# Approximate analytical solution of the quantum-mechanical three-body Coulomb continuum problem

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In this work a symmetric representation of the three-body Coulomb continuum wave function is constructed that represents an exact asymptotic solution of the many-body Schrödinger equation on a five-dimensional hypersphere of large hyperradius. Consequently, the wave function is shown to satisfy the Kato cusp conditions at all three two-body collision points. At finite distances the proposed solution is designed to account for properties of the total potential surface. In particular, dynamical stabilization due to the presence of ridge structure in the total potential (Wannier ridge) is encompassed in the present treatment. The behavior of the wave function at the total dissociation threshold is investigated. In order to allow for three-body interactions we linearly expand each two-body Coulomb potential in terms of all three two-body potentials. The expansion coefficients determine the amount of distortion of each two-body subsystem by the presence of the third particle and thus give direct information on the strength of three-body interactions.

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The study of the dynamics of three charged particles moving in the three-body continuum is one of the fundamental outstanding questions in atomic, molecular, and nuclear physics. The simple analytic dependence of Coulomb potentials and the small number of particles involved are in great contrast to the complexity of this process. The main difficulty arises from the infinite range of Coulomb forces which forbids free asymptotic states of charged particles. Hence, a three-body Coulomb continuum state remains a correlated one in the whole Hilbert space. This brings about principle as well as practical problems. Standard methods of scattering theory assume, in general, short-range forces, and therefore are not applicable to Coulomb systems. The evaluation of transition amplitudes for reactions involving charged particles requires then the knowledge of a many-body wave function whose exact form is unknown. Much theoretical effort has been thus devoted to finding approximate expressions for this wave function. An important prototype of such a problem is the motion of two electrons in the field of a nucleus which is the final state achieved in electron-impact ionization and double photoionization of atomic systems. The traditional, more practical, approach has been to break down the three-body system into two two-body subsystems which are uncoupled in the configuration space. The correlation between these two subsystems is then accounted for parametrically, e.g., by the use of momentum-dependent effective product charges [1–3]. In other words the six-dimensional wave function of the three-body continuum is expressed in the coordinates $\mathbf{r}_a, \mathbf{r}_b$ of two electrons $a,b$ with respect to the nucleus. No explicit dependence on the electron coordinate $\mathbf{r}_{ab}=\mathbf{r}_a-\mathbf{r}_b$ is included. Although this approach has rendered possible the calculation of ionization amplitudes which are to some extent in agreement with experimental data, its range of validity is difficult to estimate. In addition, such schemes are still unsatisfactory from a fundamental point of view. For example, wave functions provided by such methods do not satisfy the Kato cusp conditions at the electron-electron collision point and are inconsistent with the boundary condition of the Schrödinger equation, as will be shown below. Mathematically, the three-body Schrödinger equation constitutes an elliptical partial differential equation in six variables with nondenumerable infinity of solutions. Hence, appropriate boundary conditions prescribed on an asymptotic five-dimensional closed manifold $\mathscr{M}$ are needed to fix the wave function describing the process under consideration. Unfortunately, the specification of such asymptotic states is an involved task. Redmond [4] and others [5–7] proposed asymptotic scattering states valid in a subspace of $\mathscr{M}$ in which all interparticle distances tend to infinity. Only recently Alt and Mukhamedzhanov [8] showed that a correct description of the whole asymptotic region $\mathscr{M}$ requires the introduction of local relative momenta. It should be borne in mind, however, that such asymptotic states are crucial as boundary conditions to be imposed on acceptable solutions of the Schrödinger equation. From a practical point of view, they are of limited value since evaluation of ionization amplitudes involves integration over configuration space in domains outside the asymptotic region $\mathscr{M}$. For example, reaction zones most important for such amplitudes are often confined to a small region around the origin where all particles are close together. Hence, a proper description of continuum states resulting from such processes requires wave functions such that their range of validity goes beyond asymptotic regions. In other words, a propagation of asymptotic states to finite distances must be compatible with properties of the potential surface which is known to control the fragmentation dynamics [9].

In this work a strategy is developed to construct three-body continuum states which are, to leading order, exact asymptotic solutions on the manifold $\mathscr{M}$. The Kato-cusp conditions are then satisfied at all three two-body collision points. At finite distances, the back-to-back configuration $\mathbf{r}_a=-\mathbf{r}_b$ (Wannier configuration) is correctly described by the proposed function. This configuration is of particular interest since the potential surface contains a saddle structure

 

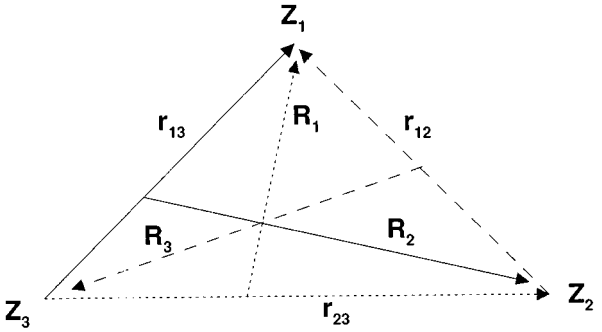


FIG. 1. The Jacobi coordinates as used in the text.

in this subspace which strongly influences the correlated dynamics of the system [12,9]. In addition, the behavior of the wave function at the three-body dissociation threshold is studied and shown to be regular. An approximate version of the wave function derived here has already been employed for the description of two continuum electrons following electron-impact single ionization of helium and atomic hydrogen. Preliminary results for the cross section of these processes turn out to be in good agreement with experimental findings over a wide range of collision geometry [13,14]. The paper is organized as follows. In Sec. I we investigate the asymptotic behavior of the Schrödinger equation and the range of validity of asymptotic wave functions and heuristically introduce the idea of this work. In Sec. II the scattering problem is reformulated in curvilinear coordinates in which the separation of the internal, body-fixed degrees of freedom from the space-fixed degrees of freedom is more transparent. Further, three-body interactions are explicitly introduced by an expansion of each two-body potential as a linear combination of all three two-body interactions. Section III deals with an application of the model where a wave function describing two continuum electrons in the field of a nucleus is derived. Threshold behavior, Kato-cusp conditions, and asymptotic behavior are analyzed. In addition, the uniqueness of this procedure is discussed. Conclusions are drawn in Sec. IV. Atomic units are used throughout.

## I. ASYMPTOTIC BEHAVIOR

In the center-of-mass system the internal motion of three charged particles with masses $m_i$ and charges $Z_i; i \in \{1,2,3\}$ can be described by each of the three Jacobi coordinates $(\mathbf{r}_{ij},\mathbf{R}_k); i,j,k \in \{1,2,3\}; \epsilon_{ijk} \neq 0; j>i$ (see Fig. 1). The three sets of Jacobi coordinates can be employed equivalently. They are connected with each other by the transformation

$$\begin{pmatrix} \mathbf{r}_3 \\ \mathbf{R}_2 \end{pmatrix} = \mathbf{D}_1 \begin{pmatrix} \mathbf{r}_{23} \\ \mathbf{R}_1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathbf{r}_{12} \\ \mathbf{R}_3 \end{pmatrix} = \mathbf{D}_2 \begin{pmatrix} \mathbf{r}_{23} \\ \mathbf{R}_1 \end{pmatrix}, \tag{1}$$

where

$$\mathbf{D}_1 = \begin{pmatrix} \mu_{23}/m_3 & 1 \\ 1-\mu_{13}\mu_{23}/m_3^2 & -\mu_{13}/m_3 \end{pmatrix},$$

$$\mathbf{D}_2 = \begin{pmatrix} -\mu_{23}/m_2 & 1 \\ -1+\mu_{12}\mu_{23}/m_2^2 & -\mu_{12}/m_2 \end{pmatrix}. \tag{2}$$

The reduced masses are defined as $\mu_{ij} = m_i m_j/(m_i+m_j); i,j \in \{1,2,3\}; j>i$. Accordingly, the momenta conjugate to $(\mathbf{r}_{ij},\mathbf{R}_k)$ are defined as $(\mathbf{k}_{ij},\mathbf{K}_k)$. These momenta are related to each other by

$$\begin{pmatrix} \mathbf{k}_{23} \\ \mathbf{K}_1 \end{pmatrix} = \mathbf{D}_2^t \begin{pmatrix} \mathbf{k}_{12} \\ \mathbf{K}_3 \end{pmatrix} = \mathbf{D}_1^t \begin{pmatrix} \mathbf{k}_{13} \\ \mathbf{K}_2 \end{pmatrix}, \tag{3}$$

where $\mathbf{D}_1^t$ and $\mathbf{D}_2^t$ are transposed matrices of $\mathbf{D}_1$ and $\mathbf{D}_2$, respectively. The scalar product

$$(\mathbf{r}_{ij},\mathbf{R}_k) \cdot \begin{pmatrix} \mathbf{k}_{ij} \\ \mathbf{K}_k \end{pmatrix}$$

is invariant for all three sets of Jacobi coordinates. The kinetic energy operator $H_0$ is then diagonal and reads

$$H_0 = -\frac{1}{2\mu_{ij}}\Delta_{\mathbf{r}_{ij}} - \frac{1}{2\mu_k}\Delta_{\mathbf{R}_k}, \quad \forall(\mathbf{r}_{ij},\mathbf{R}_k), \tag{4}$$

where $\mu_k = m_k(m_i+m_j)/(m_1+m_2+m_3)$. The eigenenergy of (4) is then given as

$$E_0 = \frac{\mathbf{k}_{ij}^2}{2\mu_{ij}} + \frac{\mathbf{K}_k^2}{2\mu_k}, \quad \forall(\mathbf{r}_{ij},\mathbf{R}_k). \tag{5}$$

The time-independent Schrödinger equation of the system reads

$$\left[ H_0 + \sum_{\substack{i,j \\ j>i}}^{3} \frac{Z_{ij}}{r_{ij}} - E \right] \langle \mathbf{r}_{kl},\mathbf{R}_m | \Psi \rangle = 0. \tag{6}$$

Here we defined a product charge $Z_{ij} = Z_i Z_j; j>i \in \{1,2,3\}$. The relative coordinates $r_{ij}$ occurring in the Coulomb potentials have to be expressed in terms of the appropriately chosen set $(\mathbf{r}_{kl},\mathbf{R}_m)$.

