Parabolic-hyperspherical approach to the fragmentation of three-particle Coulomb systems

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In this work the three-body Coulomb continuum problem is reformulated in a set of parabolic-hyperspherical coordinates. It is shown how this procedure yields additional information on the angular and radial behavior of correlated three-body Coulomb continuum wave functions. For two electrons receding from a nucleus it is shown that three-body coupling is essential in describing the dependence of the fragmentation dynamics on the ratio of the electronic distances from the nucleus whereas the angular distribution of these electrons is less sensitive to this coupling. The spin asymmetry in the total cross section for electron-impact ionization of atomic hydrogen is analyzed and found to be sensitive to the radial correlation of the outgoing electrons. [S1050-2947(96)08308-4]

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I. INTRODUCTION

The correlated motion of three particles interacting via Coulomb forces has been described within a variety of coordinate systems. A widely used approach considers the three-body Coulomb problem in hyperspherical coordinates in which the overall size of the system is characterized by one coordinate, the hyper-radius ρ. The remaining five dimensionless coordinates, collectively denoted by Ω, parametrize the five-dimensional manifold defined by a constant hyper-radius [1–4]. A major advantage of this concept is its flexibility to take into account various physical aspects of three-body systems. For example, the fact that the total Coulomb potential depends only on the space-fixed triangle formed by the three particles and scales as the size of this triangle can be accounted for by choosing two of the five dimensionless coordinates to parametrize the shape of this triangle while its size is characterized by ρ. The remaining three coordinates describe then the orientation of this triangle in space and hence the rotational coupling between internal, body-fixed motion and external degrees of freedom. Often, Euler angles are employed for these three coordinates. On the other hand, it has been shown [5] that the formulation of the three-body Coulomb continuum problem in a new set of coordinates leads to a useful insight into the mathematical and physical properties of the correlated motion of Coulomb particles in the continuum. In the latter frame of reference the internal, body-fixed motion is characterized by the three interparticle distances. The remaining three coordinates needed to describe the system are chosen as the parabolic coordinates associated with the three two-body Coulomb systems. It has been pointed out [5] that within this frame of reference the (nonrelativistic) time-independent Schrödinger equation breaks down into two parametrically coupled differential operators: a parabolic differential operator and an operator differential in internal coordinates only. In addition, a third operator results from the off-diagonal elements of the metric tensor and plays the role of a rotational coupling term in a hyperspherical treatment. Furthermore, exact eigenfunctions Ψ_{DS3C}, where DS3C means dynamically screened three-body Coulomb function, of the parabolic differential operator have been identified and successfully applied to physical situations [6,7]. Since this approach and hyperspherical methods are quite similar in that dynamical and kinematical properties are disentangled by introducing internal and external coordinates and a vast amount of information already exists on three-body systems in hyperspherical coordinates [4], it is worthwhile to reveal the connection between these two approaches. In particular, it will be shown that further insight into correlated three-body continuum wave function can be gained by unraveling the part of the hyperspherical Hamiltonian diagonalized by these wave functions. To this end a parabolic-hyperspherical frame of reference is introduced in Sec. II, in which the directions associated with the parabolic coordinates play the role of Euler angles. The connection to the grand-angular momentum is revealed as well as the part of the Hamiltonian diagonalized by the three-body wave function Ψ_{DS3C} and its subderivatives. In Sec. III properties of these wave functions are studies and compared with experimental and theoretical finding on the dynamic of electron-impact ionization of atomic hydrogen. Atomic units are used throughout.

II. PARABOLIC-HYPERSPHERICAL COORDINATES FOR COULOMB SYSTEMS IN THE CONTINUUM

We consider the time-independent Schrödinger equation of three charged particles of masses m_i and charges $Z_i; i \in 1,2,3$ moving above the total dissociation threshold. In the center-of-mass system the internal motion is described by a set of Jacobi coordinates $(\mathbf{r}_{ij},\mathbf{R}_k), i,j,k \in \{1,2,3\}; \epsilon_{ijk} \neq 0, j>i$ where $\mathbf{r}_{ij}$ is the relative coordinate between particles i and j and $\mathbf{R}_k$ refers to particle k with respect to the center of mass of the other two particles [4]. An advantageous property of the Jacobi coordinates is that the kinetic energy operator is diagonal. Hence the time-independent Schrödinger equation, at a given total energy E of the system, reads

$$\left[-\frac{1}{2\mu_{ij}}\Delta_{\mathbf{r}_{ij}}-\frac{1}{2\mu_k}\Delta_{\mathbf{R}_k}+\sum_{\substack{i,j\\ j>i}}^{3}\frac{Z_{ij}}{r_{ij}}-E\right]\langle \mathbf{r}_{kl},\mathbf{R}_m|\Psi\rangle = 0 \quad \forall(\mathbf{r}_{ij},\mathbf{R}_k). \tag{1}$$

Here we defined product charges as $Z_{ij}=Z_iZ_j$, $j>i \in\{1,2,3\}$. The reduced masses occurring in Eq. (1) are given by $\mu_{ij}=m_im_j/(m_i+m_j)$ and $\mu_k=m_k(m_i+m_j)/(m_1+m_2+m_3)$ where $j>i\in\{1,2,3\}$, $j\neq k\neq i$. The Coulomb potentials in Eq. (1) have to be expressed in terms of the appropriately chosen set $(\mathbf{r}_{kl},\mathbf{R}_m)$.

