Modification of the quantum mechanical flux formula for electron-hydrogen ionization through Bohm's velocity field

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For the single differential cross section (SDCS) for hydrogen ionization by electron impact (*e*-H problem), we propose a correction to the flux formula given by R. Peterkop [*Theory of Ionization of Atoms by Electron Impact* (Colorado Associated University Press, Boulder, 1977)]. The modification is based on an alternative way of defining the kinetic energy fraction, using Bohm's definition of velocities instead of the usual asymptotic kinematical, or geometrical, approximation. It turns out that the solution-dependent, modified energy fraction is equally related to the components of the probability flux. Compared to what is usually observed, the correction yields a finite and well-behaved SDCS value in the asymmetrical situation where one of the continuum electrons carries all the energy while the other has zero energy. We also discuss, within the *S*-wave model of the *e*-H ionization process, the continuity of the SDCS derivative at the equal energy sharing point, a property not so clearly observed in published benchmark results obtained with integral and *S*-matrix formulas with unequal final states.

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I. INTRODUCTION

In the past decades, several numerical approaches to evaluating the solution of the quantum three-body Coulomb breakup problem have been introduced (see, e.g., [1–5]). The single ionization of atomic hydrogen by electron impact was one of the first fundamental three-body Coulomb problems solved [2,6], showing a remarkably good agreement with the available experimental data [7]. Over the years, particular attention has been paid to the *S*-wave approximation, also known as the Temkin-Poet model [5,8–10]; although simpler than the physical one, it is a nontrivial problem that contains the major difficulties, i.e., the long-range character of the Coulomb interactions. The Temkin-Poet model has been systematically used as a test bed for the development of theoretical and numerical methods. In this work we use it to show that, even in this simplified scattering problem, the task of extracting the single differential cross section (SDCS) directly from the asymptotic behavior of the wave function is not trivial because of the long-range nature of the interaction.

It is well known that transition amplitudes which characterize a scattering problem can be obtained from the asymptotic part of the wave function, as prescribed by scattering theory, which is well established for short-range potentials (and extended to Coulomb ones). It is also well known that all channels are entangled when the Schrödinger equation is exactly solved. In the case of electron impact ionization of atomic hydrogen, elastic, excitation, and ionization channels are coupled in the collision. Numerical solutions of the three-body scattering problem are nowadays available through several methods. Such solutions are evaluated in finite, though large, regions of the configuration space, the restrictions being mainly determined by computational capabilities (size and speed). In spite of the long-range nature of the Coulomb scattering problem, these large domains (several hundreds atomic units) have proved to be generally sufficient to calculate—through integral formulas—the end product, i.e., the cross section. If, however, the asymptotic part of the solutions is employed explicitly, one should be sure that the true Coulomb asymptotic behavior is reached, and care is needed.

There exist several ways to extract the SDCS from quantum mechanical calculations. Among them, the method designed by Peterkop [11] of counting particles by means of the quantum mechanical probability current stands out and has been tested thoroughly [12,13]. Contrary to integral formulas, this flux formula procedure does not depend on the chosen description of the final states, which, for long-range interactions, usually has a certain arbitrariness. The flux formula is formally correct and is somehow similar to a measurement; as it corresponds to counting particles, it can be applied in both finite and infinite domains, the evaluation at infinite distances providing the true answer. Practically, the usual technique to extract the differential cross sections consists in extrapolating the results obtained from a finite domain to the infinite one. However, after the appearance of unsatisfactory cross sections [13], the flux procedure has been questioned. It has been said that the ionization flux at finite distances is populated by discrete—excitation—channels which lead to unphysical behavior of the SDCS in very asymmetric energy regimes [12]; we note, however, that the flux approach in hyperspherical coordinates gave good results for double-photoionization of helium in asymmetric regimes [14]. In the end, the advantages of the integral formulas have been reinforced [15] over the flux formula, which was finally abandoned for all practical purposes for the *e*-H problem. This paper essentially aims to "rescue" the flux formula procedure.

Since the counting of "asymptotic" particles can be considered a realistic approach to the scattering problem, we believe that there is something missing in the interpretation of the flux formula rather than the "counting" approach itself. The aim of this work is to show that the reason behind the apparent

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flux formula failure is due to the way in which the continuum electron energy sharing is approximated at finite distances, and not because of the contribution of discrete channels (which indeed should be present and coupled to ionization). The idea is to correct the energy fraction definition to take into account finite-distance (Coulomb interaction) effects. For this purpose, we introduce an alternative and more realistic (solution-dependent) energy fraction; the modified definition involves the kinetic energy arising from Bohm's velocity field evaluated in the asymptotic region, rather than from the usual (free-wave) geometrical assumption,

$$\mathbf{r} \simeq t\,\mathbf{k}, \tag{1}$$

which, for Coulomb interactions, is valid only at infinite distances. It turns out that our proposal is equivalent to the ratio of flux components, thus providing some further physical interpretation. Once modified, the definition of energy sharing leads to a different picture by removing the previously observed unphysical behaviors, thus rehabilitating the flux formula approach.

We also study another interesting and somewhat not fully clear issue. In some benchmark calculations a sharp change of slope was observed in the Temkin-Poet SDCS at equal energy sharing. We show that this feature is not exactly what is expected from the continuity of the asymptotic scattering wave function and its derivative when it perpendicularly crosses the curve $r_1 = r_2$: the slope of the SDCS at that point must be continuous and 0. This property is always fulfilled when using the flux formula, but not necessarily with other methods. In the S-matrix method [8] or with integral formulas [16], one makes use of free states for the faster electron and Coulomb states for the slower one, and its interchange of coordinates when crossing the equal energy sharing value. These final states, which are employed to avoid phase divergences in the SDCS integral formulas, seem to be responsible for a surprisingly sharp change of slope.

