Correlated scattering states of N-body Coulomb systems

Jamal Berakdar
Atomic and Molecular Physics Laboratories, Research School of Physical Sciences and Engineering, Australian National University, Canberra, Australian Capital Territory 0200, Australia
(Received 8 July 1996)

For N charged particles of equal masses moving in the field of a heavy residual charge, an approximate analytical solution of the many-body time-independent Schrödinger equation is derived at a total energy above the complete fragmentation threshold. All continuum particles are treated on equal footing. The proposed correlated wave function represents, to leading order, an exact solution of the many-body Schrödinger equation in the asymptotic region defined by large interparticle separations. Thus, in this asymptotic region the N-body Coulomb modifications to the plane-wave motion of free particles are rigorously estimated. It is shown that the Kato cusp conditions are satisfied by the derived wave function at all two-body coalescence points. An expression of the normalization of this wave function is also given. To render possible the calculations of scattering amplitudes for transitions leading to a four-body scattering state, an effective-charge method is suggested in which the correlations between the continuum particles are completely subsumed into effective interactions with the residual charge. Analytical expressions for these effective interactions are derived and discussed for physical situations. [S1050-2947(97)01103-7]

PACS number(s): 34.80.Dp, 34.10.+x, 25.10.+s

I. INTRODUCTION

Many-body Coulomb scattering states arise in various fundamental reactions in atomic and molecular physics. Although the Coulomb interactions governing the motion of charged particles possess a simple analytical dependence, the theoretical treatment of Coulomb scattering states is a challenging task even in the asymptotic region. The main difficulties in the theoretical description of such states arise from the infinite-range behavior of the Coulomb interaction. This is already revealed in the exactly solvable two-body (Kepler) problem in which case the asymptotic free motion in the relative coordinate is modified by the notorious Coulomb phase. For the three-body system the theoretical treatment is much more involved due to the nonseparability of the many-body Schrödinger equation. Asymptotic states for the three-body problem have been reported at large interparticle separations [1–4]. Only recently [5,6] have asymptotic three-body scattering states been derived that are valid in the entire asymptotic region defined by large hyperradius. The introduction of coupling between individual two-body subsystems (in the form of local relative momenta in Ref. [5] and local Sommerfeld parameters in the case of Ref. [6]) in deriving these asymptotic states underlines the complexity in the theoretical descriptions of Coulomb systems in the continuum. For systems with more than three particles in the continuum only little is known. Employing hyperspherical coordinates in the $3N$-configuration space, Peterkop [2] has derived an estimate of the Coulomb phase modification to an outgoing $(3N-1)$-dimensional spherical free wave of N electrons receding from a massive nucleus. The Coulomb phase modifications to the asymptotic plane-wave motion of the individual N electrons as well as the propagation of such asymptotic scattering states to finite distances have not been given. Due to unpublished work by Redmond, an expression for the Coulomb distortions of the asymptotic plane-wave relative motions in N-body Coulomb scattering systems has been reported in Ref. [1], however, without derivation.

In this work we derive an approximate analytical expression for the solution of the non-relativistic, time-independent Schrödinger equation of N charged particles moving in the field of a residual ion. The total energy of the system is assumed to be above the complete breakup threshold. The study is restricted to continuum particles with comparable masses and, with respect to these masses, a very heavy mass of the residual charge so that mass-polarization terms can be neglected and the center-of-mass motion can be separated out in a relative-coordinate frame of reference. The wave function is determined by separately solving for the N-independent Coulomb particle motion in the residual ion field and the correlated motion between the continuum particles with disregard of the residual-charge field. These two solutions are then subsequently coupled by an arbitrary function that is determined from the Schrödinger equation of the system. The derived correlated N-body wave function coincides with known expressions [4,6–8] in the case of three-body system and, for a two-body system, with the exact two-body Coulomb wave function. It is shown that the proposed wave function constitutes an exact solution of the many-body problem in the asymptotic region of large interparticle distances. In this region the asymptotic expression of the derived wave function tends to the asymptotic form suggested in Ref. [1], hence providing the proof for this suggestion. In addition, the normalization of the proposed wave function is derived by requiring that the total flux, generated by the wave function derived here, through a large multidimensional manifold defined by large, but constant, interparticle separations should be the same as the flux due to normalized N plane waves of the receding particles.

The inclusion of the correlations between the continuum particles presents an obstacle in actual calculations of scattering amplitudes using the derived wave function since in this case a $3N$-dimensional integral has to be evaluated. The reactions for which such Coulomb scattering amplitudes are

currently needed are the double ionization of atomic systems upon charged particle impact and the electron-impact single ionization of atomic inner shells followed by an Auger decay [9]. Both of these processes lead to a four-body Coulomb continuum states in the final channel. Measurements of such reactions have already been performed [10–14,16,15]. In light of the absence of theoretical descriptions under situations where the four-body problem cannot be reduced to three-body one using the Born approximation, it appears timely to investigate methods of simplifying the proposed wave function such that reaction cross sections can be calculated. In a method proposed in Ref. [17] the correlations between the continuum particles are taken into account as an effective interaction between the continuum particles and the nucleus. However, as shown below, the effective product charges given by the method of Ref. [17] exhibit some undesirable features. Therefore, maintaining the philosophy of effective charges, an alternative set of effective product charges is derived by requiring that the many-body wave function constructed by this method should analytically match the known solution of the many-body Schrödinger equation in some limiting cases. The derived product charges are then well behaved. Properties of the proposed effective product charges are discussed in the case of positron-impact double ionization of He($^1S^e$) . Using the method developed in this work, pilot calculations for the multiple differential cross sections of the electron- and positron-impact double ionization of He($^1S^e$) have already been reported [18].

The plan of the paper is as follows. In Sec. II, after formulating the theoretical framework, the correlated many-body wave function is derived and the asymptotic behavior of the Schrödinger equation is investigated. In Sec. III the proposed wave function is shown to satisfy the Kato cups conditions [19] at all $N(N-1)/2$ two-body collision points. Section IV deals with the normalization of the derived wave function, whereas in Sec. V the method is applied to the four-body Coulomb continuum problem. To render possible the calculations of scattering amplitudes, the proposed wave functions is simplified using a method based on the effective-product-charge method. Conclusions are drawn in Sec. VI. Atomic units are used throughout.

II. FORMULATION OF THE PROBLEM AND ASYMPTOTIC SCATTERING STATES

We consider N charged particles of equal masses m and with charges Z_j, $j\in[1,N]$ moving in the field of a residual charge Z. The mass M of the charge Z is assumed to be much larger than m ($M\gg m$). In this work only continuum states are considered, i.e., the total energy E of the system is larger than the complete fragmentation-threshold energy. Neglecting terms of the orders m/M, the center-of-mass system and the laboratory frame of reference can be chosen to be identical. The nonrelativistic time-independent Schrödinger equation of the N-body system can then be formulated in the relative-coordinate representation as

$$\left[H_0+\sum_{j=1}^{N}\frac{ZZ_j}{r_j}+\sum_{\substack{i,j\\ j>i=1}}^{N}\frac{Z_iZ_j}{r_{ij}}-E\right]\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)=0, \tag{1}$$

where $\mathbf{r}_j$ is the position of particle j with respect to the residual charge Z and $\mathbf{r}_{ij}:=\mathbf{r}_i-\mathbf{r}_j$ denotes the relative coordinate between particles i and j. The kinetic-energy operator H_0 has the form (in the limit $m/M\to 0$) $H_0=-\Sigma_{L=1}^{N}\Delta_L/2m$, where Δ_L is the Laplacian with respect to the coordinate $\mathbf{r}_L$. We note here that for a system of general masses the problem is complicated by an additional mass-polarization term that arises in Eq. (1). Upon introduction of N-body Jacobi coordinates, H_0 becomes diagonal; however, the potential terms acquire a much more complex form. Assuming the continuum particles to escape with relative asymptotic momenta $\mathbf{k}_j$ (with respect to the charge Z), it has been suggested in Ref. [1], due to unpublished work by Redmond, that for large interparticle distances the wave function $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ takes on the form

