Three-potential formalism for the three-body scattering problem with attractive Coulomb interactions

Z. Papp,[1,2] C-.Y. Hu,[1] Z. T. Hlousek,[1] B. Kónya,[2] and S. L. Yakovlev[3]
[1]*Department of Physics and Astronomy, California State University, Long Beach, California 90840*
[2]*Institute of Nuclear Research of the Hungarian Academy of Sciences, Debrecen, Hungary*
[3] *Department of Mathematical and Computational Physics, St. Petersburg State University, St. Petersburg, Russia*
(Received 9 February 2001; published 16 May 2001)

A three-body scattering process in the presence of Coulomb interaction can be decomposed formally into two-body single channel scattering, two-body multichannel scattering, and genuine three-body scattering. The corresponding integral equations are coupled Lippmann-Schwinger and Faddeev-Merkuriev integral equations. We solve these by applying the Coulomb-Sturmian separable expansion method. We present elastic scattering and reaction cross sections of the $e^+ + H$ system both below and above the $H(n=2)$ threshold. We find excellent agreements with previous calculations in most cases.

DOI: 10.1103/PhysRevA.63.062721 PACS number(s): 34.10.+x, 31.15.−p, 34.85.+x, 21.45.+v

The three-body Coulomb scattering problem is one of the most challenging long-standing problems of nonrelativistic quantum mechanics. The source of the difficulties is related to the long-range character of the Coulomb potential. In standard scattering theory it is supposed that particles move freely asymptotically. This is not the case if Coulombic interactions are involved. As a result, the fundamental equations of the three-body problems, the Faddeev equations, become ill behaved if they are applied for Coulomb potentials in a straightforward manner.

The first, and most formally exact, approach was proposed by Noble [1]. His formulation was designed to solve the nuclear three-body Coulomb problem, where all Coulomb interactions are repulsive. The interactions were split into short and long-range Coulomb-like parts and the long-range parts were formally included in the ''free'' Green's operator. Therefore, the corresponding Faddeev-Noble equations become mathematically well-behaved, and in the absence of Coulomb interaction fell back to the standard equations. However, the associated Green's operator was not known. This formalism, as presented at that time, was not suitable for practical calculations.

In Noble's approach the separation of the Coulomb-like potential into short and long-range parts was carried out in two-body configuration space. Merkuriev extended the idea of Noble by performing the splitting in three-body configuration space. This was a crucial development, since it made it possible to treat attractive Coulomb interactions on an equal footing with repulsive ones. This theory was developed using integral equations with connected (compact) kernels, and transformed into configuration-space differential equations with asymptotic boundary conditions [2]. In practical calculations, so far only the latter version of the theory was considered. The primary reason is that the more complicated structure of the Green's operators in the kernels of the Faddeev-Merkuriev integral equations has not yet allowed any direct solution. However, use of integral equations is a very appealing approach, since no boundary conditions are required.

Recently, one of us developed a method for treating the three-body problem with repulsive Coulomb interactions in three-potential picture [3]. In this approach a three-body Coulomb scattering process can be decomposed formally into two-body single channel scattering, two-body multichannel scattering, and genuine three-body scattering. The corresponding integral equations are coupled Lippmann-Schwinger and Faddeev-Noble integral equations, which were solved using the Coulomb-Sturmian separable expansion method. The approach was tested first for bound-state problems [4] with repulsive Coulomb plus nuclear potentials. Then it was extended to calculate p-d scattering at energies below the breakup threshold [3]. More recently we used this method to calculate resonances of three-α systems [5]. Also, atomic bound-state problems with attractive Coulomb interactions were considered [6]. These calculations showed an excellent agreement with the results of other well-established methods. The efficiency and the accuracy of the method was demonstrated.

The aim of this paper is to generalize this method for solving the three-body Coulomb problem with repulsive and attractive Coulomb interactions. We combine the concept of three-potential formalism with Merkuriev's splitting of the interactions, and solve the resulting set of Lippmann-Schwinger and Faddeev-Merkuriev integral equations by applying the Coulomb-Sturmian separable expansion method. In this paper we restrict ourselves to energies below the three-body breakup threshold.

I. INTEGRAL EQUATIONS OF THE THREE-POTENTIAL PICTURE

We consider a three-body system with a Hamiltonian,

$$H = H^0 + v_\alpha^C + v_\beta^C + v_\gamma^C, \tag{1}$$

where H^0 is the three-body kinetic-energy operator, and v_α^C denotes the Coulomb-like interaction in subsystem α. The potential v_α^C may have a repulsive or attractive Coulomb tail and any short-range component. We use the typical configuration-space Jacobi coordinates x_α and y_α; x_α is a coordinate between the pair (β,γ), and y_α is a coordinate between the particle α and the center of mass of the pair

 ©2001 The American Physical Society

(β,γ). Thus the potential v_α^C, the interaction of the pair (β,γ), appears as $v_\alpha^C(x_\alpha)$. We also use the notation $X=\{x_\alpha,y_\alpha\}\in\mathbf{R}^6$.

A. Merkuriev's cut of the Coulomb potential

Hamiltonian (1) is defined in the three-body Hilbert space. The two-body potential operators are formally embedded in the three-body Hilbert space

$$v^C=v^C(x)\mathbf{1}_{y)}, \tag{2}$$

where $\mathbf{1}_y$ is a unit operator in the two-body Hilbert space associated with the y coordinate. Faddeev and Merkuriev introduced a separation of the three-body configuration space into different asymptotic regions. The two-body asymptotic region Ω_α is defined as a part of the three-body configuration space where the conditions

$$|x_\alpha|<x_\alpha^0(1+|y_\alpha|/y_\alpha^0)^{1/\nu}, \tag{3}$$

with $x_\alpha^0,y_\alpha^0>0$ and $\nu>2$, are satisfied. They proposed splitting the Coulomb interaction in the three-body configuration space into short and long-range terms,

$$v_\alpha^C=v_\alpha^{(s)}+v_\alpha^{(l)}, \tag{4}$$

where the superscripts s and l indicate the short- and long-range attributes, respectively. The splitting is carried out with the help of a splitting function ζ:

$$v^{(s)}(x,y)=v^C(x)\zeta(x,y), \tag{5}$$

$$v^{(l)}(x,y)=v^C(x)[1-\zeta(x,y)]. \tag{6}$$

The function ζ is defined such that

$$\zeta(x,y)\xrightarrow{X\to\infty}\begin{cases}1, & X\in\Omega_\alpha\\ 0 & \text{otherwise.}\end{cases} \tag{7}$$

In practice, in the configuration-space differential equation approaches, usually the functional form

$$\zeta(x,y)=2/\{1+[(x/x^0)^\nu/(1+y/y^0)]\} \tag{8}$$

was used.

The long-range Hamiltonian is defined as

$$H^{(l)}=H^0+v_\alpha^{(l)}+v_\beta^{(l)}+v_\gamma^{(l)}, \tag{9}$$

and its resolvent operator is

$$G^{(l)}(z)=(z-H^{(l)})^{-1}. \tag{10}$$

Then the three-body Hamiltonian takes the form

$$H=H^{(l)}+v_\alpha^{(s)}+v_\beta^{(s)}+v_\gamma^{(s)}. \tag{11}$$

In the conventional Faddeev theory the wave-function components are defined by

$$|\psi_\alpha\rangle=(z-H^0)^{-1}v_\alpha|\Psi\rangle, \tag{12}$$

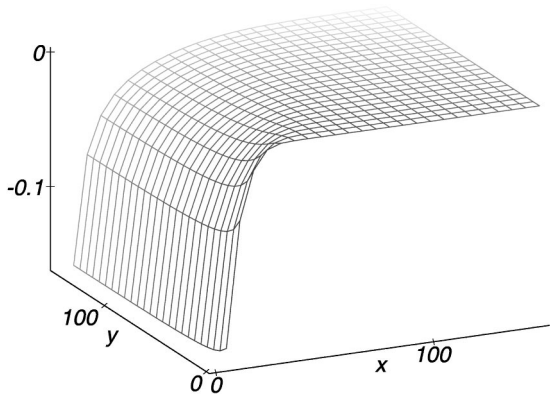

FIG. 1. The short-range part $v^{(s)}$ of the $-1/x$ attractive Coulomb potential.

where v_α is a short-range potential and $|\psi_\alpha\rangle$ is the Faddeev component of the total wave function $|\Psi\rangle$. While the total wave function $|\Psi\rangle$, in general, has three different kind of two-body asymptotic channels, $|\psi_\alpha\rangle$ possesses only α-type two-body asymptotic channels. The other channels are suppressed by the short-range potential v_α. This procedure is called asymptotic filtering, and it guarantees the asymptotic orthogonality of the Faddeev components [7].