Asymptotic scattering solutions of (6) for large interparticle distances $\mathbf{r}_{ij}$, hereafter referred to as *Redmond asymptotic*, have the form [4–7,15]:

$$\lim_{\substack{r_{ij}\to\infty \\ R_k\to\infty}} \Psi(\mathbf{r}_{ij},\mathbf{R}_k) \to (2\pi)^{-3} \exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij} + i\mathbf{K}_k\cdot\mathbf{R}_k) \prod_{\substack{i,j=1 \\ j>i}}^{3} \times \exp[\pm i\alpha_{ij} \ln(k_{ij}r_{ij} \pm \mathbf{k}_{ij}\cdot\mathbf{r}_{ij})], \quad \forall(\mathbf{r}_{ij},R_k). \tag{7}$$

The + and − signs refer to outgoing and incoming boundary conditions, respectively. The Sommerfeld parameter $\alpha_{ij}$ are defined as follows:

$$\alpha_{ij} = \frac{Z_{ij}\mu_{ij}}{k_{ij}}. \tag{8}$$

The asymptotic form (7) is the generalization of the familiar two-body (Kepler) case to three-body systems. However, unlike the situation in two-body scattering, in three-body systems other types of asymptotics are present where, in a certain set $(\mathbf{r}_{ij},\mathbf{R}_k)$, one Jacobi coordinate tends to infinity whereas the other coordinate remains finite [8]. Therefore, we define the following asymptotic regions:

$$\mathscr{S}:=\{\mathbf{r}_{ij},\mathbf{R}_k;r_{ij}\to\infty \quad \text{and} \quad R_k\to\infty, \quad \forall(\mathbf{r}_{ij},\mathbf{R}_k)\}, \tag{9}$$

$$\mathscr{S}_\alpha:=\left\{\mathbf{r}_{ij},\mathbf{R}_\alpha;\frac{r_{ij}}{R_\alpha}\to 0 \quad \text{and} \quad R_\alpha\to\infty, \quad \forall(\mathbf{r}_{ij},\mathbf{R}_\alpha)\right\}, \tag{10}$$

$$\mathscr{S}_{ij}:=\left\{\mathbf{r}_{ij},\mathbf{R}_k;\frac{R_k}{r_{ij}}\to 0 \quad \text{and} \quad r_{ij}\to\infty, \quad \forall(\mathbf{r}_{ij},\mathbf{R}_k)\right\}. \tag{11}$$

The Redmond asymptotic is valid in $\mathscr{S}$ and $\mathscr{S}_{ij}$, but not in $\mathscr{S}_\alpha$, as will be explicitly shown below. In fact, the relation $\mathscr{S}_{ij}\subset\mathscr{S}$ holds (but not the converse). Hence, we restrict the treatment to the subspaces $\mathscr{S}$ and $\mathscr{S}_\alpha$. The asymptotic form of the wave function in $\mathscr{S}_\alpha$ is readily derived. To leading order Eq. (6) in $\mathscr{S}_\alpha$ takes on the form

$$\left(H_0+\frac{Z_{ij}}{r_{ij}}+\frac{Z_\alpha(Z_i+Z_j)}{R_\alpha}-E\right)\psi_\alpha^{as}=0, \quad \forall(\mathbf{r}_{ij},\mathbf{R}_\alpha)\in\mathscr{S}_\alpha. \tag{12}$$

Equation (12) is separable in the coordinates $(\mathbf{r}_{ij},\mathbf{R}_\alpha)$. Solutions of (12) satisfying outgoing boundary conditions read:

$$\begin{aligned}\psi_\alpha^{as}=&(2\pi)^{-3/2}\exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}+i\mathbf{K}_\alpha\cdot\mathbf{R}_\alpha)N_{ij}\\ &\times {}_1F_1(i\alpha_{ij},1,-i[k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}])\\ &\times\exp[i\bar{\gamma}_\alpha\ln(K_\alpha R_\alpha+\mathbf{K}_\alpha\cdot\mathbf{R}_\alpha)],\end{aligned} \tag{13}$$

where

$$\bar{\gamma}_\alpha:=\frac{Z_\alpha(Z_i+Z_j)\mu_\alpha}{K_\alpha},$$

$$N_{ij}:=(2\pi)^{-3/2}e^{-\pi\alpha_{ij}/2}\Gamma(1-i\alpha_{ij}). \tag{14}$$

The confluent hypergeometric function and the gamma function are denoted by ${}_1F_1(a,b,z)$ and $\Gamma(z)$, respectively. The existence of a global analytic asymptotic defined on $\mathscr{M}=\mathscr{S}_\alpha\cup\mathscr{S}_{ij}$ derives from the fact that the regions $\mathscr{S}_\alpha$ and $\mathscr{S}_{ij}$ are not disjoint. In order to find such an asymptotic form and to facilitate the derivation of wave functions valid at finite distances, we consider the propagation of the asymptotic (7) to finite distances, as proposed in Refs. [16,7,17,15]:

$$\Psi(\mathbf{r}_{ij},\mathbf{R}_k)\approx\Psi_{3C}(\mathbf{r}_{ij},\mathbf{R}_k):=(2\pi)^{3/2}\exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}+i\mathbf{K}_k\cdot\mathbf{R}_k)\prod_{\substack{m,n=1\\ n>m}}^{3}N_{mn}\,{}_1F_1(i\alpha_{mn},1,-i[k_{mn}r_{mn}+\mathbf{k}_{mn}\cdot\mathbf{r}_{mn}]). \tag{15}$$

To show explicitly the range of validity of (15) we make, for the exact solution of (6), the general ansatz:

$$\Psi(\mathbf{r}_{ij},\mathbf{R}_k)=\Psi_{3C}(\mathbf{r}_{ij},\mathbf{R}_k)[1-f(\mathbf{r}_{ij},\mathbf{R}_k)]. \tag{16}$$

To be specific we choose the set $(\mathbf{r}_{13},\mathbf{R}_2)$ and insert (16) in (6) to arrive at the differential equation

$$\begin{aligned}&\left[\frac{1}{2\mu_{13}}\Delta_{\mathbf{r}_{13}}+\frac{1}{\mu_{13}}(i\mathbf{k}_{13}+\alpha_{13}k_{13}\mathbf{F}_{13}+\alpha_{12}k_{12}\mathbf{F}_{12})\nabla_{\mathbf{r}_{13}}\right]f\\ &+\left[\frac{1}{2\mu_{23}}\Delta_{\mathbf{r}_{23}}+\frac{1}{\mu_{23}}(i\mathbf{k}_{23}+\alpha_{23}k_{23}\mathbf{F}_{23}-\alpha_{12}k_{12}\mathbf{F}_{12})\cdot\nabla_{\mathbf{r}_{23}}\right]f-\alpha_{12}k_{12}\mathbf{F}_{12}\cdot(Z_{13}\mathbf{F}_{13}-Z_{23}\mathbf{F}_{23})(1-f)=D_{pol}(f),\end{aligned} \tag{17}$$

where

$$\mathbf{F}_{ij}:=\frac{{}_1F_1(1+i\alpha_{ij},2,-i[k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}])}{{}_1F_1(i\alpha_{ij},1,-i[k_{ij}r_{ij}+\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}])}(\hat{\mathbf{k}}_{ij}+\hat{\mathbf{r}}_{ij}). \tag{18}$$

For the derivation of (17) we factor out the plane-wave part of (16) in Jacobi coordinates and then transform to relative coordinates $(\mathbf{r}_{13},\mathbf{r}_{23})$. This introduces the mass-polarization term $D_{pol}$ in (17), which has the form

$$D_{pol}(f):=\frac{1}{m_3}[D_1(f-1)+D_2 f], \tag{19}$$

where

$$D_2:=[\alpha_{13}k_{13}\mathbf{F}_{13}+\alpha_{12}k_{12}\mathbf{F}_{12}]\cdot\nabla_{\mathbf{r}_{23}}+[\alpha_{23}k_{23}\mathbf{F}_{23}-\alpha_{12}k_{12}\mathbf{F}_{12}]\cdot\nabla_{\mathbf{r}_3}+\nabla_{\mathbf{r}_{23}}\cdot\nabla_{\mathbf{r}_3} \tag{20}$$

and

$$\begin{aligned}D_1:=&(\alpha_{13}k_{13})(\alpha_{23}k_{23})\mathbf{F}_{13}\cdot\mathbf{F}_{23}-(\alpha_{13}k_{13})(\alpha_{12}k_{12})\mathbf{F}_{13}\cdot\mathbf{F}_{12}+(\alpha_{23}k_{23})(\alpha_{12}k_{12})\mathbf{F}_{23}\cdot\mathbf{F}_{12}+2k_{12}(\alpha_{12}k_{12})(i-\alpha_{12})(1+\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{r}}_{12})\\ &\times\frac{{}_1F_1(2+i\alpha_{12},3,-i[k_{12}r_{12}+\mathbf{k}_{12}\cdot\mathbf{r}_{12}])}{{}_1F_1(i\alpha_{12},1,-i[k_{12}r_{12}+\mathbf{k}_{12}\cdot\mathbf{r}_{12}])}+(\alpha_{12}k_{12})\frac{{}_1F_1(1+i\alpha_{12},2,-i[k_{12}r_{12}+\mathbf{k}_{12}\cdot\mathbf{r}_{12}])}{{}_1F_1(i\alpha_{12},1,-i[k_{12}r_{12}+\mathbf{k}_{12}\cdot\mathbf{r}_{12}])}\frac{2}{r_{12}}.\end{aligned} \tag{21}$$

Note that when dealing with continuum states resulting from ionization of atomic systems we take $m_3$ to be the mass of the nucleus and $m_1$ to be the mass of the particle initially bound. In this case the polarization term (19) is negligible $(m_1/m_3 \to 0)$.