$$\lim_{\substack{r_{lm}\to\infty\\ r_n\to\infty}}\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\to(2\pi)^{-3N/2}\prod_{s=1}^{N}\xi_s(\mathbf{r}_s)\psi_s(\mathbf{r}_s)\times\prod_{\substack{i,j=1\\ j>i}}^{N}\psi_{ij}(\mathbf{r}_{ij})\qquad\forall l,m,n\in[1,N];\ m>l, \tag{2}$$

where the functions $\xi_j(\mathbf{r}_j),\psi_j(\mathbf{r}_j),\psi_{ij}(\mathbf{r}_{ij})$ are defined as

$$\xi_j(\mathbf{r}_j):=\exp(i\mathbf{k}_j\cdot\mathbf{r}_j), \tag{3}$$

$$\psi_j(\mathbf{r}_j):=\exp[\mp i\alpha_j\ln(k_jr_j\pm\mathbf{k}_j\cdot\mathbf{r}_j)], \tag{4}$$

$$\psi_{ij}(\mathbf{r}_{ij}):=\exp[\mp i\alpha_{ij}\ln(k_{ij}r_{ij}\pm\mathbf{k}_{ij}\cdot\mathbf{r}_{ij})]\ . \tag{5}$$

The + and − signs refer to outgoing and incoming boundary conditions, respectively, and $\mathbf{k}_{ij}$ is the momentum conjugate to $\mathbf{r}_{ij}$, i.e., $\mathbf{k}_{ij}:=(\mathbf{k}_i-\mathbf{k}_j)/2$. The Sommerfeld parameters α_j,α_{ij} are given by

$$\alpha_{ij}=\frac{Z_iZ_j}{v_{ij}},\quad \alpha_j=\frac{ZZ_j}{v_j}. \tag{6}$$

In Eq. (6) v_j denotes the velocity of particle j relative to the residual charge, whereas $\mathbf{v}_{ij}:=\mathbf{v}_i-\mathbf{v}_j$. In this work we restrict the considerations to outgoing-wave boundary conditions. The treatment of incoming-wave boundary conditions runs along the same lines. The total energy of the system E is given by

$$E=\sum_{l=1}^{N}E_l\quad\text{where}\quad E_l=\frac{k_l^2}{2m}. \tag{7}$$

To derive asymptotic scattering states in the limit of large interparticle separations and their propagations to finite distances we assume for $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ the ansatz

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\mathcal{N}\Phi_I(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Phi_{II}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\times\chi(\mathbf{r}_1,\ldots,\mathbf{r}_N), \tag{8}$$

where Φ_I,Φ_{II} are appropriately chosen functions, $\mathcal{N}$ is a normalization constant, and $\chi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is a function of an arbitrary form. The function Φ_I is chosen to describe the

motion of N-independent Coulomb particles moving in the field of the charge Z at the total energy E, i.e., Φ_I is determined by the differential equation

$$\left(H_0+\sum_{j=1}^{N}\frac{ZZ_j}{r_j}-E\right)\Phi_I(\mathbf{r}_1,\ldots,\mathbf{r}_N)=0. \tag{9}$$

Since we are interested in scattering solutions with outgoing-wave boundary conditions that describe N particles escaping with asymptotic momenta $\mathbf{k}_j, j\in[1,N]$, it is appropriate to factor out the plane-wave part and write for Φ_I

$$\Phi_I(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\overline{\Phi}_I(\mathbf{r}_1,\cdots,\mathbf{r}_N)\prod_{j=1}^{N}\xi_j(\mathbf{r}_j). \tag{10}$$

Upon substitution of the ansatz (10) into Eq. (9) it is readily concluded that Eq. (9) is completely separable and the regular solution Φ_I can be written in closed form

$$\Phi_I(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\prod_{j=1}^{N}\xi_j(\mathbf{r}_j)\varphi_j(\mathbf{r}_j), \tag{11}$$

where $\varphi_j(\mathbf{r}_j)$ is a confluent-hypergeometric function in the notation of Ref. [20]

$$\varphi_j(\mathbf{r}_j)={}_1F_1[\alpha_j,1,-i(k_jr_j+\mathbf{k}_j\cdot\mathbf{r}_j)]. \tag{12}$$

The function Φ_I describes the motion of the continuum particles in the extreme case of very strong coupling to the residual ion, i.e., $|ZZ_j|\gg|Z_jZ_i|\forall i,j\in[1,N]$. In order to incorporate the other extreme case of strong correlations among the continuum particles ($|Z_jZ_i|\gg|ZZ_j|\forall i,j\in[1,N]$) we choose Φ_{II} to possess the form

$$\Phi_{II}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\overline{\Phi}_{II}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\prod_{j=1}^{N}\xi_j(\mathbf{r}_j), \tag{13}$$

with

$$\overline{\Phi}_{II}(\mathbf{r}_1,\ldots,\mathbf{r}_N):=\prod_{j>i=1}^{N}\varphi_{ij}(\mathbf{r}_{ij}), \tag{14}$$

where $\varphi_{ij}(\mathbf{r}_{ij}):={}_1F_1[\alpha_{ij},1,-i(k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij})]$. It is straightforward to show that the expression $\varphi_{ij}(\mathbf{r}_{ij})\Pi_{l=1}^{N}\xi_l(\mathbf{r}_l)$ solves for the Schrödinger equation (1) in the case of extreme correlations between particle i and particle j, i.e., $|ZZ_l|\ll|Z_iZ_j|\gg|Z_mZ_n|\forall l,m,n\neq i,j$. In terms of differential equations this means

$$\left(H_0+\frac{Z_iZ_j}{r_{ij}}-E\right)\varphi_{ij}(\mathbf{r}_{ij})\prod_{j=1}^{N}\xi_j(\mathbf{r}_j)=0. \tag{15}$$

It should be stressed, however, that the function (13) does not solve for Eq. (1) in the case of weak coupling to the residual ion ($Z\to0$), but otherwise comparable strength of correlations between the continuum particles. This is due to the fact that two-body subsystems formed by the continuum particles are coupled to each other. To derive an expression for this coupling term we note first that

$$\Delta_m\overline{\Phi}_{II}=\sum_{l=1}^{m-1}\Delta_m\varphi_{lm}\prod_{\substack{j>i\\ i\neq l}}^{N}\varphi_{ij}+\sum_{n=m+1}^{N}\Delta_m\varphi_{mn}\prod_{\substack{j>i\\ j\neq n}}^{N}\varphi_{ij}+A_m,\quad m\in[1,N], \tag{16}$$

where the differential operator A_m has the form

$$\begin{aligned}A_m=&2\sum_{l=1}^{m-1}\left[(\boldsymbol{\nabla}_m\varphi_{lm})\cdot\left(\sum_{n=m+1}^{N}\boldsymbol{\nabla}_m\varphi_{mn}\right)\right]\prod_{\substack{j>i\\ j\neq n,i\neq l}}^{N}\varphi_{ij}\\&+\sum_{l=1}^{m-1}\left[(\boldsymbol{\nabla}_m\varphi_{lm})\cdot\left(\sum_{l\neq s=1}^{m-1}\boldsymbol{\nabla}_m\varphi_{sm}\right)\right]\prod_{\substack{j>i\\ s\neq i\neq l}}^{N}\varphi_{ij}\\&+\sum_{n=m+1}^{N}\left[(\boldsymbol{\nabla}_m\varphi_{mn})\cdot\left(\sum_{\substack{t=m+1\\ t\neq n}}^{N}\boldsymbol{\nabla}_m\varphi_{mt}\right)\right]\prod_{\substack{j>i\\ j\neq t\neq n}}^{N}\varphi_{ij},\quad m\in[1,N].\end{aligned} \tag{17}$$