The scattering state $|\Psi\rangle$ has to satisfy the Sommerfeld-Abstrahlung conditions which can be formulated as

$$\lim_{r_{ij}\to\infty}\nabla_{\mathbf{r}_{ij}}\ln\Psi(\mathbf{r}_{ij},\mathbf{R}_k)=\pm i\mathbf{k}_{ij},$$

$$\lim_{R_k\to\infty}\nabla_{\mathbf{R}_k}\ln\Psi(\mathbf{r}_{ij},\mathbf{R}_k)=\pm i\mathbf{K}_k, \tag{2}$$

where $\mathbf{k}_{ij}$ and $\mathbf{K}_k$ are the momenta conjugate to $\mathbf{r}_{ij}$ and $\mathbf{R}_k$, respectively, with $E=K_k^2/\mu_k+k_{ij}^2/\mu_{ij}$. Now in order to decouple dynamical from kinematical properties we make use of the fact that the total potential is invariant under overall rotations and introduce internal, body-fixed hyperspherical coordinates. To emphasize the importance of parabolic direction we choose, in addition, three dimensionless coordinates associated with parabolic directions:

$$\xi_1^{\pm}=\frac{1}{r_{23}}(r_{23}\pm\hat{\mathbf{k}}_{23}\cdot\mathbf{r}_{23}),$$

$$\xi_2^{\pm}=\frac{1}{r_{13}}(r_{13}\pm\hat{\mathbf{k}}_{13}\cdot\mathbf{r}_{13}),$$

$$\xi_3^{\pm}=\frac{1}{r_{12}}(r_{12}\pm\hat{\mathbf{k}}_{12}\cdot\mathbf{r}_{12}),$$

$$\varphi=\tan^{-1}\frac{\overline{r_{ij}}}{\overline{R}_k},$$

$$\gamma=\overline{\mathbf{R}}_k\cdot\overline{\mathbf{r}}_{ij},$$

$$\rho=(\overline{R}_k^2+\overline{r}_{ij}^2)^{1/2}. \tag{3}$$

In order to simplify the structure of the Schrödinger equation, reformulated in the coordinates given by (3), we introduced mass-dependent Jacobi coordinates as

$$\overline{\mathbf{r}}_{ij}=\mu_{ij}^{1/2}\mathbf{r}_{ij},\quad \overline{\mathbf{R}}_k=\mu_k^{1/2}\mathbf{R}_k. \tag{4}$$

The $\pm$ sign occurring in Eqs. (3) means to take the plus (minus) sign if outgoing (incoming) boundary conditions are required. To simplify notation, hereafter we confine the treatment to outgoing waves and exclude the singular directions $\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{k}}_{ij}=-1$ which corresponds to incoming waves. The coordinates $\xi_i, i\in\{1,2,3\}$ play the role of Euler angles in a hyperspherical treatment. A relationship between Euler angles and the coordinates given by Eq. (3) can be derived using symbolic computational programs [8]. The laboratory frame of reference is naturally given by two of the relative momenta, say $(\mathbf{k}_{12},\mathbf{k}_{13})$, usually measured in a scattering process. Since we are dealing with continuum solution at fixed total energy E under the constraint (2), the following ansatz for the solution of (1) is appropriate:

$$\Psi(\mathbf{r}_{ij},\mathbf{R}_k)=\exp(i\mathbf{r}_{ij}\cdot\mathbf{k}_{ij}+i\mathbf{R}_k\cdot\mathbf{K}_k)\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_k). \tag{5}$$

Thus the function $\overline{\Psi}(\mathbf{r}_{ij},\mathbf{R}_k)$ is a measure for the amount of distortion of free scattering waves caused by the presence of the total potential $\Sigma_{j>i}Z_{ij}/r_{ij}$. Transforming (1) into the coordinates (4) and making the ansatz (5) we end up with the expression

$$\left[\Delta_{\bar{\mathbf{r}}_{ij}}+\Delta_{\bar{\mathbf{R}}_k}+2i\left(\frac{1}{\sqrt{\mu_{ij}}}\mathbf{k}_{ij}\cdot\nabla_{\bar{\mathbf{r}}_{ij}}+\frac{1}{\sqrt{\mu_k}}\mathbf{K}_k\cdot\nabla_{\bar{\mathbf{R}}_k}\right)-2\sum_{\substack{m,n\\ n>m}}^{3}\frac{q_{mn}}{\overline{r}_{mn}}\right]\overline{\Psi}(\bar{\mathbf{r}}_{ij},\bar{\mathbf{R}}_k)=0, \tag{6}$$

with $q_{mn}=\mu_{ij}^{1/2}Z_{ij}$. Now we transform further to the coordinates (3). The Jacobi determinant scales as $\rho^5\sin^2 2\varphi/4$ and does not vanish except for cases where a pair of the three vectors $\mathbf{k}_{ij}$ or $\overline{\mathbf{r}}_{ij}$ and $\overline{\mathbf{R}}_k$ are linearly dependent, as to be expected. In the curvilinear coordinates (3) the six-dimensional Laplacian $\Delta:=\Delta_{\bar{\mathbf{r}}_{ij}}+\Delta_{\bar{\mathbf{R}}_k}$ is the sum of a hyperradial kinetic energy term and a centrifugal term:

$$\Delta:=\rho^{-5}\partial_\rho\rho^5\partial_\rho-\frac{\mathbf{\Lambda}^2}{\rho^2}. \tag{7}$$

