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SDCS quantum mechanical flux formula revisited for electron-hydrogen ionization

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Abstract. Through a simple, classical, energy conservation analysis, we propose a finite distance reinterpretation of the standard energy fraction definition used for the single differential cross section (SDCS) for the electron-hydrogen S wave ionization process. The energy modification is due to the fact that, at finite distances from the nucleus, the continuum electrons have to overcome the remaining potential energy to be completely free. As a consequence, the flux formula for extracting - at finite distances - SDCS is also modified. Differently from the usual observations, the proposed corrections yield finite and well behaved SDCS values also at the asymmetrical situation where one of the continuum electrons carries all the energy while the other has zero energy. Results of calculations performed at various impact energies, for both singlet and triplet symmetry, are presented and compared favorably with benchmark theoretical data. Although we do not know how, we believe that finite distance effects should strongly affect the evaluation of the flux and consequently the SDCS, also in the full electron-hydrogen case.

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Key words: ionization, flux formula, differential cross section

1 Introduction

The solution of the quantum three-body Coulomb break-up problem is notoriously difficult both from a scattering theory and a numerical point of view. In the last decade, several numerical approaches have been put forward [1–8] to deal, in particular, with

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the single ionization of atomic hydrogen by electron impact: remarkable good agreement between several theoretical results, and with the available experimental data, was observed.

The present work aims to investigate some issues related to the extraction of cross sections from the asymptotic part of the (numerically evaluated) scattered wave function. While numerical solutions of the Coulomb three-body problem are now available with different methods, they are generally restricted to finite regions of the configurations space; this is directly associated to the computer clusters size. The main difficulty is to ensure that the appropriate asymptotic behavior is reached, and this requires very large domains (several hundreds atomic units, see e.g. [7]). Besides, some difficulties occur because all the channels are entangled when solving the Schrödinger equation. In the particular case of the ionization of hydrogen by electron impact, the elastic, excitation, and the ionization channels are all present and coupled. Investigating and comparing extractions procedures is of interest also for more complicated break up problems, the e-H case serving as benchmark test.

Different strategies have been used to extract ionization cross sections from the computed solutions. One of them is based on the counting of particles by means of the quantum mechanical probability current designed by Peterkop and his coworkers [9–11]. This flux formula procedure has two main advantages. First of all, it is independent of the description of the electrons in the final state which, for long range interactions, has a certain arbitrariness. Secondly, since the flux formula corresponds to counting particles, it is adequate not only for infinite, but also, for finite domains (which is always the case for numerical solutions). The usual technique to extract differential cross sections consists in extrapolating to infinity the results obtained on a finite domain (the infinite domain corresponds to the exact solution, which can be compared with the experimental macroscopic domains). In spite of these advantages, the flux formula has been somehow abandoned because it yielded a bad e-H SDCS behavior for extreme unequal energy sharing [10]. This unphysical behavior has been associated [11] to the fact that the ionization flux at finite distances is contaminated by discrete –excitation– channels. Other procedures to calculate cross sections use integral formulae; they do not present any difficulties associated to the finite domains as they yield convergent results. For this reason, integral formulae have been favoured [12], and the flux formula has been finally discarded. In this contribution, we revisit the flux formula: in a specific, benchmark, case we will show that it can be successfully used if an appropriate finite distances' correction is taken into account, and that the contribution of discrete two-body channels (which indeed should be present and coupled to the ionization channel) is not, to our mind, responsible for the failure of the procedure.

The Temkin-Poet (TP) model [14, 15] of e-H scattering provides an ideal test of any method that aims to study the problem of ionization. This simplified S wave model, in which angular momentum is neglected (the electron-electron repulsion is spherically averaged), contains all the complexities of a three-body Coulomb problem, in particular the long range nature of the Coulomb interactions. The TP model has been systematically

used as a benchmark to test different numerical approaches (see [5, 7, 16–19] and references therein). Here we will consider it to discuss the use of the flux formula to extract the scattering information from the wave function evaluated on finite domains. For the present purpose, the latter is calculated within a Sturmian approach (see [5, 16, 20] and references therein).

There may be several reasons for what is seemingly a failure of the flux formula. One reason may be associated to the usual geometrical/kinematical assumption that, at large distances, the electrons' coordinates and momenta are proportional to each other (free electrons); this is actually never true for Coulomb potentials because of their long range. Geometrical and flux directions considerations have been investigated in a separate contribution [13]. Another possible reason is related to the way in which the energy sharing is defined at finite distances (the particles kinetic energy differs whether considered at finite or infinite distances).

In this contribution, we introduce, within the TP e-H problem, an alternative and more realistic definition of the energy sharing value for finite domain calculations. It takes into account the finite-distance effect that the particles have to overcome: the remaining Coulomb potential "tail". Consequently, the energy fraction evaluated at finite distances differs from that usually associated to the particles reaching freely the asymptotic region. The proposed classical energy correction modifies also the expression providing the SDCS. We will see that our simple reinterpretation (i) clearly shows that finite distance effects are present; (ii) improves the overall results and (iii) removes the unphysical behavior of the S wave e-H SDCS evaluated with the flux formula.