To obtain the differential operator that couples the two-body subsystems in the absence of the charge Z we neglect in Eq. (1) the interactions between the residual charge and the continuum particles ($Z=0$) and substitute the function (13) into Eq. (1). Making use of the relation (16) it is straightforward, however cumbersome, to show that the coupling term that prevents separability has the form

$$A=\sum_{m=1}^{N}A_m. \tag{18}$$

Equations (17) and (18) warrant comment. The term A_m is a mixing operator. It couples an individual two-body subsystem formed by two continuum particles to all other two-body subsystems formed by the continuum particles in the absence of the residual ion. Hence it is clear that all the terms in the sum (17) vanish for the case of the three-body system since in this case only one two-body system exists in the field of the residual charge. The second remark concerns the structure of A_m and hence A. From Eq. (16) it is evident that the remainder term (17) is part of the kinetic-energy operator. Thus it is expected that, under certain circumstances, this term has a finite range, which indicates that asymptotic separability, in the sense specified below, exists for many-body continuum Coulomb systems. In fact, as the functional form of $\varphi_{ij}(\mathbf{r}_{ij})$ is known, the term A can be calculated explicitly, which will be done below.

Now with Φ_I and Φ_{II} determined, the exact wave function (8) is given by the expression $\chi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$. Upon substitution of the expressions (13) and (11) into the ansatz (8) and inserting in the Schrödinger equation (1), a differential equation for the determination of $\chi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is derived

$$\left\{H_0-\frac{A}{\overline{\Phi}_{II}}-\sum_{L=1}^{N}\left[(\boldsymbol{\nabla}_L\ln\Phi_I+\boldsymbol{\nabla}_L\ln\Phi_{II})\cdot\boldsymbol{\nabla}_L+(\boldsymbol{\nabla}_L\ln\Phi_I)\cdot(\boldsymbol{\nabla}_L\ln\Phi_{II})\right]+E\right\}\chi(\mathbf{r}_1,\ldots,\mathbf{r}_N)=0\ . \tag{19}$$

From the derivation of the functions Φ_I and Φ_{II} [Eqs. (9) and (13)] it is clear that all long-range two-body Coulomb interactions have already been diagonalized by Φ_I and Φ_{II} because the total potential is exactly treated by these wave functions. Hence the function χ, to be determined here, contains information on many-body couplings, which are, under certain conditions (see below), of finite range. To explicitly show that, and due to flux arguments we write the function χ in the form

$$\chi(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\prod_{j=1}^{N}\xi^*(\mathbf{r}_j)[1-f(\mathbf{r}_1,\ldots,\mathbf{r}_N)], \quad (20)$$

where $f(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is a function of an arbitrary structure. Inserting the form (20) into Eq. (19) we arrive, after much differential analysis, at the inhomogeneous differential equation

$$\left\{H_0-\sum_{L=1}^{N}[\boldsymbol{\nabla}_L(\ln\Phi_I+\ln\Phi_{II})+i\mathbf{k}_L]\cdot\boldsymbol{\nabla}_L\right\}f+\mathcal{R}(1-f)=0, \quad (21)$$

where the inhomogeneous term $\mathcal{R}$ is given by

$$\begin{aligned}\mathcal{R}:=\sum_{m=1}^{N}\Bigg\{&(\boldsymbol{\nabla}_m\ln\overline{\Phi_I})\cdot(\boldsymbol{\nabla}_m\ln\overline{\Phi_{II}})\\&+\sum_{l=1}^{m-1}\sum_{p=m+1}^{N}(\nabla_m\ln\varphi_{lm})\cdot(\nabla_m\ln\varphi_{mp})\\&+\frac{1}{2}\sum_{l=1}^{m-1}\sum_{s\neq l}^{m-1}(\nabla_m\ln\varphi_{lm})\cdot(\nabla_m\ln\varphi_{sm})\\&+\frac{1}{2}\sum_{n=m+1}^{N}\sum_{n\neq q=m+1}^{N}(\nabla_m\ln\varphi_{mn})\cdot(\nabla_m\ln\varphi_{mq})\Bigg\}.\end{aligned} \quad (22)$$

It is the inhomogeneous term $\mathcal{R}$ that contains the coupling between all individual two-particle subsystems. For example, the first term in Eq. (22) describes the coupling of a two-body subsystems formed by particles i and j to all two-body subsystems formed by the individual continuum particles and the residual ion. The second term originates from Eq. (18) and, as explained above, is a measure for the coupling among two-body subsystems of the continuum particles (in the absence of Z). To these couplings to be negligible the norm of the term $\mathcal{R}$ must be small. To get some insight into the functional form of $\mathcal{R}$, given by Eq. (22), we note that

$$\boldsymbol{\nabla}_L\ln\overline{\Phi_I}=\alpha_L k_L\mathbf{F}_L(\mathbf{r}_L), \quad (23)$$

where

$$\mathbf{F}_L(\mathbf{r}_L):=\frac{{}_1F_1[1+i\alpha_L,2,-i(k_Lr_L+\mathbf{k}_L\cdot\mathbf{r}_L)]}{{}_1F_1[i\alpha_L,1,-i(k_Lr_L+\mathbf{k}_L\cdot\mathbf{r}_L)]}(\hat{\mathbf{k}}_L+\hat{\mathbf{r}}_L)\ . \quad (24)$$

In addition, we remark that

$$\begin{aligned}\nabla_m\ln\overline{\Phi_{II}}&=\sum_{n=m+1}^{N}\nabla_m\ln\varphi_{mn}+\sum_{l=1}^{m-1}\nabla_m\ln\varphi_{lm}\\&=\sum_{n=m+1}^{N}\alpha_{mn}k_{mn}\mathbf{F}_{mn}(\mathbf{r}_{mn})-\sum_{l=1}^{m-1}\alpha_{lm}k_{lm}\mathbf{F}_{lm}(\mathbf{r}_{lm}),\end{aligned} \quad (25)$$

where

$$\mathbf{F}_{ij}(\mathbf{r}_{ij}):=\frac{{}_1F_1[1+i\alpha_{ij},2,-i(k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij})]}{{}_1F_1[i\alpha_{ij},1,-i(k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij})]}(\hat{\mathbf{k}}_{ij}+\hat{\mathbf{r}}_{ij})\ . \quad (26)$$

Thus the behavior of the coupling term $\mathcal{R}$ is controlled by the generalized functions $\mathbf{F}_{ij}(\mathbf{r}_{ij}),\mathbf{F}_l(\mathbf{r}_l)$ since Eq. (22) can be written in the form

$$\begin{aligned}\mathcal{R}:=\sum_{m=1}^{N}\Bigg\{&\alpha_m k_m\mathbf{F}_m(\mathbf{r}_m)\cdot\Bigg[\sum_{n=m+1}^{N}\alpha_{mn}k_{mn}\mathbf{F}_{mn}(\mathbf{r}_{mn})\\&-\sum_{s=1}^{m-1}\alpha_{sm}k_{sm}\mathbf{F}_{sm}(\mathbf{r}_{sm})\Bigg]\\&-\sum_{l=1}^{m-1}\sum_{p=m+1}^{N}\alpha_{lm}\alpha_{mp}k_{lm}k_{mp}\mathbf{F}_{lm}\cdot\mathbf{F}_{mp}\\&+\frac{1}{2}\sum_{l=1}^{m-1}\sum_{s\neq l}^{m-1}\alpha_{lm}\alpha_{sm}k_{lm}k_{sm}\mathbf{F}_{lm}\cdot\mathbf{F}_{sm}\\&+\frac{1}{2}\sum_{n=m+1}^{N}\sum_{n\neq q=m+1}^{N}\alpha_{mn}\alpha_{mq}k_{mn}k_{mq}\mathbf{F}_{mn}\cdot\mathbf{F}_{mq}\Bigg\}.\end{aligned} \quad (27)$$