The differential operator $\mathbf{\Lambda}^2$ is a self-adjoint scalar operator defined in the Hilbert space $L_2(\omega,d\omega)$, on the domain $\omega=[0,2]\times[0,2]\times[0,2]\times[0,\pi/2]\times[-1,1]$ where $\omega\equiv\{\xi_1,\xi_2,\xi_3,\varphi,\gamma\}$. Since this domain is compact the operator $\mathbf{\Lambda}^2$ has a discrete spectrum and is associated with the grand-angular momentum [Casimir operator of the $O(6)$ group] which is well known from the hyperspherical approach. The differential operator $\mathbf{\Lambda}^2$ can be decomposed as

$$\mathbf{\Lambda}^2=\mathbf{\Lambda}_{\rm in}^2+\mathbf{\Lambda}_{\rm ext}^2+\mathbf{\Lambda}_{\rm mix}^2. \tag{8}$$

The operator $\mathbf{\Lambda}_{\rm in}^2$ is being differential in internal angles $\{\varphi,\gamma\}$ only whereas $\mathbf{\Lambda}_{\rm ext}^2$ operates on $\{\xi_i;i=1,2,3\}$ only. The operator $\mathbf{\Lambda}_{\rm mix}^2$ contains the mixed derivatives resulting from off-diagonal elements of the metric tensor and couples internal to external motion (rotational coupling). The explicit form of these operators is

$$\begin{aligned}\mathbf{\Lambda}_{\rm in}^2:&=-\frac{4}{\sin^2 2\varphi}[-2\gamma\partial_\gamma+(1-\gamma)\partial_\gamma^2\\&\quad+\sin 2\varphi\,\cos 2\varphi\partial_\varphi+\tfrac{1}{4}\sin^2 2\varphi\partial_\varphi^2]\\&=-\frac{4}{\sin^2 2\varphi}[\partial_{2\varphi}\sin^2 2\varphi\partial_{2\varphi}-\hat{\mathbf{L}}_\gamma^2].\end{aligned} \tag{9}$$

Here $\hat{\mathbf{L}}_\gamma^2$ denotes the operator of the squared orbital angular momentum of particle k with respect to the center of mass of the pair ij. This can be immediately deduced when $\mathbf{\Lambda}_{\rm in}^2$ is expressed in terms of $\theta:=\arccos\gamma$ in which case it reads

$$\hat{\mathbf{L}}_\gamma^2=-\sin^{-1}\theta\partial_\theta\sin\theta\partial_\theta. \tag{10}$$

The differential operator $\mathbf{\Lambda}_{\rm ext}^2$ has the form

$$\Lambda^2_{\rm ext}:=-\rho^2\Bigg\{\frac{1}{r^2_{23}\mu_{23}}[2\partial_{\xi_1}\xi_1\partial_{\xi_1}-\partial_{\xi_1}\xi_1^2\partial_{\xi_1}]\times\frac{1}{r^2_{13}\mu_{13}}[2\partial_{\xi_2}\xi_2\partial_{\xi_2}-\partial_{\xi_2}\xi_2^2\partial_{\xi_2}]\times\frac{1}{r^2_{12}\mu_{12}}[2\partial_{\xi_3}\xi_1\partial_{\xi_3}-\partial_{\xi_3}\xi_3^2\partial_{\xi_3}]\Bigg\}. \quad (11)$$

The coupling term $\Lambda^2_{\rm mix}$ is determined by the off-diagonal elements of the metric,

$$\Lambda^2_{\rm mix}:=-\rho^2\sum_{u\neq v}\{(\nabla_{\bar{\mathbf{r}}_{ij}}u)\cdot(\nabla_{\bar{\mathbf{r}}_{ij}}v)+(\nabla_{\bar{\mathbf{R}}_k}u)\cdot(\nabla_{\bar{\mathbf{R}}_k}v)\}\partial_u\partial_v,$$
$$u,v\in\{\xi_1,\xi_2,\xi_3,\varphi,\gamma,\rho\}. \quad (12)$$

An essential feature of the operator $\Lambda^2_{\rm ext}$ (11) is that it depends *parametrically* on internal coordinates since r_{ij} are functions of (φ,γ,ρ) only,

$$r_{13}=\rho\ \sin\varphi,$$
$$r_{23}=\rho\left[\cos^2\varphi+\left(\frac{m_1}{m_1+m_3}\right)^2\sin^2\varphi+\gamma\ \sin 2\varphi\right]^{1/2},$$
$$r_{12}=\rho\left[\cos^2\varphi+\left(\frac{m_3}{m_1+m_3}\right)^2\sin^2\varphi-\gamma\ \sin 2\varphi\right]^{1/2}. \quad (13)$$