Our proposal of the energy sharing reinterpretation at finite distances is strictly applicable only to the S wave model. Indeed, in this case, the interaction potentials are separable and it is possible to clearly attribute the energy to each electron: one electron is fast and free, while the other one is slow and feels the nuclear potential. A similar screening approximation is used when SDCS are evaluated with integral formulae, where the final state is considered to be a product of a Coulomb function for the slower electron and a free spherical wave for the faster one [19]. While our classical, screening, approach cannot be applied to the full physical e-H problem, finite distance effects are necessarily present. Indeed, the inter electronic potential energy is again shared between the two electrons but a simple classical energy analysis is obviously not feasible; knowing how this occurs is equivalent to solving the quantum mechanical problem itself. In fact we believe that a solution-dependent definition of the energy sharing fraction is possible and adequate to the rescue of Peterkop's flux formula [13]. We do not aim to provide here a prescription on how to do it, we believe that finite distance effects should strongly affect the evaluation of the flux and consequently the SDCS, also in the real case, and should be taken into account also in integral formulae. This contribution illustrates the sensitivity to neglecting the Coulomb potential barrier when a finite domain calculation is performed. For the complete problem, such a potential energy exists, and ignoring it can be the cause of serious differences in cross sections evaluations.

Another issue of interest, within the TP model, is what happens for the SDCS at the

equal energy fraction value. Indeed, the extraction of that magnitude from the scattering wave function (whatever the way it is evaluated) with a s-matrix representation [7] or some integral formulae [19] involves a free state for the faster electron and a Coulombic one for the slower one. When crossing the equal energy sharing value, an interchange of coordinates occurs and we have a potential discontinuity. As a consequence of the discontinuous final state description, a sharp slope of the singlet SDCS is observed at the symmetric energy fraction value. In contrast with this inconsistent observation, the application of the flux formula (Exterior Complex Scaling (ECS) [11] or Sturmian results) yields the correct continuous (zero valued) slope. This property is a direct consequence of the expected continuity of the asymptotic scattering wave function and its derivative when one perpendicularly crosses the surface $r_1 = r_2$.

The rest of this paper is organized as follows. In Section 2, we present the model equation, the usual SDCS definition through the flux formula given by Peterkop and the corrections based on a classical energy conservation analysis. In Section 3, results are presented and compared to benchmark data for several energies, and for both singlet and triplet symmetries. A small summary is given in Section 4.

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

2 Theory

Let Ψ^+ be the three-body solution of the Schrödinger equation for hydrogen ionization by electron impact:

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

where $\mathbf{r}_i$ ($i = 1,2$) denote the electrons coordinates and $r_{12} = |\mathbf{r_1} - \mathbf{r_2}|$ is the inter electronic distance. We set the function Ψ^+ as $\Psi^+ = \Psi_{sc}^+ + \Psi_0$, where Ψ_0 represents the prepared collisional state and Ψ_{sc}^+ the scattering wave function which contains all the physical information about the collision process. According to Pauli exclusion principle, we have the symmetry condition $\Psi^+(\mathbf{r}_1,\mathbf{r}_2) = (-1)^S\Psi^+(\mathbf{r}_2,\mathbf{r}_1)$ depending on whether the two electrons form a singlet ($S = 0$) or a triplet ($S = 1$) spin state. As in Ref. [16] (and references therein), we will consider an initial state:

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

where $k_i = \sqrt{2(E-(-0.5))}$, i.e. the symmetrized/antisymmetrized product of a plane wave times an hydrogenic bound state. The scattering function Ψ_{sc}^+ satisfies the non ho-

mogeneous Schrödinger equation:

$$\left[-\frac{1}{2}\nabla_{r_1}^2-\frac{1}{2}\nabla_{r_2}^2-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{r_{12}}-E\right]\Psi_{sc}^{+}(\mathbf{r}_1,\mathbf{r}_2)=$$
$$-\frac{1}{\sqrt{2}}\left[\left(\frac{1}{r_{12}}-\frac{1}{r_2}\right)\frac{1}{\sqrt{\pi}}e^{-r_1}e^{i\mathbf{k}_i.\mathbf{r}_2}+(-1)^S(1\leftrightarrow 2)\right], \tag{2}$$

where E is the total energy of the system.

Let ρ and α be the hyperspherical coordinates defined through $r_1=\rho\cos\alpha$ and $r_2=\rho\sin\alpha$ ($0\leq\rho\leq\infty$, $0\leq\alpha\leq\pi/2$). Equation (2) must be solved together the following boundary condition

$$\lim_{\rho\to\infty}\Psi_{sc}^{+}(\mathbf{r}_1,\mathbf{r}_2)=A(\omega_5)\rho^{-5/2}e^{i\left(K\rho-\frac{C(\omega_5)}{K}\log[2K\rho]\right)}, \tag{3}$$

where $A(\omega_5)$ is the scattering amplitude; ω_5 represents the five hyperangular coordinates. The factor $C(\omega_5)$, which can be considered as an angular dependent Coulomb charge, is defined as:

$$C(\omega_5)=-\frac{Z}{\cos\alpha}-\frac{Z}{\sin\alpha}+\sum_{l=0}^{\infty}\frac{4\pi}{2l+1}\sum_{m=-l}^{l}(-1)^m Y_{-m}^{l}(\hat{\mathbf{r}}_2)Y_m^l(\hat{\mathbf{r}}_1)\left\{\begin{array}{c}\sec\alpha\tan^l\alpha\\ \csc\alpha\cot^l\alpha\end{array}\right\},$$

where the upper (lower) value is for $\alpha<\pi/4$ ($\alpha>\pi/4$).

The scattering amplitude $A(\omega_5)$ is related to the single differential cross section through $|A(\omega_5)|^2$ and corresponds to finding – asymptotically – the two electrons in directions $\hat{\mathbf{r}}_i$ with kinetic energies $E_1=E\cos^2\alpha$ and $E_2=E\sin^2\alpha$ ($E=E_1+E_2$).