The solution of (6) is thus reduced to the solution of Eq. (17). The function $f=1$ solves (17) but leads, however, to the trivial solution $\Psi=0$. The exact solution $\Psi(\mathbf{r}_{ij},\mathbf{R}_k)$ can only be replaced by $\Psi_{3C}(\mathbf{r}_{ij},\mathbf{R}_k)$ if the function $f=0$ is a solution of (17). This can only be the case when the inhomogeneous term

$$\mathscr{R} := \mu_{12} Z_{12} \mathbf{F}_{12} \cdot (Z_{13}\mathbf{F}_{13} - Z_{23}\mathbf{F}_{23}) + \frac{1}{m_3} D_1 \tag{22}$$

vanishes (in principle we arrive at a manifold of solutions $f=\text{const}$. Due to flux argument, however, only the solution $f=0$ is acceptable). The behavior of the expression $\mathscr{R}$ in Eq. (22) is dictated by the generalized functions $\mathbf{F}_{ij}$ (18), which exhibit the asymptotic form

$$\lim_{r_{ij}\to\infty} |\mathbf{F}_{ij}| \to \left| \frac{\hat{\mathbf{k}}_{ij} + \hat{\mathbf{r}}_{ij}}{\mathbf{k}_{ij} \cdot (\hat{\mathbf{k}}_{ij} + \hat{\mathbf{r}}_{ij}) r_{ij}} \right| + O(|k_{ij} r_{ij} + \mathbf{k}_{ij} \cdot \mathbf{r}_{ij}|^{-2}). \tag{23}$$

It should be emphasized that the functions $\mathbf{F}_{ij}$ and $\mathscr{R}$ are to be understood in the distributive sense, i.e., asymptotically only terms of $\mathbf{F}_{ij}$ which fall off faster than the Coulomb potentials can be disregarded. Consequently, the expression $\mathscr{R}$ (22) is asymptotically negligible only in the case when two independent Jacobi coordinates tend to infinity, or, equivalently, $r_{ij}\to\infty \forall i,j \in \{1,2,3\}; j>i$, for in this case we have

$$\lim_{\substack{r_{ij}\to\infty \\ R_k\to\infty}} \mathscr{R} \to O(|k_{ij} r_{ij} + \mathbf{k}_{ij} \cdot \mathbf{r}_{ij}|^{-2}), \quad \forall \mathbf{r}_{ij}, \mathbf{R}_k \in \mathscr{S}, \tag{24}$$

as is evident from (23). That means only in the subspaces $\mathscr{S}$ and $\mathscr{S}_{ij}$ is the wave function $\Psi_{3C}$ an asymptotic eigenstate of the Schrödinger equation (6), in agreement with [4–8]. In the asymptotic subspace $\mathscr{S}_\alpha$, however, the term $\mathscr{R}$ (22) is of the order of the Coulomb potential and hence cannot be neglected. Accordingly, $f=0$ does not solve (17) and $\Psi_{3C}$ is not a global asymptotic solution of (6) in $\mathscr{M}$. Asymptotic solutions valid in $\mathscr{M}$ have been proposed in Ref. [8]. In order to obtain solutions whose validity range extends to regions inside and outside $\mathscr{M}$ the function $f$, defined by Eq. (17), is required. Formally this function is determined by

$$f = f_0 - \int d^3 r'_{13} \int d^3 r'_{23} G(\mathbf{r}_{13} - \mathbf{r}'_{13}, \mathbf{r}_{23} - \mathbf{r}'_{23}) \mathscr{R}(\mathbf{r}'_{13}, \mathbf{r}'_{23}), \tag{25}$$

where the Green function $G(\mathbf{r}_{13},\mathbf{r}_{23})$ is given by

$$\begin{aligned} \Big[ \frac{1}{2\mu_{13}} \Delta_{\mathbf{r}_{13}} + \frac{1}{2\mu_{23}} \Delta_{\mathbf{r}_{23}} + \frac{1}{\mu_{13}} (i\mathbf{k}_{13} + \alpha_{13} k_{13} \mathbf{F}_{13} \\ + \alpha_{12} k_{12} \mathbf{F}_{12}) \cdot \nabla_{\mathbf{r}_{13}} + \frac{1}{\mu_{23}} (i\mathbf{k}_{23} + \alpha_{23} k_{23} \mathbf{F}_{23} \\ - \alpha_{12} k_{12} \mathbf{F}_{12}) \cdot \nabla_{\mathbf{r}_{23}} - \frac{1}{m_3} D_2 \Big] G(\mathbf{r}_{13}, \mathbf{r}_{23}) \\ = \delta^3(\mathbf{r}_{13}) \delta^3(\mathbf{r}_{23}). \end{aligned} \tag{26}$$

The following boundary conditions then have to be imposed:

$$f(\mathbf{r}_{ij},\mathbf{R}_k) = 0, \quad \forall \mathbf{r}_{ij}, \mathbf{R}_k \in \mathscr{S}, \tag{27}$$

$$f(\mathbf{r}_{ij},\mathbf{R}_k) = 1 - \frac{\psi^{as}_\alpha}{\Psi_{3C}}, \quad \forall \mathbf{r}_{ij}, \mathbf{R}_\alpha \in \mathscr{S}_\alpha. \tag{28}$$

From (27) we deduce $f_0=0$. However, finding the Green function $G(\mathbf{r}_{13},\mathbf{r}_{23})$ could be quite an involved task. In order to derive approximate analytical expression for the wave function we consider, instead, the functional dependence of the inhomogeneous term $\mathscr{R}$ (22). Let us assume for the moment the product charges $Z_{ij}$ to be position dependent and consider $\mathscr{R}$ as function of $Z_{ij}$. The decisive point is now to find product charges which leave the total potential, and hence the Schrödinger equation, invariant, i.e.,

$$\sum_{\substack{i,j \\ j>i}}^{3} \frac{\bar{Z}_{ij}}{r_{ij}} \equiv \sum_{\substack{i,j \\ j>i}}^{3} \frac{Z_{ij}}{r_{ij}}, \tag{29}$$

where the position-dependent product charges are denoted by $\bar{Z}_{ij}$. Subject to condition (29) the treatment remains exact. In addition to (29) we require

$$\mathscr{R}(\bar{Z}_{ij}) \to 0, \quad \forall \mathbf{r}_{ij}, \mathbf{R}_\alpha \in \mathscr{S}_\alpha, \tag{30}$$

$$\bar{Z}_{ij} \text{ finite}, \quad \forall \mathbf{r}_{ij}, \mathbf{R}_k \in \mathscr{S}. \tag{31}$$

Further, assume the solution of (6) to have the same analytical form as (15), however, with product charges satisfying (30) and (31), i.e.,

$$\Psi(\mathbf{r}_{ij},\mathbf{R}_k) \approx \Psi_{DS3C}(\mathbf{r}_{ij},\mathbf{R}_k) := \exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij} + i\mathbf{K}_k\cdot\mathbf{R}_k) \bar{N} \prod_{\substack{m,n=1 \\ n>m}}^{3} {}_1F_1(i\beta_{mn}, 1, -i[k_{mn} r_{mn} + \mathbf{k}_{mn}\cdot\mathbf{r}_{mn}]), \tag{32}$$

where the normalization constant is denoted by $\bar{N}$ and position-dependent Sommerfeld parameters have been introduced as

$$\beta_{mn} = \frac{\bar{Z}_{mn} \mu_{mn}}{k_{mn}}. \tag{33}$$

Now the main conjecture is, if the wave function (32) leads to the remainder (17) when making the ansatz (16) and inserting in (6), then the expression (32) is an exact asymptotic in $\mathscr{L}_\alpha$ [because of (30) and (22)] and in $\mathscr{L}$ and $\mathscr{L}_{ij}$ [because of (31) and (24)]. From the above treatment, however, it is not obvious that such a procedure would be justifiable, since kinetic energy operators would operate then on the product charges $\bar{Z}_{ij}$. Thus, we are obliged to decouple kinematical from dynamical properties, as will be done in the next section.

It is remarkable that familiar treatments by Peterkop [2] and Rudge and Seaton [1,18] (see also [3]) of the two-electron wave function in the double continuum derive from (30), (31), and (29) as a special case $\bar{Z}_{12}=0$ where the interelectronic coordinate is chosen to be $\mathbf{r}_{12}$. In this case and under the assumption $\mathbf{r}_{ij}\propto\mathbf{k}_{ij}$, Eq. (29) reduces the well known *Peterkop-Rudge-Seaton relation*

$$\frac{\bar{Z}_{13}}{k_{13}}+\frac{\bar{Z}_{23}}{k_{23}}=\sum_{\substack{i,j\\ j>i}}^{3}\frac{Z_{ij}}{k_{ij}}, \tag{34}$$

where the product charges $\bar{Z}_{ij}$ now depend on the momenta rather than positions. Solutions of (6) with $\bar{Z}_{12}=0$ and $\bar{Z}_{13},\bar{Z}_{23}$ satisfying (34) are readily established:

$$\Psi_{\mathrm{DS3C}}(\mathbf{r}_{ij},\mathbf{R}_k)\Big|_{\bar{Z}_{12}=0}=\exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}+i\mathbf{K}_k\cdot\mathbf{R}_k)\bar{N}_{13}\,{}_1F_1(i\beta_{13},1,-i[k_{13}r_{13}+\mathbf{k}_{13}\cdot\mathbf{r}_{13}])\bar{N}_{23}\,{}_1F_1(i\beta_{23},1,-i[k_{23}r_{23}+\mathbf{k}_{23}\cdot\mathbf{r}_{23}]), \tag{35}$$

where $\bar{N}_{ij}:=(2\pi)^{-3/2}\exp(-\pi\beta_{ij}/2)\Gamma(1-i\beta_{ij})$. From the structure of Eqs. (35) and (15) it is obvious that the solution (35) is asymptotically exact only in a limited subspace of $\mathscr{M}$.

## II. CURVILINEAR COORDINATES FOR COULOMB SYSTEMS IN THE CONTINUUM

In this section position-dependent product charges are derived by decoupling dynamical from kinematical properties. The total potential is invariant under overall rotations, hence dynamical properties will depend on body-fixed (or internal) coordinates only, i.e., on coordinates parametrizing the triangle formed by the three particles regardless of its orientation in space. In addition, product charges $\bar{Z}_{ij}$ measuring the strength of interaction between particles $i$ and $j$ are known to depend on the shape of this triangle but not on its size [9,11]. This indicates a special functional dependence of product charges $\bar{Z}_{ij}$, to be introduced.