In addition, Eq. (11) is exactly separable in the coordinates $\{\xi_j,j=1,2,3\}$. This separability is directly reflected in the Schrödinger equation (6) since gradient terms introduce no additional coupling;

$$2i\left(\frac{1}{\sqrt{\mu_{ij}}}\mathbf{k}_{ij}\cdot\nabla_{\bar{\mathbf{r}}_{ij}}+\frac{1}{\sqrt{\mu_k}}\mathbf{K}_k\cdot\boldsymbol{\nabla}_{\bar{\mathbf{R}}_k}\right)=D_{\rm ext}+D_{\rm in}, \quad (14)$$

where

$$D_{\rm ext}:=2i\left(\frac{k_{23}}{r_{23}\mu_{23}}(2\xi_1-\xi_1^2)\partial_{\xi_1}+\frac{k_{13}}{r_{13}\mu_{13}}(2\xi_2-\xi_2^2)\partial_{\xi_2}+\frac{k_{12}}{r_{12}\mu_{12}}(2\xi_3-\xi_3^2)\partial_{\xi_3}\right). \quad (15)$$

The differential operator $D_{\rm in}$ depends on internal coordinates only:

$$D_{\rm in}:=2i\left[\frac{1}{\sqrt{\mu_{ij}}}\mathbf{k}_{ij}\cdot\nabla_{\bar{\mathbf{r}}_{ij}}u+\frac{1}{\sqrt{\mu_k}}\mathbf{K}_k\cdot\nabla_{\bar{\mathbf{R}}_k}u\right]\partial_u,$$
$$u\in\{\varphi,\gamma,\rho\}. \quad (16)$$

Now we are able to rewrite the Schrödinger equation (1) as the sum of internal and external differential operators with an additional mixing term:

$$\left[H_{\rm in}+H_{\rm ext}-\frac{\Lambda^2_{\rm mix}}{\rho^2}\right]\overline{\Psi}(\xi_1,\xi_2,\xi_3,\varphi,\gamma,\rho)=0. \quad (17)$$

The differential operator $H_{\rm in}$ depends on body-fixed degrees of freedom:

$$H_{\rm in}:=\rho^{-5}\partial_\rho\rho^5\partial_\rho-\frac{\Lambda^2_{\rm in}}{\rho^2}+D_{\rm in}, \quad (18)$$

whereas the external differential operator takes on the form

$$H_{\rm ext}:=-\frac{\Lambda^2_{\rm ext}}{\rho^2}+D_{\rm ext}-2\sum_{\substack{m,n\\ n>m}}^{3}\frac{q_{mn}}{\overline{r_{mn}}}. \quad (19)$$

In Eq. (19) the total potential has been added to the external part as we intend below to solve for the eigenfunction of $H_{\rm ext}$. It is important to recognize that the eigenfunctions of the operator $H_{\rm ext}$, and in fact of Eq. (17), are invariant under any transformation of the total potential, provided this transformation depends on internal coordinates only and it does not affect the sum occurring in Eq. (19). This is due to the fact that Eq. (19) contains the internal coordinates parametrically. We make use of this additional freedom by using a transformation similar to that given in Ref. [5]. We introduce two-body-type potentials $V_{ij}=Z_{ij}/r_{ij}$ as the most general linear superposition of all three physical two-body potentials $V_{ij}=Z_{ij}/r_{ij}$ with coefficient a_{ij} dependent on internal coordinates only, i.e.,

$$\begin{pmatrix}\overline{V_{23}}\\ \overline{V_{13}}\\ \overline{V_{12}}\end{pmatrix}=\mathcal{A}\begin{pmatrix}V_{23}\\ V_{13}\\ V_{12}\end{pmatrix}, \quad (20)$$

where $\mathcal{A}(\varphi,\gamma)$ is a 3×3 matrix with elements $a_{ij}=a_{ij}(\varphi,\gamma)$. An equivalent relation for $\overline{Z}_{ij}(\varphi,\gamma)$ can immediately be deduced from (20).

The invariance of the sum, i.e., the total potential, occurring in Eq. (19) under the transformation (20) requires

$$\sum_{i=1}^{3}a_{ij}=1,\quad j=1,2,3. \quad (21)$$

It should be emphasized that within the condition (21) the treatment is still exact. In addition to (21), six further conditions have to be imposed to uniquely define the transformation (20). These relations can be chosen according to practical considerations as well as to the specific type of three particles under investigation, an example of this has been given in Ref. [5]. The physical interpretation of the transformation (20) is quite obvious. According to Eq. (20) the strength of interaction of two individual particles i and j is no longer determined by their product charges Z_iZ_j as is the case in two-body Rutherford scattering. The product charges $\overline{Z_{ij}}$ depend rather dynamically on the shape of triangle formed by the three particles. This functional dependence is given by the coefficients a_{ij} which indicate the amount of distortion of a two-body subsystem due to the presence of a third charged particle. Hence these coefficients can be identified as a direct measure for three-body interactions.

In atomic and molecular physics three-body continuum systems arise as final states achieved in charged particle-impact ionization and photo double ionization. Estimates of

