving integral equations it is especially advantageous if one uses such a representation where the Green’s operator is simple. The free Green’s operator takes a very simple form in momentum representation. This is the main reason why for the solution of Faddeev equations, in the presence of short-range interactions, momentum-representation techniques are performing so successfully (see for a recent review Ref. [13]). Since the momentum representation is a continuous representation, to solve the equation one needs also some kind of discretization.

For the two-body Coulomb Green’s operator there exists a Hilbert-space basis in which its representation is very simple, it is the Coulomb-Sturmian (CS) basis. In this representation space the Coulomb Green’s operator can be given by simple and well-computable analytic functions [14]. This basis is a countable set. If we represent the interaction term on a finite subset of the basis it looks like a kind of separable expansion of the potential, so the integral equation becomes an algebraic equation. The completeness of the basis ensures the convergence of the method.

In the past few years along this idea we have developed a quantum-mechanical approximation method for treating Coulomb-like interactions in two-body calculations. Bound- and resonant-state calculations were presented first [14], then the method was extended to scattering states [15] and multi-channel problems [16]. Since only the asymptotically irrelevant short range interaction is approximated, the correct (two-body) Coulomb asymptotics is guaranteed. The corresponding computer codes for solving two-body bound-, resonant-, and scattering-state problems were also published [17].

Recently the CS separable expansion approach was applied for solving the three-body bound-state problem in the presence of short-range plus repulsive Coulomb interactions [18]. The homogeneous Faddeev-Noble integral equations were solved by expanding only the short-range part of the interaction in a separable form while treating the long-range part in an exact manner. The efficiency of the method was

demonstrated in benchmark calculations of the three-body bound-state problem without and with Coulomb interactions. In both cases the solution showed a rapid convergence and, whenever comparisons were possible to existing results in the literature, correct predictions for the binding energies and wave functions were achieved. The method was also applied in realistic calculations [19].

In Sec. III A below we will define the basis states in two- and three-particle Hilbert space. In Sec. III B below we recapitulate some of the most important formulas of the two-body problem (the details are given in Refs. [14,15,17]), while in Sec. III C below the solution of the three-body Coulomb scattering problem along the CS separable expansion technique is presented.

A. Basis states

The CS functions, which are the solutions of the Sturm-Liouville problem of hydrogenic systems [20], in some angular momentum state l are defined in configuration and momentum space as

$$\langle r | nl \rangle = \left[\frac{n!}{(n+2l+1)!} \right]^{1/2} (2br)^{l+1} e^{-br} L_n^{2l+1}(2br) \quad (27)$$

and

$$\langle p | nl \rangle = \frac{2^{l+3/2} l! (n+l+1) \sqrt{n!}}{\sqrt{\pi} (n+2l+1)!} \frac{b(2bp)^{l+1}}{(p^2+b^2)^{2l+2}} \times G_n^{l+1} \left(\frac{p^2-b^2}{p^2+b^2} \right), \quad (28)$$

respectively, and $n=0,1,2, \dots$. Here, L and G represent the Laguerre and Gegenbauer polynomials, respectively, and b relates to the energy in the Sturm-Liouville equation. We take b as a fixed real parameter, thus working with energy-independent bound state CS functions. In an angular momentum subspace they form a complete set

$$\mathbf{1} = \lim_{N \rightarrow \infty} \sum_{n=0}^N |\tilde{n}l\rangle \langle nl| = \lim_{N \rightarrow \infty} \mathbf{1}_N, \quad (29)$$

where $|\tilde{n}l\rangle$ in configuration-space representation reads

$$\langle r | \tilde{n}l \rangle = \frac{1}{r} \langle r | nl \rangle. \quad (30)$$