The simplest approximation is to neglect the term $\mathcal{R}$ altogether. In this case the function $f=0$ solves for Eq. (21). Then the solution of Eq. (1) takes on the approximate form

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\approx\mathcal{N}\prod_{m>l,j=1}^{N}\xi_j(\mathbf{r}_j)\varphi_j(\mathbf{r}_j)\varphi_{lm}(\mathbf{r}_{lm}). \quad (28)$$

Thus the justification of the approximation (28) reduces to the validity of neglecting the inhomogeneous term (27). One region in which this term can be disregarded is the asymptotic region of large interparticle separations. This is immediately deduced from the asymptotic behavior of the generalized functions $\mathbf{F}_{ij}(\mathbf{r}_{ij}),\mathbf{F}_l(\mathbf{r}_l)$, which dictate the asymptotic properties of $\mathcal{R}$, as readily concluded from Eq. (27). From the asymptotic expansion of the hypergeometric functions [20] we infer that

$$\begin{aligned}\lim_{r_{ij}\to\infty}|\mathbf{F}_{ij}(\mathbf{r}_{ij})|\to&\left|\frac{\hat{\mathbf{k}}_{ij}+\hat{\mathbf{r}}_{ij}}{\mathbf{k}_{ij}\cdot(\hat{\mathbf{k}}_{ij}+\hat{\mathbf{r}}_{ij})r_{ij}}\right|\\&+O(|k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}|^{-2})\ .\end{aligned} \quad (29)$$

An asymptotic relation similar to Eq. (29) holds for $\mathbf{F}_l(\mathbf{r}_l)$. It should be noted that the functions $\mathbf{F}_{ij}(\mathbf{r}_{ij}),\mathbf{F}_l(\mathbf{r}_l)$ have to be considered in a distributive (operator) sense, which means that, asymptotically, only terms of $\mathbf{F}_{ij},\mathbf{F}_l$ that fall off faster

than the Coulomb potentials can be disregarded. Since $\mathcal{R}$ is essentially a sum of products of $\mathbf{F}_{ij},\mathbf{F}_l$, the expression $\mathcal{R}$ is of finite range, in the sense that it diminishes faster than the Coulomb potential in the asymptotic regime, only in the case where all particles are far apart from each other, i.e.,

$$\lim_{\substack{r_{ij}\to\infty \\ r_l\to\infty}} \mathcal{R} \;\to\; O(|k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}|^{-2},|k_l r_l+\mathbf{k}_l\cdot\mathbf{r}_l|^{-2})$$

$$\forall j>i,l\in[1,N]. \tag{30}$$

Therefore, in the limit (30), the term $\mathcal{R}$ can be asymptotically neglected and the approximation (28) is justified. In fact, it is straightforward to show that the wave function (28) tends to the asymptotic form (2) in the limit of large interparticle separations, which proves the assumption made in Ref. [1]. However, if two particles are close together, regardless of whether all other particles are well separated, the coupling term is of infinite range, as seen from Eqs. (29) and (27). In this case the relation (30) does not hold. Consequently, the wave function (28) is not an exact asymptotic eigenfunction of the total Hamiltonian in this limit. It is important to note that the limit Eq. (30) is energy dependent. With increasing momenta of the escaping particles the asymptotic region, i.e., the limit Eq. (30), is reached faster. In other words, at a certain interparticle separations, the remainder term $\mathcal{R}$, which has been neglected to arrive at the approximate form (28), diminishes with increasing velocities of the emerging particles. In this sense the approximation leading to the wave function (28) is a high-energy approximation.

III. TWO-BODY CUSP CONDITIONS

In the preceding section it has been shown that the approximation (28) is, to leading order, exact for large particles' separation. In addition, it is concluded below that this function exhibits a behavior compatible with Eq. (1) at all two-body coalescence points $r_{ij}\to 0, r_l\to 0$, with $j>i,l\in[1,N]$. To guarantee regular behavior of the wave function at these collision points, at which the corresponding Coulomb two-body potential is divergent, the solution $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ of Eq. (1) must satisfy the Kato cusp conditions [19,21] (provided the solution does not vanish at these points). At a collision point $r_i\to 0$ these conditions are

$$\left[\frac{\partial\ \widetilde{\Psi}(\mathbf{r}_1,\ldots,\mathbf{r}_N)}{\partial r_i}\right]_{r_i=0} = k_i\alpha_i\Psi(\mathbf{r}_1,\ldots,r_i=0,\ldots,\mathbf{r}_N)$$

$$\forall(r_i/r_j)\to 0,(r_i/r_{lm})\to 0;\ \ m>l,\ \ i\neq j\in[1,N]\ . \tag{31}$$

The quantity $\widetilde{\Psi}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ is the wave function $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ averaged over a sphere of small radius $r_\delta\ll 1$ around the singularity $r_i=0$. A relation similar to Eq. (31) holds in the case of the coalescence points $r_{ij}\to 0$. To prove that the wave function (28) satisfies the conditions (31) we linearize $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ around $r_i=0$ and average over a sphere of small radius $r_\delta\ll 1$ to arrive at

$$\widetilde{\Psi}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\mathcal{N}\ D(\mathbf{r}_i)\prod_{\substack{i\neq j=1 \\ l>m}}^{N}\xi_j\varphi_j(\mathbf{r}_j)\varphi_{lm}(\mathbf{r}_{lm}),\epsilon_{ilm}\neq 0, \tag{32}$$

where

$$D(\mathbf{r}_i)=\frac{2\pi}{4\pi r_\delta^2}\int_{-1}^{1} r_\delta^2 d\cos\theta[1+ik_i\cos\theta+\alpha_i k_i r_i(1+\cos\theta)]$$
$$=1+\alpha_i k_i r_i\,. \tag{33}$$

To arrive at Eq. (33) one takes the z axes as $\mathbf{k}_i$ and defines $\cos\theta=\hat{\mathbf{k}}_i\cdot\hat{\mathbf{r}}_i$. From Eqs. (33) and (32) it is obvious that

$$\left[\frac{\partial\ \widetilde{\Psi}(\mathbf{r}_1,\ldots,\mathbf{r}_N)}{\partial r_i}\right]_{r_i=0} = \alpha_i k_i\mathcal{N}\prod_{\substack{i\neq j=1 \\ l>m}}^{N}\xi_j\varphi_j(\mathbf{r}_j)\varphi_{lm}(\mathbf{r}_{lm})$$
$$=\alpha_i k_i\Psi(\mathbf{r}_1,\ldots,r_i=0,\ldots,\mathbf{r}_N),$$

$$\epsilon_{ilm}\neq 0. \tag{34}$$

In deriving Eq. (34) we made use of the fact that in the limit $(r_i/r_{ij}\to 0)$ the distance r_{ij} tends to r_j. The proof that the wave function (28) fulfills the cusp conditions at the collision points of two continuum particles $(r_{ji}\to 0)$ runs along the same lines. Finally, we remark that the wave function (28) is not compatible with the expansion of the exact solution of the Schrödinger equation (1) at the three-body collision points (e.g., $r_i\to 0$ and $r_j\to 0, j\neq i$) since in this case the exact wave function is known to satisfy a Fock expansion [22] in the coordinate $\rho:=\sqrt{(r_i^2+r_j^2)}$, which contains, in addition to powers in ρ, logarithmic terms in ρ, whereas the wave function (28) possesses a regular power-series expansion around $r_i\to 0$ and $r_j\to 0$.