cross sections for these processes require the knowledge of the wave function (5). Using a multiple scattering model Garibotti and Miraglia [9] have derived an approximate expression for (5), hereafter Ψ_{3C}, which has been employed for the calculations of ionization cross sections for proton- and antiproton-impact ionization of atomic hydrogen and helium. The wave function Ψ_{3C} treats all particles in the continuum on equal footing and, as pointed out in Ref. [5], satisfies the Kato-cusp conditions [11] when two particles come close together (in configuration space). Later it has been realized [10] that this wave function satisfies the Schrödinger equation (1) for large interparticle separations. The wave function Ψ_{3C} has then been extensively employed for the description of final states achieved by various scattering reactions [10,12–14]. An important feature of Ψ_{3C} is that it employs the coupling matrix $\mathcal{A}=\mathbb{1}$. Thus, according to the interpretations of $\mathcal{A}$, by approximating the final-state wave function by Ψ_{3C} the three-body system is considered as three noninteracting two-body subsystems. Three-body coupling can be introduced by making use of Eq. (20). For two electrons moving in the double continuum of a nucleus a scattering three-body wave function, hereafter Ψ_{DS3C}, has recently been constructed [5] which is similar to Ψ_{3C} in philosophy, in fact it encompasses Ψ_{3C} as a special case ($\mathcal{A}=\mathbb{1}$). The explicit form of Ψ_{DS3C} expressed in the coordinates of Eq. (3) is

$$\overline{\Psi}_{\mathrm{DS3C}}(\xi_1,\xi_2,\xi_3,\varphi,\gamma,\rho)={}_1F_1(i\beta_{23}(\varphi,\gamma),1,-i[k_{23}r_{23}\xi_1])\,{}_1F_1(i\beta_{13}(\varphi,\gamma),1,-i[k_{13}r_{13}\xi_2])\,{}_1F_1(i\beta_{12}(\varphi,\gamma),1,-i[k_{12}r_{12}\xi_3]), \tag{22}$$

where the relative coordinates r_{ij} are given by (13). Note, that taking (13) into account the whole solution Ψ_{DS3C} can be written in terms of (3) because the plane-wave argument can be expressed as

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

The Sommerfeld parameters appearing in Eq. (22) have the form

$$\beta_{ij}(\varphi,\gamma):=\frac{\overline{Z_{ij}}\mu_{ij}}{k_{ij}}, \tag{24}$$

where $\overline{Z_{ij}}$ are determined from Eq. (20) using the matrix $\mathcal{A}$ given in Refs. [5,15]. The wave function Ψ_{3C} derives from Eq. (22) in the special case $Z_{ij}=Z_iZ_j$, i.e., for $\mathcal{A}=\mathbb{1}$. From previous derivation it was, however, not clear which part of the grand-angular momentum is diagonalized by the wave functions Ψ_{DS3C} and Ψ_{3C}. Upon inspection of Eq. (19) the part H_{DS3C} of which Ψ_{DS3C} is the regular exact eigenfunction with zero eigenvalue is readily identified:

$$H_{\mathrm{ext}}=H_{\mathrm{DS3C}}+H_{\mathrm{rem}}, \tag{25}$$

where

$$\begin{aligned}H_{\mathrm{DS3C}}:=&\frac{2}{r_{23}^2\mu_{23}}[\partial_{\xi_1}\xi_1\partial_{\xi_1}+ik_{23}r_{23}\xi_1\partial_{\xi_1}-\mu_{23}\overline{Z_{23}}r_{23}]\\&+\frac{2}{r_{13}^2\mu_{13}}[\partial_{\xi_2}\xi_2\partial_{\xi_2}+ik_{13}r_{13}\xi_2\partial_{\xi_2}-\mu_{13}\overline{Z_{13}}r_{13}]\\&+\frac{2}{r_{12}^2\mu_{12}}[\partial_{\xi_3}\xi_3\partial_{\xi_3}+ik_{12}r_{12}\xi_3\partial_{\xi_3}-\mu_{12}\overline{Z_{12}}r_{12}]\end{aligned} \tag{26}$$

in which case

$$H_{\mathrm{DS3C}}\overline{\Psi}_{\mathrm{DS3C}}=0.$$

III. REMARKS ON THE WAVE FUNCTIONS Ψ_{3C} AND Ψ_{DS3C}

From Eq. (26) it is clear that only the total potential, part of Λ^2_{ext}, and a part of the gradient terms are taken into account when employing the approximation $H=H_{DS3C}$ where H is the total Hamiltonian. The whole body-fixed kinetic energy operator and H_{rem} are still to be considered. In the case of $\mathcal{A}=\mathbb{1}$ ($\Psi\approx\Psi_{3C}$) these operators are simply neglected. In contrast, the wave function Ψ_{DS3C} is determined according to a coupling matrix $\mathcal{A}$ which minimizes the part $H-H_{DS3C}$ in some region of the Hilbert space (the five-dimensional manifold defined by large constant ρ and the Wannier configuration). On the other hand, it has been shown in Ref. [5] that the wave function $\overline{\Psi}_{DS3C}$ ($\overline{\Psi}_{3C}$) solves the Schrödinger equation in the whole asymptotic region (for large interparticle separations). This has important implications. As the coordinate important for Coulomb scattering is of the parabolic type $k_{ij}(r_{ij}+\hat{\mathbf{k}}_{ij}\cdot\hat{\mathbf{r}}_{ij})$ the asymptotic region is reached faster, i.e., at smaller ρ, for higher energies than is the case for lower energies. Thus at threshold the validity of the approximation $\overline{\Psi}\approx\overline{\Psi}_{3C}$ is not clear. Indeed, at lower excess energies the radial part of $\overline{\Psi}_{3C}$ shows a behavior not compatible with the total potential [5]. This fact also signifies the importance of the part of H at lower energies which is not diagonalized by $\overline{\Psi}_{3C}$. In the case of Ψ_{DS3C} this deficiency is partly dealt with by choosing the transformation