The three-body Hilbert space is a direct sum of two-body Hilbert spaces. Thus, the appropriate basis in angular momentum representation (omitting the explicit spin and isospin dependence from our notation) should be defined as the direct product

$$|n\nu l \lambda\rangle_\alpha = |nl\rangle_\alpha \otimes |\nu \lambda\rangle_\alpha, \quad (n, \nu=0,1,2, \dots), \quad (31)$$

with the CS states from Eq. (27) or Eq. (28). Here l and λ denote the angular momenta of the two-body pair (β, γ) and of the third particle α relative to the center of mass of the

pair, respectively. Now the completeness relation takes the form (with angular momentum summation implicitly included)

$$\mathbf{1} = \lim_{N \rightarrow \infty} \sum_{n, \nu=0}^N |\widetilde{n\nu l \lambda}\rangle_{\alpha\alpha} \langle n\nu l \lambda| = \lim_{N \rightarrow \infty} \mathbf{1}_N^{\alpha}, \quad (32)$$

where the configuration-space representation in terms of Jacobi coordinates ξ_{α} and η_{α} reads

$$\langle \xi_{\alpha} \eta_{\alpha} | \widetilde{n\nu l \lambda} \rangle_{\alpha} = \frac{1}{\xi_{\alpha} \eta_{\alpha}} \langle \xi_{\alpha} \eta_{\alpha} | n\nu l \lambda \rangle_{\alpha}. \quad (33)$$

It should be noted that in the three-particle Hilbert space we can introduce three equivalent bases which belong to fragmentation α , β , and γ .

B. Coulomb-Sturmian separable expansion in two-body problems

Let us study a two-potential case of short-range plus Coulomb-like interactions

$$v_l = v_l^s + v^C \quad (34)$$

and consider the inhomogeneous Lippmann-Schwinger equation for the scattering state $|\psi_l\rangle$ in some partial wave l

$$|\psi_l\rangle = |\phi_l^C\rangle + g_l^C(E) v_l^s |\psi_l\rangle. \quad (35)$$

Here $|\phi_l^C\rangle$ is the regular Coulomb function, $g_l^C(E)$ is the two-body Coulomb Green's operator

$$g_l^C(E) = (E - h_l^0 - v^C)^{-1} \quad (36)$$

with the free Hamiltonian denoted by h_l^0 . We make the following approximation on Eq. (35)

$$|\psi_l\rangle = |\varphi_l^C\rangle + g_l^C(E) \mathbf{1}_N v_l^s \mathbf{1}_N |\psi_l\rangle, \quad (37)$$

i.e., we approximate the short-range potential v_l^s by a separable form

$$v_l^s \approx \sum_{n, n'=0}^N |\widetilde{nl}\rangle v_l^s \langle \widetilde{n'l}|, \quad (38)$$

where

$$\underline{v}_l^s = \langle nl | v_l^s | n'l \rangle. \quad (39)$$

Multiplied with the CS states $\langle \widetilde{n'l}|$ from the left, Eq. (37) turns into a linear system of equations for the wave-function coefficients $\underline{\psi}_{ln} = \langle \widetilde{n'l} | \psi_l \rangle$

$$[(g_l^C(E))^{-1} - \underline{v}_l^s] \underline{\psi}_l = \underline{\varphi}_l^C, \quad (40)$$

where

$$\underline{\varphi}_{ln}^C = \langle \widetilde{n'l} | \varphi_l^C \rangle \quad (41)$$

and

$$\underline{g}_{lnn'}^C(E) = \langle \widetilde{n'l} | g_l^C(E) | \widetilde{n'l} \rangle. \quad (42)$$

While the matrix elements of the potential may be evaluated (numerically) for any given short-range potential either in configuration or in momentum space, the matrix elements (42) and the overlap (41) can be calculated analytically [14]; the corresponding computer code is available from Ref. [17]. This fact then also allows to calculate the matrix elements of the full Green's operator in the whole complex plane,

$$\underline{g}_l(z) = \{[\underline{g}_l^C(z)]^{-1} - \underline{v}_l^s\}^{-1}, \quad (43)$$

this will be needed later on in the solution of the three-body problem with charged particles. Of course, bound-state solutions can also be generated by solving the homogeneous version of Eq. (40).