The organization of the paper is as follows. In Sec. II we present the model equation, the usual definition of the SDCS through the flux formula given by Peterkop, and the theoretical correction to the energy sharing definition; we also show that the SDCS should have a continuous derivative under the equal energy sharing regime. Then, in Sec. III, these theoretical points are illustrated through numerical calculations; cross-section results are presented and analyzed in detail for an impact energy of 54.4 eV (results for energies of 40.817 and 150 eV are also reported). Finally, some conclusions are drawn in Sec. IV.

We employ atomic units ($m = \hbar = e = 1$) throughout, which means distances in units of a_0, energy in hartree, and the SDCS in units of πa_0^2.

II. THEORY

Consider the Schrödinger equation for hydrogen ionization by electron impact,

$$\left[-\frac{1}{2}\nabla_{r_1}^2 - \frac{1}{2}\nabla_{r_2}^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} - E\right]\Psi^+(\mathbf{r}_1,\mathbf{r}_2) = 0, \tag{2}$$

where E is the total energy of the system, $\mathbf{r_i}$ $(i = 1,2)$ denote the electron coordinates, and $r_{12} = |\mathbf{r_1} - \mathbf{r_2}|$ is the interelectronic distance. The solution Ψ^+ may be separated into two terms, $\Psi^+ = \Psi_{\rm sc}^+ + \Psi_0$, where Ψ_0 represents the prepared collision state and $\Psi_{\rm sc}^+$ the scattering wave function, which contains all the physical information about the collision process. Depending on whether the two electrons form a singlet ($S = 0$) or a triplet ($S = 1$) spin state, we have the symmetry condition $\Psi^+(\mathbf{r}_1,\mathbf{r}_2) = (-1)^S\Psi^+(\mathbf{r}_2,\mathbf{r}_1)$. For simplicity, throughout this work, we consider only singlet spin symmetry (all results are applicable to triplet symmetry also).

For the initial channel, we choose the approximate wave function

$$\Psi_0(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}[\pi^{-1/2}e^{-r_1}e^{i\mathbf{k_i}\cdot\mathbf{r}_2} + (1 \leftrightarrow 2)],$$

where $k_i = \sqrt{2(E-(-0.5))}$. This leads to the following nonhomogeneous Schrödinger equation for the scattering wave function $\Psi_{\rm sc}^+$:

$$\left[-\frac{1}{2}\nabla_{r_1}^2 - \frac{1}{2}\nabla_{r_2}^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} - E\right]\Psi_{sc}^+(\mathbf{r}_1,\mathbf{r}_2) = -\left[\left(\frac{1}{r_{12}} - \frac{1}{r_2}\right)\Psi_0(\mathbf{r}_1,\mathbf{r}_2) + (1 \leftrightarrow 2)\right]. \tag{3}$$

At long distances ($r_1, r_2 \to \infty$) the solution of this equation must behave as [11]

$$\lim_{\rho\to\infty}\Psi_{\rm sc}^+(\mathbf{r}_1,\mathbf{r}_2) = A(\omega_5)\rho^{-5/2}e^{i(K\rho - \frac{C(\omega_5)}{K}\ln(2K\rho))}, \tag{4}$$

with $K = \sqrt{2E}$, and where we have used the hyperspherical coordinates α and ρ defined through $r_1 = \rho\cos\alpha$ and $r_2 = \rho\sin\alpha$. In Eq. (4), $A(\omega_5)$ represents the scattering amplitude depending on the five hyperangular coordinates $(\alpha,\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)$, and the angular-dependent charge $C(\omega_5)$ is defined as

$$C(\omega_5) = -\frac{Z}{\cos\alpha} - \frac{Z}{\sin\alpha} + \sum_{l=0}^{\infty}\frac{4\pi}{2l+1} \times \sum_{m=-l}^{l}(-1)^m Y_l^{-m}(\hat{\mathbf{r}}_2)Y_l^m(\hat{\mathbf{r}}_1)\begin{Bmatrix}\sec\alpha\tan^l\alpha\\ \csc\alpha\cot^l\alpha\end{Bmatrix}, \tag{5}$$

where the upper (lower) value in curly braces corresponds to $\alpha < \pi/4$ ($\alpha > \pi/4$).

The scattering amplitude $A(\omega_5)$ is related to the SDCS for finding, in the asymptotic region, two electrons with energies $E_1 = E\cos^2\alpha$ and $E_2 = E\sin^2\alpha$ and pointing in the directions $\hat{\mathbf{r}}_i$ $(i = 1,2)$. The relation reads

$$\frac{d^5\sigma}{d\hat{\mathbf{k}}_1 d\hat{\mathbf{k}}_2 dE_2} \propto |A(\omega_5)|^2. \tag{6}$$

The link between the energies of the electrons and the coordinate α comes from the formal theory of ionization, which states that relation (1) is valid in the asymptotic region. We refer to this relation as the *geometrical approximation*.