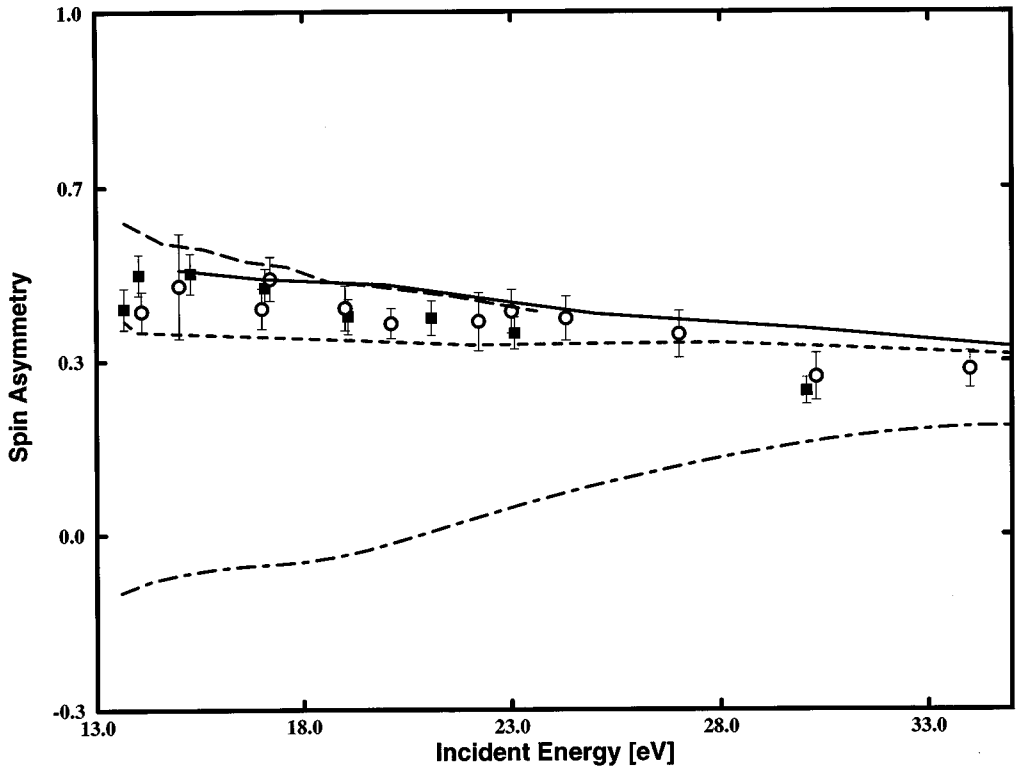

FIG. 1. The spin asymmetry [Eq. (27)] in the total cross section for the electron-impact ionization of atomic hydrogen. The curves show the results of the hidden crossing theory [19] (long-dashed curve) and the CCC method (solid curve). Representing the final state by Ψ_{3C} yields for the spin asymmetry the results shown by the dot-dashed curve. The results of using Ψ_{DS3C} and assuming the total potential to be conserved along the paths of free particles [compare Eq. (21)] are represented by the short-dashed curve. The experimental data are taken from Ref. [28] (full squares) and Ref. [27] (open circles).

(20) in a way which accounts for the part not diagonalized by Ψ_{3C}. For this reason the wave functions Ψ_{DS3C} and Ψ_{3C} are expected to show a completely different radial behavior at lower excess energies. In fact, the wave function Ψ_{3C} possesses an asymptotically diverging radial behavior at threshold [5] which results in its normalization being exponentially decreasing with declining low excess energies. This is in stark contrast to Ψ_{DS3C}, which remains asymptotically bound at threshold [5,6].

A way of directly testing the radial parts of Ψ_{3C} and Ψ_{DS3C} is offered by comparing with spin-asymmetry measurements in the total cross sections of electron-impact ionization of atomic hydrogen which is defined as

$$A := \frac{\sigma^s - \sigma^t}{\sigma^s + 3\sigma^t}, \tag{27}$$

where σ^s and σ^t are the total ionization cross sections for singlet and triplet scatterings, respectively. The spin asymmetry A is a dynamical quantity. It does not depend on the normalization of the wave function Ψ_{DS3C} since this wave function contains the momenta of the outgoing electrons in a symmetrical way and near to threshold the spatial part of Ψ_{DS3C} becomes energy independent [5]. Thus A tests for the radial parts of this wave function. The original version of the Wannier theory [23] has been formulated for $^1S^e$ states of the final-state electrons. Thus no estimate of the spin states occupied by the electrons in the final channel has been provided. A subsequent extension of the Wannier treatment to arbitrary L,S, and π states (total angular momentum, total spin, and parity) [16] has revealed that all L states have the same energy dependence at threshold and nearly all $LS\pi$-states (in particular, singlet and triplet states) possess the same threshold law. The implication of these conclusions for the spin asymmetry is that A does not depend on the excess energy near threshold although an exact value of A cannot be given. Careful analysis of recent measurements of A at threshold reveals, however, a slightly positive slope of the spin asymmetry with increasing excess energies [17] which indicates that σ^s and σ^t have slightly different analytical dependence on the excess energy near to threshold. The arguments of Ref. [16] can be reversed to conclude from a constant A that at threshold σ^s and σ^t differ only by an excess-energy-independent factor. The results for A when representing the two-electron continuum final state by Ψ_{3C} and Ψ_{DS3C} are depicted in Fig. 1 along with the results of the convergent-close-coupling calculations (CCC) [18] and the method using hidden-crossing theory [19]. Although the last three theories are in reasonable agreement with experimental finding the positive slope of A at threshold is not reproduced. Calculations using the CCC method could not be performed directly at threshold due to the increasing number of pseudostates needed to achieve convergence. From Fig. 1 it is clear that describing the final state by Ψ_{3C} leads to a completely wrong behavior of the spin asymmetry whereas this shortcoming is corrected for by employing Ψ_{DS3C}. We can