The aim of the Merkuriev procedure was to formally obtain a three-body Hamiltonian with short-range potentials $v^{(s)}$ and a long-range Hamiltonian $H^{(l)}$, in order that we could repeat the procedure of the conventional Faddeev theory. The total wave function $|\Psi\rangle$ is split into three components,

$$|\Psi\rangle=|\psi_\alpha\rangle+|\psi_\beta\rangle+|\psi_\gamma\rangle, \tag{13}$$

with components defined by

$$|\psi_\alpha\rangle=G^{(l)}v_\alpha^{(s)}|\Psi\rangle. \tag{14}$$

This procedure is an example of asymptotic filtering. The short-range potential $v_\alpha^{(s)}$ acting on $|\Psi\rangle$ suppresses the possible β and γ asymptotic two-body channels, provided $G^{(l)}$ itself does not introduce any new two-body asymptotic channels. With the Merkuriev splitting this is avoided, because $H^{(l)}$ does not have two-body asymptotic channels even if some of the long-range potentials have an attractive Coulomb tail. In the attractive case $v^{(l)}$ appears as a valley along the $y=x^\nu$ parabolalike curve, with a Coulomb-like asymptotic behavior in x at any finite y (see Figs. 1 and 2 for the short- and long-range parts, respectively). However, as $y\to\infty$ the depth of the valley goes to zero, and consequently the two-body bound states are pushed up, and finally the system does not have any two-body asymptotic channels. We note that the Merkuriev formalism contains Noble's formalism in the limit $y^0\to\infty$.

B. Three-potential picture

In Ref. [3] the three-body scattering problem with repulsive Coulomb interactions was considered in the three-potential picture. In this picture the scattering process can be decomposed formally into three consecutive scattering pro-

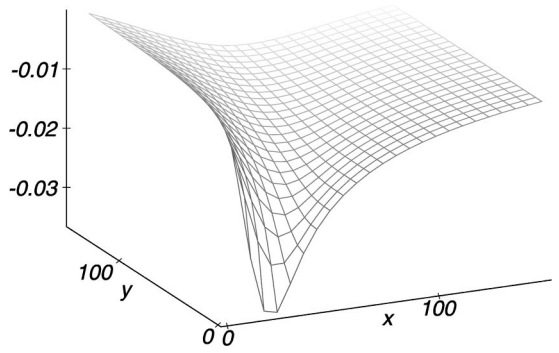

FIG. 2. The long-range part $v^{(l)}$ of the $-1/x$ attractive Coulomb potential.

cesses: two-body single channel, two-body multichannel scattering and genuine three-body scattering. This formalism also provides the integral equations and the method of constructing the S matrix. Below we adapt this formalism to attractive Coulomb interactions using the Faddeev-Merkuriev approach.

The asymptotic Hamiltonian is defined as

$$H_\alpha = H^0 + v_\alpha^C, \tag{15}$$

and the asymptotic states are the eigenstates of H_α,

$$H_\alpha |\Phi_\alpha\rangle = E|\Phi_\alpha\rangle, \tag{16}$$

where $\langle x_\alpha y_\alpha|\Phi_\alpha\rangle = \langle y_\alpha|\chi_\alpha\rangle\langle x_\alpha|\phi_\alpha\rangle$ is a product of a scattering state in coordinate y_α and a bound state in the two-body subsystem x_α.

We define the two asymptotic long-range Hamiltonians as

$$H_\alpha^{(l)} = H^0 + v_\alpha^C + v_\beta^{(l)} + v_\gamma^{(l)} \tag{17}$$

and

$$\tilde{H}_\alpha = H^0 + v_\alpha^C + u_\alpha^{(l)}, \tag{18}$$

where $u_\alpha^{(l)}$ is an auxiliary potential in coordinate y_α, and it is required to have the asymptotic form

$$u_\alpha^{(l)} \sim Z_\alpha (Z_\beta + Z_\gamma)/y_\alpha \tag{19}$$

as $y_\alpha \to \infty$. In fact, $u_\alpha^{(l)}$ is an effective Coulomb-like interaction between the center of mass of the subsystem α (with charge $Z_\beta + Z_\gamma$) and the third particle (with charge Z_α). We introduced this potential in order that we compensate for the long-range Coulomb tail of $v_\beta^{(l)} + v_\gamma^{(l)}$ in Ω_α.

Let us introduce the resolvent operators

$$G(z) = (z - H)^{-1}, \tag{20}$$

$$G_\alpha^{(l)}(z) = (z - H_\alpha^{(l)})^{-1}, \tag{21}$$

$$\tilde{G}_\alpha(z) = (z - \tilde{H}_\alpha)^{-1}. \tag{22}$$

The operator $G_\alpha^{(l)}$ is the long-range channel Green's operator, and $\tilde{G}_\alpha$ is the channel-distorted long-range Green's operator. These operators are connected via the resolvent relations

$$G(z) = G_\alpha^{(l)}(z) + G_\alpha^{(l)}(z) V^\alpha G(z), \tag{23}$$

$$G_\alpha^{(l)}(z) = \tilde{G}_\alpha(z) + \tilde{G}_\alpha(z) U^\alpha G_\alpha^{(l)}(z), \tag{24}$$

where $V^\alpha = v_\beta^{(s)} + v_\gamma^{(s)}$ and $U^\alpha = v_\beta^{(l)} + v_\gamma^{(l)} - u_\alpha^{(l)}$.

The scattering state, which evolves from the asymptotic state $|\Phi_\alpha\rangle$ under the influence of H, is given as

$$|\Psi_\alpha^{(\pm)}\rangle = \lim_{\varepsilon \to 0} i\varepsilon G(E_\alpha \pm i\varepsilon)|\Phi_\alpha\rangle. \tag{25}$$

Similarly, we can define the following scattering states

$$|\Phi_\alpha^{(l)(\pm)}\rangle = \lim_{\varepsilon \to 0} i\varepsilon G_\alpha^{(l)}(E \pm i\varepsilon)|\Phi_\alpha\rangle \tag{26}$$

and

$$|\tilde{\Phi}_\alpha^{(\pm)}\rangle = \lim_{\varepsilon \to 0} i\varepsilon \tilde{G}_\alpha(E \pm i\varepsilon)|\Phi_\alpha\rangle, \tag{27}$$

which describe scattering processes due to Hamiltonians $H_\alpha^{(l)}$ and $\tilde{H}_\alpha$, respectively.

The S-matrix elements of the scattering processes are obtained from the resolvent of the total Hamiltonian by the reduction technique [8]

$$S_{\beta j,\alpha i} = \lim_{t \to \infty} \lim_{\varepsilon \to 0} i\varepsilon e^{i(E_{\beta j} - E_{\alpha i})t} \langle \Phi_{\beta j}| G(E_{\alpha i} + i\varepsilon)|\Phi_{\alpha i}\rangle. \tag{28}$$

The subscript i and j denotes the ith and jth eigenstates of the corresponding subsystems, respectively. If we substitute Eq. (23) into Eq. (28) we obtain the following two terms:

$$S_{\beta j,\alpha i}^{(1,2)} = \lim_{t \to \infty} \lim_{\varepsilon \to 0} i\varepsilon e^{i(E_{\beta j} - E_{\alpha i})t} \langle \Phi_{\beta j}| G_\alpha^{(l)}(E_{\alpha i} + i\varepsilon)|\Phi_{\alpha i}\rangle \tag{29}$$

$$S_{\beta j,\alpha i}^{(3)} = \lim_{t \to \infty} \lim_{\varepsilon \to 0} i\varepsilon e^{i(E_{\beta j} - E_{\alpha i})t} \langle \Phi_{\beta j}| G_\alpha^{(l)}(E_{\alpha i} + i\varepsilon) V^\alpha \times G(E_{\alpha i} + i\varepsilon)|\Phi_{\alpha i}\rangle. \tag{30}$$