Within the Temkin-Poet S wave model, angular momentum is neglected, and $1/r_{12}$ is replaced by $1/r_>$ where $r_>=\mathrm{Max}[r_1,r_2]$. In this case for $\alpha<\pi/4$ (respectively $\alpha>\pi/4$), the $-1/r_1$ (respectively $-1/r_2$) potential is removed from the left-hand-side of Eq. (1) or (2). The boundary condition (3) becomes

$$\lim_{\rho\to\infty}\Psi_{sc}^{+}(\mathbf{r}_1,\mathbf{r}_2)=A(\alpha)\rho^{-5/2}e^{i\left(K\rho-\frac{\gamma(\alpha)}{K}\log[2K\rho]\right)}, \tag{4}$$

where $K=\sqrt{2E}$, $A(\alpha)$ is the scattering amplitude and the factor $\gamma(\alpha)$ is defined as:

$$\gamma(\alpha)=\left\{\begin{array}{ll}-\frac{1}{\sin\alpha} & \text{if } \alpha<\pi/4\\ -\frac{1}{\cos\alpha} & \text{if } \alpha>\pi/4\end{array}\right..$$

Consequently the SDCS

$$\frac{d\sigma}{dE_2}\propto|A(\alpha)|^2 \tag{5}$$

now depends only on α which defines not only the coordinates r_1 and r_2 but also measures, in the asymptotic region, the ratio $\tan\alpha=k_2/k_1$ between the local momenta of

the electrons. SDCS are usually shown as a function of the energy fraction defined as $\epsilon = \sin^2\alpha = E_2/E$ (the same results would be obtained by using E_1/E). Since the SDCS is symmetric with respect to $\alpha = \pi/4$, only half of the range, i.e. $0 \leq \epsilon \leq 0.5$, needs to be considered.

2.1 Flux formula for the single differential cross section

For the electron-hydrogen scattering problem (full problem or TP model), the single differential cross section is defined as the ratio between the number of electrons which populate a given final continuum state by the incident flux of particles:

$$d\sigma = \frac{dN}{k_i}. \tag{6}$$

The quantity dN can be calculated as [9]

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

where $d\hat{\Omega}$ is the (five dimensional) solid angle element

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

J_ρ is the flux density in the radial hyperspherical direction, which can be written as

$$J_\rho = \Im\left\{ \left(\Psi^+_{sc}\right)^* \frac{\partial \Psi^+_{sc}}{\partial \rho} \right\} = \frac{1}{2i}\left[\left(\Psi^+_{sc}\right)^* \bigtriangledown \Psi^+_{sc} - \Psi^+_{sc} \left(\bigtriangledown \Psi^+_{sc}\right)^* \right].(\cos\alpha, \sin\alpha) \tag{7}$$

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

$$\frac{d\sigma}{dE_2} = \frac{(4\pi)^2}{k_0 2E} J_\rho \rho^5 \sin\alpha\cos\alpha. \tag{8}$$

This flux formula has been applied [10] to evaluate the SDCS, from the scattered wave function at finite distances ρ and for values of α which are far enough from 0 and $\pi/2$. Extrapolating procedures have been applied to obtain, on one hand, the flux value at infinite ρ values and, on the other hand, to obtain its values for the energy sharing corresponding to $\alpha = 0$ and $\alpha = \pi/2$.

2.2 Reinterpretation of the energy fraction

In this section we introduce a correction for extracting the SDCS which takes into account that the evaluation is performed at finite values of the hyperspherical coordinate ρ, when the two escaping electrons are still interacting with the nucleus.

The proposed modification consists in reinterpreting the continuum energy fraction value at finite distances. Consider first the case $\alpha < \pi/4$, i.e. $r_1 > r_2$. Electron 1 is free. At finite distances, electron 2 feels the Coulomb potential, and since the total energy E is conserved we can write

$$E = \mathcal{E} - \frac{1}{\rho \sin\alpha} \tag{9}$$

where $\mathcal{E} > E$ is the effective kinetic energy (see Fig. 1). The two electrons share this finite-distance kinetic energy with the proportions $\mathcal{E}_1 = \mathcal{E}\cos^2\alpha$ and $\mathcal{E}_2 = \mathcal{E}\sin^2\alpha$ (note that $\mathcal{E}_1 + \mathcal{E}_2 = \mathcal{E}$).

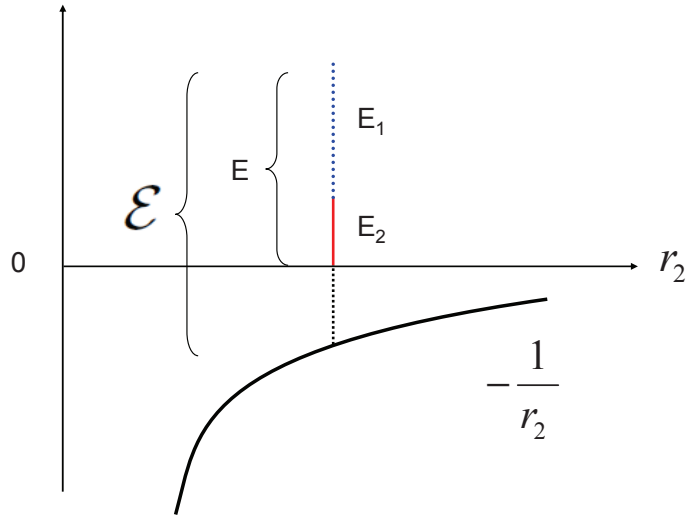

Figure 1: (Color online) Energy representation in the case $\alpha < \pi/4$. Usually, the kinetic energy E is considered as shared (E_1 and E_2) by the two escaping electrons. Taking into account the Coulomb barrier ($-1/r_2$), at finite distances, the effective kinetic energy to be considered is $\mathcal{E}$ (see text).