now reverse the arguments and deduce that the spin asymmetry A is highly sensitive to the part of the Hamiltonian neglected by Ψ_{3C} and accounted for by using Ψ_{DS3C}. The spin asymmetry calculated with Ψ_{DS3C} is not a constant function of the excess energy at threshold, as seen in Fig. 1. Thus describing the two final-state electrons by Ψ_{DS3C} results in an excess-energy dependence of singlet and triplet states which is not compatible with the Wannier theory analysis.

Another important point to be emphasized is the following. When employing Ψ_{3C} for the description of two-electron final states following one-photon two-electron transitions and electron-impact ionization, the angular distributions for these electrons turn out to be well reproduced in many situations even at lower excess energies [20,12]. This behavior has been traced to the inclusion of the normalization factor (N_{ee}) of the radial part of the two-body Coulomb wave function which represents the (isolated) electron-electron subsystem and indeed only this normalization factor (also called the Gamov factor) has then been used to simulate the measured angular distribution of ejected electrons following electron-impact ionization of atomic hydrogen [21,22]. It should be stressed, however, that this normalization factor originates from the radial part, which is the cause for the wrong radial behavior exposed in Fig. 1 and thus its normalization cannot be correct. This conclusion is reinforced by the fact that inclusion of $|N_{ee}|$ in theoretical calculations results in a spurious behavior of the magnitude of the cross sections.

The above analysis offers a possible way of explaining why the Ψ_{3C} is capable of reproducing the measured angular distributions. To this end we remark that the approximation $H=H_{DS3C}$ which results in the approximations $\bar{\Psi}=\bar{\Psi}_{DS3C}$ means that the variation in internal coordinates is negligibly small compared with that of the external coordinates $\xi_{1,2,3}$, i.e., the coordinates ρ,φ, and γ are treated adiabatically. The validity of this adiabatic approach is readily derived from properties of the (total) potential surface. As pointed out by many authors [23,16], at lower excess energies the variation in γ is much smaller than that in φ. In fact, the Wannier ionization mode [23,16], which dominates at threshold, occurs at a stable equilibrium in γ and is unstable in the coordinate φ. Hence, at lower excess energies, treating γ adiabatically is more reasonable than considering φ to vary slowly, or in fact to be frozen as assumed by Ψ_{3C}. As the angular distribution is determined by the γ degree of freedom it is expected that Ψ_{3C} would provide a better description for the angular than for the radial correlations. The latter correlation controls the excess-energy sharing of the two electrons. In fact, using the Ψ_{3C} final state at lower excess energies results (Fig. 2) in an energy distribution sharply peaked around equal-energy sharing which is at variance with experimental finding [24,25] and the Wannier theory prediction which indicate basically a flat energy distribution at threshold. The same behavior as shown in Fig. 2 has been observed for one-photon double ionization [8]. Although Ψ_{DS3C} indicates a flatter energy distribution which is slightly peaked around equal-energy sharing the variation in this distribution is still much higher than that anticipated by the Wannier theory which indicates a shortcoming of Ψ_{DS3C} in fully accounting for the variation in the coordinate φ.

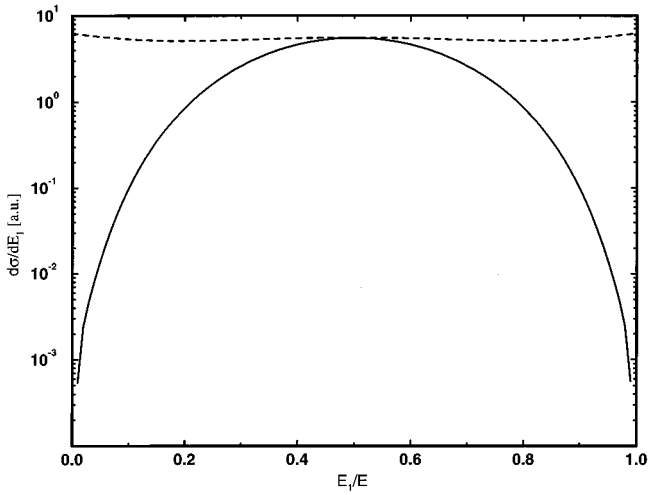

FIG. 2. The single differential cross section for the electron-impact ionization of atomic hydrogen as a function of the ratio E_1/E where E_1 is the energy of one of the final-state electrons and E is the total excess energy which is chosen as $E=200$ meV. Using the Ψ_{DS3C} approximation yields the dotted curve whereas the solid curve represents the results when employing Ψ_{3C} for the final state. The results of Ψ_{3C} have been multiplied by a factor of 10^{13}.