Substituting Eq. (24) into Eq. (29), the first term yields two more terms

$$S_{\beta j,\alpha i}^{(1)} = \lim_{t \to \infty} \lim_{\varepsilon \to 0} i\varepsilon e^{i(E_{\beta j} - E_{\alpha i})t} \langle \Phi_{\beta j}| \tilde{G}_\alpha(E_{\alpha i} + i\varepsilon)|\Phi_{\alpha i}\rangle \tag{31}$$

$$S_{\beta j,\alpha i}^{(2)} = \lim_{t \to \infty} \lim_{\varepsilon \to 0} i\varepsilon e^{i(E_{\beta j} - E_{\alpha i})t} \langle \Phi_{\beta j}| \tilde{G}_\alpha(E_{\alpha i} + i\varepsilon) \times U^\alpha G_\alpha^{(l)}(E_{\alpha i} + i\varepsilon)|\Phi_{\alpha i}\rangle. \tag{32}$$

Using the properties of the resolvent operators, the limits can be performed, and we arrive at the following, physically

plausible, result. The first term, $S^{(1)}_{\beta j,\alpha i}$, is the S matrix of a two-body single-channel scattering on the potential $u^{(l)}_{\alpha}$:

$$S^{(1)}_{\beta j,\alpha i}=\delta_{\beta\alpha}\delta_{ji}S(u^{(l)}_{\alpha}). \tag{33}$$

If $u^{(l)}_{\alpha}$ is a pure Coulomb interaction, $S(u^{(l)}_{\alpha})$ falls back to the S matrix of the Rutherford scattering; if $u^{(l)}_{\alpha}$ is identically zero, $S^{(1)}_{\beta j,\alpha i}$ is equal to unity. The second term $S^{(2)}_{\beta j,\alpha i}$ describes a two-body multichannel scattering on the potential U^{α}:

$$S^{(2)}_{\beta j,\alpha i}=-2\pi i\,\delta_{\beta\alpha}\delta(E_{\beta j}-E_{\alpha i})\langle\tilde{\Phi}^{(-)}_{\beta j}|U^{\alpha}|\Phi^{(l)(+)}_{\alpha i}\rangle. \tag{34}$$

The third term takes account of the complete three-body dynamics:

$$S^{(3)}_{\beta j,\alpha i}=-2\pi i\,\delta(E_{\beta j}-E_{\alpha i})\langle\Phi^{(l)(-)}_{\beta j}|V^{\alpha}|\Psi^{(+)}_{\alpha i}\rangle. \tag{35}$$

C. Lippmann-Schwinger integral equation for $|\Phi^{(l)}_{\alpha}\rangle$

Starting from the definition of $|\Phi^{(l)}_{\alpha}\rangle$ [Eq. (26)], by utilizing resolvent relation (24) and definition (27), we easily derive a Lippmann-Schwinger equation

$$|\Phi^{(l)(\pm)}_{\alpha}\rangle=|\tilde{\Phi}^{(\pm)}_{\alpha}\rangle+\tilde{G}_{\alpha}(E\pm i\epsilon)U^{\alpha}|\Phi^{(l)(\pm)}_{\alpha}\rangle, \tag{36}$$

where $|\tilde{\Phi}^{(\pm)}_{\alpha}\rangle$ are given by

$$|\tilde{\Phi}^{(\pm)}_{\alpha}\rangle=|\tilde{\chi}^{(\pm)}_{\alpha}\rangle|\phi_{\alpha}\rangle. \tag{37}$$

The state $|\tilde{\chi}^{(\pm)}_{\alpha}\rangle$ is a scattering state in the Coulomb-like potential $u^{(l)}_{\alpha}(y_{\alpha})$.

D. Faddeev-Merkuriev integral equations for the wave-function components

The integral equations for the wave function $|\Psi^{(\pm)}_{\alpha}\rangle$ are arrived at by combining the resolvent relation [Eq. (23)] and Eq. (25). In this case, however, we have three resolvent relations, and therefore we obtain a triad of Lippmann-Schwinger equations:

$$|\Psi^{(\pm)}_{\alpha}\rangle=|\Phi^{(l)(\pm)}_{\alpha}\rangle+G^{(l)}_{\alpha}(E\pm i0)V^{\alpha}|\Psi^{(\pm)}_{\alpha}\rangle, \tag{38}$$

$$|\Psi^{(\pm)}_{\alpha}\rangle=G^{(l)}_{\beta}(E\pm i0)V^{\beta}|\Psi^{(\pm)}_{\alpha}\rangle, \tag{39}$$

$$|\Psi^{(\pm)}_{\alpha}\rangle=G^{(l)}_{\gamma}(E\pm i0)V^{\gamma}|\Psi^{(\pm)}_{\alpha}\rangle. \tag{40}$$

Although these three equations together provide unique solutions [9], their kernels are not connected; therefore they cannot be solved by iterations. The way out of the problem is to use the Faddeev decomposition, which leads to equations with connected kernels; thus they are effectively Fredholm-type integral equations.

Multiplying each elements of the triad from left by $G^{(l)}v^{(s)}_{\alpha}$, and utilizing Eq. (14), we obtain a set of Faddeev-Merkuriev integral equations for the components:

$$|\psi^{(\pm)}_{\alpha}\rangle=|\Phi^{(l)(\pm)}_{\alpha}\rangle+G^{(l)}_{\alpha}(E\pm i0)v^{(s)}_{\alpha}[|\psi^{(\pm)}_{\beta}\rangle+|\psi^{(\pm)}_{\gamma}\rangle], \tag{41}$$

$$|\psi^{(\pm)}_{\beta}\rangle=G^{(l)}_{\beta}(E\pm i0)v^{(s)}_{\beta}[|\psi^{(\pm)}_{\alpha}\rangle+|\psi^{(\pm)}_{\gamma}\rangle], \tag{42}$$

$$|\psi^{(\pm)}_{\gamma}\rangle=G^{(l)}_{\gamma}(E\pm i0)v^{(s)}_{\gamma}[|\psi^{(\pm)}_{\alpha}\rangle+|\psi^{(\pm)}_{\beta}\rangle]. \tag{43}$$

Merkuriev showed that, after a certain number of iterations, these equations were reduced to Fredholm integral equations of the second kind with compact kernels for all energies, including energies below ($E<0$) and above ($E>0$) the three-body breakup threshold [2]. Thus all the nice properties of the original Faddeev equations established for short-range interactions also remain valid for the case of Coulomb-like potentials. We note that the triad of Lippmann-Schwinger equations and the set of Faddeev-Merkuriev equations describe the same physics, the equations have identical spectra and in fact, the Faddeev-Merkuriev equations are the adjoint representations of the triad of Lippmann-Schwinger equations [10].

Utilizing the properties of the Faddeev components, the matrix elements in Eq. (35) can be rewritten in a form better suited for numerical calculations:

$$\langle\Phi^{(l)(-)}_{\beta j}|V^{\alpha}|\Psi^{(+)}_{\alpha i}\rangle=\sum_{\gamma\neq\beta}\langle\Phi^{(l)(-)}_{\beta j}|v^{(s)}_{\beta}|\psi^{(+)}_{\gamma i}\rangle. \tag{44}$$

Summarizing, in the three-potential formalism, starting from $|\tilde{\Phi}^{(\pm)}_{\alpha}\rangle$, by solving a Lippmann-Schwinger equation, we determine $|\Phi^{(l)(\pm)}_{\alpha}\rangle$. Then, from $|\Phi^{(l)(+)}_{\alpha}\rangle$, by solving the set of Faddeev-Merkuriev equations, we determine the components $|\psi^{(+)}_{\alpha}\rangle$. Finally using Eqs. (34) and (44) we construct the S matrix.

II. COULOMB-STURMIAN SEPARABLE EXPANSION APPROACH TO THE THREE-BODY INTEGRAL EQUATIONS

In order 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 a representation where the Green's operator is simple. For the two-body Coulomb Green's operator there exists a Hilbert-space basis in which its representation is very simple. This 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 [11]. This basis forms 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, and so the integral equation becomes a set of algebraic equations which can then be solved without any further approximation. The completeness of the basis ensures the convergence of the method.

This approximation scheme was thoroughly tested in two-body calculations. Bound- and resonant-state calculations were presented first [11]. Then the method was extended to scattering states [12]. Since only the asymptotically irrelevant short-range interaction is approximated, the correct Coulomb asymptotic is guaranteed [13]. A recent account of

this method was presented in Ref. [14]. The method also proved to be very efficient in solving three-body Faddeev-Noble integral equations for bound- [4] and scattering-state [3] problems with repulsive Coulomb interactions.