IV. NORMALIZATION

The knowledge of the normalization factor $\mathcal{N}$ of the wave function (28) is imperative for the evaluation of scattering amplitudes using the wave function (28) as a representation of scattering states. In principle, $\mathcal{N}$ is derived from a $3N$-dimensional integral over the norm of the function (28) which, for large N, is an inaccessible task. Thus, for the determination of $\mathcal{N}$ we resort to the requirement that the flux through an asymptotic manifold defined by a constant large interparticle separations should be the same in the case of the wave function (28) and a normalized plane-wave representation of the scattering state, i.e.,

$$\mathbf{J}_{\mathrm{PW}}=\mathbf{J}_\Psi\,, \tag{35}$$

where the plane-wave flux is given by

$$\mathbf{J}_{\mathrm{PW}}=-\frac{i}{2}(2\pi)^{-3N}\left[\prod_l^N \xi_l^*(\mathbf{r}_l)\boldsymbol{\nabla}\prod_l^N \xi_l(\mathbf{r}_l) - \prod_l^N \xi_l(\mathbf{r}_l)\boldsymbol{\nabla}\prod_l^N \xi_l^*(\mathbf{r}_l)\right] = (2\pi)^{-3N}\sum_{l=1}^N \mathbf{k}_l . \tag{36}$$

In Eq. (36) the total gradient $\boldsymbol{\nabla}:=\Sigma_{l=1}^N \boldsymbol{\nabla}_l$ has been introduced. To evaluate the flux generated by the wave function (28) we note that, by taking advantage of Eqs. (23) and (25), we can write for the total gradient of the wave function (28)

$$\nabla\Psi := P\mathcal{N}\sum_{m=1}^N \left\{ i\mathbf{k}_m\Psi + \alpha_m k_m \mathbf{F}_m\Psi + \left[\sum_{n=m+1}^N \alpha_{mn}k_{mn}\bar{\mathbf{F}}_{mn}(\mathbf{r}_{mn})\prod_{\substack{j>i\\ j\neq n}}^N \varphi_{ij} - \sum_{l=1}^{m-1}\alpha_{lm}k_{lm}\bar{\mathbf{F}}_{lm}(\mathbf{r}_{lm})\prod_{\substack{j>i\\ i\neq l}}^N \varphi_{ij}\right]\prod_{s=1}^N \xi_s(\mathbf{r}_s)\varphi_s(\mathbf{r}_s)\right\}, \tag{37}$$

where $\bar{\mathbf{F}}_{mn}$ is given by $\mathbf{F}_{mn}\varphi_{mn}$. The decisive point now is that since we are considering the flux at large interparticle distances only the first term of Eq. (37) is relevant. This is readily deduced from Eqs. (24) and (26) which state that all other terms in Eq. (37), except for the first term, can be neglected asymptotically. Note, in this context, that terms in the wave function that are asymptotically of the order $O(1/r_j,1/r_{lm})$ correspond to parts of the Hamiltonian falling off faster than the Coulomb potentials and hence can be disregarded in the asymptotic regime. Now making use of the asymptotic expansion of the confluent hypergeometric function [20] and taking leading order in the interparticle distances, the flux $\mathbf{J}_\Psi$ can be deduced

$$\mathbf{J}_\Psi=\mathcal{N}^2\prod_{j=1}^N \frac{\exp(\pi\alpha_j)}{\Gamma(1-i\alpha_j)\Gamma^*(1-i\alpha_j)} \times\prod_{m>l=1}^N \frac{\exp(\pi\alpha_{lm})}{\Gamma(1-i\alpha_{lm})\Gamma^*(1-i\alpha_{lm})}\sum_{n=1}^N \mathbf{k}_n , \tag{38}$$

where $\Gamma(x)$ is the Gamma function. From Eqs. (35), (36), and (38) it follows that

$$\mathcal{N}=(2\pi)^{-3N/2}\prod_{j=1,m>l=1}^N \exp[-\pi(\alpha_{lm}+\alpha_j)/2] \times\Gamma(1-i\alpha_j)\Gamma(1-i\alpha_{lm}). \tag{39}$$

For two charged particles moving in the field of a heavy nucleus the wave function (28) with the normalization, given by Eq. (39), simplifies to the three-body wave function proposed in Refs. [4,7].

V. APPLICATION TO THE FOUR-BODY COULOMB CONTINUUM PROBLEM

Apart from the Rutherford scattering, the simplest application of the theory presented in the previous sections is the description of three-body Coulomb continuum states that are, for example, achieved as final states of electron-impact ionization and doublephoto ionization of atomic and molecular systems. In this case the wave function (28) simplifies to the three-body wave function proposed in Refs. [4,7] and extensively used by various authors. The second step in complexity is the description of the four-body scattering states. These states arise in the final channel of various reactions such as the double ionization of atomic systems by electron and positron impact as well as the triplephoto ionization. Experimentally there has been an increased interest in such reactions due to recent advances in coincidence-detection techniques [10–13]. The measurement of fully differential cross sections of reactions leading to four-body Coulomb continuum states was reported in Refs. [10,11]. In this study argon and krypton targets have been double ionized by a fast projectile electron under conditions where little momentum is being transferred to the target atoms. To describe the final state, the standard theoretical treatment [23–30] has been to reduce the four-body Coulomb continuum problem to a three-body problem by employing a first-order Born-type approximation (FBA) in the projectile-target potential, which is justified for the conditions under which the experiment has been performed. Recently, measurements for electron-impact double ionization have been performed at intermediate incident energies using the cold-target recoil-ion momentum spectroscopy [12,14]. In this case the FBA model is inappropriate. The last statement was also inferred from recent measurements [15] of the cross section for the double ionization of magnesium by electron impact at moderate incident energy. In view of these recent experiments and the absence of adequate theoretical models it appears timely to consider the applicability of the theory developed in the previous sections for the case of the four-body problem.

A. Product charges according to Jetzke and Faisal

For N continuum particles the wave function (28) describes $N(N-1)/2$ two-body Coulomb subsystems. The coupling between these two-body subsystems through the relative coordinates presents a serious problem for the calculations of scattering amplitudes. To overcome these difficulties further simplifications are needed. In Ref. [17] a procedure has been proposed in which the correlations between the continuum particles are completely subsumed in an effective interactions of each continuum particle with the nucleus. This is achieved by rewriting the total Coulomb potential in the form

$$\sum_{j=1}^N \frac{ZZ_j}{r_j} + \sum_{\substack{i,j\\ j>i=1}}^N \frac{Z_iZ_j}{r_{ij}} = \sum_i^N \frac{Z_i^{\mathrm{JF}}}{r_i}, \tag{40}$$

where the local product charges Z_i^{JF} are given by

$$Z_i^{\mathrm{JF}}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=ZZ_i+\sum_{j\neq i}^N Z_iZ_j\frac{\mathbf{r}_i\cdot\mathbf{r}_{ij}r_i}{r_{ij}^3}. \tag{41}$$

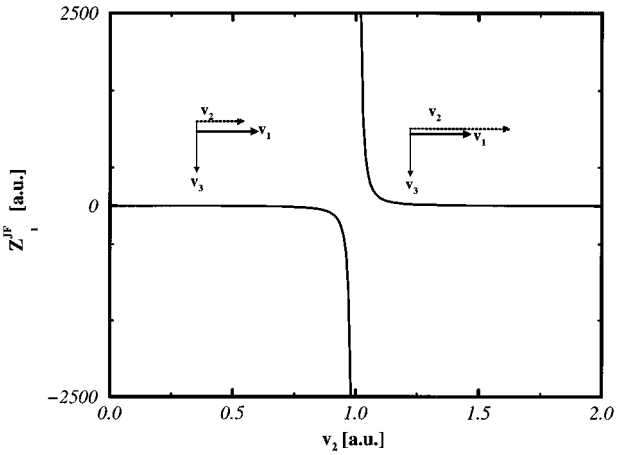

FIG. 1. Case where one positron and two electrons are moving in a nuclear field of a charge $Z=2$. The velocity vectors of all particles lie in the same plane. One electron, particle 2, and the positron, particle 1, are assumed to escape in the same direction with the positron having a fixed velocity $v_1=1$ a.u. The remaining electron, particle 3, is ejected in a direction perpendicular to $\mathbf{v}_1$, i.e., $\hat{\mathbf{v}}_1\cdot\hat{\mathbf{v}}_3=0$, with a fixed velocity $v_3=1$ a.u. The positron-nucleus product charge Z_1^{eff}, determined according to Eq. (42), is studied as function of v_2.