As electron 2 reaches infinity, it has to overcome the remaining Coulomb potential barrier, so that it possesses asymptotically a kinetic energy of

$$\hat{E}_2 = \mathcal{E}\sin^2\alpha - \frac{1}{\rho\sin\alpha}; \tag{10}$$

note that the full energy is conserved as $\hat{E}_1 + \hat{E}_2 = E$ ($\hat{E}_1 = \mathcal{E}_1$ as electron 1 is free). In summary, according to this picture, the usual energy fraction $\epsilon = E_2/E = \sin^2\alpha$, should be replaced by

$$\begin{aligned} \epsilon \to \hat{\epsilon} = \frac{\hat{E}_2}{E} &= \frac{\mathcal{E}}{E}\sin^2\alpha - \frac{1}{E\rho\sin\alpha} \\ &= \sin^2\alpha - \frac{\cos^2\alpha}{E\rho\sin\alpha}. \end{aligned} \tag{11}$$

Consider now the case $\alpha > \pi/4$, i.e. $r_2 > r_1$. At finite distance the kinetic energy is now $\bar{\mathcal{E}} = E + 1/(\rho\cos\alpha)$. This time electron 2 is free, and it is electron 1 which has to overcome the Coulomb barrier, so that

$$\bar{E}_1 = \bar{\mathcal{E}}\cos^2\alpha - \frac{1}{\rho\cos\alpha}, \tag{12}$$

and therefore $\bar{E}_2 = E - \bar{E}_1 = \sin^2\alpha[E + 1/(\rho\cos(\alpha)]$ by energy conservation. The energy fraction associated to electron 2 is

$$\epsilon \to \hat{\epsilon} = \frac{\bar{E}_2}{E} = \sin^2\alpha + \frac{\sin^2\alpha}{E\rho\cos\alpha}. \tag{13}$$

Three major observations stem from the new definition. First, there is a shift with respect to the usual energy fraction: for a given $\alpha < \pi/4$, the energy fraction $\hat{\epsilon} < \epsilon$ while for $\alpha > \pi/4$, $\hat{\epsilon} > \epsilon$. Secondly, the zero of the new variable $\hat{\epsilon}$ does not correspond to $\alpha = 0$; at finite distances, and depending on the value of E, the domain $0 < \alpha < \delta(\rho) \simeq \arcsin([\rho E]^{-1/3})$ yields a negative $\hat{\epsilon}$ which is unphysical and is discarded (similarly, for $\alpha > \pi/4$ the domain $\pi/2 > \alpha > \pi/2 - \delta(\rho)$ is discarded). As illustrated in Fig. 2, the zero energy fraction value for finite domains is approximated by Eqs. (11) or (13) by potential curves in the (r_1, r_2) plane; this allow us to identify, for a given energy E, the ionization region. Finally, as α approaches $\pi/4$ (from below or above), the equal energy sharing value $\hat{\epsilon} = 0.5$ is not reached at finite distances. Setting $\alpha = \pi/4$ in (11) and (13) we have:

$$\begin{aligned} \hat{\epsilon}_l\left(\frac{\pi}{4}\right) &= \frac{1}{2}\left(1 - \frac{\sqrt{2}}{E\rho}\right) < 0.5 \\ \hat{\epsilon}_r\left(\frac{\pi}{4}\right) &= \frac{1}{2}\left(1 + \frac{\sqrt{2}}{E\rho}\right) > 0.5. \end{aligned}$$

We therefore have a left-right jump of $\sqrt{2}/(E\rho)$ which is directly related to the discontinuity of $r_>$ in the TP model. Due to the finite value of ρ, the new energy fraction is limited to the domain $0 < \hat{\epsilon} < \hat{\epsilon}_l\left(\frac{\pi}{4}\right)$ and $\hat{\epsilon}_r\left(\frac{\pi}{4}\right) < \hat{\epsilon} < \frac{\pi}{2}$. As $\rho \to \infty$, the shift (and hence the jump) in the energy fraction disappears, as expected, and one recovers the usual picture over the whole domain $0 < \epsilon < 0.5$. It is worth noting that it is not ρ and E separately, but the product ρE that intervenes in the modification.

Moreover, as a consequence of the newly defined asymptotic kinetic energy $\hat{E}_2$, dE_2 has to be replaced by $d\hat{E}_2$ leading to a structural modification of the SDCS given by Eq. (8) which has to be replaced by

$$\frac{d\sigma}{dE_2} \to \frac{d\sigma}{d\hat{E}_2} = \frac{d\sigma}{dE_2} f(\alpha, \rho E) \tag{14}$$

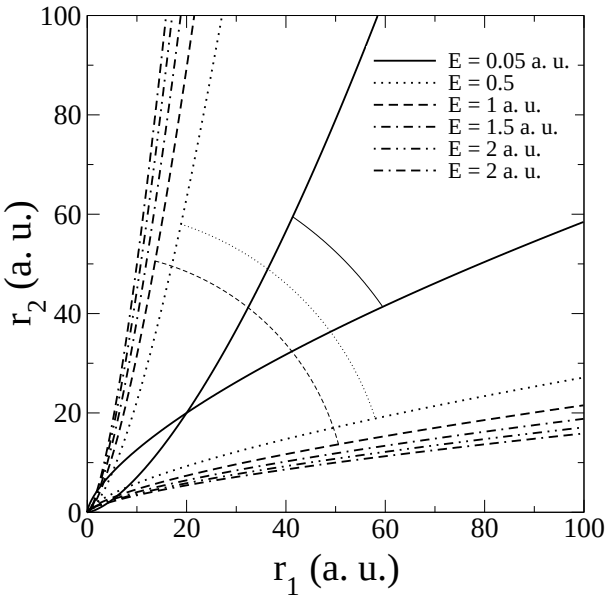

Figure 2: Ionisation threshold contours for different energy values E according to the new definition of the energy-sharing given by Eqs. (11) and (13). The arcs at fixed hyperradius values ρ show the angular regions considered when counting ionized electrons.