In Sec. II A we define the basis states in two- and three-particle Hilbert space. In Sec. II B we review some of the most important formulas of the two-body problem. In Secs. II C and II D we describe the calculation of the S matrix and the solution of the Faddeev-Merkuriev integral equations. We follow the line presented in Ref. [3].

A. Basis states

The Coulomb-Sturmian functions [15] in some angular momentum state l are defined as

$$\langle r|nl\rangle=\left[\frac{n!}{(n+2l+1)!}\right]^{1/2}(2br)^{l+1}\exp(-br)L_n^{2l+1}(2br), \tag{45}$$

where $n=0,1,2,\ldots$. Here L represents the Laguerre polynomials, and b is a fixed parameter. In an angular momentum subspace they form a complete set

$$\mathbf{1}=\lim_{N\to\infty}\sum_{n=0}^{N}|\widetilde{nl}\rangle\langle nl|=\lim_{N\to\infty}\mathbf{1}_N, \tag{46}$$

where $|\widetilde{nl}\rangle$, in a configuration-space representation, reads $\langle r|\widetilde{nl}\rangle=\langle r|nl\rangle/r$.

The three-body Hilbert space is a direct sum of two-body Hilbert spaces. Thus the appropriate basis in an angular momentum representation should be defined as a direct product

$$|n\nu l\lambda\rangle_\alpha=|nl\rangle_\alpha\otimes|\nu\lambda\rangle_\alpha\quad(n,\nu=0,1,2,\ldots) \tag{47}$$

with the CS states of Eq. (45). Here l and λ denote the angular momenta associated with Jacobi coordinates x and y, respectively. In our three-body Hilbert space basis, we take the bipolar harmonics in the angular variables, and CS functions in the radial coordinates. The completeness relation takes the form (with angular momentum summation implicitly included)

$$\mathbf{1}=\lim_{N\to\infty}\sum_{n,\nu=0}^{N}|\widetilde{n\nu l\lambda}\rangle_{\alpha\alpha}\langle n\nu l\lambda|=\lim_{N\to\infty}\mathbf{1}_N^\alpha, \tag{48}$$

where $\langle x_\alpha y_\alpha|\widetilde{n\nu l\lambda}\rangle_\alpha=\langle x_\alpha y_\alpha|n\nu l\lambda\rangle_\alpha/(x_\alpha y_\alpha)$. It should be noted that in three-particle Hilbert space we can introduce three equivalent basis sets which belong to fragmentations α, β and γ.

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

Let us study a two-body case of short-range interaction plus Coulomb-like interaction,

$$v_l=v_l^{(s)}+v^C \tag{49}$$

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

$$|\psi_l\rangle=|\phi_l^C\rangle+g_l^C(E)v_l^{(s)}|\psi_l\rangle. \tag{50}$$

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

$$g_l^C(E)=(E-h_l^0-v^C)^{-1} \tag{51}$$

with a free Hamiltonian h_l^0. We make the following approximation for Eq. (50):

$$|\psi_l\rangle=|\varphi_l^C\rangle+g_l^C(E)\mathbf{1}_Nv_l^{(s)}\mathbf{1}_N|\psi_l\rangle, \tag{52}$$

i.e., we approximate the short-range potential $v_l^{(s)}$ by a separable form

$$v_l^{(s)}=\lim_{N\to\infty}\mathbf{1}_Nv_l^{(s)}\mathbf{1}_N\approx\mathbf{1}_Nv_l^{(s)}\mathbf{1}_N=\sum_{n,n'=0}^{N}|\widetilde{nl}\rangle\underline{v}_l^{(s)}\langle\widetilde{n'l}|, \tag{53}$$

where the matrix

$$\underline{v}_{l\,nn'}^{(s)}=\langle nl|v_l^{(s)}|n'l\rangle. \tag{54}$$

These matrix elements can always be calculated (numerically) for any reasonable short-range potential. In practice, we use a Gauss-Laguerre quadrature, which is well suited to the CS basis.

Multiplied by the CS states $\langle\widetilde{nl}|$ from the left, Eq. (52) turns into a linear system of equations for the wave-function coefficients $\underline{\psi}_{l_n}=\langle\widetilde{nl}|\psi_l\rangle$,

$$[(\underline{g}_l^C(E))^{-1}-\underline{v}_l^{(s)}]\underline{\psi}_l=(\underline{g}_l^C(E))^{-1}\underline{\varphi}_l^C, \tag{55}$$

where the underlined quantities are matrices with the following elements:

$$\underline{\varphi}_{l_n}^C=\langle\widetilde{nl}|\varphi_l^C\rangle \tag{56}$$

and

$$\underline{g}_{l\,nn'}^C(E)=\langle\widetilde{nl}|g_l^C(E)|\widetilde{n'l}\rangle. \tag{57}$$

1. Matrix elements $\langle\widetilde{nl}|g_l^C(z)|\widetilde{n'l}\rangle$

The key point in the whole procedure is an exact and analytical calculation of the CS matrix elements of the Coulomb Green's operator and of the overlap of the Coulomb and CS functions. For the Green's matrix we have developed two independent, analytical approaches. Both are based on the observation that the Coulomb Hamiltonian possesses an infinite symmetric tridiagonal (Jacobi) matrix structure on the CS basis.

Let us consider the radial Coulomb Hamiltonian

$$h_l^C=-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{l(l+1)}{r^2}\right)+\frac{Z}{r}, \tag{58}$$

where m, l, and Z stand for the mass, angular momentum, and charge, respectively. The matrix $\underline{J}^{\mathrm{C}}_{nn'}=\langle n|(z-h^{\mathrm{C}}_l)|n'\rangle$ possesses a Jacobi structure,

$$\underline{J}^{\mathrm{C}}_{nn}=2(n+l+1)(k^2-b^2)\frac{\hbar^2}{4mb}-Z \tag{59}$$

and

$$\underline{J}^{\mathrm{C}}_{nn-1}=-[n(n+2l+1)]^{1/2}(k^2+b^2)\frac{\hbar^2}{4mb}, \tag{60}$$

where $k=(2mz/\hbar^2)^{1/2}$ is the wave number. The main result of Ref. [16] is that for Jacobi matrix systems the Nth leading submatrix $\underline{g}^{\mathrm{C}(N)}_{nn'}$ of the infinite Green's matrix can be determined by the elements of the Jacobi matrix,

$$\underline{g}^{\mathrm{C}(N)}_{nn'}=[\underline{J}^{\mathrm{C}}_{nn'}+\delta_{nN}\delta_{n'N}\underline{J}^{\mathrm{C}}_{NN+1}C]^{-1}, \tag{61}$$

where C is a continued fraction,

$$C=-\cfrac{u_N}{d_N+\cfrac{u_{N+1}}{d_{N+1}+\cfrac{u_{N+2}}{d_{N+2}+\cdots}}}, \tag{62}$$

with coefficients

$$u_n=-\underline{J}^{\mathrm{C}}_{n,n-1}/\underline{J}^{\mathrm{C}}_{n,n+1}, \quad d_n=-\underline{J}^{\mathrm{C}}_{n,n}/\underline{J}^{\mathrm{C}}_{n,n+1}. \tag{63}$$

In Ref. [16] it was shown that although the continued fraction C is convergent only on the upper-half k plane, it can be continued analytically to the whole k plane. This is because the u_n and d_n coefficients satisfy the limit properties

$$u\equiv\lim_{n\to\infty}u_n=-1, \tag{64}$$

$$d\equiv\lim_{n\to\infty}d_n=2(k^2-b^2)/(k^2+b^2). \tag{65}$$

Then the continued fraction appears as

$$C=-\cfrac{u_N}{d_N+\cfrac{u_{N+1}}{d_{N+1}+\cdots+\cfrac{u}{d+\cfrac{u}{d+\cdots}}}}. \tag{66}$$

Therefore, the tail w of C satisfies the implicit relation

$$w=\frac{u}{d+w}, \tag{67}$$

which is solved by

$$w_{\pm}=(b\pm ik)^2/(b^2+k^2). \tag{68}$$

Replacing the tail of the continued fraction by its explicit analytical form $w_{\pm}$, we can speed up the convergence and, more importantly, turn a nonconvergent continued fraction into a convergent one [17]. Analytic continuation is achieved by using $w_{\pm}$ instead of the nonconverging tail. In Ref. [16], it was shown that w_+ provides an analytic continuation of the Green's matrix to the physical, and w_- does the same to the unphysical Riemann sheet. This way Eq. (62), together with Eq. (61) provides the CS basis representation of the Coulomb Green's operator on the whole complex k plane. We note here that with the choice of $Z=0$ the Coulomb Hamiltonian [Eq. (58)] reduces to the kinetic-energy operator, and our formulas provide the CS basis representation of the Green's operator of the free particle as well. We emphasize that this procedure does not truncate the Coulomb Hamiltonian, because all the higher $J_{nn'}$ matrix elements are implicitly contained in the continued fraction.