For the Temkin-Poet S-wave model, $1/r_{12}$ is replaced by $1/r_>$, where $r_> = \max[r_1,r_2]$. In this case for $\alpha < \pi/4$ ($\alpha > \pi/4$) the $-1/r_1$ ($-1/r_2$) potential is removed from the left-hand-side of Eq. (2) or (3). The asymptotic behavior

corresponding to the TP model is similar to (4),

$$\lim_{\rho\to\infty}\Psi^{+}_{\rm sc}(r_1,r_2)=A(\alpha)\rho^{-5/2}e^{i(K\rho-\frac{\gamma(\alpha)}{K}\ln(2K\rho))}, \tag{7}$$

with the scattering amplitude $A(\alpha)$ depending only on the angle α and the charge $\gamma(\alpha)$ defined as

$$\gamma(\alpha)=\begin{cases}-\frac{1}{\sin\alpha} & \text{if} \quad \alpha<\pi/4,\\ -\frac{1}{\cos\alpha} & \text{if} \quad \alpha>\pi/4.\end{cases}$$

Since the geometrical approximation, (1), also relates α to the ratio between the local momenta of the electrons, through $\tan\alpha=k_2/k_1$, the scattering amplitude—and thus the SDCS $\propto|A(\alpha)|^2$—can be considered a function of the energy fraction, defined as

$$\epsilon\equiv\sin^2\alpha=\frac{E_2}{E}. \tag{8}$$

The SDCS is typically U shaped; since it is symmetric with respect to $\alpha=\pi/4$, only half of the range, i.e., $0\leqslant\epsilon\leqslant 0.5$, needs to be considered.

It should be noted that the relation between α and ϵ is strictly valid only for $\rho\to\infty$, where the hyperangular structure of the scattering wave function is smooth enough, i.e., where it behaves locally as a pure hyperspherical wave. In spite of this, when numerical calculations are performed in finite domains, the same energy fraction formula is taken: this can affect the shape of the SDCS and even lead to wrong results. This finite-versus-infinite ρ-domain issue constitutes the starting point of the present investigation, which leads to our correction proposal.

A. Flux formula for the single differential cross section

The SDCS for the electron-hydrogen scattering problem is defined as the ratio between the number of electrons which populate a given final continuum state and the incident flux of particles,

$$d\sigma=\frac{dN}{k_0}, \tag{9}$$

where dN can be calculated as [1]

$$dN=J_\rho d\hat{\Omega}$$

and $d\hat{\Omega}$ is the (five-dimensional) element of the solid angle:

$$d\hat{\Omega}=\rho^5\sin^2\alpha\cos^2\alpha d\alpha\sin\theta_1 d\theta_1 d\varphi_1\sin\theta_2 d\theta_2 d\varphi_2.$$

J_ρ is the flux density along the hyperradial coordinate direction $d\hat{\rho}$, which can be written as

$$\begin{aligned}J_\rho&=\mathrm{Im}\left\{(\Psi^{+}_{\rm sc})^*\frac{\partial\Psi^{+}_{\rm sc}}{\partial\rho}\right\}\\&=\frac{1}{2i}[(\Psi^{+}_{\rm sc})^*\bigtriangledown\Psi^{+}_{\rm sc}-\Psi^{+}_{\rm sc}(\bigtriangledown\Psi^{+}_{\rm sc})^*].(\cos\alpha,\sin\alpha),\end{aligned} \tag{10}$$

where the dot in the second equality indicates a scalar product. Taking into account the expression $dE_2=2E\sin\alpha\cos\alpha$ and integrating over the angles θ_i and φ_i $(i=1,2)$, the cross section reads

$$\frac{d\sigma}{dE_2}=\frac{(4\pi)^2}{k_0 2E}J_\rho\rho^5\sin\alpha\cos\alpha. \tag{11}$$

In Ref. [13], the authors applied Eq. (11) to evaluate the SDCS at finite distances and for values of α which are far from 0 and $\pi/2$. Extrapolating procedures have been implemented, on one hand, to obtain, the value of the flux at infinite ρ values and, on the other hand, to derive its values for extremely unequal energy sharing ($\alpha=0$ and $\alpha=\pi/2$). However, this flux formula produces bad results close to these two limits, a feature associated with the contamination of the ionization flux by discrete channels contribution [12]; for this reason the flux formula was thereafter abandoned for the e-H problem.

B. Correction for the flux formula and properties of the single differential cross section

In this section we introduce our proposal to redefine the energy fraction and provide some justifications. Also, making use of the asymptotic condition, (7), we study analytically the derivative of the SDCS as a function of ϵ and show that it should be 0 at $\alpha=\pi/4$. This is in contrast with the observations in benchmark calculations in which the SDCS is evaluated with integral formulas or the S-matrix system of equations, with asymmetric final states.

1. Bohm's velocity field for assignation of the kinetic energy fraction

As it is necessary to correct the approximate values of the electron momenta given by the geometrical approximation, we propose making use of Bohm's velocity field associated with the scattering wave function:

$$\dot{\mathbf{r}}_\mathbf{i}=\frac{\hbar}{m}\mathrm{Im}\left\{\frac{\bigtriangledown_{\mathbf{r}_\mathbf{i}}\Psi^{+}_{\rm sc}}{\Psi^{+}_{\rm sc}}\right\}\quad(i=1,2). \tag{12}$$

Each of the vectors gives, with the direction and magnitude, the velocity of the particle when it is passing through a given point of space. For a steady state the trajectories do not cross each other, and the velocity field takes only one value at each coordinate. Recalling that the energy fraction, (8), is the kinetic energy ratio $E_2/E=E_2/(E_1+E_2)$, it makes sense to consider the alternative quantity,

$$\frac{\dot{\mathbf{r}}_\mathbf{2}^{\,2}}{\dot{\mathbf{r}}_\mathbf{1}^{\,2}+\dot{\mathbf{r}}_\mathbf{2}^{\,2}}. \tag{13}$$

For the S-wave problem, we thus define a modified energy fraction

$$\tilde{\epsilon}=\sin^2\theta\equiv\frac{\dot{r}_2^{\,2}}{\dot{r}_1^{\,2}+\dot{r}_2^{\,2}}. \tag{14}$$

Our proposal consists of replacing the angle α, which is considered the indicator of the energy sharing between electrons, with the angle θ, defined by Eq. (14). Note that our definition is solution dependent since it involves Bohm's velocities, (12); the angle θ depends not only on α but also on the hyperradius ρ at which one counts the particles and evaluates the SDCS.