A natural space-fixed system is provided by momenta $(\mathbf{k}_{ij},\mathbf{K}_k)$, usually determined in scattering experiment. The orientation of the aforementioned triangle in space is then commonly described by Euler angles. However, these angles are of no direct physical meaning to our problem. On the contrary, the analytical form of (7) and the two-body Coulomb continuum wave function suggest that coordinates relevant to the motion of Coulomb particles are the parabolic coordinates $\xi^{\pm}:=r_{ij}\pm\hat{\mathbf{k}}_{ij}\cdot\mathbf{r}_{ij}$. Thus, it appears worthwhile to reformulate the scattering problem in the curvilinear coordinates

$$\begin{aligned}\xi_1^{\pm}&=r_{23}\pm\hat{\mathbf{k}}_{23}\cdot\mathbf{r}_{23},\\ \xi_2^{\pm}&=r_{13}\pm\hat{\mathbf{k}}_{13}\cdot\mathbf{r}_{13},\\ \xi_3^{\pm}&=r_{12}\pm\hat{\mathbf{k}}_{12}\cdot\mathbf{r}_{12},\\ \xi_4&=r_{23},\\ \xi_5&=r_{13},\\ \xi_6&=r_{12}.\end{aligned} \tag{36}$$

The coordinates $(\xi_4,\xi_5,\xi_6)$ parametrize the shape and size of the triangle spanned by the three particles whereas the orientation of this triangle in space is described by $(\xi_1,\xi_2,\xi_3)$. Indeed, a relationship between the quantities $\xi_k/r_{ij};\epsilon_{ijk}\neq 0,j>i\in\{1,2,3\}$ and Euler angles is readily established [19]. The uniqueness of the transformations (36) is indicated by the Jacobi determinant

$$\frac{d\xi_1^+\wedge d\xi_2^+\wedge d\xi_3^+\wedge d\xi_4\wedge d\xi_5\wedge d\xi_6}{d^3\mathbf{r}_{ij}\wedge d^3\mathbf{R}_k}\propto\{(\hat{\mathbf{k}}_{12}\times\hat{\mathbf{k}}_{23})\cdot\mathbf{r}_{23}[\hat{\mathbf{k}}_{13}\cdot(\mathbf{r}_{13}\times\mathbf{r}_{23})]+(\hat{\mathbf{k}}_{13}\times\hat{\mathbf{k}}_{12})\cdot\mathbf{r}_{13}[\hat{\mathbf{k}}_{23}\cdot(\mathbf{r}_{13}\times\mathbf{r}_{23})]\}\frac{1}{r_{23}r_{13}r_{12}}, \tag{37}$$

where $\wedge$ signifies the outer product of differential operators. From (37) it is evident that the Jacobi determinant is dimensionless and the transformation (36) is unique if, e.g., $|\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{k}}_{23}|\neq 1$. The $\pm$ sign in (36) implies that one takes the plus (minus) sign if outgoing (incoming) boundary conditions are required. To simplify notation, hereafter we confine the treatment to outgoing waves and write $\xi_j^+\equiv\xi_j$. Further, we exclude singular directions $\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{k}}_{ij}=-1$ which corresponds to incoming waves. Treatment of scattering systems with incoming boundary conditions runs along the same lines.

Since we are dealing with continuum solutions at fixed total energy (5) the following ansatz for the wave function is appropriate:

$$\Psi(\mathbf{r}_{ij},\mathbf{R}_k)=N\exp(i\mathbf{r}_{ij}\cdot\mathbf{k}_{ij}+i\mathbf{R}_k\cdot\mathbf{K}_k)\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_k). \tag{38}$$

Inserting the ansatz (38) into the Schrödinger equation (6) leads to the equation

$$\left[\frac{1}{\mu_{ij}}\Delta_{\mathbf{r}_{ij}}+\frac{1}{\mu_k}\Delta_{\mathbf{R}_k}+2i\left(\frac{1}{\mu_{ij}}\mathbf{k}_{ij}\cdot\boldsymbol{\nabla}_{\mathbf{r}_{ij}}+\frac{1}{\mu_k}\mathbf{K}_k\cdot\boldsymbol{\nabla}_{\mathbf{R}_k}\right)-2\sum_{\substack{m,n\\n>m}}^{3}\frac{Z_{ij}}{r_{mn}}\right]\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_k)=0. \tag{39}$$

In terms of the coordinates (36) Eq. (39) casts

$$[H_{\rm par}+H_{\rm in}+H_{\rm mix}]\overline{\Psi}(\xi_1,\ldots,\xi_6)=0. \tag{40}$$

The operator $H_{\rm par}$ is differential in parabolic (external) coordinates $(\xi_1,\xi_2,\xi_3)$ only:

$$\begin{aligned}H_{\rm par}:=&\frac{2}{\mu_{23}\xi_4}[\partial_{\xi_1}\xi_1\partial_{\xi_1}+ik_{23}\xi_1\partial_{\xi_1}-\mu_{23}Z_{23}]\\&+\frac{2}{\mu_{13}\xi_5}[\partial_{\xi_2}\xi_2\partial_{\xi_2}+ik_{13}\xi_2\partial_{\xi_2}-\mu_{13}Z_{13}]\\&+\frac{2}{\mu_{12}\xi_6}[\partial_{\xi_3}\xi_3\partial_{\xi_3}+ik_{12}\xi_3\partial_{\xi_3}-\mu_{12}Z_{12}],\end{aligned} \tag{41}$$

whereas the operator $H_{\rm in}$ is differential in internal coordinates only:

$$\begin{aligned}H_{\rm in}:=&\frac{1}{\mu_{23}}\left[\frac{1}{\xi_4^2}\partial_{\xi_4}\xi_4^2\partial_{\xi_4}+2ik_{23}\frac{\xi_1-\xi_4}{\xi_4}\partial_{\xi_4}\right]\\&+\frac{1}{\mu_{13}}\left[\frac{1}{\xi_5^2}\partial_{\xi_5}\xi_5^2\partial_{\xi_5}+2ik_{13}\frac{\xi_2-\xi_5}{\xi_5}\partial_{\xi_5}\right]\\&+\frac{1}{\mu_{12}}\left[\frac{1}{\xi_6^2}\partial_{\xi_6}\xi_6^2\partial_{\xi_6}+2ik_{12}\frac{\xi_3-\xi_6}{\xi_6}\partial_{\xi_6}\right].\end{aligned} \tag{42}$$

The remainder term $H_{\rm mix}$ contains mixed derivatives resulting from off-diagonal elements of the metric tensor and couples internal to external motion

$$\begin{aligned}H_{\rm mix}:=&\sum_{u\neq v=1}^{6}\{(\boldsymbol{\nabla}_{\mathbf{r}_{ij}}\xi_u)\cdot(\boldsymbol{\nabla}_{\mathbf{r}_{ij}}\xi_v)\\&+(\boldsymbol{\nabla}_{\mathbf{R}_k}\xi_u)\cdot(\boldsymbol{\nabla}_{\mathbf{R}_k}\xi_v)\}\partial_{\xi_u}\partial_{\xi_v}.\end{aligned} \tag{43}$$

Now the decisive point is that the operator $H_{\rm par}$ (41) depends *parametrically* on internal coordinates $(\xi_4,\xi_5,\xi_6)$ and is exactly separable for a given set of "parameters" $(\xi_4,\xi_5,\xi_6)$. This feature of $H_{\rm par}$ remains unaffected in the case where the product charges $Z_{ij}$ are position dependent, provided they depend on internal coordinate $(\xi_4,\xi_5,\xi_6)$ only. Thus, we make use of this additional freedom and assume $Z_{ij}=Z_{ij}(\xi_4,\xi_5,\xi_6)$. The exact functional dependence will be investigated below. With these product charges $Z_{ij}$, the regular exact eigenfunction of (41) with zero eigenvalue can be given in closed form:

$$\begin{aligned}&\overline{\Psi}_{\rm DS3C}(\xi_1,\xi_2,\xi_3)|_{(\xi_4,\xi_5,\xi_6)}\\&\quad={}_1F_1(i\beta_{23}(\xi_4,\xi_5,\xi_6),1,-ik_{23}\xi_1)\\&\qquad\times{}_1F_1(i\beta_{13}(\xi_4,\xi_5,\xi_6),1,-ik_{13}\xi_2)\\&\qquad\times{}_1F_1(i\beta_{12}(\xi_4,\xi_5,\xi_6),1,-ik_{12}\xi_3),\end{aligned} \tag{44}$$

where $\beta_{ij}$ are given by (33). It should be emphasized that the wave function (44) originates from an intrinsic separation of the total Hamiltonian as given by (40) and is not enforced, e.g., by some ansatz for the wave function.

The structure of the differential equation (41) and its eigenfunction (44) resemble similar situations encountered in adiabatic treatments where some degrees of freedom are varied parametrically, or even "frozen." This suggests for the wave function (38) the approximation

$$\overline{\Psi}(\xi_1,\ldots,\xi_6)\approx\overline{\Psi}_{\rm DS3C}(\xi_1,\xi_2,\xi_3)|_{(\xi_4,\xi_5,\xi_6)}. \tag{45}$$

Note that the whole solution (38) can then be written in terms of the coordinates (36) because the plane-wave argument can be expressed as

$$\begin{aligned}\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}+\mathbf{K}_k\cdot\mathbf{R}_k=&\sum_{j>i=1}^{3}\frac{m_i+m_j}{m_1+m_2+m_3}\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}\\=&\frac{\mu_1}{m_1}k_{23}(\xi_1-\xi_4)+\frac{\mu_2}{m_2}k_{13}(\xi_2-\xi_5)\\&+\frac{\mu_3}{m_3}k_{12}(\xi_3-\xi_6).\end{aligned} \tag{46}$$