with the correction factor

$$f(\alpha,\rho E)=\left[1+\frac{1+\sin^2\alpha}{2E\rho\sin^3\alpha}\right]^{-1}. \tag{15}$$

For all values of α, the modified SDCS are affected (diminished) by this factor which is always smaller than 1. The correction is particularly strong for small α values, as $f(\alpha\to 0,\rho E)\to 0$. In the illustration below, we will see that the energy fraction shift, together with the modified SDCS formula, modifies the SDCS extracted at finite distances, and remove the unphysical behavior close to the zero energy fraction value.

The energy fraction reinterpretation discussed above is only applicable within the TP approximation, since the interaction potentials are separable. We consider that the faster electron is free while the slower is the one which has to overcome the Coulomb tail barrier (a similar approximation is used when SDCS are evaluated with integral formulas where final states are Coulombic or free depending of the electrons' velocities [19]). Similarly to the model, for the complete physical problem, the two electrons need to overcome the nuclear potential, and when reaching the asymptotic region they share the inter electronic potential energy term (which is finite at finite distances, except at the electron-electron cusp). However, as the system is correlated, it is not possible to state how this occurs. This said, similarly to what happens for the S wave model, a modification of the energy fraction should be taken into account at finite distances. As illustrated below such a modification has very important effects in the extraction of SDCS results.

To conclude this section, let us make some comments on what happens at equal energy sharing ($\alpha = \pi/4$). As already mentioned in the Introduction, in some numerical evaluations [7,8] of the singlet SDCS for the e-H process, a discontinuity in the derivative is observed at $\alpha = \pi/4$:

$$\lim_{x\to 0} \frac{d}{dE_2}\left(\frac{d\sigma}{dE_2}\right)\bigg|_{E/2-x} = -\lim_{x\to 0} \frac{d}{dE_2}\left(\frac{d\sigma}{dE_2}\right)\bigg|_{E/2+x} \tag{16}$$

The jump is related to the final state used in such calculations, i.e. a simple product of continuum waves (a Coulomb wave for the slower electron and a free one for the faster one). This final state has the advantage of having well defined momenta and correspond to an exact solution of the equation when all the particles are far from each other. Besides, it avoids the divergency of the transition amplitude phase [21]. However, it introduces an "if" behavior in the α-coordinate which causes the unphysical abrupt change in the SDCS slope. Assuming the asymptotic region is reached, one may use the asymptotic relation (4) and the cross section definition (5) to demonstrate formally that such behavior should not be present. Indeed, using the continuity of the wave function and its derivative when crossing perpendicularly the surface $r_1 = r_2$, one finds [13] that $|A(\alpha)|^2$, and consequently also the SDCS, have a zero slope at $\pi/4$ when represented as a function of α, or as a function of the variable $\sin^2\alpha$.

3 Results

We have solved the inhomogeneous Schrödinger Eq. (2) using a Sturmian approach (see details in Ref. [5, 16, 20] where the capability of the method is shown). Essentially, we use a double expansion on Sturmian functions for each radial coordinate r_i $(i = 1,2)$; all basis functions are regular at $r_i = 0$ and they all possess the same outgoing flux boundary condition. The scattering wave function is used to calculate the flux J_ρ at several finite distances ρ according to expression (7).

Below, we will present spin-weighted SDCS results for both the singlet and the triplet solution of the TP e-H process. We start with a detailed analysis of the SDCS (uncorrected and corrected) at total energy E of 1.5 a.u. (corresponding to an impact energy of 2 a.u. (54.422 eV)). We then present the final (corrected) results also for other energies, i.e., at 1 a.u. (impact energy of 1.5 a.u. (40.817 eV)) and 5.01248 a.u. (impact energy of 5.51248 a.u. (150 eV)). In all cases, benchmark results are available and shown for comparison. We have considered different finite values of ρ running from 1λ up to 41λ by steps of λ, where $\lambda = 2\pi/\sqrt{2E}$ corresponds to the wavelength of the hyperspherical outgoing wave given by Eq. (4). The largest ρ value considered are about 182 a.u. for $E = 1$ a.u., 150 a.u. for $E = 1.5$ a.u., and 81 a.u. for $E = 5.01248$ a.u.

3.1 Uncorrected results

We start from the singlet and triplet SDCS results for an energy $E=1.5$ a.u. obtained from the standard flux formula Eq.(8) calculated at 36 finite values of ρ. They are shown as a function of the standard energy fraction value $\epsilon=\sin^2\alpha$, in Fig. 3 (singlet) and Fig. 4 (triplet). Since the results are symmetric with respect to $\epsilon=0.5$, only half of the (typical U-shaped) curve is shown. The extrapolated SDCS ($\rho\to\infty$) is also shown (solid dots with line), and should be compared to the benchmark results of S. Jones and A. Stelbovics [7] (dashed line) obtained with the Finite Element Method (FEM).

Several observations can be made: (i) all our calculated SDCS present a zero slope at $\alpha=\pi/4$ (as it should be); (ii) one clearly observes unphysical (oscillations and divergence) behaviors near $\epsilon\simeq 0$ (the same behavior is found for $\epsilon\simeq 1$), even for quite large ρ values; (iii) due to the large oscillations, the present extrapolated SDCS results can be considered as accurate only for $\epsilon\gtrsim 0.05$.