C. Coulomb-Sturmian separable expansion approach to three-body Coulomb scattering problems

In the set of Faddeev-Noble equations (17) we make the following approximation:

$$|\psi_{\alpha}\rangle = \delta_{\beta\alpha} |\Phi_{\alpha m}^C\rangle + G_{\alpha}^C [\mathbf{1}_N v_{\alpha}^s \mathbf{1}_N^{\beta} |\psi_{\beta}\rangle + \mathbf{1}_N v_{\alpha}^s \mathbf{1}_N^{\gamma} |\psi_{\gamma}\rangle], \quad (44)$$

i.e., we approximate the short-range potential v_{α}^s in the three-body Hilbert space by a separable form

$$v_{\alpha}^s \approx \sum_{n, \nu, n', \nu'=0}^N |\widetilde{n\nu l \lambda}\rangle_{\alpha} v_{\alpha\beta}^s \langle \widetilde{n' \nu' l' \lambda'} |, \quad (45)$$

where

$$\underline{v}_{l\alpha\lambda\alpha n\nu, l'\beta\lambda'\beta n'\nu'}^s = (1 - \delta_{\alpha\beta})_{\alpha} \langle n\nu l \lambda | v_{\alpha}^s | n' \nu' l' \lambda' \rangle_{\beta}. \quad (46)$$

In Eq. (45) the ket and bra states are in different fragmentation depending on the environments of the potential operators in the equations.

Multiplying with the CS states ${}_{\alpha} \langle \widetilde{n\nu l \lambda} |$ from the left, Eqs. (44) turn into a linear system of equations for the coefficients of the Faddeev components $\underline{\psi}_{l\alpha\lambda\alpha n\nu} = {}_{\alpha} \langle \widetilde{n\nu l \lambda} | \psi_{\alpha} \rangle$:

$$[(G^C)^{-1} - \underline{v}^s] \underline{\psi} = \underline{\Phi}^C, \quad (47)$$

with

$$\underline{G}_{l\alpha\lambda\alpha n\nu, l'\alpha\lambda'\alpha n'\nu'}^C = \delta_{\alpha\beta} {}_{\alpha} \langle \widetilde{n\nu l \lambda} | G_{\alpha}^C | \widetilde{n' \nu' l' \lambda'} \rangle_{\alpha} \quad (48)$$

and

$$\underline{\Phi}_{l\alpha\lambda\alpha n\nu}^C = {}_{\alpha} \langle \widetilde{n\nu l \lambda} | \Phi_{\alpha}^C \rangle. \quad (49)$$

Notice that the matrix elements of the Green's operator are needed only between the same partition α whereas the matrix elements of the potentials occur only between different partitions α and β . The latter may again be evaluated numerically either in configuration or momentum space by making use of the transformation of Jacobi coordinates [21].

Unfortunately neither the matrix elements (48) nor the overlap (49) are known. However, Eqs. (11) and (13), which are, in fact, two-body Lippmann-Schwinger equations, link them to relatively simpler quantities. If we perform again the

separable approximation on potential U^α with the help of the formal solution of Eq. (11) we may now express the inverse matrix $[\underline{G}_\alpha^C(E)]^{-1}$ as

$$(\underline{G}_\alpha^C)^{-1} = (\underline{\tilde{G}}_\alpha)^{-1} - \underline{U}^\alpha, \quad (50)$$

where

$$\underline{\tilde{G}}_{l_\alpha \lambda_\alpha n v, l'_\alpha \lambda'_\alpha n' v'} = {}_\alpha \langle n v l \lambda | \underline{\tilde{G}}_\alpha | n' v' l' \lambda' \rangle_\alpha \quad (51)$$

and

$$\underline{U}_{l_\alpha \lambda_\alpha n v, l'_\alpha \lambda'_\alpha n' v'}^\alpha = {}_\alpha \langle n v l \lambda | U^\alpha | n' v' l' \lambda' \rangle_\alpha. \quad (52)$$