To remain in the adiabatic picture, let us assume the operators $H_{\rm par}$ and $H_{\rm mix}$ commute for a fixed set of parameters $(\xi_j,j=4,5,6)$ (which is, in general, not the case). The approximation (45) means then that, in a fragmentation process, for example, the variation in internal coordinates $(\xi_4,\xi_5,\xi_6)$ is negligibly small compared with the variation in parabolic coordinates $(\xi_j,j=1,2,3)$. Physically, this is not justifiable for arbitrary choice of $\mathbf{k}_{ij},\mathbf{K}_k$. It is important to recognize that parabolic coordinates $(\xi_j,j=1,2,3)$ can also be adiabatically treated since they enter parametrically in the differential operator $H_{\rm in}$ [see Eq. (42)]. A comparative study in which either $(\xi_j,j=1,2,3)$ or $(\xi_j,j=4,5,6)$ are considered adiabatically would reveal direct information on the motion of Coulomb particles. Now, in analogy to an adiabatic approach one could proceed by expanding the exact wave function of the system (38) in the basis (44). Then, in a standard way, the Schrödinger equation (40) reduces to an infinite set of integrodifferential equations for the coefficients of the

adiabatic expansion. Details of such an expansion and its implications will be presented elsewhere. Here we adopt a different strategy motivated by the physical interpretation of Eq. (44). According to Eq. (44) the motion of three Coulomb particles propagates along parabolic coordinates. The strength of interaction between two individual particles $i$ and $j$ is no longer determined by their product charges $Z_iZ_j$ as is the case in two-body scattering or in $\Psi_{3C}$ (16). The product charges $\bar{Z}_{ij}(\xi_4,\xi_5,\xi_6)$ depend rather dynamically on the shape of the triangle formed by the three particles. This functional dependence can now be designed to account for correct boundary conditions on $\mathscr{M}$ and, if possible, to minimize the part not diagonalized by (44). An natural way of introducing the functions $\bar{Z}_{ij}(\xi_4,\xi_5,\xi_6)$ while preserving scaling properties of the Schrödinger Eq. (6) is to split the total potential in three two-body-type potentials $\bar{V}_{ij}=\bar{Z}_{ij}/r_{ij}$ and to assume each of these potentials to be the most general linear superposition of the three physical two-body potentials $V_{ij}:=Z_iZ_j/r_{ij}$ with coefficients $\bar{a}_{ij}$ dependent on internal coordinates only, i.e.,

$$\begin{pmatrix} \bar{V}_{23} \\ \bar{V}_{13} \\ \bar{V}_{12} \end{pmatrix} = \bar{\bar{\mathscr{A}}} \begin{pmatrix} V_{23} \\ V_{13} \\ V_{12} \end{pmatrix}, \tag{47}$$

where $\bar{\bar{\mathscr{A}}}(\xi_4,\xi_5,\xi_6)$ is a $3\times3$ matrix with elements $\bar{a}_{ij}=\bar{a}_{ij}(\xi_{4\cdots6})$:

$$\bar{\bar{\mathscr{A}}} = \begin{pmatrix} \bar{a}_{11}\bar{a}_{12}\bar{a}_{13} \\ \bar{a}_{21}\bar{a}_{22}\bar{a}_{23} \\ \bar{a}_{31}\bar{a}_{32}\bar{a}_{33} \end{pmatrix}. \tag{48}$$

Taking into account that $\bar{Z}_{ij}=\bar{V}_{ij}r_{ij}$, an equivalent relation for $\bar{Z}_{ij}(\xi_4,\xi_5,\xi_6)$ can immediately be deduced from (47). Note that Eq. (47), an essential result of this work, introduces three-body interactions automatically and in an obvious way.

The invariance of the total potential under the transformation (47) requires that

$$\sum_{i=1}^{3} \bar{a}_{ij}=1; \quad j=1,2,3. \tag{49}$$

Within the condition (49) our treatment is exact. To uniquely fix the coefficients $\bar{a}_{ij}$ there are, in addition to (49), six further conditions to be imposed. These conditions can be freely chosen according to practical considerations as well as to the specific type of three-particle system under investigation. An example of this will be given below. It should be mentioned here that the simplest choice of the matrix $\bar{\bar{\mathscr{A}}}$ compatible with (49) is $\bar{\bar{\mathscr{A}}}=\mathbb{1}$. In this case the wave function $\Psi_{DS3C}$ reduces to $\Psi_{3C}$ (16). According to Eq. (47) $\bar{\bar{\mathscr{A}}}=\mathbb{1}$ means, however, that coupling (in the configuration space) between any of three two-body subsystems is disregarded. This is consistent with the Hamiltonian $H_{par}$ [Eq. (41)] being the sum of three position-decoupled two-body Hamiltonians. In this sense the wave function $\Psi_{3C}$, the eigenfunction of $H_{par}$, is actually *uncorrelated*.

## III. DYNAMICALLY COUPLED WAVE FUNCTION OF TWO ELECTRONS IN THE FIELD OF A NUCLEUS

In the preceding section we outlined how additional freedom in constructing three-body wave functions of the form (44) can be gained be choosing appropriate coordinates. In this section it will be shown how the coefficients $\bar{a}_{ij}$ can be designed to construct a wave function describing two continuum electrons in the field of a nucleus with the following properties.

(i) It is, to leading order, an exact asymptotic solution of Eq. (6) on $\mathscr{M}$.

(ii) The motion of electrons escaping on the potential ridge is correctly described.

(iii) The behavior of the wave function at total breakup threshold is regular.

(iv) The two electrons are described on equal footing.

To account for the symmetry of the final state with respect to the two electrons, it is customary in the literature on electron-atom ionizing collisions to designate the relative coordinates of the electrons with respect to the nucleus by $\mathbf{r}_a$ and $\mathbf{r}_b$; hereafter we adopt this notation and choose $m_3$ to be the mass of the nucleus. The coordinates $\mathbf{r}_{13}\equiv\xi_2$, $\mathbf{r}_{23}\equiv\xi_1$, and $\mathbf{r}_{12}\equiv\xi_3$ become then $\mathbf{r}_b$, $\mathbf{r}_a$, and $\mathbf{r}_{ba}:=\mathbf{r}_b-\mathbf{r}_a$, respectively. Conjugate momenta, product charges, and Sommerfeld parameters are then correspondingly renamed. The nucleus is assumed infinitely massive.

### A. Effective product charges

Condition (49), which ensures the conservation of the total potential under (47), requires the coefficients $\bar{a}_{ij}$ to be finite in the whole phase space. Disregarding terms of the order $1/m_3$ the asymptotic conditions, Eq. (13), reduce in the case of two electrons in the field of a nucleus of charge $Z$ to

$$\lim_{\substack{r_a\to\infty \\ (r_b/r_a)\to0}} \psi_2^{as} = (2\pi)^{-3/2} N_b \exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}+i\mathbf{K}_\alpha\cdot\mathbf{R}_\alpha) \times {}_1F_1(i\alpha_b,1,-ik_b\xi_2) \times \exp\left[-i\frac{Z-1}{k_a}\ln k_a\xi_1\right] \tag{50}$$

and

$$\lim_{\substack{r_b\to\infty \\ (r_a/r_b)\to0}} \psi_1^{as} = (2\pi)^{-3/2} N_a \exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}+i\mathbf{K}_\alpha\cdot\mathbf{R}_\alpha) \times {}_1F_1(i\alpha_a,1,-ik_a\xi_1) \times \exp\left[-i\frac{Z-1}{k_b}\ln k_b\xi_2\right]. \tag{51}$$

Further, we treat the two electrons on equal footing and take first-order terms to arrive at the relation

$$\lim_{\substack{R_3\to\infty \\ (r_{ba}/R_3)\to0}} (K_3R_3+\mathbf{K}_3\cdot\mathbf{R}_3)^{i\bar{\gamma}_3} = (k_br_b+\mathbf{k}_b\cdot\mathbf{r}_b)^{i\bar{\gamma}_3/2} 2^{i\bar{\gamma}_3} (k_ar_a+\mathbf{k}_a\cdot\mathbf{r}_a)^{i\bar{\gamma}_3/2}. \tag{52}$$

From Eq. (52) and Eq. (13) we deduce

$$\lim_{\substack{R_3\to\infty \\ (r_{ba}/R_3)\to 0}} \psi_3^{as} = 2^{i\bar{\gamma}_3}(2\pi)^{-3/2} N_{ba} \times \exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij} + i\mathbf{K}_\alpha\cdot\mathbf{R}_\alpha) \times {}_1F_1(i\alpha_{ba},1,-ik_{ba}\xi_3) \times \exp[i\alpha_b \ln k_b\xi_2 + i\alpha_a \ln k_a\xi_1]. \quad (53)$$

An important feature of the total potential which is known to dominate the correlated dynamic of two electrons escaping from positively charged particles is the presence of a ridge structure in the subspace $\mathbf{r}_a = -\mathbf{r}_b$ [9,10]. In this configuration the force exerted on the two-electron system vanishes. The Schrödinger equation reduces in this case to [9]

$$\left[H_0 + \frac{1-4Z}{4r_a} + \frac{1-4Z}{4r_b} - E\right]\Psi_{col}(\mathbf{r}_{ij},\mathbf{R}_k) = 0. \quad (54)$$

Solutions of Eq. (54) describing a two-electron continuum state can be immediately deduced:

$$\Psi_{col}(\mathbf{r}_a,\mathbf{r}_b) = \exp(i\mathbf{k}_b\cdot\mathbf{r}_b + i\mathbf{k}_a\cdot\mathbf{r}_a)\bar{N}_a \times {}_1F_1(i\gamma_a,1,-i[k_a r_a + \mathbf{k}_a\cdot\mathbf{r}_a])\bar{N}_b \times {}_1F_1(i\gamma_b,1,-i[k_b r_b + \mathbf{k}_b\cdot\mathbf{r}_b]), \quad (55)$$

where

$$\gamma_a = \frac{1-4Z}{4k_a}, \quad \gamma_b = \frac{1-4Z}{4k_b}. \quad (56)$$

Asymptotically, the collinear configuration ($\mathbf{r}_a = -\mathbf{r}_b$) is contained in the space $\mathscr{S}_{ij} \subset \mathscr{S}$. In fact, it can be shown that the solution $\Psi_{col}(\mathbf{r}_{ij},\mathbf{R}_k)$ (55) and the wave function $\Psi_{3C}$ (15), apart from an irrelevant constant phase, are asymptotically identical in the collinear configuration. At finite distances, however, $\Psi_{3C}$ does not satisfy Eq. (54). Upon comparison of Eq. (55) with the wave function $\Psi_{DS3C}$, given by Eq. (32), we deduce the relation

$$\lim_{\mathbf{r}_a=-\mathbf{r}_b} \{\bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = -Z+\tfrac{1}{4}; \quad \bar{Z}_b(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = -Z+\tfrac{1}{4}; \quad \bar{Z}_{ba}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = 0\}, \quad (57)$$

which ensure that the two electrons escaping along the potential saddle have the behavior given by Eqs. (55) and (54). It should be emphasized that asymptotic arguments are irrelevant in concluding Eq. (57). Asymptotic conditions, as given by Eqs. (50), (51), and (53), can be accounted for by demanding the product charges $\bar{Z}_j; j = a,b,ba$, and hence the Sommerfeld parameters $\beta_j; j = a,b,ba$, to satisfy the relations

$$\lim_{\substack{r_b\to 0 \\ r_a\to\infty}} \left\{\beta_b(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \alpha_b; \quad \beta_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \frac{(-Z+1)}{k_a}; \quad \beta_{ba}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = 0\right\}, \quad (58)$$

$$\lim_{\substack{r_a\to 0 \\ r_b\to\infty}} \left\{\beta_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \alpha_a; \quad \beta_b(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \frac{(-Z+1)}{k_b}; \quad \beta_{ba}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = 0\right\}, \quad (59)$$

$$\lim_{\substack{r_{ba}\to 0 \\ r_a,r_b\to\infty}} \{\beta_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \alpha_a; \quad \beta_b(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \alpha_b; \quad \beta_{ba}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \alpha_{ba}\}. \quad (60)$$