Several arguments support the choice of this modified definition. First, the same definition is obtained from the ratio of probability currents (or flux)

$$\sin^2\theta=\frac{J_2^2}{J_1^2+J_2^2}, \tag{15}$$

where J_i are the (S-wave) components of the flux operator:

$$J_i = \frac{1}{2i}\left[(\Psi_{sc}^{+})^{*}\frac{\partial \Psi_{sc}^{+}}{\partial r_i} - \Psi_{sc}^{+}\frac{\partial (\Psi_{sc}^{+})^{*}}{\partial r_i}\right] \quad (i = 1,2). \quad (16)$$

Equivalently, one may write $\tan\theta = J_2/J_1$, which can be put in relation to $\tan\alpha = r_2/r_1$ and thus to $\tan\alpha = k_2/k_1 = E_2/E_1$ by using the geometrical assumption, (1).

Second, the velocity components give a measure of the energy fraction $\tilde{\epsilon}$, which differs from the geometrical definition ϵ at finite distances but matches it at $\rho \to \infty$. To show this, we can use the asymptotic functional form, (7), to evaluate the ratio, (14). Retaining the leading asymptotic orders [more important than $O(\rho^{-1})$], it is rather easy to show that ($\hbar = 1$)

$$m\dot{r_1} \simeq K\cos\alpha + \gamma'(\alpha)\sin(\alpha)\frac{\ln(2K\rho)}{K\rho}, \quad (17a)$$

$$m\dot{r_2} \simeq K\sin\alpha - \gamma'(\alpha)\cos(\alpha)\frac{\ln(2K\rho)}{K\rho}. \quad (17b)$$

Clearly, in the $\rho \to \infty$ limit, the Bohm velocities, (17a) and (17b), lead to an energy fraction, (14), that matches the geometrical definition. At finite distances, on the other hand, we have the influence of the Coulomb interaction through an $O(\ln(\rho)/\rho)$ correction term.

Third, the new energy fraction—again calculated with the asymptotic form, (7)—reads

$$\tilde{\epsilon} \simeq \sin^2\alpha - \frac{2}{K}\sin\alpha\cos\alpha\gamma'(\alpha)\frac{\ln(2K\rho)}{K\rho}, \quad (18)$$

where $\gamma'(\alpha)$ is the derivative of the charge $\gamma(\alpha)$; as for the velocities, the new energy fraction matches the geometrical definition at infinite ρ values but involves a correction at finite distances.

From result (18), we find that the equal energy regime is not reached at finite distances, say at ρ_0. Indeed we find a value smaller than 0.5 (larger than 0.5) when evaluating $\tilde{\epsilon}$ at $\alpha = \pi/4$ from the left (the right):

$$\tilde{\epsilon}_{<}|_{\alpha=\pi/4} \simeq \frac{1}{2}\left[1 - \frac{2\sqrt{2}}{K}\frac{\ln(2K\rho_0)}{\rho_0}\right], \quad (19a)$$

$$\tilde{\epsilon}_{>}|_{\alpha=\pi/4} \simeq \frac{1}{2}\left[1 + \frac{2\sqrt{2}}{K}\frac{\ln(2K\rho_0)}{\rho_0}\right]. \quad (19b)$$

Although with a different interpretation, we observed the same phenomenon in a semiclassical definition of the energy fraction [17]. Note that with the exact solution, however, this limitation does not occur; we see below that if ρ is large enough the energy fraction defined by Eq. (14) reaches all possible values between 0 and 1 when one moves through a constant-value hyperradial contour of the (r_1,r_2) plane, without being too close to the axes. Thus, the conflicting regions (the one which gives unphysical "counting" of particles for the SDCS with the *geometrical* definition) become naturally excluded.

In Fig. 1, we have plotted, in the (r_1,r_2) plane, hyperspherical constant-phase contours for the free wave (circles of radii ρ) and for the Coulomb behavior of Eq. (7). The direction normal to these contours indicates the two-dimensional momenta (k_1,k_2); their directions are clearly modified by the Coulomb interactions. Also, the horizontal (vertical) axis, which corresponds to an energy fraction of 0 (1) in the case of a free wave, is replaced with one of the dashed lines in the Coulomb case.

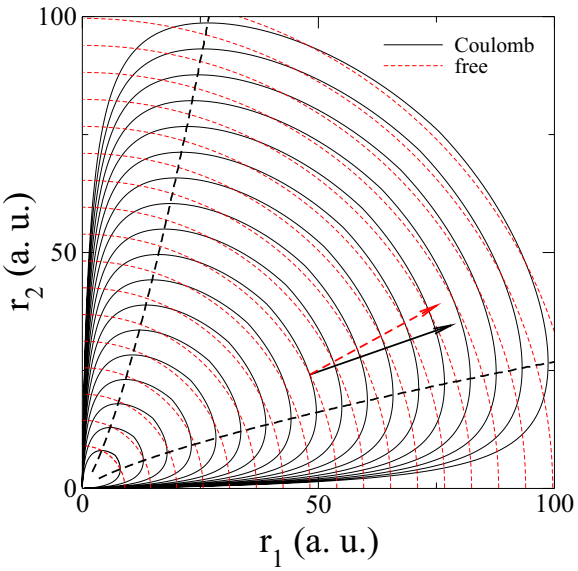

FIG. 1. (Color online) Constant phase contours for the free [dashed (red) lines] and Coulomb (solid black lines) hyperspherical waves. The direction perpendicular to these lines is the one followed by the local momentum vector (k_1,k_2). The red and black normal arrows have the same origin at the intersection of two Coulomb- and free-wave constant phase contours, respectively, highlighting the differences between the Coulomb and the geometrical definition of the asymptotic momenta. While zero-energy-fraction values follow the axes in the case of the free wave, for the Coulomb wave it is the one indicated by dashed black lines.