A further point concerns the wave function Ψ_{DS3C} and its subderivatives at vanishing hyper-radius, i.e., the three-body collision point. These functions do not take into account the hyper-radial kinetic energy term which is known to dominate the total Hamiltonian for small hyper-radius. Thus it is conceivable that wave functions of the form (22) reveal a behavior not compatible with the Schrödinger equation for small hyper-radius. In fact, solutions of Eq. (1) for $\rho\rightarrow 0$ are known to have a Fock expansion [26] in the hyper-radius which contains power and logarithmic terms in ρ whereas the wave functions Ψ_{3C} and Ψ_{DS3C} possess a regular power-series expansion in small hyper-radius. For large ρ the potential term dominates and Ψ_{DS3C} and Ψ_{3C} become adequate descriptions. Hence the wave functions Ψ_{DS3C} and Ψ_{3C} satisfy the Kato-cusp conditions to be imposed when two particles come close together since in this case ρ is large even though one interparticle distance is very small.

The last remark concerns the treatment of partial waves by Ψ_{3C}. Since the operator $\mathbf{\Lambda}_{in}^2$ given by Eq. (9), is not treated by Ψ_{3C} this wave function provides a better approximation to the exact solution when $\mathbf{\Lambda}_{in}^2$ is minimized. This is the case for vanishing angular momentum $\hat{\mathbf{L}}_{\gamma}^2$ as can be immediately deduced from Eq. (9).

IV. CONCLUSIONS

In this work the three-body Coulomb continuum problem has been reformulated in a parabolic-hyperspherical coordinate system. It has been shown how additional information on three-body Coulomb wave functions can be gained through this procedure. Various aspects of Coulomb wave functions have been critically analyzed in light of spin-asymmetry measurements, angle, and energy distribution of two electrons moving in a nuclear field. It has been argued that at threshold Ψ_{3C} provides an adequate description for

the angular correlations since the variation in the corresponding degree of freedom is slow whereas it fails in simulating the energy distribution due to the rapid variation in the ratio of the electronic distances from the nucleus. As this shortcoming is partly removed by Ψ_{DS3C} we deduce that this ratio is very sensitive to three-body coupling. It has been suggested that the correct description of the dynamic with varying φ is sufficient to explain the behavior of the spin asymmetry shown in Fig. 1.

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[1] T.H. Gronwall, Phys. Rev. **51**, 655 (1937).
[2] V.A. Fock, Izv. Akad. Nauk. SSSR Ser. Fiz. **18**, 161 (1954).
[3] J.H. Macek, J. Phys. B **1**, 831 (1968).
[4] C.D. Lin, Phys. Rep. **257**, 1 (1995).
[5] J. Berakdar, Phys. Rev. A **53**, 2314 (1996).
[6] J. Berakdar and J.S. Briggs, Phys. Rev. Lett. **72**, 3799 (1994).
[7] J. Berakdar and J.S. Briggs, J. Phys. B **27**, 4271 (1994).
[8] J. Berakdar (unpublished).
[9] G. Garibotti and J.E. Miraglia, Phys. Rev. A **21**, 572 (1980).
[10] M. Brauner, J.S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[11] T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957).
[12] F. Maulbetsch and J.S. Briggs, J. Phys. B **26**, 1679 (1993).
[13] J. Berakdar, J.S. Briggs, and H. Klar, Z. Phys. D **24**, 351 (1992).
[14] J. Berakdar and H. Klar, J. Phys. B **26**, 4219 (1993).
[15] J. Berakdar, Aust. J. Phys. (to be published).
[16] C.H. Greene and A.R.P. Rau, Phys. Rev. Lett. **48**, 533 (1982).
[17] X.Q. Guo, D.M. Crowe, M.S. Lubell, F.C. Tang, A. Vasilakis, J. Slevin, and M. Eminyan, Phys. Rev. Lett. **15**, 1857 (1990).
[18] B. Igor and A.T. Stelbovics, Phys. Rev. Lett. **70**, 746 (1993).
[19] J.H. Macek and S.Yu. Ovchinnikov, Phys. Rev. Lett. **74**, 4631 (1995).
[20] M. Brauner, J.S. Briggs, H. Klar, J.T. Broad, T. Rösel, K. Jung, and H. Ehrhardt, J. Phys. B **24**, 657 (1991).
[21] C.T. Whelan, R.J. Allan, J. Rasch, H.R.J. Walters, X. Zhang, J. Röder, K. Jung, and H. Ehrhardt, Phys. Rev. A **50**, 4394 (1994).
[22] J. Botero and J.H. Macek, Phys. Rev. Lett. **68**, 576 (1992).
[23] G. Wannier, Phys. Rev. **90**, 817 (1953).
[24] S. Cvejanović and F.H. Read, J. Phys. B **7**, 1841 (1974).
[25] P. Lablanquie, K. Ito, P. Morin, I. Nenner, and J.H.D. Eland, Z. Phys. D **16**, 77 (1990).
[26] V.A. Fock, K. Nor. Vidensk. Selsk. Forh. **31**, 138 (1958).
[27] D.M. Crowe, X.Q. Guo, M.S. Lubell, J. Slevin, and M. Eminyan, J. Phys. B **23**, L325 (1990).
[28] G.D. Fletcher, M.J. Alguard, T.J. Gay, V.W. Hughes, P.F. Wainwright, M.S. Lubell, and W. Raith, Phys. Rev. A **31**, 2854 (1985).