Further, a symmetrical treatment of the two electrons requires

$$\bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \bar{Z}_b(\mathbf{r}_b,\mathbf{r}_a,\mathbf{r}_{ab}), \quad (61)$$

$$\bar{Z}_{ba}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = \bar{Z}_{ba}(\mathbf{r}_b,\mathbf{r}_a,\mathbf{r}_{ab}). \quad (62)$$

Now, to determine the product charges $\bar{Z}_j$, $j = a,b,ba$, which satisfy Eqs. (57)–(62), we proceed as follows. First we determine $\bar{Z}_a$. The charge $\bar{Z}_b$ can then be obtained using Eq. (61). Taking Eq. (49) into account, $\bar{Z}_{ba}$ is then deduced. According to Eq. (47), $\bar{Z}_a$ has the form

$$\bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = -Z\bar{a}_{11} + \bar{a}_{12}\frac{r_a}{r_{ba}} - Z\bar{a}_{13}\frac{r_a}{r_b}. \quad (63)$$

Condition (59) imposed on $\bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ leads to $a_{11} = 1$. To ensure $\bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ being finite in the limits given by Eqs. (58) and (60) we make for the coefficients $\bar{a}_{12},\bar{a}_{13}$ the ansatz

$$\bar{a}_{12} = a_{12}\left(\frac{3-\cos 4\alpha}{4}\,\frac{r_{ba}}{r_a+r_b}\right)^2 \frac{r_a}{r_a+r_b}, \qquad \bar{a}_{13} = a_{13}\left(\frac{r_b}{r_a+r_b}\right)^m, \quad (64)$$

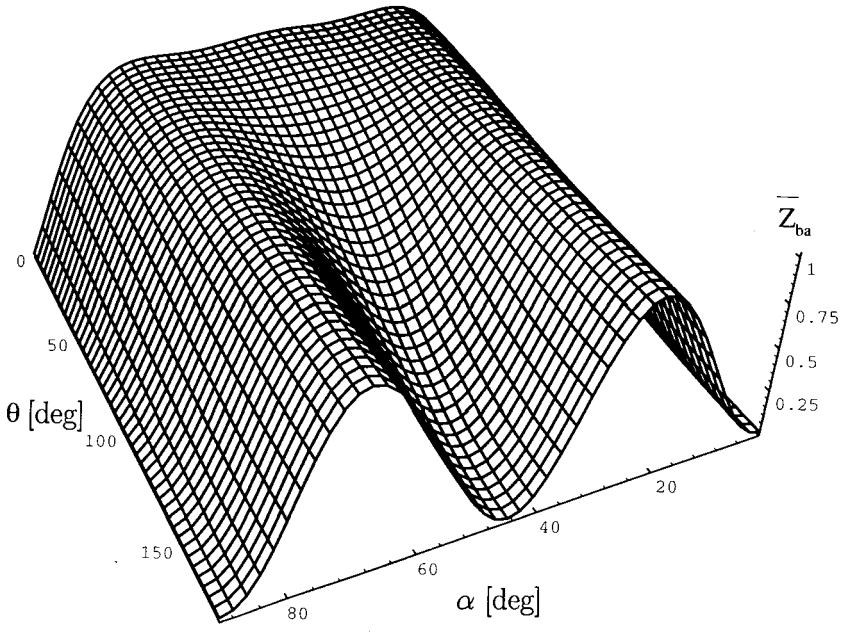


FIG. 2. The charge $\bar{Z}_{ba}$, as given by Eq. (69), depicted in hyperspherical coordinates.

where $a_{12}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}), a_{13}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ are arbitrary functions, $\cos\alpha = r_b/\sqrt{(r_a^2+r_b^2)}$, and $m>1$ is an arbitrary positive real number. Subject to condition (58), $\bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ has to satisfy the relation (note $m>1$):

$$\lim_{\substack{r_b\to 0\\ r_a\to\infty}} \bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = -Z+1 = -Z+a_{12}, \tag{65}$$

which requires $a_{12}=1$. In addition, relation (57) imposed on (63) leads to

$$\lim_{\mathbf{r}_b\to\mathbf{r}_a} \bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = -Z+\frac{1}{4} = -Z+\frac{1}{4}+a_{13}2^{-m} \tag{66}$$

and hence $a_{13}=0$. Thus, the charge $\bar{Z}_a$ reads:

$$\bar{Z}_a(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = -Z+\left(\frac{3+\cos 4^2\alpha}{4}\,\frac{r_{ba}}{r_a+r_b}\right)^2 \frac{r_a^2}{(r_a+r_b)r_{ba}}. \tag{67}$$

The analytical form of $\bar{Z}_b(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ derives from Eqs. (67) and (61) to

$$\bar{Z}_b(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) = -Z+\left(\frac{3+\cos 4^2\alpha}{4}\,\frac{r_{ba}}{r_a+r_b}\right)^2 \frac{r_b^2}{(r_a+r_b)r_{ba}}. \tag{68}$$

Finally, the interelectronic charge $\bar{Z}_{ba}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ is obtained using Eq. (49), which can be formulated in the form

$$\begin{aligned}\bar{Z}_{ba}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba}) &= -Z\frac{r_{ba}}{r_a}-Z\frac{r_{ba}}{r_b}+1-\bar{Z}_a\frac{r_{ba}}{r_a}-\bar{Z}_b\frac{r_{ba}}{r_b}\\ &= 1-\left(\frac{3+\cos 4^2\alpha}{4}\,\frac{r_{ba}}{r_a+r_b}\right)^2\end{aligned} \tag{69}$$

It is readily established that the conditions given by Eqs. (49) and (57)–(62) are satisfied by the product charges determined above. The uniqueness of this procedure will be discussed below.

### B. Physical interpretations

According to $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ constructed with product charges given by Eqs. (67)–(69) the motion of Coulomb particles proceeds along parabolic coordinates $\xi_{1\ldots3}$, as is the case with $\Psi_{3\mathrm{C}}(\mathbf{r}_a,\mathbf{r}_b)$. In contrast to $\Psi_{3\mathrm{C}}(\mathbf{r}_a,\mathbf{r}_b)$ however, the wave function $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ does not separate into a product of three two-body Coulomb continuum states as it might appear at first glance. Rather, it is a product of three functions each of them is a three-body function. To see this directly we introduce hyperspherical coordinates $\rho := \sqrt{r_a^2+r_b^2}$, $\tan\alpha = r_a/r_b$, $\cos\theta = \hat{\mathbf{r}}_a\cdot\hat{\mathbf{r}}_b$. Now consider for example the part of $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ depending on the interelectronic parabolic coordinates $\xi_3$. The charge $\bar{Z}_{ba}$ and thus the strength of repulsion between the electrons, is dependent on the shape of the triangle formed by the three particles, as shown in Fig. 2, whereas in the $\Psi_{3\mathrm{C}}$ approximation $Z_{ba}$ would be a constant surface at $Z_{ba}=1$. Now if the two electrons emerge in the same direction $\mathbf{r}_{ba}\to 0$ the electron-electron interaction is fully switched on. As the two electrons move away from each other their mutual repulsive interaction is gradually screened by the nucleus. For example, if one electron is far away from the nucleus whereas the other is near the nucleus then the electron-electron interaction is totally switched off due to screening and the electron nearby the nucleus experiences the full nuclear charge, whereas the other electron 'sees' merely an effective charge of $Z-1$ [compare Eqs. (67) and (68)]. When the two electrons travel outward on opposite sides of and equal distances from the nucleus, i.e., in the Wannier configuration, the electron-electron repulsion possesses a local minimum and is subsumed completely in an effective electron-nuclear interaction. Considering the back-to-back configuration ($\hat{\mathbf{r}}_a = -\hat{\mathbf{r}}_b$) and varying the ratio $\alpha$, the electron-electron in-

teraction is slowly switched on. The electron nearby the nucleus becomes more attracted the closer it approaches the nucleus whereas the other electron is increasingly screened from the nucleus. This mechanism closely resembles the stability analyses by the Wannier theory for low energetic three-body break up [12,21–28]. We remark, however, that the Wannier theory deduces the energy functional dependence of the total ionization cross section at the three-particle fragmentation threshold from the volume of the phase space available for double escape of the two electrons. In the Wannier theory and its modifications [12,21–25] the total potential is expanded around the Wannier configuration. In contrast, in the present treatment the total potential is exactly diagonalized because of Eq. (49) whereas parts of the kinetic energy are neglected (as shown below). Hence, a direct link between this work and the Wannier theory is not obvious. In particular, it is not clear whether the theory presented in this work would lead to the Wannier threshold law for the total cross section. In a forthcoming work we will show, however, how the Wannier threshold law can be explicitly implemented when constructing the dynamical product charges $\bar{Z}_j, j=a,b,ba$.