In a similar way, with the help of the formal solution of Eq. (13) we get

$$\underline{\Phi}_\alpha^C = [(\underline{\tilde{G}}_\alpha)^{-1} - \underline{U}^\alpha]^{-1} (\underline{\tilde{G}}_\alpha)^{-1} \underline{\tilde{\Phi}}_\alpha, \quad (53)$$

where

$$\underline{\tilde{\Phi}}_\alpha = {}_\alpha \langle n v l \lambda | \underline{\tilde{\Phi}}_\alpha \rangle. \quad (54)$$

The state $|\underline{\tilde{\Phi}}_\alpha\rangle$, in fact, is a product of a two-body bound-state wave function in coordinate ξ_α and a two-body scattering-state wave function in coordinate η_α . Their CS representations are known from the two-particle case of the previous section [cf. Eq. (40)].

For the calculation of the matrix elements in Eq. (51) we proceed in a similar way as in the case of three-body bound states [18]. Since in $\underline{\tilde{H}}_\alpha$ of Eq. (5) we can write the three-particle free Hamiltonians as a sum of two-particle free Hamiltonians

$$H^0 = h_{\xi_\alpha}^0 + h_{\eta_\alpha}^0, \quad (55)$$

the Hamiltonian $\underline{\tilde{H}}_\alpha$ appears as a sum of two Hamiltonians acting on different coordinates

$$\underline{\tilde{H}}_\alpha = h_{\xi_\alpha} + h_{\eta_\alpha}, \quad (56)$$

with $h_{\xi_\alpha} = h_{\xi_\alpha}^0 + v_\alpha^s(\xi_\alpha) + v_\alpha^C(\xi_\alpha)$ and $h_{\eta_\alpha} = h_{\eta_\alpha}^0 + u_\alpha^C(\eta_\alpha)$, which, of course, commute. Thus we can apply the convolution theorem [22]

$$\begin{aligned} \underline{\tilde{G}}_\alpha(z) &= (z - h_{\xi_\alpha} - h_{\eta_\alpha})^{-1} \\ &= \frac{1}{2\pi i} \oint_C dw (z - w - h_{\eta_\alpha})^{-1} (w - h_{\xi_\alpha})^{-1}. \end{aligned} \quad (57)$$

Here the contour C should encircle, in positive direction, the spectrum of h_{ξ_α} without penetrating into the spectrum of h_{η_α} . For scattering-state energies at real z these singularities overlap. To find the correct path one should take the $z = E + i\varepsilon$ case with finite ε . Now the condition on C can easily be fulfilled and then, one should take the $\varepsilon \rightarrow 0$ limit allowing only analytic deformation for the contour C [see Fig. 1].

After sandwiching the above Green's operator between the CS states, the integral in Eq. (57) appears in the form

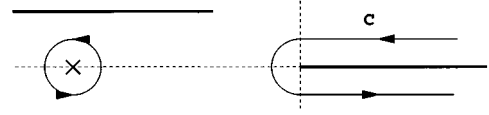


FIG. 1. Contour C for the integral for $\underline{\tilde{G}}_\alpha(E + i\varepsilon)$ in case of the three-body scattering problem. The contour C encircles the continuous and discrete spectrum of h_{ξ_α} . In the $\varepsilon \rightarrow 0$ limit the topology of the contour should be kept.

$$\begin{aligned} &\underline{\tilde{G}}_{l_\alpha \lambda_\alpha n v, l'_\alpha \lambda'_\alpha n' v'}(E + i0) \\ &= \frac{1}{2\pi i} \oint_C dw {}_\alpha \langle \tilde{v} \lambda | (E + i0 - w - h_{\eta_\alpha})^{-1} | \tilde{n} v' \lambda' \rangle_\alpha \\ &\quad \times {}_\alpha \langle \tilde{\eta} l | (w - h_{\xi_\alpha})^{-1} | \tilde{n}' l' \rangle_\alpha, \end{aligned} \quad (58)$$

where both matrix elements occurring in the integrand are known from the two-particle case [cf. Eq. (43)].