3.2 Corrected results

After applying the kinematical correction given by Eq. (11) and using the modified differential cross section formula (14), the data of Fig. 3 are shown on Fig. 5 as a function of the new energy fraction $\hat{\epsilon}$. As indicated above, for finite values of ρ the equal energy fraction value cannot be reached (dotted line on the right of the figure corresponding to $\hat{\epsilon}_l\left(\frac{\pi}{4}\right)$); as the product ρE increases the excluded domain clearly decreases, and disappears in the limit of infinite distance. The corrected results show a significant modification close to zero energy sharing, where the curves are closer to each other for all ρ values (note that the vertical scale differs from that of Fig. 3). The correction related to the factor $f(\alpha,\rho E)$, is strongest for small energy fractions. The unphysical amplitudes close to the axes have clearly been wiped out. This seems to indicate that the divergence observed close to $\epsilon=0$ are not to be attributed to any specific physics (coupling to discrete channels), but rather to an inappropriate definition of the energy fraction when calculating over finite ρ domains. Actually, for small values of α, some electrons considered to be in the continuum with the usual definition, within our reinterpretation they are treated as not reaching their escape velocity (although they can be very far from the nucleus). At the same time, close to strongly asymmetric energy sharing, the correction factor $f(\alpha,\rho E)$ yields a decreasing SDCS, in contrast to the benchmark observation; this may possibly be related to the intrinsic way of counting the particles through the flux formula.

We have extrapolated to infinity the SDCS calculated at finite values of ρ; simultaneously, the equal energy value is also reached. The results (solid dots with line, labelled SF(1) in Fig. 5) give an overall good agreement with the benchmark curve (dashed line). For energy fractions in the range $(0.15,0.5)$ the new data are very close to the benchmark values. A fair agreement is observed also quite close to asymmetrical energy sharing

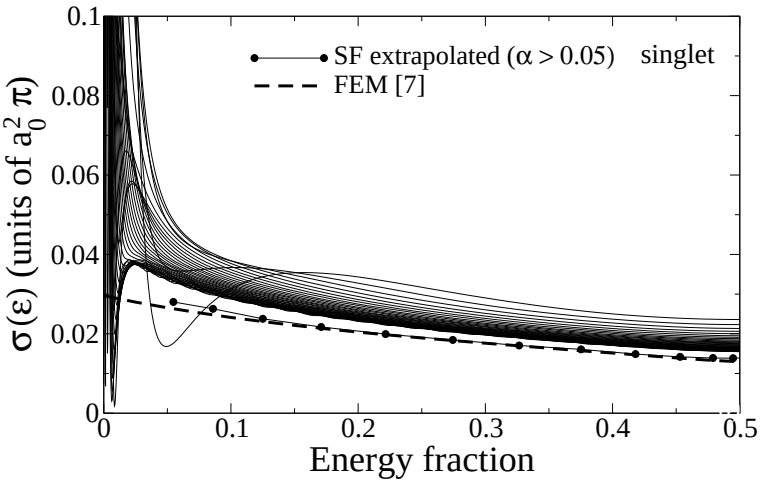

Figure 3: Singlet SDCS for the e-H processes at $E=1.5$ a.u. Dashed line: results from Jones and Stelbovics [7]. Solid lines: our evaluation of the flux formula approximation given by Eq. (8) as a function of $\epsilon=\sin^2\alpha$, for different values of ρ from 5λ up to 41λ in steps of λ (see text). Solid dots with line: our extrapolated results in the range $0.05<\epsilon<0.5$.

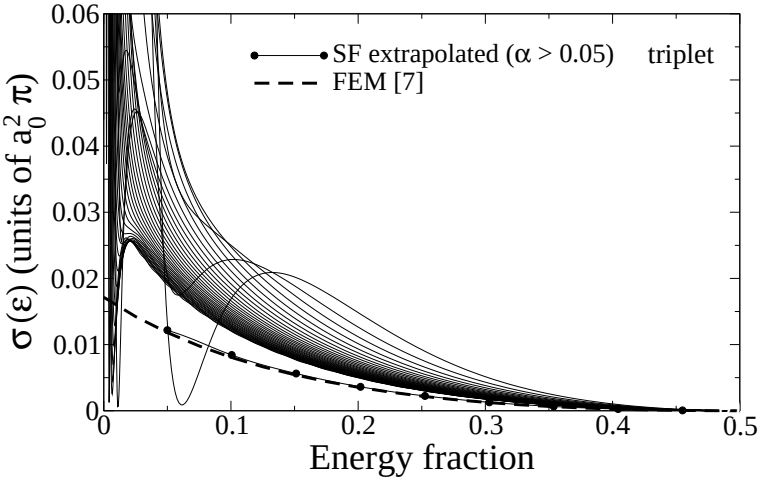

Figure 4: Same as Fig. 3 but for the triplet symmetry.

where there subsists a slight difference between our extrapolated results and the reference value given by Jones and Stelbovics. The discrepancy can be probably attributed to the fact that we are only considering domains up to 150 a.u. for each radial coordinate, while 500 a.u. were used within the FEM method [7]. For comparison, we have also included in the figure the ECS result [11] (open symbols with lines); our data practically coincide with these for energy fractions in the range $(0.05,0.5)$. It should be noted that for small energy fractions the ECS data were extrapolated linearly from the smallest value calculated directly (this will be called hereafter ECS technique). In the inset of Fig.