### C. Threshold behavior

It is established that the wave function $\Psi_{3C}(\mathbf{r}_a,\mathbf{r}_b)$, when employed to describe a continuum final state resulting from an ionization process, leads to ionization cross sections exponentially decreasing with decreasing small excess energy [20], a fact which is at variance with the Wannier theory and experimental finding. Here the origin of this shortcoming is investigated and it is shown how the coupling introduced by $\bar{Z}_j, j=a,b,ba$, removes this deficiency. To this end we introduce hyperspherical momenta

$$K:=(k_a^2+k_b^2)/2=E, \quad \tan\beta=\frac{k_a}{k_b}, \quad \text{and} \quad \cos\Theta_k=\hat{\mathbf{k}}_a\cdot\hat{\mathbf{k}}_b. \tag{70}$$

From Eqs. (68), (69), and (61) it is clear that the product charges, given by Eqs. (67)–(69) are limited to the intervals $\bar{Z}_a,\bar{Z}_b\in[-Z,0]; \bar{Z}_{ba}\in[0,1]$, i.e., a two-body interaction can be screened by the presence of a third charged particle but does not change sign. Thus, expanding the wave function $\bar{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ [see Eq. (44)] in terms of Bessel functions [29,30] and, for small excess energies $E\to 0$, taking leading order terms in excess energy we obtain

$$\lim_{E\to 0}\bar{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b) = J_0(2\sqrt{-\bar{Z}_a\xi_1})J_0(2\sqrt{-\bar{Z}_b\xi_2})I_0(\sqrt{2\bar{Z}_{ba}\xi_3}), \tag{71}$$

where $J_0(x), I_0(x)$ are Bessel and modified Bessel functions, respectively. A similar equation applies to $\Psi_{3C}(\mathbf{r}_a,\mathbf{r}_b)$ with the replacement $\bar{Z}_a=-Z=\bar{Z}_b, \bar{Z}_{ba}=1$. The Bessel function $J_0(x)$ has an oscillatory bound asymptotic behavior whereas the modified Bessel function $I_0(x)$, corresponding to the electron-electron interaction, is unbound for large arguments $x$. Hence, to account for this behavior, the normalization $|N_{ee}|^2$ of the electron-electron Coulomb wave must decrease exponentially with vanishing excess energy. The ionization cross section declines then exponentially at lower excess energy. This behavior is consistent within a two-body electron-electron Rutherford scattering. Since the wave function $\Psi_{3C}(\mathbf{r}_a,\mathbf{r}_b)$ describes the three-particle system as three non-interacting two-body systems (as shown above) it is comprehensible that properties of the electron-electron Rutherford scattering are directly reflected into the behavior of the whole system. It should be noted, however, that in a three-body continuum the two electrons are subject to the total potential, which is totally different from their mutual repulsive two-body interaction. Thus, even though the normalization factor (also called the Gamov factor) $|N_{ee}|$ of the electron-electron interaction, occurring, for example, in $\Psi_{3C}(\mathbf{r}_a,\mathbf{r}_b)$, can sometimes be useful in simulating electron-electron repulsion in the continuum [31,32] it originates from a wrong behavior of the corresponding radial part. Since the product charges $\bar{Z}_a,\bar{Z}_b,\bar{Z}_{ba}$ are designed to account for properties of the *total* potential it is expected that $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ has a drastically different threshold behavior than $\Psi_{3C}(\mathbf{r}_a,\mathbf{r}_b)$. In fact, the argument $\sqrt{2\bar{Z}_{ba}\xi_3}$ of the modified Bessel function in Eq. (71) remains limited when $\xi_3$ tends to infinity since then $\bar{Z}_{ba}$ becomes zero. This can be seen when rewriting Eq. (69) in the Jacobi coordinates $(\mathbf{R}_3,\mathbf{r}_{12})$ and considering $r_{12}\equiv\xi_3\to\infty$. Therefore, the exponential decrease of ionization cross sections when employing $\Psi_{3C}(\mathbf{r}_a,\mathbf{r}_b)$ final state is removed by using $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ to describe the state of the final channel [13,14]. Investigation of the exact threshold behavior of the total cross section for two-electron escape using $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ for the final state is a mathematically involved task since in this case the normalization of $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ is required. Details of such a study are planned to be published elsewhere.

### D. Kato-cusp conditions

The normalization of an eigenfunction $\Psi(\mathbf{r}_{ij},\mathbf{R}_k)$ of the Schrödinger equation requires the function $\Psi(\mathbf{r}_{ij},\mathbf{R}_k)$ to be bound in the whole six-dimensional space $(\mathbf{r}_{ij},\mathbf{R}_k)$, i.e., $||\Psi(\mathbf{r}_{ij},\mathbf{R}_k)||<\epsilon$. On the other hand, Coulomb potentials $Z_{ij}/r_{ij}$ are singular at the two-body collision points $r_{ij}\to 0$. Hence, the wave function $\Psi(\mathbf{r}_{ij},\mathbf{R}_k)$ must reveal certain properties to be regular (at $r_{ij}\to 0$) and normalizable. In case $\Psi(\mathbf{r}_{ij},\mathbf{R}_k)$ does not vanish at the two-body coalescence points, these conditions are known as the Kato-cusp conditions [33,34],

$$\left(\frac{\partial\tilde{\Psi}(\mathbf{r}_{ij},\mathbf{R}_k)}{\partial r_{ij}}\right)_{r_{ij}=0}=Z_{ij}\mu_{ji}\Psi(r_{ij}=0,\mathbf{R}_k), \quad \forall(\mathbf{r}_{ij},\mathbf{R}_k), \tag{72}$$

where $\tilde{\Psi}(\mathbf{r}_{ij},\mathbf{R}_k)$ is the wave function averaged over a sphere of small radius $r_\epsilon\ll 1$ around the singularity $r_{ij}=0$. Now we show that the wave function $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ as derived in previous sections does satisfy the conditions (72). To obtain an expression for $\tilde{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ at, e.g., the collision point $(r_b=0, r_a/r_b\to\infty)$, we linearize $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b)$ around $r_b=0$,

$$\tilde{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_b,\mathbf{r}_a)=\mathcal{N}\exp(i\mathbf{k}_a\cdot\mathbf{r}_a)\times {}_1F_1(i\beta_a,1,-i[k_a r_a+\mathbf{k}_a\cdot\mathbf{r}_a])\times {}_1F_1(i\beta_{ba},1,-i[k_{ba}r_{ba}+\mathbf{k}_{ba}\cdot\mathbf{r}_{ba}])\times D(\mathbf{r}_b), \tag{73}$$

where $\mathcal{N}=(2\pi)^{3/2}\Pi_j\bar{N}_j, j=a,b,ba,$ and

$$D(\mathbf{r}_b)=\frac{2\pi}{4\pi r_\epsilon^2}\int_{-1}^{1} r_\epsilon^2 d\cos\theta[1+ik_b\cos\theta+\alpha_b k_b r_b(1+\cos\theta)]$$

$$=1+\alpha_b k_b r_b. \tag{74}$$

In deriving Eq. (74) we take the $z$ axes as $\mathbf{k}_b$ and define $\cos\theta=\hat{\mathbf{k}}_b\cdot\hat{\mathbf{r}}_b$. Note that in the limit $(r_b\to 0; r_a/r_b\to\infty)$ and to leading order the Sommerfeld parameter $\beta_b$ tends to $\alpha_b$ [see Eq. (58)]. Therefore, we arrive at

$$\left(\frac{\partial\tilde{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_b,\mathbf{r}_a)}{\partial r_b}\right)_{r_b=0}$$
$$=Z_b\mathcal{N}\exp(i\mathbf{k}_a\cdot\mathbf{r}_a)\times {}_1F_1(i\beta_a,1,-i[k_a r_a+\mathbf{k}_a\cdot\mathbf{r}_a])\times {}_1F_1(i\beta_{ba},1,-i[k_{ba}r_{ba}+\mathbf{k}_{ba}\cdot\mathbf{r}_{ba}])$$
$$=Z_b\Psi_{\mathrm{DS3C}}(r_b=0,\mathbf{r}_a). \tag{75}$$

The Kato-cusp conditions at $(r_a=0, r_b/r_a\to\infty)$ and $(r_{ba}=0, R_3/r_{ba}\to\infty)$ can be shown to be fulfilled in an analogous way. Two important remarks are due here. Following the procedure above, the wave function $\Psi_{3\mathrm{C}}(\mathbf{r}_b,\mathbf{r}_a)$ is shown to satisfy the Kato-cusp conditions and hence exposes a regular behavior at all two-body collision points. This is a direct consequence of all two-body interactions being accounted for to infinite order by $\Psi_{3\mathrm{C}}(\mathbf{r}_b,\mathbf{r}_a)$ on the two-body energy shell, as shown above and in Refs. [17,35,36].

The second remark concerns wave functions $\Psi_{unkor}$ which do not contain an explicit dependence on the interelectronic coordinates $\mathbf{r}_{ba}$, e.g., the wave function given by Eq. (35). Strictly speaking, these wave functions do not satisfy the Kato-cusp condition at the electron-electron collision point $r_{ba}=0$ since $\partial\Psi_{unkor}/\partial r_{12}=0$.

### E. Asymptotic behavior

From the asymptotic properties of the product charges $\bar{Z}_j, j=a,b,ba$ [Eqs. (58)–(60)] it is obvious that the constructed wave function $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ takes asymptotically the forms given by Eqs. (50), (51), and (53), in the respective limits and hence solves the corresponding asymptotic Schrödinger equations (12). The same asymptotic conditions, as given by Eq. (12), have been imposed on the wave function derived in Ref. [8]. Hence, the wave function presented here and that given in Ref. [8] differ only with a constant phase factor in the subspaces $\mathcal{S}_\alpha$. To explicitly show that the part of the three-body Schrödinger equation not diagonalized by $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})$ falls faster than the Coulomb potential in the asymptotic region $\mathcal{S}$ we drop the approximation (45) and write instead for the exact solution the general ansatz:

$$\overline{\Psi}(\xi_1,\ldots,\xi_6)=\overline{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})(1-F). \tag{76}$$

Upon substitution of (76) in Eq. (40) a differential equation is obtained for the arbitrary function $F(\xi_1,\ldots,\xi_6)$,

$$\left\{\frac{(H_{\mathrm{in}}+H_{\mathrm{mix}})\overline{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})}{\overline{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})}\right\}(1-F)-2\left[\frac{\Delta}{2}+\boldsymbol{\nabla}_1\ln\overline{\Psi}_{\mathrm{DS3C}}\cdot\boldsymbol{\nabla}_1+\boldsymbol{\nabla}_2\ln\overline{\Psi}_{\mathrm{DS3C}}\cdot\boldsymbol{\nabla}_2+i(\mathbf{k}_a\cdot\boldsymbol{\nabla}_1+\mathbf{k}_b\cdot\boldsymbol{\nabla}_2)\right]F=0. \tag{77}$$