We note that $\underline{g}^C$ has been calculated before [11]. From the J-matrix structure a three-term recursion relation follows for the matrix elements $\underline{g}^C_{nn'}$. This recursion relation is solvable if the first element $\underline{g}^C_{00}$ is known. It is given in a closed analytical form

$$\underline{g}^C_{00}=\frac{4mb}{\hbar^2}\frac{1}{(b-\mathrm{i}k)^2}\frac{1}{l+\mathrm{i}\eta+1}\times{}_2F_1\left[-l+\mathrm{i}\eta,1;l+\mathrm{i}\eta+2,\left(\frac{b+\mathrm{i}k}{b-\mathrm{i}k}\right)^2\right], \tag{69}$$

where $\eta=Zm/(\hbar^2k)$ is the Coulomb parameter, and ${}_2F_1$ is the hypergeometric function. For those cases where the first or second indexes of ${}_2F_1$ are equal to unity, there exists a continued fraction representation, which is very efficient in practical calculations. It was shown that the two methods lead to numerically identical results for all energies, and our numerical continued fraction representation possesses all the analytical properties of g^C. An exact analytical knowledge of g^C allows us to calculate the matrix elements of the full Green's operator in the whole complex plane:

$$\underline{g}_l(z)=\{[\underline{g}^C_l(z)]^{-1}-\underline{v}^{(s)}_l\}^{-1}. \tag{70}$$

The overlap vector of CS and the Coulomb functions $\langle\widetilde{nl}|\varphi^C_l\rangle$ is known analytically [12]. It can be calculated by a three-term recursion, derived from the J matrix, using the starting value

$$\langle\widetilde{0l}|\varphi^C_l\rangle=\exp(2\eta\arctan(k/b))\sqrt{\frac{2\pi\eta}{\exp(2\pi\eta)-1}}\times\left(\frac{2k/b}{1+k^2/b^2}\right)^{l+1}\prod_{i=1}^{l}\left(\frac{\eta^2+i^2}{i(i+1/2)}\right)^{1/2}. \tag{71}$$

C. Calculation of the three-body S matrix

The aim of any scattering calculation is to determine the S-matrix elements. In our case we need to calculate terms (33), (34), and (44) of the three-potential picture.

The term $S^{(1)}_{\beta j,\alpha i}$ is trivial because it is just the two-body S matrix of the Coulomb-like potential $u^{(l)}_\alpha$.

To calculate the second term, $S^{(2)}_{\beta j,\alpha i}$ of Eq. (34), the matrix elements $\langle\tilde{\Phi}^{(-)}_{\alpha j}|U^{\alpha}|\Phi^{(l)(+)}_{\alpha i}\rangle$ are needed. Since $\langle\tilde{\Phi}^{(-)}_{\alpha j}|$ contains a two-body bound-state wave function in coordinate x_α this matrix element is confined to Ω_α, where U^α is of short-range type. Therefore, a separable approximation is justified,

$$\langle\tilde{\Phi}^{(-)}_{\alpha j}|U^{\alpha}|\Phi^{(l)(+)}_{\alpha i}\rangle\approx\langle\tilde{\Phi}^{(-)}_{\alpha j}|\mathbf{1}^{\alpha}_{N}U^{\alpha}\mathbf{1}^{\alpha}_{N}|\Phi^{(l)(+)}_{\alpha i}\rangle, \quad (72)$$

i.e., in this matrix element, we can approximate U^α by a separable form

$$\begin{aligned} U^{\alpha} &= \lim_{N\to\infty}\mathbf{1}^{\alpha}_{N}U^{\alpha}\mathbf{1}^{\alpha}_{N} \\ &\approx \mathbf{1}^{\alpha}_{N}U^{\alpha}\mathbf{1}^{\alpha}_{N} \\ &\approx \sum_{n,\nu,n',\nu'=0}^{N} |\widetilde{n\nu l}\lambda\rangle_{\alpha}\,\underline{U}^{\alpha}{}_{\alpha}\langle\widetilde{n'\nu'l'}\lambda'|, \end{aligned} \quad (73)$$

where

$$\underline{U}^{\alpha}_{n\nu l\lambda,n'\nu'l'\lambda'} = {}_{\alpha}\langle n\nu l\lambda|U^{\alpha}|n'\nu'l'\lambda'\rangle_{\alpha}. \quad (74)$$

The matrix element appears as

$$\begin{aligned} \langle\tilde{\Phi}^{(-)}_{\alpha j}|U^{\alpha}|\Phi^{(l)(+)}_{\alpha i}\rangle \approx \sum^{N} & \langle\tilde{\Phi}^{(-)}_{\alpha j}|\widetilde{n\nu l}\lambda\rangle_{\alpha} \\ & \times\underline{U}^{\alpha}{}_{\alpha}\langle\widetilde{n'\nu'l'}\lambda'|\Phi^{(l)(+)}_{\alpha i}\rangle. \end{aligned} \quad (75)$$

In calculating the third term $S^{(3)}_{\beta j,\alpha i}$ of Eq. (44), we have matrix elements of the type $\langle\tilde{\Phi}^{l(-)}_{\alpha j}|v^{(s)}_{\alpha}|\psi^{(+)}_{\beta i}\rangle$. Here again we can approximate the short-range potential $v^{(s)}_\alpha$ in the three-body Hilbert space by a separable form

$$\begin{aligned} v^{(s)}_{\alpha} &= \lim_{N\to\infty}\mathbf{1}^{\alpha}_{N}v^{(s)}_{\alpha}\mathbf{1}^{\beta}_{N} \\ &\approx \mathbf{1}^{\alpha}_{N}v^{(s)}_{\alpha}\mathbf{1}^{\beta}_{N} \\ &\approx \sum_{n,\nu,n',\nu'=0}^{N} |\widetilde{n\nu l}\lambda\rangle_{\alpha}\,\underline{v}^{(s)}_{\alpha\beta}\,{}_{\beta}\langle\widetilde{n'\nu'l'}\lambda'|, \end{aligned} \quad (76)$$

where

$$\underline{v}^{(s)}_{\alpha\beta\,n\nu l\lambda,n'\nu'l'\lambda'} = {}_{\alpha}\langle n\nu l\lambda|v^{(s)}_{\alpha}|n'\nu'l'\lambda'\rangle_{\beta}. \quad (77)$$

In Eq. (76) the ket and bra states belong to different fragmentations depending on the neighbors of the potential operators in the matrix elements. Finally, the matrix elements take the form

$$\begin{aligned} \langle\Phi^{l(-)}_{\alpha j}|v^{(s)}_{\alpha}|\psi^{(+)}_{\beta i}\rangle \approx \sum^{N} & \langle\Phi^{l(-)}_{\alpha j}|\widetilde{n\nu l}\lambda\rangle_{\alpha} \\ & \times\underline{v}^{(s)}_{\alpha\beta}\,{}_{\beta}\langle\widetilde{n'\nu'l'}\lambda'|\psi^{(+)}_{\beta i}\rangle. \end{aligned} \quad (78)$$

We conclude that to calculate the S matrix of the three-potential formulas we need the CS matrix elements [Eqs. (74) and (77)], which can always be evaluated numerically by using the transformation of Jacobi coordinates [18]. In addition we need the CS wave-function components ${}_{\alpha}\langle\widetilde{n\nu l}\lambda|\tilde{\Phi}^{(\pm)}_{\alpha i}\rangle$, ${}_{\alpha}\langle\widetilde{n\nu l}\lambda|\Phi^{l(\pm)}_{\alpha i}\rangle$, and ${}_{\alpha}\langle\widetilde{n\nu l}\lambda|\psi^{(+)}_{\alpha}\rangle$. We determine these in Sec. II D by solving Lippmann-Schwinger and Faddeev-Merkuriev integral equations.