In summary, for given values of α and ρ, we propose considering the quantity $\tilde{\epsilon} = \sin^2\theta$ instead of $\epsilon = \sin^2\alpha$ as the local value of the kinetic energy fraction. Our approximation is based on the physical information carried by the flux and is of general application; i.e., it is valid for any kind of scattering problem and can be applied beyond the TP approximation.

2. *Continuity of the wave function at* $\alpha = \pi/4$

Let us now analyze the shape properties of the SDCS as a function of the energy fraction for values close to 0.5. We start from the asymptotic behavior of the scattering wave function given by Eq. (7). At $\alpha = \pi/4$, the logarithmic phase is continuous as a function of α but the derivative is not; intuitively, this discontinuity must be balanced by a property of $A(\alpha)$ at that point. For a given large value of ρ we ask for continuity of the wave function and its derivative with respect to α. Suppose that $A(\alpha)$ takes two different functional forms: $A_{<}(\alpha)$ for $\alpha < \pi/4$ and $A_{>}(\alpha)$ for $\alpha > \pi/4$. Taking the derivative of Eq. (7) with respect to α we find

$$\frac{\partial \Psi_{sc}}{\partial \alpha} \simeq \rho^{-5/2}e^{i\left(K\rho + \frac{1}{K\sin\alpha}\ln(2K\rho)\right)} \times\left[A'_{<}(\alpha) + A_{<}(\alpha)\frac{i}{K}\ln(2K\rho)\left(\frac{-\cos\alpha}{\sin^2\alpha}\right)\right], \quad \alpha < \pi/4; \quad (20a)$$

$$\frac{\partial \Psi_{sc}}{\partial \alpha} \simeq \rho^{-5/2} e^{i(K\rho + \frac{1}{K\cos\alpha}\ln(2K\rho))} \times \left[A'_{>}(\alpha) + A_{>}(\alpha)\frac{i}{K}\ln(2K\rho)\left(\frac{\sin\alpha}{\cos^2\alpha}\right)\right], \quad \alpha > \pi/4. \tag{20b}$$

Matching the expressions at $\alpha = \pi/4$ and simplifying we get

$$A'_{<}(\pi/4) - A'_{>}(\pi/4) \simeq (A_{>}(\pi/4) + A_{<}(\pi/4))\frac{i\sqrt{2}}{K}\ln(2K\rho).$$

By continuity of the wave function and singlet spin symmetry we, respectively, have $A_{>}(\pi/4) = A_{<}(\pi/4)$ and $A'_{<}(\pi/4) = -(-1)^S A'_{>}(\pi/4)$. This means that

$$A'_{<}(\pi/4) \simeq A_{<}(\pi/4)\frac{i\sqrt{2}}{K}\ln(2K\rho) \tag{21}$$

for $S = 0$, and $A_{<}(\pi/4) = A_{>}(\pi/4) = 0$ for $S = 1$. Now we can use Eq. (21) and its conjugate to calculate the derivative of the SDCS as a function of α:

$$\left.\frac{d|A_{<}(\alpha)|^2}{d\alpha}\right|_{\alpha=\pi/4} = \left.\frac{d}{d\alpha}(A_{<}(\alpha)A^*_{<}(\alpha))\right|_{\alpha=\pi/4} = A'_{<}(\alpha)A^*_{<}(\alpha) + A_{<}(\alpha)(A'_{<}(\alpha))^*\big|_{\alpha=\pi/4} = 0. \tag{22}$$

Consequently, the slope of the curve $|A_{<}(\alpha)|^2$ with respect to the variable $\sin^2\alpha$ is also 0.

III. RESULTS

In this section we present SDCS results for the singlet e-H process at an impact energy of 2 a.u. (54.422 eV) and discuss them in view of the geometrical and new energy fraction definition. Then we present results also for impact energies of 1.5 and 5.012 48 a.u. (40.817 and 150 eV). Since for singlet states SDCSs are symmetric with respect to $\epsilon = 0.5$, only half of the curve is shown.

The numerical technique to be used to solve the inhomogeneous Schrödinger equation, (3), is based on a configuration-interaction-type expansion using Sturmian functions with outgoing flux boundary conditions for each radial coordinate. Details of the methodology can be found in Refs. [5] and [18], where the capability of the method is demonstrated. Once the scattering wave function Ψ^+_{sc} is obtained, we evaluate—at fixed finite values of ρ—the SDCS through the flux formula given by Eqs. (10) and (11).

A. Uncorrected results

In Fig. 2 we show, as a function of the usual energy fraction $\epsilon = \sin^2\alpha$, the SDCS for the singlet solution of the e-H processes for an impact energy equal to 2 a.u. Benchmark results were provided by Jones and Stelbovics [8] with the Finite Element Method (FEM). We plot our results obtained for different values of ρ, from 10λ up to 40λ ($\simeq$150 a.u. for $E = 1.5$ a.u.), in steps of 2λ, where $\lambda = 2\pi/\sqrt{2E}$ corresponds to the wavelength of the hyperspherical outgoing wave given by Eq. (7). The extrapolation to $\rho \to \infty$ is shown by filled circles.