IV. TESTS OF THE METHOD

In this section we demonstrate the performance of the method in calculations of three-body short-range and Cou-

TABLE I. Convergence of the ${}^2\delta_{\text{nd}}$ phase shifts for three-nucleon system interacting via the MT I-III potential at various energies, with increasing basis for the separable expansion. N denotes the maximum number of basis states employed for n and v . The phase shifts are in degrees.

N	${}^2\delta_{\text{nd}}$		
	0.1 MeV	1.0 MeV	2.18 MeV
10	-4.0908	-20.704	-32.896
11	-3.6803	-20.330	-33.596
12	-3.8876	-20.450	-33.599
13	-3.4583	-20.630	-33.901
14	-3.5189	-20.562	-33.963
15	-3.3917	-20.629	-33.834
16	-3.3434	-20.653	-33.723
17	-3.3293	-20.636	-33.594
18	-3.2914	-20.660	-33.525
19	-3.2940	-20.652	-33.341
20	-3.2764	-20.654	-33.282
21	-3.2783	-20.656	-33.267
22	-3.2709	-20.653	-33.290
23	-3.2715	-20.655	-33.326
24	-3.2688	-20.654	-33.377
25	-3.2688	-20.654	-33.424
26	-3.2681	-20.654	-33.460
27	-3.2678	-20.654	-33.483
28	-3.2678	-20.654	-33.491
29	-3.2676	-20.654	-33.486
30	-3.2676	-20.654	-33.473
31	-3.2675	-20.654	-33.456
32	-3.2675	-20.654	-33.438
33	-3.2675	-20.654	-33.423
34	-3.2675	-20.654	-33.413

TABLE II. Convergence of the ${}^2\delta_{pd}$ phase shifts for three-nucleon system interacting via the MT I-III potential at various energies, with increasing basis for the separable expansion. N denotes the maximum number of basis states employed for n and ν . The phase shifts are in degrees.

N	${}^2\delta_{pd}$		
	0.1 MeV	1.0 MeV	2.0 MeV
10	-0.9485	-16.376	-28.405
11	-0.7947	-15.924	-28.659
12	-0.8794	-16.089	-28.564
13	-0.6721	-16.195	-28.847
14	-0.7015	-16.138	-28.874
15	-0.6241	-16.210	-28.840
16	-0.5962	-16.226	-28.865
17	-0.5817	-16.216	-28.840
18	-0.5575	-16.241	-28.802
19	-0.5572	-16.232	-28.800
20	-0.5446	-16.238	-28.774
21	-0.5455	-16.238	-28.767
22	-0.5390	-16.236	-28.764
23	-0.5394	-16.238	-28.761
24	-0.5362	-16.236	-28.765
25	-0.5363	-16.237	-28.768
26	-0.5350	-16.237	-28.772
27	-0.5349	-16.237	-28.776
28	-0.5345	-16.237	-28.778
29	-0.5343	-16.237	-28.780
30	-0.5342	-16.237	-28.780
31	-0.5341	-16.237	-28.780
32	-0.5341	-16.237	-28.779
33	-0.5340	-16.237	-28.778
34	-0.5340	-16.237	-28.778

lombic scattering phase shifts at energies below the breakup threshold. We have selected cases that serve as benchmarks for various three-body scattering calculations. As an example we take a model three-nucleon problem with s -wave Malfliet-Tjon (MT) I-III potential, acting in singlet and triplet states, as parametrized in Ref. [6]. We have calculated quartet and doublet n - d and p - d phase shifts and compare them to the results of the configuration-space Faddeev calculations of Ref. [6].

Before presenting the final results, let us demonstrate the convergence of the results for scattering phase shifts at various energies. We take extreme cases, one is at very low energy, another one is just below the breakup threshold, the third one is in between. We select two-channel doublet n - d and p - d cases, because this case is more complicated than the one-channel quartet case. Tables I and II show that convergence up to four significant digits can comfortably be achieved with $N=30$ terms applied for n and ν in the separable expansion. Remarkably, the speed of convergence is everywhere similar, irrespective of energy and whether or not Coulomb forces are present.