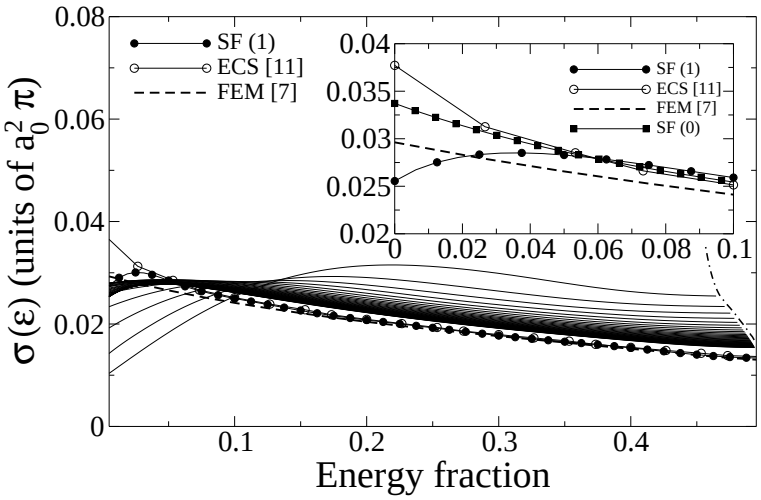

Figure 5: Our singlet SDCS data of Fig. 3, corrected according to the kinematical correction given by Eq. (11) and using the modified differential cross section formula (14). Extrapolated data (SF(1)) are shown by solid dots with line. The benchmark data [7] (dashed line) are the same as in Fig. 3. The ECS results [11] are also included (open symbols with line); using a similar extrapolation technique, our results extrapolated to zero energy fraction (labelled SF(0)), are shown by solid squares with line in the inset.

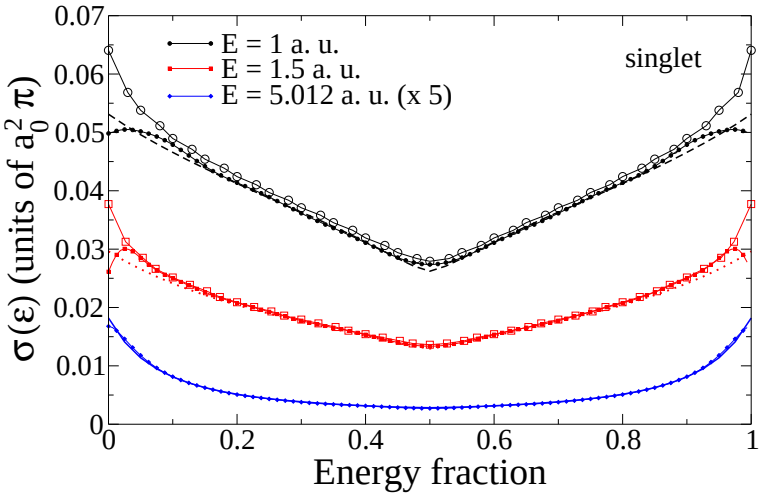

Figure 6: (Color online) Singlet SDCS for the e-H process, for three energies $E=1$ a.u. (top curves), 1.5 a.u. (middle curves) and 5.0124 a.u. (bottom curves)). Results from Jones and Stelbovics [7] (dashed, dotted and continuous thick lines, respectively) and Baertschy *et al.* [11] (open symbols with lines) are compared with our (corrected and extrapolated) results (filled symbols with line). For illustration purposes the 5.012 a.u. data are multiplied by 5.

5, the results are shown in the range $(0,0.1)$. Our uncorrected results, extrapolated to zero energy fraction (labelled SF(0)), are shown by solid squares with line and should be compared only to the ECS data.

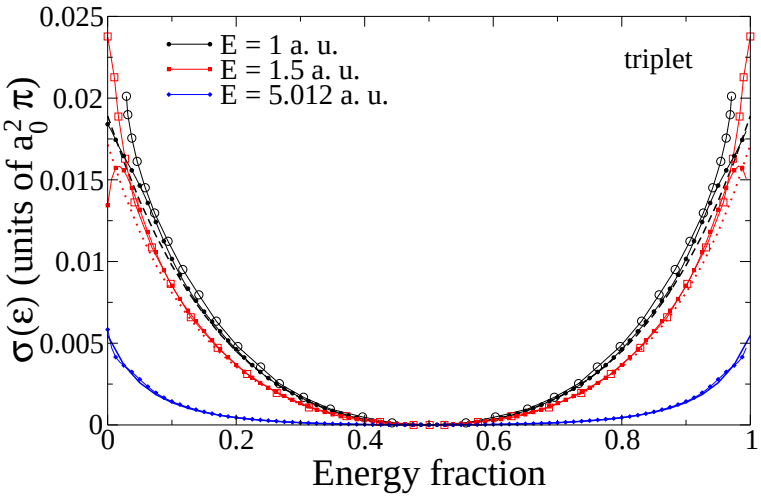

Figure 7: (Color online) Same as Fig. 6 for triplet symmetry. No multiplying factor was introduced for the 5.012 a.u. data.

We have considered two other energy values (1 and 5.0124 a.u.) for which benchmark values are also available. Our corrected and extrapolated SDCS results are presented in Figs. 6 and 7 for the singlet and triplet symmetry respectively. The singlet SDCS decrease as the incident energy increases; this monotonicity trend is not valid for the triplet case (see analysis in [7]). The singlet benchmark data with the FEM method [7] are also shown and present a discontinuous slope at equal energy sharing. On the other hand, our SDCS obtained using the flux formula at finite values of ρ (not shown) and subsequently the extrapolated curves (shown) always present a zero slope at equal energy sharing. This correct behavior is also observed in the ECS results [11] (line with open symbols, for the two lower energies only) obtained with the flux formula with a $\rho \to \infty$ extrapolation.