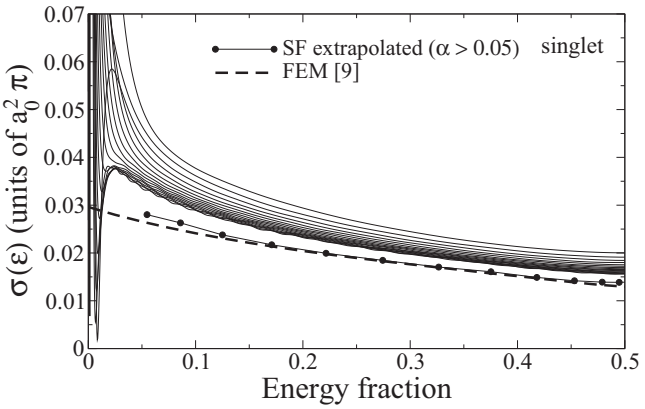

FIG. 2. SDCS for the e-H process for an impact energy of 2 a.u. as a function of the energy fraction $\epsilon = \sin^2\alpha$. Thick dashed line: FEM results [19]. Solid lines: Sturmian function evaluation and flux formula given by Eq. (11), for different values of ρ from 10λ up to 40λ in steps of 2λ. Filled circles: extrapolated flux formula result.

It is clear that the flux formula results show unphysical behavior near $\epsilon \simeq 0$ (by symmetry, the same behavior is found for $\epsilon \simeq 1$) which constitutes the apparent failure of the extraction technique. The extrapolated result (which depends on the finite domain used) is much smoother but can be considered accurate only for $\epsilon > 0.05$.

B. Correction of the energy fraction value

The proposed correction consists of considering, as the argument of the SDCS, the energy fraction $\tilde{\epsilon} = \sin^2\theta$ defined by Eq. (14) instead of $\epsilon = \sin^2\alpha$. Before applying the recipe to cross-section results, let us first analyze how the two definitions are related. For this purpose, we plot in Fig. 3 the value of $\sin^2\theta$ as a function of $\sin^2\alpha$ for different values of ρ. We observe a peak structure which develops in a region of small values of $\sin^2\alpha$, which we characterize by $\alpha < \alpha_c(\rho)$. This region reflects the strong distortion observed close to the $r_2 = 0$ axis and becomes smaller as ρ increases. Beyond $\alpha_c(\rho)$, $\sin^2\theta$ behaves almost linearly, with a slope which tends to 1 as ρ increases; this behavior indicates that $\sin^2\theta$ is equal to $\sin^2\alpha$ at $\rho \to \infty$. Furthermore, at finite but sufficiently large values of ρ, the modified energy fraction (i) is smaller than $\sin^2\alpha$; (ii)

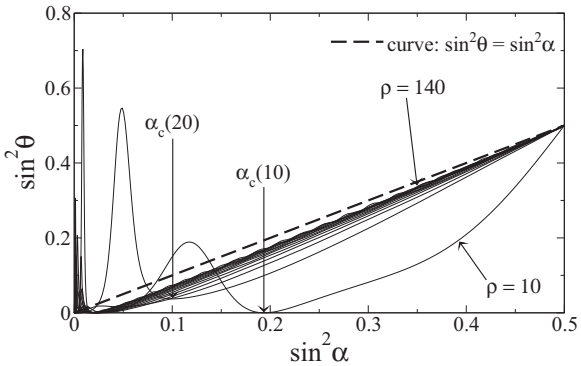

FIG. 3. $\sin^2\theta$ calculated with Eq. (14) as a function of $\sin^2\alpha$, for different values of $\rho = 10, 20, \ldots, 140$.

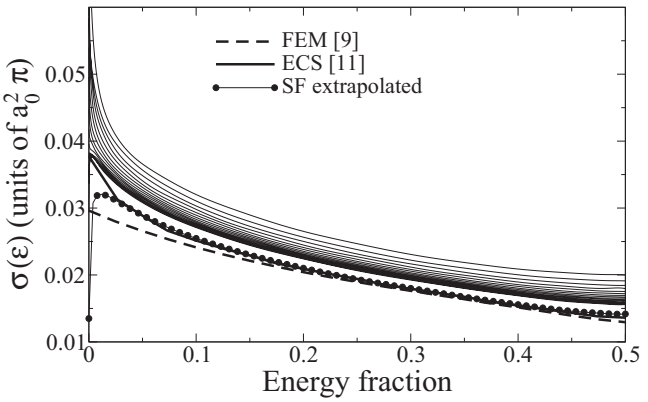

FIG. 4. Same SDCS as in Fig. 2 but presented as a function of the new energy fraction $\sin^2\theta$ calculated through Bohm's velocities.

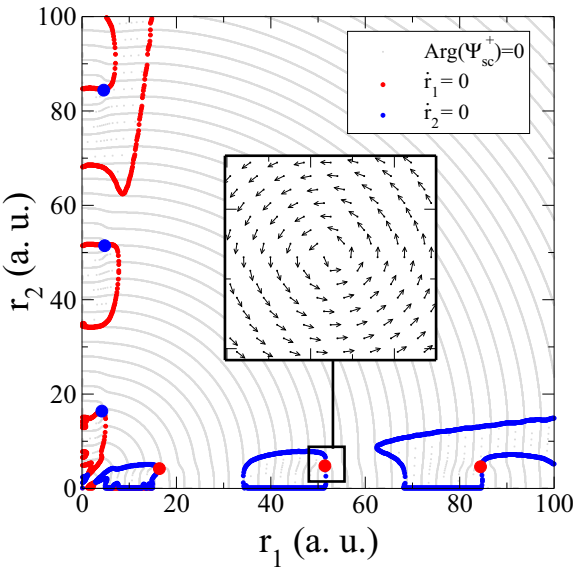

FIG. 5. (Color online) Light (gray) circles: zero phase contours of Ψ_{sc}^+ for 40.8 eV. Darker (red) circles along vertical axis: $\dot{r}_1 = 0$ points. Darker (blue) circles along horizontal axis: $\dot{r}_2 = 0$ points. Inner box: velocity vectors normalized to unity surrounding a point (large circle) where $\dot{r}_1 = \dot{r}_2 = 0$.

vanishes at $\sin\alpha_c$ (for $\rho < 20$ a.u. it has a small finite value but zero slope at a value of α_c which is close to $\alpha = 0$); and (iii) from $\alpha = \alpha_c$ to $\alpha = \pi/4$ takes all possible values between 0 and 0.5. The latter property indicates that the new energy fraction is a mathematically acceptable variable for the SDCS.