In Tables III and IV we compare our converged results to the configuration-space Faddeev calculations of the Los Alamos-Iowa group [6]. We can report perfect agreements in all cases.

In Tables II and IV and also in Ref. [6] the Coulomb

TABLE III. ${}^4\delta_{nd}$ and ${}^2\delta_{nd}$ phase shifts for three-nucleon system interacting via the MT I-III potential at various energies. The phase shifts are in degrees.

E	${}^4\delta_{nd}$		${}^2\delta_{nd}$	
	Ref. [6]	This work	Ref. [6]	This work
0.001	-2.09	-2.092	-0.230	-0.229
0.05	-14.6	-14.62	-1.99	-1.988
0.1	-20.4	-20.44	-3.28	-3.267
0.2	-28.3	-28.29	-5.68	-5.670
0.3	-34.0	-33.98	-7.95	-7.944
0.4	-38.5	-38.54	-10.1	-10.09
0.5	-42.4	-42.37	-12.1	-12.12
0.6	-45.7	-45.69	-14.0	-14.03
0.7	-48.6	-48.63	-15.8	-15.83
0.8	-51.2	-51.27	-17.5	-17.53
0.9	-53.6	-53.66	-19.1	-19.13
1.0	-55.8	-55.86	-20.7	-20.65
1.633	-66.7	-66.72	-28.6	-28.60
2.180	-73.6	-73.6	-33.6	-33.4

modified phase shift from short-range plus polarization potential ($\delta^{c,ps}$) were presented, and the corresponding values were used in the calculation of the scattering lengths $a_{pd}^{c,ps}$. However, since our three-potential formalism allows a unique separation of these two effects we can also calculate the Coulomb plus polarization modified short-range phase shift $\delta^{cp,s}$ and the corresponding scattering lengths $a_{pd}^{cp,s}$. Theoretically the scattering length should be calculated from $\delta^{cp,s}$ since $a_{pd}^{c,ps}$ is minus infinite [23]. In practical calculations the extrapolation to zero energy were made from higher energy and this minus infinity limit were not seen. Careful analyses of low-energy p - d calculations indicated that in these condition $a_{pd}^{c,ps}$ is a good approximation to $a_{pd}^{cp,s}$ [6,8,23,24]. We have calculated the scattering length from

TABLE IV. ${}^4\delta_{pd}$ and ${}^2\delta_{pd}$ phase shifts for three-nucleon system interacting via the MT I-III potential at various energies. The phase shifts are in degrees.

E	${}^4\delta_{pd}$		${}^2\delta_{pd}$	
	Ref. [6]	This work	Ref. [6]	This work
0.001	0.0	0.0	0.0	0.0
0.05	-2.69	-2.694	-0.113	-0.112
0.1	-7.46	-7.458	-0.537	-0.534
0.2	-15.6	-15.56	-1.96	-1.949
0.3	-21.9	-21.86	-3.73	-3.720
0.4	-27.0	-27.00	-5.62	-5.612
0.5	-31.3	-31.34	-7.53	-7.520
0.6	-35.1	-35.11	-9.40	-9.394
0.7	-38.4	-38.43	-11.2	-11.21
0.8	-41.4	-41.40	-13.0	-12.96
0.9	-44.1	-44.09	-14.6	-14.63
1.0	-46.5	-46.55	-16.2	-16.24
0.667	-37.3	-37.37	-10.6	-10.62
1.333	-53.5	-53.49	-21.1	-21.08
2.0	-63.8	-63.74	-28.8	-28.78

both phase shifts using the formula of Ref. [23]

$$a = \lim_{k \rightarrow 0} a(k) = \lim_{k \rightarrow 0} -\frac{\tan \delta(k)}{kC^2(k)}, \quad (59)$$

where k is the wave number and

$$C^2(k) = \frac{2\pi\eta}{e^{2\pi\eta} - 1} \quad (60)$$

with $\eta = me^2/\hbar k$, m being the reduced mass. From $a(k)$ values corresponding to energies down to 0.01 MeV in the doublet case and to 0.001 MeV in the quartet case, where the phase shift still can reliably be calculated, we extrapolated to zero energy. The results are given in Table V. We can see that the effect of the polarization potential can really be neglected in the calculation of the p - d scattering lengths.