It should be noted that approximations (73) and (76) used in calculating matrix elements (75) and (78) become equalities as N goes to infinity. In practical calculations we increase N until we observe a numerical convergence in scattering observables.

D. Solution of the three-body integral equations

In the set of Faddeev-Merkuriev equations [Eqs. (41)–(43)], we make approximation of Eq. (76):

$$|\psi_{\alpha}\rangle = |\Phi^{(l)}_{\alpha i}\rangle + G^{(l)}_{\alpha}[\mathbf{1}^{\alpha}_{N}v^{(s)}_{\alpha}\mathbf{1}^{\beta}_{N}|\psi_{\beta}\rangle + \mathbf{1}^{\alpha}_{N}v^{(s)}_{\alpha}\mathbf{1}^{\gamma}_{N}|\psi_{\gamma}\rangle], \quad (79)$$

$$|\psi_{\beta}\rangle = G^{(l)}_{\beta}[\mathbf{1}^{\beta}_{N}v^{(s)}_{\beta}\mathbf{1}^{\alpha}_{N}|\psi_{\alpha}\rangle + \mathbf{1}^{\beta}_{N}v^{(s)}_{\beta}\mathbf{1}^{\gamma}_{N}|\psi_{\gamma}\rangle], \quad (80)$$

$$|\psi_{\gamma}\rangle = G^{(l)}_{\gamma}[\mathbf{1}^{\gamma}_{N}v^{(s)}_{\gamma}\mathbf{1}^{\alpha}_{N}|\psi_{\alpha}\rangle + \mathbf{1}^{\gamma}_{N}v^{(s)}_{\gamma}\mathbf{1}^{\beta}_{N}|\psi_{\beta}\rangle]. \quad (81)$$

Multiplied by the CS states ${}_{\alpha}\langle\widetilde{n\nu l}\lambda|$, ${}_{\beta}\langle\widetilde{n\nu l}\lambda|$, and ${}_{\gamma}\langle\widetilde{n\nu l}\lambda|$, respectively, from the left the set of integral equations turns into a linear system of algebraic equations for the coefficients of the Faddeev components $\underline{\psi}_{\alpha_{n\nu l\lambda}} = {}_{\alpha}\langle\widetilde{n\nu l}\lambda|\psi_{\alpha}\rangle$,

$$[(\underline{G}^{(l)})^{-1} - \underline{v}^{(s)}]\underline{\psi} = (\underline{G}^{(l)})^{-1}\underline{\Phi}^{(l)}, \quad (82)$$

with

$$\underline{G}^{(l)}_{\alpha_{n\nu l\lambda,n'\nu'l'\lambda'}} = {}_{\alpha}\langle\widetilde{n\nu l}\lambda|G^{(l)}_{\alpha}|\widetilde{n'\nu'l'}\lambda'\rangle_{\alpha}, \quad (83)$$

and

$$\underline{\Phi}^{(l)}_{\alpha_{n\nu l\lambda}} = {}_{\alpha}\langle\widetilde{n\nu l}\lambda|\Phi^{(l)}_{\alpha}\rangle. \quad (84)$$

Note 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.

1. Matrix elements ${}_{\alpha}\langle\widetilde{n\nu l\lambda}|G^{(l)}_{\alpha}|\widetilde{n'\nu'l'\lambda'}\rangle_{\alpha}$ and ${}_{\alpha}\langle\widetilde{n\nu l\lambda}|\Phi^{(l)}_{\alpha}\rangle$

Unfortunately neither the matrix element [Eq. (83)] nor the overlap [Eq. (84)] is known. The appropriate Lippmann-Schwinger equation for $G^{(l)}_\alpha$ was proposed by Merkuriev [2],

$$G^{(l)}_{\alpha}(z) = G^{as}_{\alpha}(z) + G^{as}_{\alpha}(z)V^{as}_{\alpha}G^{(l)}_{\alpha}(z), \quad (85)$$

where G_α^{as} and V_α^{as} are the asymptotic channel Green's operator and potential, respectively. A similar equation is valid for $|\Phi_\alpha^{(l)}\rangle$:

$$|\Phi_\alpha^{(l)}\rangle = |\Phi_\alpha^{as}\rangle + G_\alpha^{as}(z) V_\alpha^{as} |\Phi_\alpha^{(l)}\rangle. \tag{86}$$

Both $G_\alpha^{(l)}$ and $|\Phi_\alpha^{(l)}\rangle$ are genuine three-body quantities. One may wonder why a single Lippmann-Schwinger equation suffices. The Hamiltonian $H_\alpha^{(l)}$ has a peculiar property—it has only α-type two-body asymptotic channels. For such systems a single Lippmann-Schwinger equation provides a unique solution [19].

The objects G_α^{as}, V_α^{as}, and Φ_α^{as} are very complicated. Their leading-order terms were constructed in configuration spaces in different asymptotic regions. The potential V^{as}, as $|X| \to \infty$, decays faster than the Coulomb potential in all directions of the three-body configuration space: $V^{as} \sim \mathcal{O}(|X|^{-1-\epsilon})$, where $\epsilon > 0$ [2]. Therefore, we may express the solutions of Eqs. (85) and (86) formally as

$$(\underline{G}_\alpha^{(l)})^{-1} = (\underline{G}_\alpha^{as})^{-1} - \underline{V}_\alpha^{as} \tag{87}$$

and

$$[(\underline{G}_\alpha^{as})^{-1} - \underline{V}_\alpha^{as}] \underline{\Phi}_\alpha^{(l)} = (\underline{G}_\alpha^{as})^{-1} \underline{\Phi}_\alpha^{as}, \tag{88}$$

respectively, where

$$\underline{G}^{as}_{\alpha_{n\nu l\lambda, n'\nu' l'\lambda'}} = {}_\alpha\langle \widetilde{n\nu l\lambda} | G_\alpha^{as} | \widetilde{n'\nu' l'} \lambda' \rangle_\alpha, \tag{89}$$

$$\underline{V}^{as}_{\alpha_{n\nu l\lambda, n'\nu' l'\lambda'}} = {}_\alpha\langle n\nu l\lambda | V_\alpha^{as} | n'\nu' l'\lambda' \rangle_\alpha \tag{90}$$

and

$$\underline{\Phi}^{as}_{\alpha_{n\nu l\lambda}} = {}_\alpha\langle \widetilde{n\nu l\lambda} | \Phi_\alpha^{as} \rangle. \tag{91}$$

Here G_α^{as}, V_α^{as}, and Φ_α^{as} appear between finite number of square-integrable CS states, which confine the domain of integration to Ω_α. In this region, however, G_α^{as} coincides with $\tilde{G}_\alpha$, V_α^{as} with U^α and Φ_α^{as} with $\tilde{\Phi}_\alpha$ [2]. Finally we have

$$(\underline{G}_\alpha^{(l)})^{-1} = (\underline{\tilde{G}}_\alpha)^{-1} - \underline{U}^\alpha, \tag{92}$$

where

$$\underline{\tilde{G}}_{\alpha_{n\nu l\lambda, n'\nu' l'\lambda'}} = {}_\alpha\langle \widetilde{n\nu l\lambda} | \tilde{G}_\alpha | \widetilde{n'\nu' l'} \lambda' \rangle_\alpha \tag{93}$$

and

$$\underline{U}^\alpha_{n\nu l\lambda, n'\nu' l'\lambda'} = {}_\alpha\langle n\nu l\lambda | U^\alpha | n'\nu' l'\lambda' \rangle_\alpha. \tag{94}$$

In a similar way,

$$[(\underline{\tilde{G}}_\alpha)^{-1} - \underline{U}^\alpha] \underline{\Phi}_\alpha^{(l)} = (\underline{\tilde{G}}_\alpha)^{-1} \underline{\tilde{\Phi}}_\alpha, \tag{95}$$

where

$$\underline{\tilde{\Phi}}_{\alpha_{n\nu l\lambda}} = {}_\alpha\langle \widetilde{n\nu l\lambda} | \tilde{\Phi}_\alpha \rangle. \tag{96}$$

We note that from Eq. (92) it follows that the left side of Eq. (95) is just the inhomogeneous term of Eq. (82). Both Eqs. (95) and (82) are solved with the same inhomogeneous term.