What happens for $\alpha < \alpha_c$ and finite ρ values may be physically interpreted in the following way. The continuum electron with the lower energy is strongly affected by the central potential; in order to conserve its total energy the kinetic energy increases. While the usual definition $\epsilon = \sin^2\alpha$ of the energy fraction maintains a reasonable value, counting of the electrons by means of the flux formula, (11), becomes incorrect in that region (overestimating it in its major part). Besides, small α values correspond to the region where the initial-channel wave function is nonnegligible. Since it is the "source" of the electrons, this region is not adequate to perform the "measurement" of continuum electrons, since they are in the processes of being "created." The flux component sometimes becomes negative for $\alpha < \alpha_c$ (in fact, the sign alternates with increasing ρ values) and reaches very high values close to $\alpha = 0$.

The contour through which we evaluate the flux is a constant ρ surface. It should be noted, however, that, in principle, any curve covering the $\sin^2\theta$ range [0,0.5] which satisfies $\alpha > \alpha_c$ would be valid. In practice, for each fixed ρ contour we need only the domain $\alpha_c < \alpha < \pi/4$.

Figure 4 shows the SDCS results presented in Fig. 2, but as a function of $\sin^2\theta$. We see that after redefining the abscissas, the unphysical amplitudes close to the asymmetric energy sharing situation are no longer present. The SDCS can now be considered acceptable in the complete energy fraction domain, and the $\rho \to \infty$ extrapolation can be performed for all their values. In this way the flux formula procedure is clearly rehabilitated.

It is noteworthy that the $\epsilon = 0$ extrapolated value yields a very small SDCS value. This fact is observed also for other energies, as we see in next section, where we discuss its origin and try to understand whether this collapse is the true physical behavior or an incorrect artifact of the novel energy fraction definition. But first let us mention a possible connection with vortices. In the small energy fraction region, one may observe periodic nodal structure in the scattering wave function. These points correspond to sites where Bohm's velocities (evaluated with the numerical scattering wave function obtained as described in Sec. III) vanish and have a definite circulation [20]. They are marked with darker circles in a two-dimensional radial domain (see Fig. 5). As a visual reference, lighter circles indicate constant phase contours of Ψ_{sc}^+; these approximately follow the dashed circular lines in Fig. 1 representing free hyperspherical waves. We also plot the velocity field in the inset.

Since the scattering state is a superposition of outgoing waves with nonzero modulus, vortices appear as an interference process between waves of different periodicities, in our case the double-continuum and the discrete channels. If we considered elastic scattering, we would observe the interference pattern between waves of momenta K and k_i, thus a periodicity $\lambda = 2\pi/(K - k_i)$. For the energy (40.8 eV) chosen for Ψ_{sc}^+ in Fig. 5, one gets $\lambda \simeq 23$ a.u., which is of the order of magnitude of the observed distance between the nodes. Differences could be explained by contributions from excitation channels with which higher values of λ are associated. Recall that exact zero interference patterns occur with waves of the same amplitude. Modulation of the outgoing waves associated with the discrete channels by the bound states in the other coordinate may provide coincident amplitude values.

It is known [21–23] that vortices in atomic wave functions have observable consequences. In recent studies [24,25] Navarrete and collaborators associated vortex lines with 0's in the transition matrix element for positron-impact ionization of hydrogen. Because of the dimensionality of our problem vortices are related to points which are well located in the two-dimensional domain. Without any evidence, we suggest that their periodic appearance may be connected with a vanishing extrapolated SDCS value at zero energy sharing.

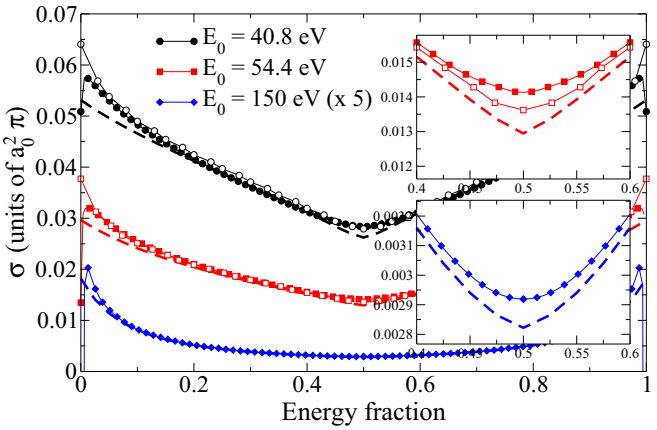

FIG. 6. (Color online) Results of SDCS for incident energy values equal to 40.8 eV (top, black lines), 54.4 eV [middle (red) lines], and 150 eV [bottom (blue) lines; multiplied by 5]. Dashed lines: FEM results [8]. Open symbols with lines: ECS results [12] with the uncorrected flux formula (only for 40.8- and 54.4-eV incident energies) and with a linear extrapolation to reach zero energy fraction. Filled symbols with lines: present Sturmian function results with the corrected flux formula. Insets: For the 54.4- and 150-eV cases, the details close to equal energy sharing.