Besides the number of terms in the expansion there is only one parameter in the method, the b parameter of the basis. This should be chosen according to the range of the potential. We have found that the converged results do not depend on b and for a wide range of reasonable values even the speed of the convergence is rather insensitive to the choice of b . In all calculations presented the same value was applied ($b = 1 \text{ fm}^{-1}$).

V. CONCLUSION

We have proposed a three-potential formalism for treating the three-body Coulomb scattering problem. In absence of Coulomb interactions the formalism falls back to the usual short-range formalism. According to the three-potential picture the three-body Coulomb scattering starts with a two-body single channel Coulomb scattering, then it goes over to a two-body multichannel scattering on the intermediate-range polarization potential, finally comes the three-body scattering due to the short-range potentials. This formalism preserves the mathematical correctness of the Noble's approach, and along the idea of channel distorted formalism of Bencze, without neglecting important terms, gives solvable equations.

These "solvable" equations are certainly too complicated for most of the numerical methods available in the literature, but the Coulomb-Sturmian separable expansion method can cope with them. It solves the three-body integral equations by expanding only the short-range part of the interaction in a separable form on a Hilbert-space basis while treating the long-range part in an exact manner via a proper integral representation of the three-body channel distorted Coulomb Green's operator. As a consequence the method has good

TABLE V. p - d scattering lengths for three-nucleon system interacting via the MT I-III potential.

	This work	Ref. [6]
$^4\delta_{pd}^{c,ps}$	13.76	13.8
$^4\delta_{pd}^{cp,s}$	13.79	
$^2\delta_{pd}^{c,ps}$	0.161	0.17
$^2\delta_{pd}^{cp,s}$	0.195	

convergence properties and can in practice be made arbitrarily accurate by employing an increasing number of terms in the expansion. The usage of the Coulomb-Sturmian basis is essential as it allows an exact analytic representation of the two-body Green's operator, and thus the contour integral for the channel distorted Coulomb Green's operator can be calculated also in the practice.

We have presented below-breakup calculations and got perfect agreements with existing benchmark results. We have observed a fast convergence with respect to increasing the number of terms in the expansion. Using high rank expansion we got very accurate results. The quality of the convergence is practically the same in the short-range and Coulomb cases, Coulombic calculations need only roughly 30% more computer time. Although the example presented here is rather simple, but not unrealistic, the method can handle more complicated potentials, as were demonstrated in bound state calculations [18,19].

Certainly, the toughest problems in nonrelativistic three-body scattering are the above-breakup calculations with Coulomb interactions. In this respect, the method presented here, is very promising since the equations used are mathematically well behaved also for this case. The extension of the contour integral for above-breakup energies is straightforward. The only foreseeable problem is, that the interaction volume is much bigger and one needs much higher terms in the expansion. Indeed, test calculations show that for energies just a little bit above the breakup threshold with terms up to $N=34$ we can reach acceptable convergence and good agreements with benchmark results [25], but the method fails to reach convergence for higher energies. This indicates that the mathematical formulation is correct, but the available computing power is not sufficient. So, the method needs some more polishing and we have to think a little bit further.

ACKNOWLEDGMENTS

This work has been supported by OTKA under Contract No. T17298.

- [1] E. O. Alt, in *Few-Body Methods: Principles and Applications*, edited by T. K. Lim *et al.* (World Scientific, Singapore, 1986), p. 239.
 [2] C. Chandler, Nucl. Phys. **A463**, 181c (1987).
 [3] Gy. Bencze, P. Doleshall, C. Chandler, A. G. Gibson, and D. Walliser, Phys. Rev. C **43**, 992 (1991).
 [4] S. P. Merkuriev, C. Gignoux, and A. Laverne, Ann. Phys.