2. Matrix elements ${}_\alpha\langle \widetilde{n\nu l\lambda} | \tilde{G}_\alpha | \widetilde{n'\nu' l'} \lambda' \rangle_\alpha$ and ${}_\alpha\langle \widetilde{n\nu l\lambda} | \tilde{\Phi}_\alpha \rangle$

The three-particle free Hamiltonian can be written as a sum of two-particle free Hamiltonians

$$H^0 = h^0_{x_\alpha} + h^0_{y_\alpha}. \tag{97}$$

Then the Hamiltonian $\tilde{H}_\alpha$ of Eq. (18) appears as a sum of two Hamiltonians acting on different coordinates,

$$\tilde{H}_\alpha = h_{x_\alpha} + h_{y_\alpha}, \tag{98}$$

with $h_{x_\alpha} = h^0_{x_\alpha} + v^C_\alpha(x_\alpha)$ and $h_{y_\alpha} = h^0_{y_\alpha} + u^{(l)}_\alpha(y_\alpha)$, which, of course, commute. The state $|\tilde{\Phi}_\alpha\rangle$, which is an eigenstate of $\tilde{H}_\alpha$, is a product of a two-body bound-state wave function in coordinate x_α and a two-body scattering-state wave function in coordinate y_α. Their CS representations are known from the two-particle case described above.

The matrix elements of $\tilde{G}_\alpha$ can be determined by making use of the convolution theorem,

$$\begin{aligned} \tilde{G}_\alpha(z) &= (z - h_{x_\alpha} - h_{y_\alpha})^{-1} \\ &= \frac{1}{2\pi \mathrm{i}} \oint_C dz' (z - z' - h_{x_\alpha})^{-1} (z' - h_{y_\alpha})^{-1}. \end{aligned} \tag{99}$$

The contour C should encircle, in a positive direction, the spectrum of h_{y_α} without penetrating into the spectrum of h_{x_α}.

The convolution theorem follows from a more general formula. A function of a self-adjoint operator h is defined as

$$f(h) = \frac{1}{2\pi \mathrm{i}} \oint_C dz f(z) (z - h)^{-1}, \tag{100}$$

where C is a contour around the spectrum of h and f should be analytic on the region encircled by C.

In the following we suppose that $u^{(l)}$ either vanishes or is a repulsive Coulomb-like potential. This assumption is not necessary, but it greatly simplifies the analysis below. Numerical examples show that there are a great many physical three-body systems where this condition is satisfied. This condition ensures that h_y does not have bound states.

To examine the analytical structure of integrand (99) let us shift the spectrum of g_{x_α} by taking $z = E + i\varepsilon$, with positive ε. In doing so, the two spectra become well separated and the spectrum of g_{y_α} can be encircled. The contour C is deformed analytically in such a way that the upper part descends to the unphysical Riemann sheet of g_{y_α}, while the lower part of C can be detoured away from the cut (see Fig. 3). The contour still encircles the branch cut singularity of g_{y_α}, but in the $\varepsilon \to 0$ limit avoids the singularities of g_{x_α}. Thus the mathematical conditions for the contour integral

TABLE I. Convergence of $e^+ + H \to e^+ + H$ elastic scattering (σ_{11}) and $e^+ + H \to p + \mathrm{Ps}$ positronium formation (σ_{12}) cross sections (in πa_0^2) with respect to N, the number of CS functions in the expansion, and with respect to increasing the angular momentum channels ($l_{\max}$) in the bipolar basis.

	$l_{\max}=6$		$l_{\max}=8$		$l_{\max}=10$	
N	σ_{11}	σ_{12}	σ_{11}	σ_{12}	σ_{11}	σ_{12}
	$k_1=0.71$, Ref. [20]: $\sigma_{11}=0.025$, $\sigma_{12}=0.0038$					
12	0.02662	0.00423	0.02664	0.00397	0.02665	0.00393
13	0.02608	0.00424	0.02609	0.00398	0.02610	0.00394
14	0.02581	0.00423	0.02582	0.00398	0.02583	0.00394
15	0.02562	0.00424	0.02561	0.00398	0.02562	0.00395
16	0.02548	0.00425	0.02546	0.00400	0.02547	0.00396
17	0.02541	0.00426	0.02539	0.00401	0.02539	0.00397
18	0.02532	0.00427	0.02529	0.00401	0.02530	0.00398
19	0.02528	0.00427	0.02524	0.00402	0.02525	0.00398
20	0.02522	0.00428	0.02517	0.00403	0.02518	0.00399
	$k_1=0.75$, Ref. [20]: $\sigma_{11}=0.044$, $\sigma_{12}=0.0043$					
12	0.04412	0.00441	0.04412	0.00424	0.04413	0.00422
13	0.04345	0.00440	0.04344	0.00422	0.04345	0.00421
14	0.04318	0.00440	0.04317	0.00423	0.04318	0.00421
15	0.04280	0.00440	0.04278	0.00423	0.04279	0.00421
16	0.04269	0.00440	0.04265	0.00423	0.04266	0.00422
17	0.04252	0.00441	0.04248	0.00424	0.04249	0.00423
18	0.04246	0.00442	0.04240	0.00425	0.04241	0.00423
19	0.04238	0.00442	0.04232	0.00426	0.04232	0.00424
20	0.04232	0.00442	0.04225	0.00426	0.04226	0.00424
	$k_1=0.80$, Ref. [20]: $\sigma_{11}=0.063$, $\sigma_{12}=0.0047$					
12	0.06572	0.00475	0.06571	0.00467	0.06572	0.00467
13	0.06573	0.00481	0.06571	0.00473	0.06572	0.00473
14	0.06518	0.00483	0.06515	0.00475	0.06517	0.00475
15	0.06488	0.00485	0.06484	0.00477	0.06486	0.00477
16	0.06457	0.00486	0.06452	0.00478	0.06453	0.00478
17	0.06440	0.00487	0.06433	0.00479	0.06435	0.00479
18	0.06427	0.00487	0.06420	0.00479	0.06422	0.00480
19	0.06418	0.00487	0.06409	0.00480	0.06411	0.00480
20	0.06412	0.00488	0.06402	0.00480	0.06404	0.00480

representation of $\tilde{G}_\alpha(z)$ in Eq. (99) are met. The matrix elements $\underline{\tilde{G}}_\alpha$ can be cast in the form

$$\underline{\tilde{G}}_\alpha(z)=\frac{1}{2\pi i}\oint_C dz'\,\underline{g}_{x_\alpha}(z-z')\underline{g}_{y_\alpha}(z'), \tag{101}$$

where the corresponding CS matrix elements of the two-body Green's operators in the integrand are known analytically for all complex energies.

III. TEST OF THE METHOD

We demonstrate the power of our method by calculating elastic phase shifts of $e^+ + H$ scattering below the Ps($n=1$) threshold and cross sections of the $e^+ + H$ elastic scattering as well as $p^+ + \mathrm{Ps}$ reaction channels up to the Ps($n=2$) threshold. In all examples we have a total angular momentum $L=0$, and we take angular momentum channels up to $l=10$. We use atomic units.

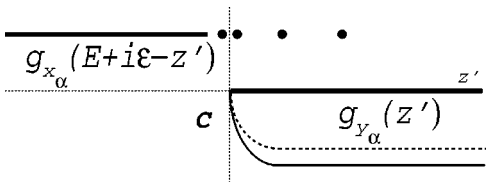

FIG. 3. Analytic structure of $g_{x_\alpha}(z-z')g_{y_\alpha}(z')$ as a function of z' with $z=E+i\varepsilon$, $E<0$, and $\varepsilon>0$. The contour C encircles the continuous spectrum of h_{y_α}. A part of this, which goes on the unphysical Riemann sheet of g_{y_α}, is shown by the broken line.

Let us numerate the particles e^+, p, and e^-, with masses $m_{e^\pm}=1m_e$ and $m_p=1836.1527m_e$, by 1, 2, and 3, respectively. In channel 3 there are no two-body asymptotic channels, since particles e^+ and p do not form bound states. Therefore, we can take $v_3^{(s)}\equiv 0$, and include the total v_3^C in the long-range Hamiltonian:

$$H=H^{(l)}+v_1^{(s)}+v_2^{(s)}, \tag{102}$$

$$H^{(l)}=H^0+v_1^{(l)}+v_2^{(l)}+v_3^C. \tag{103}$$

In this case $|\psi_3\rangle\equiv 0$, and we have set of two-component Faddeev-Merkuriev equations:

$$|\psi_1\rangle=|\phi_1^{(l)}\rangle+G_1^{(l)}v_1^{(s)}|\psi_1\rangle, \tag{104}$$

$$|\psi_2\rangle=G_2^{(l)}v_2^{(s)}|\psi_2\rangle. \tag{105}$$

The parameters of the splitting function ζ of Eq. (8) are rather arbitrary. The final converged results should be insensitive to their values; our numerical experiences confirm this expectation. For the parameters of ζ, we have taken $\nu=2.1$, $x^0=3$, and $y^0=10$, whereas for the parameters of CS functions we have taken $b=0.9$. We have seen that the rate of convergence is rather insensitive to the choice of b over a broad interval.