The differential operators appearing in Eq. (77) have the forms $\boldsymbol{\nabla}_1=\Sigma_{j=1}^6(\boldsymbol{\nabla}_a\xi_j)\partial_{\xi_j}, \boldsymbol{\nabla}_2=\Sigma_{j=1}^6(\boldsymbol{\nabla}_b\xi_j)\partial_{\xi_j}$, and $\Delta=\Sigma_{j=1}^6(\Delta_a+\Delta_b)\partial_{\xi_j}+\Sigma_{i,j=1}^6[(\boldsymbol{\nabla}_a\xi_i)\cdot(\boldsymbol{\nabla}_a\xi_j)+(\boldsymbol{\nabla}_b\xi_i)\cdot(\boldsymbol{\nabla}_b\xi_j)]\partial_{\xi_j}\partial_{\xi_i}$. The differential operator $H_{\mathrm{mix}}$ has the explicit form:

$$\frac{H_{\mathrm{mix}}}{2}=(\hat{\mathbf{k}}_{ba}+\hat{\mathbf{r}}_{ba})\cdot[(\hat{\mathbf{k}}_b+\hat{\mathbf{r}}_b)\partial_{\xi_2}-(\hat{\mathbf{k}}_a+\hat{\mathbf{r}}_a)\partial_{\xi_1}]\partial_{\xi_3}+\hat{\mathbf{r}}_{ba}\cdot[(\hat{\mathbf{k}}_b+\hat{\mathbf{r}}_b)\partial_{\xi_2}-(\hat{\mathbf{k}}_a+\hat{\mathbf{r}}_a)\partial_{\xi_1}]\partial_{\xi_6}$$
$$+(\hat{\mathbf{k}}_a+\hat{\mathbf{r}}_a)\cdot\hat{\mathbf{r}}_a\partial_{\xi_1}\partial_{\xi_4}+(\hat{\mathbf{k}}_b+\hat{\mathbf{r}}_b)\cdot\hat{\mathbf{r}}_b\partial_{\xi_2}\partial_{\xi_5}+(\hat{\mathbf{k}}_{ba}+\hat{\mathbf{r}}_{ba})\cdot[\hat{\mathbf{r}}_b\partial_{\xi_2}-\hat{\mathbf{r}}_a\partial_{\xi_1}+2\hat{\mathbf{r}}_{ba}\partial_{\xi_6}]\partial_{\xi_3}+\hat{\mathbf{r}}_{ba}\cdot(\hat{\mathbf{r}}_b\partial_{\xi_2}-\hat{\mathbf{r}}_a\partial_{\xi_1}). \tag{78}$$

The coordinates $\hat{\mathbf{r}}_j, j=a,b,ba$ occurring in Eq. (78) have to be expressed in terms of the coordinates (36), which can be done using symbolic computational programs.

The exact solution of the Schrödinger equation (40) can be replaced by $\overline{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba},)$ only if the function $F=0$ is a solution of Eq. (77), which is the case if the norm of the inhomogeneous operator in Eq. (77) is negligible. Thus, we can restrict the discussion to the study of the inhomogeneous term

$$R=\frac{(H_{\mathrm{in}}+H_{\mathrm{mix}})\overline{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})}{\overline{\Psi}_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_{ba})}. \tag{79}$$

Note that derivatives of confluent hypergeometric functions with respect to the first argument can be performed by using the series expansion, which is continuously convergent for the parameters used here and exchange summation and derivation. Now

the term $R$ depends on the product charges $\bar{Z}_j, j=a,b,ba$. The asymptotic behavior of $R$ for large interparticle separations, i.e., in the Redmond asymptotic, is controlled by the fact that the product charges $\bar{Z}_j, j=a,b,ba$ are constant in this limit. This could be immediately seen by employing the parametrization

$$r_a=\bar{r}_a t, \quad r_b=\bar{r}_b t, \quad \text{and} \quad r_{ba}=\bar{r}_{ba} t, \tag{80}$$

where $\bar{r}_a,\bar{r}_b,\bar{r}_{ba}$ are nonvanishing, positive real constants and $t$ is a positive real parameter which goes to infinity for large interparticle separation, e.g., we can take the parameter $t$ to be the hyper-radius, thus the Coulomb potential is of the order $1/t$. In the asymptotic region $\mathscr{L}$ the term $R$ has the form

$$\begin{aligned}\lim_{t\to\infty} R=\lim_{t\to\infty}\Bigg[ & \bar{Z}_b(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})(\hat{\mathbf{k}}_b+\hat{\mathbf{r}}_b)\frac{{}_1F_1(i\beta_b[\bar{Z}_b(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})]+1,2,-ik_b\xi_2)}{{}_1F_1(i\beta_b[\bar{Z}_b(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})],1,-ik_b\xi_2)} \\ & \times\bar{Z}_a(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})(\hat{\mathbf{k}}_a+\hat{\mathbf{r}}_a)\frac{{}_1F_1(i\beta_a[\bar{Z}_b(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})]+1,2,-ik_a\xi_1)}{{}_1F_1(i\beta_a[\bar{Z}_b(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})],1,-ik_a\xi_1)}\Bigg] \\ & \times\bar{Z}_{ba}(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})(\hat{\mathbf{k}}_{ba}+\hat{\mathbf{r}}_{ba})\frac{{}_1F_1(i\beta_{ba}[\bar{Z}_b(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})]+1,2,-ik_{ba}\xi_3)}{2\,{}_1F_1(i\beta_{ba}[\bar{Z}_b(\bar{r}_a,\bar{r}_b,\bar{r}_{ba})],1,-ik_{ba}\xi_3)}\to O(t^{-2}).\end{aligned} \tag{81}$$

Therefore, the wave function $\Psi_{\mathrm{DS3C}}$ is an asymptotic solution in the regime $\mathscr{L}$. To prove that the wave function is also an asymptotic solution in the subspaces $\mathscr{L}_\alpha$ one could proceed as above and investigate the term $R$ in the subspace $\mathscr{L}_\alpha$. This is straightforward but cumbersome. We investigate instead the asymptotic behavior of the wave function $\Psi_{\mathrm{DS3C}}$ in $\mathscr{L}_\alpha$. Let us consider the limit $(r_b\to\infty, r_a/r_b\to 0)$; the same consideration applies to the other limits. The wave function $\Psi_{\mathrm{DS3C}}$ expanded at $(r_a/r_b\to 0, r_b\to\infty)$ reads

$$\begin{aligned}\lim_{(r_a/r_b)\to 0,r_b\to\infty}\Psi_{\mathrm{DS3C}}= & (2\pi)^{-3/2}N_a\exp(i\mathbf{k}_{ij}\cdot\mathbf{r}_{ij}+i\mathbf{K}_\alpha\cdot\mathbf{R}_\alpha)\,{}_1F_1(i\alpha_a,1,-ik_a\xi_1) \\ & \times\exp\left[-i\frac{Z-1}{k_b}\ln k_b\xi_2\right]\left\{1+\frac{i}{2}\left[\frac{(1+\hat{\mathbf{r}}_a\cdot\hat{\mathbf{r}}_b)}{k_{ba}}\ln\xi_3-\frac{(3+\hat{\mathbf{r}}_a\cdot\hat{\mathbf{r}}_b)}{k_b}\ln\xi_2\right]\frac{r_a}{r_b}+O\left(\frac{r_a^2}{r_b^2}\right)\right\}\to\psi_1^{as}.\end{aligned} \tag{82}$$

Note that in Eq. (82) terms of the order $O(r_a/r_b)$ can be neglected since they appear in the wave function and hence correspond to terms in the Schrödinger equation falling off faster than the Coulomb potential. Concluding, it has been shown that the wave function $\Psi_{\mathrm{DS3C}}(\mathbf{r}_a,\mathbf{r}_b\mathbf{r}_{ba})|_{\bar{Z}_a,\bar{Z}_b,\bar{Z}_{ba}}$ is an asymptotic solution of the Schrödinger equation on the manifold $\mathscr{M}$.

### F. Uniqueness

This work aims at diagonalizing the total potential exactly by using wave functions of the analytical form given by Eq. (44). By doing so we are still left with an additional freedom of splitting the total potential in the way given by Eq. (47) and requiring (49). The decisive point is now each choice of the matrix $\bar{\mathscr{A}}$, given by Eq. (47), will enter in the remaining, not diagonalized, part of the kinetic energy as given by Eq. (79). In this sense, the theory presented here is a self-consistent theory; the best choice of $\bar{\mathscr{A}}$ will minimize the remainder term $R$. Hence, this work should be considered as a starting point for systematic, more elaborate models where the remainder $R$ is first minimized by the method given here and then investigated, e.g., numerically. Here we have chosen $\bar{\mathscr{A}}$ such that the remainder $R$ falls off faster than the Coulomb potential in the asymptotic region $\mathscr{M}$ and the Wannier configuration and the Kato-cusp conditions are accounted for. As our imposed conditions [Eqs. (58)–(60), and (57)] are limits, there will naturally be other different functions extrapolating between these limits. However, there is no physical or mathematical reason to believe that, for example, the simplest choice of the expansion matrix $\bar{\mathscr{A}}=\mathbb{1}$, which leads to the wave function $\Psi_{3C}$, given by Eq. (16), is more unique than the matrix used to construct the wave function $\Psi_{\mathrm{DS3C}}$.

## IV. CONCLUSIONS AND OUTLOOK

In this paper a method has been presented which, in a three-body Coulomb continuum problem, separates internal, body-fixed properties from space-fixed properties and allows for introduction of three-body interactions in a mathematical way. An example of applying the theory has been given by constructing a wave function for two continuum electrons in the field of a nucleus. It has been shown that the wave function can be designed to solve the time-independent Schrödinger equation asymptotically and to account for properties of the total potential surface. The applicability of the present model to physical reactions has already been demonstrated in a previous work [13,14] where calculations of ionization amplitudes for electron-impact ionization of atomic hydrogen and helium have been performed. Results turn out to be in good agreement with experiments over a surprisingly wide

range of collision geometries [13,14,37]. However, due to technical problems we were obliged to make the approximation that the total potential is conserved only along paths of free particles. The full numerical implementation of the wave function presented here is the subject of current research. Note that comparing results of $\Psi_{\mathrm{DS3C}}$ and $\Psi_{\mathrm{3C}}$ allows for direct estimate of the strength of three-body coupling. Besides, deviations of results obtained by employing $\Psi_{\mathrm{DS3C}}$ from experiment gives direct information on the strength of the remainder part $R$. Finally, it should be noted that the wave function derived in Sec. III is valid only for two continuum electrons in the field of a nucleus. Applications to other three-particle systems require the detailed knowledge of properties of the total potentials to be incorporated in the wave functions. This can lead to totally different analytical behavior of the effective product charges as they were introduced in Sec. II.

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