C. Results for other incident energy values

Results of the SDCS for incident energies equal to 40.8 eV (upper, black lines), 54.4 eV [middle (red) lines], and 150 eV [multiplied by 5; lower (blue) lines] are shown in Fig. 6. We show the FEM benchmark results [8] with the sharp behavior of the slope of the SDCS at $\epsilon = 0.5$. We do not include the cross sections obtained by Bartlett and Stelbovics [16] with integral formulas using asymmetrical noncorrelated final states because they coincide with the FEM calculation followed by the S-matrix formulation of the SDCS. On the other hand, we show the results of Baertschy *et al.* obtained with the exterior complex scaling (ECS) method [12]. These SDCSs were evaluated with the usual (uncorrected) flux formula, with a $\rho \to \infty$ extrapolation procedure; as the cross sections did not seem reasonable close to energy fractions of 0 and 1, a linear extrapolation in α was performed to obtain reasonable values at $\alpha = 0$ and $\alpha = \pi/2$. Finally, the results of our Sturmian function calculation, with $\rho \to \infty$ extrapolation and with the new definition of the energy fraction, are also plotted.

For an incident energy equal to 40.8 eV one can easily appreciate the discrepancies in the slope, at the equal energy sharing point, between the FEM benchmark results and those obtained with the flux formula (the ECS or ours). The difference is further illustrated in the insets, which correspond to the less evident cases with incident energies equal to 54.4 and 150 eV. Note that ECS results obtained with the uncorrected flux formula also have a zero slope at the middle point; this can be easily understood, since close to the equal energy sharing situation the corrected definition $\tilde{\epsilon}$ is not very different from the usual definition ϵ (see the linear behavior close to $\alpha = \pi/4$ in Fig. 3).

The most important discrepancies, especially for the lower-incident-energy case, appear in the very unequal energy sharing region. First, we note that the flux formula extrapolated results are larger than the FEM cross sections. Our results are similar in magnitude (although slightly lower) to those obtained with the ECS method, except that in our case the SDCS go sharply to 0 for zero energy fraction. This surprising result is a direct consequence of the behavior of the approximate SDCS values at the different ρ values and their subsequent extrapolation to $\rho \to \infty$. By performing a linear extrapolation in α in order to reach $\alpha = 0$ and $\alpha = \pi/2$—as done with the ECS results—this peculiar cross-section collapse would be hidden. The collapse of the SDCS at extreme asymmetric sharing, if it is physical, is a behavior clearly in strong contrast with the FEM benchmark results. On the other hand, we also have to admit, in favor of the FEM results, that close to $\epsilon \simeq 0$ the asymmetrical final-state approximation seems to be the most adequate representation for the final state.

One final comment. We recall that the zero slope at the points $\alpha_c(\rho)$ shown in Fig. 3 is a consequence of the competition phenomenon between an increase in the slower electron momentum due to the proximity to the nucleus and a decrease related to the hyperspherical wave behavior when $\alpha \to 0$. When changing the variable from $\sin^2\alpha$ to $\sin^2\theta$, the zero slope becomes the extreme point of the SDCS with a well-established value, which decreases as ρ increases. The zero value is emphasized and strongly determined by the extrapolation if only large ρ contours are used; this is why we do not rule out that this collapse at zero energy sharing could be the actual SDCS behavior. A similar phenomenon was found for breakup processes in scattering of particles interacting through short-range potentials [26,27] for which the asymptotic region is easily reached in not too large computational domains. An additional argument possibly supporting the SDCS collapse is that, for zero-energy ionized electrons, the single-particle density of states vanishes. Whether or not this link to the density of states is the correct justification could be investigated by solving the e-H problem in one and two dimensions, where the density of states has different properties [28].

IV. CONCLUDING REMARKS

We have studied the problem of extracting the SDCS from the scattering wave function for e-H processes in the S-wave approximation. We have focused on the flux formula proposed by Peterkop, which makes use of the quantum mechanical flux component to count the emitted particles in an element of the solid angle of the physical space. Although from the theoretical point of view this procedure resembles the experimental measurement, it gives worse results than the integral formulas associated with the transition matrix.

Rather than placing in doubt the counting of particles itself, our investigation starts by questioning the correctness of the way in which the energy sharing fraction (the argument of the SDCS) is defined. The main idea lies in the fact that the geometrical approximation of the electron momenta should not be valid for a Coulombic distorted hyperspherical wave in finite domains. In order to get a more realistic definition, we propose an alternative form to evaluate the energy fraction based on Bohm's velocity. This solution-dependent definition is equivalent to that obtained from the components of the quantum mechanical flux, as a measurement of the electron

classical "velocity." The new proposal has good properties: it matches the geometrical definition at infinite distances and avoids considering the region in which either of the two electrons is very close to the nucleus as part of the ionization region. In our opinion, the unphysical SDCS behavior appearing in the "problematic" region (very unequal energy sharing) is due to the measurement of the flux in a place which coincides with the "source" of electrons, i.e., the nonhomogeneous term of the Schrödinger equation. In fact, we have shown that at sufficiently large ρ values, the double-continuum hyperspherical wave reaches all possible energy fraction values in a hyperangle domain which excludes the discrete channel region.

As a result of modifying the definition of the energy sharing fraction, very good SDCS results are obtained at three energies. There is one exception: in very extremely unequal energy sharing regimes, where, instead of having the unphysical very high value (as observed with the geometrical approximation), it collapses to 0, in clear contradiction with benchmark FEM results. If a linear extrapolation to the $\epsilon = 0$ and $\epsilon = 1$ values is performed, as done with the ECS calculations, then this collapse will be hidden. On the other hand, if this collapsing behavior were really true and not an artifact of our new definition, it would mean that integral and *S*-matrix formulas are not correct at the 0 and 1 energy sharing values.

The study presented in this paper aimed to rescue the quantum mechanical flux procedure to extract the cross section for *e*-H ionization, a task that we believe we have achieved.

ACKNOWLEDGMENTS

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