First we examine the convergence of the results for cross sections at incident wave numbers $k_1=0.71$, 0.75, and 0.8, which correspond to scattering states in the Ore gap. Table I shows the convergence of $e^+ + H \to e^+ + H$ elastic scattering (σ_{11}) and $e^+ + H \to p^+ + \mathrm{Ps}$ positronium formation (σ_{12}) cross sections (in πa_0^2) with respect to N, the number of CS

TABLE II. Phase shifts (in rad) of $e^+ + H \to e^+ + H$ elastic scattering below the positronium formation threshold.

k	Ref. [21]	Ref. [22]	Ref. [23]	Ref. [20]	This work
0.1	0.1483	0.152	0.149	0.149	0.1480
0.2	0.1877	0.188	0.188	0.189	0.1876
0.3	0.1677	0.166	0.166	0.169	0.1673
0.4	0.1201	0.118	0.120	0.121	0.1199
0.5	0.0624	0.061	0.060	0.062	0.0625
0.6	0.0039	0.003		0.003	0.0038
0.7	−0.0512	−0.053		−0.050	−0.0513

TABLE III. Partial cross sections (in πa_0^2) in the $H(n=2)$-Ps$(n=2)$ gap (threshold energies 0.7496–8745 Ry). Numbers 1, 2, 3, and 4 denote the channels $e^+ + H(1s)$, $e^+ + H(2s)$, $e^+ + H(2p)$, and $p^+ + \mathrm{Ps}(1s)$, respectively.

E_1 (Ry)		σ_{11}	σ_{12}	σ_{13}	σ_{14}
0.77	Ref. [24]	0.090	0.000702	0.000454	0.00572
0.77	This work	0.0951	0.000673	0.000331	0.00558
0.80	Ref. [24]	0.096	0.00115	0.000364	0.00585
0.80	This work	0.1010	0.00127	0.000371	0.00563
0.83	Ref. [24]	0.0993	0.00170	0.000885	0.00581
0.83	This work	0.1063	0.00163	0.000813	0.00566
0.84	Ref. [24]	0.101	0.00190	0.00113	0.00580
0.84	This work	0.1080	0.00173	0.00105	0.00566

functions in the expansion, and with respect to increasing the angular momentum channels in the bipolar expansion. For comparison, we provide the results of Ref. [20]. We can see that very good accuracy is achieved even with relatively low N in the expansion.

In Table II we compare our converged results for phase shifts (in rad) below the Ps$(n=1)$ threshold to that of other methods. Reference [21] is the best variational calculation. In Ref. [22] the Schrödinger equation was solved by means of finite-element method. In Refs. [23] and [20] the configuration space Faddeev-Merkuriev differential equations were solved using the bipolar harmonic expansion method and in total angular momentum representation, respectively. We can report perfect agreements with previous calculations.

In Table III we present partial cross sections in the $H(n=2)-\mathrm{Ps}(n=2)$ gap (threshold energies 0.7496-0.8745 Ry). In Ref. [24] the configuration space Faddeev-Merkuriev differential equations were solved using a bipolar harmonic expansion in the angular variables and a quintic spline expansion in the radial coordinates. We can report fairly good agreements.

IV. CONCLUSION

We have extended the three-potential formalism for treating the three-body scattering problem with all kinds of Coulomb interactions including attractive ones. We adopted-Merkuriev's approach, and split the Coulomb potentials in the three-body configuration space into short-and long-range terms. In this picture the three-body Coulomb scattering process can be decomposed into single channel Coulomb scattering, two-body multichannel scattering on the intermediate-range polarization potential, and genuine three-body scattering due to the short-range potentials. The formalism provides us a set of Lippmann–Schwinger and Faddeev-Merkuriev integral equations.

These integral equations are certainly too complicated for most of the numerical methods available in the literature. The Coulomb-Sturmian separable expansion method can be successfully applied. It solves the three-body integral equations by expanding only short-range terms in a separable form on a Coulomb-Sturmian basis, while treating the long-range terms in an exact manner via a proper integral representation of the three-body channel distorted Coulomb Green's operator. The use of the Coulomb-Sturmian basis is essential, as it allows an exact analytical representation of the two-body Green's operator, and thus the contour integral for the channel distorted Coulomb Green's operator can be calculated. The method provides solutions which are asymptotically correct, at least in Ω_α, which is sufficient if the scattering process starts from a two-body asymptotic state. Since the two-body Coulomb Green's operator is calculated exactly, all thresholds are automatically in the right location irrespective of the rank of the separable approximation. The method possesses good convergence properties, and in practice can be made arbitrarily accurate by employing an increasing number of terms in the expansion. Certainly, there is plenty of room for improvement, but we are convinced that this method can be a very powerful tool for studying three-body systems with Coulomb interactions.

ACKNOWLEDGMENTS

This work was supported by NSF Grant No. Phy-0088936 and by OTKA Grant No. T026233. We also acknowledge the generous allocation of computer time at the NPACI, formerly San Diego Supercomputing Center, by the National Resource Allocation Committee, and at the Department of Aerospace Engineering of CSULB.

[1] J. V. Noble, Phys. Rev. **161**, 945 (1967).
[2] L. D. Faddeev, and S. P. Merkuriev, *Quantum Scattering Theory for Several Particle Systems* (Kluwer, Dordrecht, 1993).
[3] Z. Papp, Phys. Rev. C **55**, 1080 (1997).
[4] Z. Papp and W. Plessas, Phys. Rev. C **54**, 50 (1996).
[5] Z. Papp, I. N. Filikhin, and S. L. Yakovlev, Few-Body Syst. (to be published); e-print nucl-th/9909083.
[6] Z. Papp, Few-Body Syst. **24**, 263 (1998).
[7] V. Vanzani, *Few-Body Nuclear Physics* (IAEA, Vienna, 1978), p. 57.
[8] E. O. Alt, P. Grassberger, and W. Sandhas, Nucl. Phys. B **2**, 167 (1967).
[9] W. Glöckle, Nucl. Phys. A **141**, 620 (1970); **158**, 257 (1970).
[10] S. L. Yakovlev, Theor. Math. Phys. **107**, 835 (1996).
[11] Z. Papp, J. Phys. A **20**, 153 (1987).
[12] Z. Papp, Phys. Rev. C **38**, 2457 (1988).
[13] Z. Papp, Phys. Rev. A **46**, 4437 (1992).
[14] B. Kónya, G. Lévai, and Z. Papp, Phys. Rev. C **61**, 034302 (2000).
[15] M. Rotenberg, Ann. Phys. (N.Y.) **19**, 262 (1962); Adv. At. Mol. Phys. **6**, 233 (1970).
[16] B. Kónya, G. Lévai, and Z. Papp, J. Math. Phys. **38**, 4832 (1997).
[17] L. Lorentzen and H. Waadeland, *Continued Fractions with Applications* (North-Holland, Amsterdam, 1992).

[18] R. Balian and E. Brézin, Nuovo Cimento Soc. Ital. Fis., B **2**, 403 (1969).
[19] W. Sandhas, *Few-Body Nuclear Physics* (Ref. [7]), p. 3.
[20] A. A. Kvitsinsky, A. Wu, and C.-Y. Hu, J. Phys. B **28**, 275 (1995).
[21] A. K. Bhatia, A. Temkin, R. J. Drachman, and H. Eiserike, Phys. Rev. A **3**, 1328 (1971).
[22] F. S. Levin and J. Shertzer, Phys. Rev. Lett. **61**, 1089 (1988).
[23] A. A. Kvitsinsky, J. Carbonell, and C. Gignoux, Phys. Rev. A **51**, 2997 (1995).
[24] C.-Y. Hu, Phys. Rev. A **59**, 4813 (1999).