For our corrected SDCS, the corrections (recall that they depend on the product ρE, for a given ρ) are relatively smaller (larger) at higher (lower) incident energies. The decreasing behavior close to the asymmetric energy sharing values is observable for the two lowest incident energies but is practically absent for the largest one (5.0124 a.u.). When comparing our results with the FEM calculations, we observe an overall agreement except at strongly asymmetric energy sharing for the two lowest energies. In comparison with the ECS results [11], our SDCS have slightly smaller values and are thus closer to the benchmark values. We should recall here that the ECS data for energy sharing close to $\epsilon = 0$ and $\epsilon = 1$ were obtained through a linear extrapolation in energy fraction (ECS technique) as to eliminate the aforementioned divergences. Moreover, those results were obtained with box sizes larger than what we have used here. Hence, we may consider that our Sturmian calculation with the flux formula - once our correction procedure is implemented - provides relatively better results.

We have also considered the triplet case, and obtained also a remarkable agreement with the FEM calculations. It has to be noted that at equal energy sharing the disconti-

Table 1: Singlet total ionization cross section (units of πa_0^2) for the Temkin-Poet model of e-H scattering, calculated with different formulas and integration techniques. The SF(1), SF(0) (ECS technique) and ECS results are all obtained with the flux formula. Contrary to the SF(1) result, the integration used in SF(0) (ECS technique) and ECS involves an energy fraction extrapolation.

	Total energy E (a.u.)		
Theory	1	1.5	5.0124
FEM [7]	0.01946	0.01472	0.002926
SF(1)	0.01954	0.01507	0.002926
SF(0) ECS technique)	0.01974	0.01550	0.002994
ECS [11]	0.02036	0.01536	—-

Table 2: Same as Table 1 for triplet symmetry.

	Total energy E (a.u.)		
Theory	1	1.5	5.0124
FEM [7]	0.002473	0.003103	0.002012
SF(1)	0.002552	0.003266	0.002060
SF(0) (ECS technique)	0.002469	0.003228	0.001920
ECS [11]	0.00270	0.00339	—-

nuity of the SDCS slope is not present for the triplet symmetry neither in our results nor in other calculations; besides, the SDCS must be zero at that point. There is also better agreement at the unequal energy regime, except for $E=1.5$ a.u., for which our corrected and extrapolated result changes its slope just as in the singlet case (that phenomena is not observed at the highest energy (5.0124 a.u. as for the singlet symmetry).

For completeness, we also provide total ionization cross sections (TCS), although agreement for TCS does not guarantee good SDCS, since through integration discrepancies are partially masked. We have integrated our extrapolated SDCS, and the results are given in Tables 1 and 2 for the two symmetries. It is worth underlying that, for the two lowest energies, the singlet TCS is an order of magnitude larger than in the triplet case. When compared with benchmark values (FEM, [7]), in the worst case, we find that our Sturmian results (SF) have a relative discrepancy of about 2% (singlet) and 5% (triplet). This has to be compared with relative FEM versus ECS differences of, respectively, 4% and 8%. We have also integrated our SF SDCS using the ECS technique of extrapolating to 0 (and 1) energy fraction. By doing this we obtain results similar to the published ECS data [11].

4 Summary and concluding remarks

In summary, we may say that the flux formula for e-H SDCS may be used at finite distances, provided one modifies the energy fraction definition to take into account that

the continuum electrons have to overcome a Coulomb potential energy. This has been illustrated with the TP model for the e-H process, for both singlet and triplet symmetries, and for three incident energies. The scattered wave function, numerically evaluated with a Sturmian method, is used to calculate the flux at finite hyperradii and finally provides sensible cross sections over practically the whole energy fraction domain. The new definitions of energy fraction (11) and single differential cross section (14) eliminate the divergence close to extreme asymmetric energy fraction usually observed with finite distances calculations. Moreover, extrapolation to infinite distances yields overall good agreement with benchmark results obtained with calculations performed up to much larger distances.

In view of our results, we believe that the contribution of discrete channels is not responsible for the unphysical SDCS behavior, and the subsequent failure of the flux formula procedure. On top of that, the following simple reasoning seems to indicate the same. Suppose one may decompose the scattering wave function as the sum

$$\Psi^+_{sc} = \Psi^+_{exc} + \Psi^+_{ion} \tag{17}$$

where Ψ^+_{exc} is the excitation part and Ψ^+_{ion} the ionisation one [23, 24]. Upon replacement into the flux expression (7) we get

$$\begin{aligned} J_\rho = \quad & \Im\left\{ \left(\Psi^+_{exc}\right)^* \frac{\partial \Psi^+_{exc}}{\partial \rho} + \left(\Psi^+_{exc}\right)^* \frac{\partial \Psi^+_{ion}}{\partial \rho} \right. \\ & \left. + \left(\Psi^+_{ion}\right)^* \frac{\partial \Psi^+_{exc}}{\partial \rho} + \left(\Psi^+_{ion}\right)^* \frac{\partial \Psi^+_{ion}}{\partial \rho} \right\}. \end{aligned}$$

The nonlinearity of the flux operator as a function of Ψ^+_{sc} is such that the coupling between the excitation and ionisation channels is always present. Considering the fact that Ψ^+_{exc} includes excitation to all discrete states, and particularly to the Rydberg states with large spatial extension, the coupling to the ionisation channel should be affected on a large domain, and not only on the borders $r_1 = 0$ and $r_2 = 0$.

In the full physical problem, the inter electronic energy is also shared between the two electrons, and similar finite distance arguments apply (although a detailed analysis is not possible as the system is correlated). Hence, SDCS extracted from the flux (or any other formulae), calculated from finite distance wave functions should also be affected.

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