The position dependence of the product charges Z_i^{JF} is then converted into a velocity dependence by making use of the asymptotic approximation $\mathbf{r}_i=\mathbf{v}_i t$, where t is the time. This approximation is valid at large interparticle separations in which case Eq. (41) reduces to

$$Z_i^{\text{JF}}(\mathbf{v}_1,\ldots,\mathbf{v}_N)=ZZ_i+\sum_{j\neq i}^{N} Z_iZ_j\frac{\mathbf{v}_i\cdot\mathbf{v}_{ij}v_i}{v_{ij}^3}. \tag{42}$$

Upon substitution of Eq. (42) in Eq. (40), the differential equation (1) becomes completely separable. The solution is obtained from the function (28) in the special case $\alpha_j=Z_j^{\text{JF}}/v_j$ and $\alpha_{ij}\equiv 0$. When two continuum particles i,j approach each other in momentum space ($k_{ij}\to 0$) the effective charges, given by Eq. (41), diverge so as to simulate attractive (if $Z_iZ_j<0$) or repulsive (if $Z_iZ_j>0$) interaction between these particles. However, since these product charges contain scalar products between the velocity vectors of the escaping particles they exhibit unphysical behavior in the limit $\mathbf{v}_i\|\mathbf{v}_j$, $v_i\to v_j\pm\delta, 1\gg\delta>0$. This is clearly illustrated in Fig. 1, where we envisage the case of two electrons and one positron moving in the triple continuum of a residual charge $Z=2$. This is the final state achieved by positron-impact double ionization of He. We focus on the case in which one electron and the positron emerge in the same direction. When this electron approaches the positron (in momentum space) the positron-nucleus interaction (product charge) becomes strongly attractive in order to simulate the attractive electron-positron interaction. However, as the electron passes the positron the positron-nucleus interaction (product charge) varies rapidly from an attractive to a repulsive interaction. In other words, at the removable singularities $v_{ij}=0$ of the product charges (42) the functions $Z_i^{\text{JF}}v_{ij}^2, Z_j^{\text{JF}}v_{ij}^2$ are discontinuous in the limit $v_{ij}\to 0$. This behavior is quite unphysical and must be considered as a result of the way in which these product charges are constructed. We remark in passing that the same behavior of these product charges also arise for different charge states of the continuum particles as well as for a different number of these particles, in particular for a three-body system.

B. Product charges for the four-body Coulomb system in the continuum

In order to construct product charges $\overline{Z_j}, j\in[1,3]$, for a four-body system, that do not exhibit the unphysical behavior shown in Fig. 1, we maintain the philosophy of completely subsuming the correlations between the continuum particles into an effective interaction of these particles with the nucleus. In other words, the wave function (28) is written in the form

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)\approx\Psi^{\text{eff}}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\overline{\mathcal{N}}\prod_{j=1}^{N}\xi_j(\mathbf{r}_j)\overline{\varphi_j}(\mathbf{r}_j), \tag{43}$$

where $\overline{\varphi_j}(\mathbf{r}_j)=\varphi_j(\mathbf{r}_j)|_{\alpha_j=\overline{\alpha_j}}$ and $\overline{\mathcal{N}}=\mathcal{N}|_{\alpha_j=\overline{\alpha_j}}$, where $\overline{\alpha_j}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=Z_j(\mathbf{r}_1,\ldots,\mathbf{r}_N)/v_j$. The local product charges $Z_j(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ are then determined by requiring that the solution (43) should match the known solutions of the Schrödinger equation (1) in some limiting cases. In what follows we investigate these limiting cases of the four-body Schrödinger equation. However, for brevity, only the structure of Eq. (1) is discussed. The corresponding wave functions in these cases are easily deduced.

(a) Since all particles appear in the Schrödinger equation (1) in a symmetrical way all three continuum particles must be treated on equal footing, which results in the relations

$$\overline{Z_j}(Z_i,\mathbf{r}_i;Z_j,\mathbf{r}_j)=\overline{Z_i}(Z_j,\mathbf{r}_j;Z_i,\mathbf{r}_i). \tag{44}$$

(b) When two particles i,j approach each other ($r_{ij}\to 0, r_{ij}/r_k\to 0$) their mutual interaction increases as Z_iZ_j/r_{ij} and dominates the other interactions appearing in Eq. (1). Hence the interactions of particle i and particle j with the nucleus must change in a way that simulates their mutual Coulomb interaction regardless of the direction in which particle i is approached by particle j. The interaction of the remaining continuum particles with the nucleus must remain finite, i.e.,

$$\lim_{\substack{r_{ij}\to 0\pm\mathbf{d}\\ r_{ij}/r_l\to 0}}\overline{Z_i},\overline{Z_j}\to C\frac{Z_iZ_j}{r_{ij}},\overline{Z_l}\quad\text{finite},\quad|\mathbf{d}|\ll 0,\epsilon_{ijl}\neq 0, \tag{45}$$

where C is a positive real number. Condition (45) is violated by the product charges, given by Eq. (41).

(c) If one particle is moving in the vicinity of the nucleus it experiences the full nuclear charge. Assuming the remaining two continuum particles to be far away from the nucleus, their interaction with the nucleus must remain finite,

$$\lim_{r_i\to 0, r_i/r_j\to 0}\overline{Z_i}\to Z_iZ,\overline{Z_j}\quad\text{finite}\quad\forall\ i\neq j\in[1,3]. \tag{46}$$

(d) In order to treat the total potential V in an exact manner, V, and hence the Schrödinger equation (1), must be invariant under the local product charges Z_j,

$$\sum_{j=1}^{3} \frac{\overline{Z_j}}{r_j} = V. \tag{47}$$

(e) From the Schrödinger equation (1) it is readily concluded that if one particle, say particle l, is far away from the remaining three particles, this particle (l) experiences a net charge of $Z+Z_i+Z_j$, i.e.,

$$\lim_{\substack{r_l\to\infty \\ r_l/r_i, r_l/r_j\to\infty}} \overline{Z_l} \to Z_l(Z+Z_i+Z_j), \epsilon_{ijl}\neq 0. \tag{48}$$

In addition, if in the three-body system, formed by the nucleus, particle i, and particle j, particle i approaches the nucleus, particle j experiences a net nuclear charge of $Z+Z_i$, as immediately concluded from Eq. (1). Mathematically this condition can be formulated as

$$\lim_{\substack{r_l\to\infty \\ r_i\to 0, (r_i/r_j, r_j/r_l)\to 0}} \overline{Z_j} \to Z_j(Z+Z_i). \tag{49}$$

(f) It is established that for three electrons moving in the field of a residual positive charge Z the gradient of the total potential vanishes when the three electrons recede equidistant from the nucleus forming an equilateral triangle with the nucleus residing in the center of this triangle [31]. In this case the force exerted on the three electrons by the nucleus vanishes and the interelectronic correlations are minimized. The Schrödinger equation (1) reduces in this configuration to

$$\left[H_0 + \sum_{j=1}^{3} \frac{-Z+\frac{1}{\sqrt{3}}}{r_j} - E \right] \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 0. \tag{50}$$

The eigenfunction of Eq. (50) can be given in closed form. To account for this Wannier-type configuration [32], which is known to dominate the escape dynamics at lower excess energies E, we impose on the local charges Z_j, $j\in[1,3]$, in the case of three continuum electrons, the relations

$$\lim_{\substack{r_i\to r_j\to r_l \\ \hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j = \cos\pi/3}} \overline{Z_j} \to -Z+\frac{1}{\sqrt{3}}$$

$$\forall i,j,l\in[1,3], \quad \epsilon_{ijl}\neq 0, \quad Z_1=Z_2=Z_3=-1. \tag{51}$$