- (N.Y.) **39**, 30 (1976); L. D. Faddeev and S. P. Merkuriev, *Quantum Scattering Theory for Several Particle Systems* (Kluwer, Dordrecht, 1993).
 [5] E. O. Alt, W. Sandhas, and H. Ziegelmann, Phys. Rev. C **17**, 1981 (1978); E. O. Alt, Few-Body Syst. Suppl. **1**, 79 (1986).
 [6] C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. C **39**, 1261 (1989).

- [7] E. O. Alt, W. Sandhas, H. Zankel, and H. Ziegelmann, Phys. Rev. Lett. **37**, 1537 (1976); Yu. Kuperin, S. P. Merkuriev, and A. A. Kvitsinsky, Sov. J. Nucl. Phys. **37**, 857 (1983); E. O. Alt, W. Sandhas, and H. Ziegelmann, Nucl. Phys. **A445**, 429 (1985); G. H. Berthold, A. Stadler, and H. Zankel, Phys. Rev. Lett. **61**, 1077 (1988); Phys. Rev. C **41**, 1365 (1990); E. O. Alt and M. Rauh, Few-Body Syst. Suppl. **7**, 160 (1994); E. O. Alt and M. Rauh, Few-Body Syst. **17**, 121 (1994).
- [8] G. H. Berthold and H. Zankel, Phys. Rev. C **34**, 1203 (1986).
- [9] J. V. Noble, Phys. Rev. **161**, 945 (1967).
- [10] Gy. Bencze, Nucl. Phys. **A196**, 135 (1972).
- [11] E. O. Alt, P. Grassberger, and W. Sandhas, Nucl. Phys. **B2**, 167 (1967).
- [12] W. Glöckle, *The Quantum Mechanical Few-Body Problem* (Springer, Berlin, 1983).
- [13] W. Glöckle, H. Witała, D. Hüber, H. Hamada, and J. Golak, Phys. Rep. **274**, 107 (1996).
- [14] Z. Papp, J. Phys. A **20**, 153 (1987).
- [15] Z. Papp, Phys. Rev. C **38**, 2457 (1988); Phys. Rev. A **46**, 4437 (1992).
- [16] Z. Papp and E. W. Schmid, Few-Body Syst. **13**, 159 (1992).
- [17] Z. Papp, Comput. Phys. Commun. **70**, 426 (1992); **70**, 435 (1992).
- [18] Z. Papp and W. Plessas, Phys. Rev. C **54**, 50 (1996).
- [19] L. Ya. Glozman, Z. Papp, and W. Plessas, Phys. Lett. B **381**, 311 (1996).
- [20] M. Rotenberg, Ann. Phys. (N.Y.) **19**, 262 (1962); Adv. At. Mol. Phys. **6**, 233 (1970).
- [21] R. Balian and E. Brézin, Nuovo Cimento B **2**, 403 (1969).
- [22] L. Bianchi and L. Favella, Nuovo Cimento **6**, 6873 (1964).
- [23] Gy. Bencze, C. Chandler, J. L. Friar, A. G. Gibson, and G. L. Payne, Phys. Rev. C **35**, 1188 (1987).
- [24] H. Zankel and L. Mathelitsch, Phys. Lett. **132B**, 27 (1983); L. Tomio, A. Delfino, and S. K. Adhikari, Phys. Rev. C **35**, 441 (1987); S. K. Adhikari and T. K. Das, *ibid.* **37**, 1376 (1988).
- [25] J. L. Friar, B. F. Gibson, G. Berthold, W. Glöckle, Th. Cornelius, H. Witała, J. Haidenbauer, Y. Koike, G. L. Payne, T. A. Tjon, and W. M. Kloet, Phys. Rev. C **42**, 1838 (1990).