We note that all the conditions listed above are directly deduced from the Schrödinger equation (1) in the respective (dipole) limits. To incorporate the above relations into local product charges $\overline{Z_j}$, which are analytical functions in the whole configuration space, except for the poles given by Eq. (45), we define effective two-body potential $V_j=Z_j/r_j$ and introduce the linear transformation

$$\overline{V_j} = a_{j1}V_1 + a_{j2}V_2 + a_{j3}V_3 + a_{j4}V_{12} + a_{j5}V_{13} + a_{j6}V_{23}, \quad j\in[1,3], \tag{52}$$

where $V_i=ZZ_i/r_i$ and $V_{ij}=Z_iZ_j/r_{ij}$ are the physical two-body potentials. Equivalent transformations of the charges $Z_j=V_jr_j$ immediately derive from Eq. (52). To determine the product charges Z_j the 6×3-matrix $\mathcal{A}$ with elements a_{ij} has to be derived. The conservation of the total potential [condition d] requires

$$\sum_{i=1}^{3} a_{ij} = 1 \quad \forall j\in[1,6]. \tag{53}$$

Relation (46) implies

$$a_{ii}=1 \quad \forall i\in[1,3], \quad a_{12}=a_{13}=a_{21}=a_{23}=a_{31}=a_{32}\equiv 0. \tag{54}$$

Imposing condition (45) leads to

$$a_{16}=0, \ a_{25}=0, \ a_{34}=0. \tag{55}$$

Thus the product charges are determined by the equations

$$\overline{Z_1} = ZZ_1 + \overline{a_{14}}\frac{r_1}{r_1+r_2}\,\frac{Z_1Z_2r_1}{r_{12}} + \overline{a_{15}}\frac{r_1}{r_1+r_3}\,\frac{Z_1Z_3r_1}{r_{13}}, \tag{56}$$

$$\overline{Z_2} = ZZ_2 + \overline{a_{24}}\frac{r_2}{r_1+r_2}\,\frac{Z_1Z_2r_2}{r_{12}} + \overline{a_{26}}\frac{r_2}{r_2+r_3}\,\frac{Z_2Z_3r_2}{r_{23}}, \tag{57}$$

$$\overline{Z_3} = ZZ_3 + \overline{a_{35}}\frac{r_3}{r_1+r_3}\,\frac{Z_1Z_3r_3}{r_{13}} + \overline{a_{36}}\frac{r_3}{r_2+r_3}\,\frac{Z_2Z_3r_3}{r_{23}}, \tag{58}$$

where the coefficients a_{ij} have been transformed to $\overline{a_{ij}}$ to simplify subsequent calculations. The relations, given by Eq. (48), yield, in the limits $(r_1/r_2, r_1/r_3)\to\infty$, $(r_2/r_1, r_2/r_3)\to\infty$, and $(r_3/r_2, r_3/r_1)\to\infty$, respectively,

$$Z_1(Z_2+Z_3) = \overline{a_{14}}Z_1Z_2 + \overline{a_{15}}Z_1Z_3, \tag{59}$$

$$Z_2(Z_1+Z_3) = \overline{a_{24}}Z_1Z_2 + \overline{a_{26}}Z_2Z_3, \tag{60}$$

$$Z_3(Z_1+Z_2) = \overline{a_{35}}Z_1Z_3 + \overline{a_{36}}Z_2Z_3. \tag{61}$$

Making use of Eq. (59), relation (56) reduces to

$$\overline{Z_1} = ZZ_1 + [Z_1(Z_2+Z_3) - \overline{a_{15}}Z_1Z_3]\frac{r_1^2}{(r_1+r_2)r_{12}} + \overline{a_{15}}\frac{r_1}{r_1+r_3}\,\frac{Z_1Z_3r_1}{r_{13}}. \tag{62}$$

Now we impose condition (49) on Eq. (62) and arrive at

$$\lim_{\substack{r_2\to\infty, \ r_3\to 0 \\ r_2\gg r_1\gg r_3}} \overline{Z_1} = Z_1(Z+Z_3) = ZZ_1 + \overline{a_{15}}Z_1Z_3 \tag{63}$$

which leads to $\overline{a_{15}}=1$. From Eq. (59) we deduce that $\overline{a_{14}}=1$. Similar considerations yield $\overline{a_{24}}=\overline{a_{26}}=\overline{a_{36}}=\overline{a_{35}}=1$. Thus the final form of the product charges is

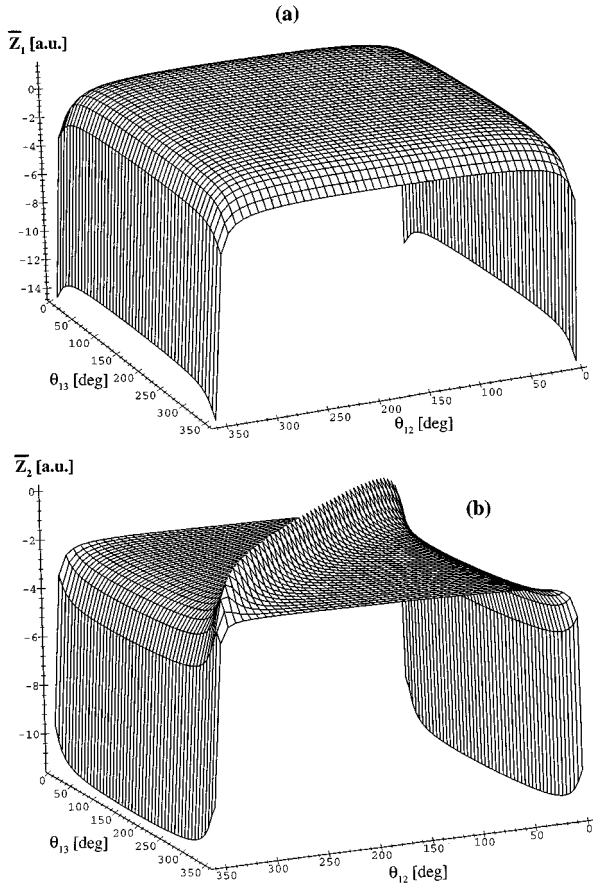

FIG. 2. For a four-body Coulomb system consisting of two electrons and one positron in the field of a residual charge $Z=2$, the effective charges, given by Eqs. (64) and (65), are depicted for the case where all particles escape in the same plane with velocities $v_1=v_2=1$ a.u. and $v_3=1.2$ a.u. The positron is taken to be particle 1. All angles are measured with respect to the direction $\hat{\mathbf{v}}_1$. (a) shows the angular dependence of the positron-nucleus effective product charge $\overline{Z}_1$, whereas in (b) the product charge of electron 1 with the nucleus ($\overline{Z}_2$) is investigated.

$$\overline{Z_1}=ZZ_1+\left[\frac{Z_1Z_2}{(r_1+r_2)r_{12}}+\frac{Z_1Z_3}{(r_1+r_3)r_{13}}\right]r_1^2, \tag{64}$$

$$\overline{Z_2}=ZZ_2+\left[\frac{Z_1Z_2}{(r_1+r_2)r_{12}}+\frac{Z_2Z_3}{(r_2+r_3)r_{23}}\right]r_2^2, \tag{65}$$

$$\overline{Z_3}=ZZ_3+\left[\frac{Z_1Z_3}{(r_1+r_3)r_{13}}+\frac{Z_2Z_3}{(r_2+r_3)r_{23}}\right]r_3^2. \tag{66}$$

It is straightforward to verify that all the conditions (44)–(51) are satisfied by the functions (64)–(66). For practical applications the position dependence of the effective charges (64)–(66) has to be converted into velocity dependence by applying the asymptotic approximation $\mathbf{r}_j=\mathbf{v}_j t$. Using this method, pilot calculations of the fully differential cross sections for the electron- and positron-impact double ionization of He($^1S^e$) have been reported [18]. A more extensive study of these reactions is in preparation [33]. For the case of positron impact the positron-nucleus product charge $\overline{Z}_1$ is depicted in Fig. 2(a), whereas Fig. 2(b) shows the electron-nucleus product charge in a typical scattering geometry where all momenta of the outgoing particles lie in the same plane. From Figs. 2(a) and 2(b) it is evident that when one of the electrons approaches the positron in velocity space the interaction of this electron with the nucleus and the positron-nucleus interaction become strongly attractive, which simulate the capture of the respective electron to the continuum of the positron. With diminishing interelectronic velocity the electron-nucleus interactions become strongly repulsive [see Fig. 2(b)] as to signify the repulsive electron-electron final-state interaction.

Three final remarks concerning the use of effective charges are due here. As our conditions (44)–(51), which have been used to determine the product charges Z_j, are limits, there will naturally be other functional forms of local product charges that smoothly connect between these limits. The procedure used here is based on the transformation (52), which is motivated by physical arguments rather than by strict mathematical reasoning. A different procedure might well lead to different product charges Z_j. Thus the benchmark for such approximate methods is that the derived effective product charges must be compatible with the physical picture of the dynamics of many-body continuum Coulomb states.

The second remark concerns the Kato cusp conditions at the collision point of two continuum particles. All effective-charge methods yield many-body wave functions of the form given by Eq. (43). Since $\partial\Psi^{\rm eff}/\partial r_{ij}=0$ such wave functions do not satisfy the Kato cups condition at the coalescence point of two continuum particles, as immediately concluded from Eq. (31).

The final remark concerns the applicability of this method for calculating scattering amplitudes. The basic idea of this work is to propagate (approximate) asymptotic solutions of the many-body Schrödinger equation to finite distances. The region around the origin where the reaction takes place, however, is not covered by this procedure. Therefore, the success or failure of employing this method to calculate reaction cross sections will decisively depend on how the process under consideration is treated at shorter distances around the origin. For example, in Refs. [34,35] the one-photon double ionization of helium has been considered. In both cases the wave function of the two electrons in the continuum of He^{2+} was taken, at large distances, in the form of Eq. (43). However, due to different treatments of the reaction around the origin, the cross section presented in Ref. [34] is in very good agreement with experimental finding, whereas the method used in Ref. [35] yielded quite disappointing results.

VI. CONCLUSION

In this work a many-body correlated scattering Coulomb wave function has been derived for N charged particles of equal masses moving in the N continuum of a massive residual charge. It has been shown that the derived wave function solves, to leading order, for the many-body Schrödinger equation in the asymptotic regime defined by large interparticle distances, which provides an expression for the asymptotic many-body Coulomb scattering states. It has been verified that the Kato cusp conditions at all two-body collision points are fulfilled by the derived wave function. In addition,

the normalization of the proposed wave function has been deduced. The developed scattering states have been considered in the case of the four-body continuum Coulomb system. A method based on the effective-product-charge strategy has been suggested to simplify the proposed wave function so as to make feasible the calculations of reaction cross sections.

ACKNOWLEDGMENTS

I would like to thank Erich Weigold and Steve Buckman for helpful suggestions and comments on the manuscript. Financial support by the Alexander von Humboldt Foundation and the Australian National University is gratefully acknowledged.

[1] L. Rosenberg, Phys. Rev. D **8**, 1833 (1973).
[2] R. K. Peterkop, *Theory of Ionization of Atoms by the Electron Impact* (Colorado Associated University Press, Boulder, 1977).
[3] S. P. Merkuriev, Theor. Math. Phys. **32**, 680 (1977).
[4] M. Brauner, J. S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[5] E. O. Alt and A. M. Mukhamedzhanov, Phys. Rev. A **47**, 2004 (1993).
[6] J. Berakdar, Phys. Rev. A **53**, 2314 (1996).
[7] G. Garibotti and J. E. Miraglia, Phys. Rev. A **21**, 572 (1980).
[8] J. S. Briggs, Phys. Rev. A **41**, 539 (1990).
[9] M. Yu. Kuchiev and S. A. Scheinerman, Usp. Fiz. Nauk. SSSR **158**, 353 (1989) [Sov. Phys. Usp. **32**, 569 (1989)].
[10] A. Lahmam-Bennani, C. Dupŕe, and A. Duguet, Phys. Rev. Lett. **63**, 1582 (1989).
[11] A. Lahmam-Bennani, A. Duguet, A. M. Grisogono, and M. Lecas, J. Phys. B **25**, 2873 (1992).
[12] R. Dörner, V. Mergel, L. Spielberger, O. Jagutzki, S. Nuttgens, M. Unverzagt, H. Schmidt-Böcking, J. Ullrich, R. E. Olson, K. Tokesi, W. E. Meyerhof, W. Wu, and C. L. Cocke, Nucl. Instrum. Methods Phys. Res. Sect. B **99**, 111 (1995).
[13] B. El Marji, A. Duguet, A. Lahmam-Bennani, M. Lecas, and H. F. Wellenstein, J. Phys. B **26**, L733 (1995).
[14] O. Jagutzki, L. Spielberger, R. Dörner, S. Nüttgens, V. Mergel, H. Schmidt-Böcking, J. Ullrich, R. E. Olson, and U. Buck, Z. Phys. D **36**, 5 (1996).
[15] M. J. Ford, J. H. Moore, M. A. Coplan, J. W. Cooper, and J. P. Doering, Phys. Rev. Lett. **77**, 2650 (1996).
[16] L. Avaldi, P. Belotti, P. Bolognesi, R. Camilloni, and G. Stefani, Phys. Rev. Lett **75**, 1915 (1995).
[17] S. Jetzke and F. H. M. Faisal, J. Phys. B **25**, 1543 (1992).
[18] J. Berakdar, Phys. Lett. A **220**, 237 (1996).
[19] T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957).
[20] M. Abramowitz and I. Stegun, *Pocketbook of Mathematical Functions* (Verlag Harri Deutsch, Frankfurt, 1984).
[21] C. R. Myers, C. J. Umrigar, J. P. Sethna, and J. D. Morgan, III, Phys. Rev. A **44**, 5537 (1991).
[22] V. A. Fock, K. Nor. Vidensk. Selsk. Frh. **31**, 138 (1958).
[23] B. Joulakian, C. Dal Cappello, and M. Brauner, J. Phys. B **25**, 2863 (1992).
[24] B. Joulakian and C. Dal Cappello, Phys. Rev. A **47**, 3788 (1993).
[25] C. Dal Cappello and H. Le Rouzo, Phys. Rev. A **43**, 1395 (1991).
[26] R. J. Tweed, J. Phys. B **6**, 270 (1973).
[27] Yu. F. Smirnov, A. V. Pavlitchenkov, V. G. Levin, and G. Neudatchin, J. Phys. B **11**, 20 (1978).
[28] J. Berakdar and H. Klar, J. Phys. B **26**, 4219 (1993).
[29] J. Berakdar, J. Phys. (France) IV **3**, C6-135 (1993).
[30] J. Berakdar, Phys. Rev. A **53**, 2281 (1996).
[31] H. Klar and W. Schlecht, J. Phys. B **9**, 1699 (1976).
[32] G. Wannier, Phys. Rev. **90**, 817 (1953).
[33] J. Berakdar and E. Weigold (unpublished).
[34] M. Pont and R. Shakeshaft, Phys. Rev. A **51**, R2676 (1995).
[35] H. Le Rouzo and C. Dal Cappello, Phys. Rev. A **43**, 318 (1991).