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Vortices in the three-body electron–positron–proton continuum system induced by the positron-impact ionization of hydrogen

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Abstract
By means of a systematic theoretical study of the transition matrix element T for the $e^{+} + \mathrm{H}$ ionization collisions in a collinear geometry, we uncover the presence of three isolated zeros at intermediate impact energies. We demonstrate that these zeros actually represent vortices in the generalized velocity field associated to T. One of these vortices is shown to be related to a deep minimum observed more than two decades ago by Brauner and Briggs in 1991 at extremely large impact energies, where the corresponding fully differential cross section was too small to be experimentally accessible. Here we elucidate that it might still be present at much smaller impact energies, thus being amenable to experimental investigation. Furthermore, we discovered that this vortex is paired with a second one of opposite circulation, in accordance with one of the scenarios for their emergence. We study the location of these vortices and find that they seem to be located at, emerge from, or move towards specific points which could be related to particular collision mechanisms, as the direct ionization and capture to the continuum cusps, or the saddle-point and Thomas processes.

Keywords: vortices, positron, Briggs, Brauner, Bohm, ionization, hydrogen

(Some figures may appear in colour only in the online journal)

1. Introduction

In 1991, Brauner and Briggs theoretically uncovered a deep minimum of about three orders of magnitude in the fully differential cross section (FDCS) for the positron impact ionization of atomic hydrogen. Since it appeared when the scattering angles of the electron and the positron were near the critical value of 45° from the forward direction, they attributed it to the interference between two double-binary scattering processes akin to the mechanism proposed by Thomas in 1927. In this mechanism, an energy-sharing binary collision of the positron and the electron is followed by the elastic reorientation of any of them by the target nucleus so as to end up moving in a collinear trajectory. Brauner and Briggs (1991) also observed that the minimum occurs at an electron velocity which is smaller than that of the positron and that this difference in speed increases for decreasing impact energies. This effect was only studied at extremely large impact energies between 10 and 100 keV where, as Brauner and Briggs (1991) pointed out, the FDCS is far too small to be measurable. This limitation might have discouraged any attempt to measure this effect in spite of its interest and oddity. In fact, up to our knowledge, this deep minimum was not experimentally observed or even searched for since its theoretical discovery more than two decades ago.

But some recent advances both in experimental and theoretical grounds might have renewed the interest in this kind of effects, and even made them experimentally accessible. On one side, the improvements in positron beam intensities and measurement techniques, as for instance the implementation of positron reaction microscopes (Williams *et al* 2010, Mueller *et al* 2012), would make the measurement of this kind of effects in positron impact ionization processes feasible. On the other hand, the presence of a vortex, i.e. a point where the transition matrix element T vanishes while the associated velocity field diverges, was recently proposed and theoretically demonstrated for the positron impact ionization of hydrogen at intermediate impact energies (Navarrete *et al* 2013). In this sense, it is akin to other effects measured in (e, 2e) collisions more than two decades ago (Murray and Read 1993), and recently recognized as vortices (Macek *et al* 2010). Note that this structure is different from the vortices that occur in superfluids, superconductors, or Bose–Einstein condensates, since it appears in a three-body wavefunction whose time-evolution is described by the Schrödinger equation with Coulomb interactions, with no need of including nonlinear terms or ad hoc potentials. Besides, its compelling analysis in the framework of Madelungs's hydrodynamic (Madelung 1926, Ghosh and Deb 1982) and Bohmian (Bohm 1952, Dürr and Teufel 2009) interpretations of quantum mechanics highlights its lure and topicality (e.g. Chattaraj 2010, Oriols and Mompart 2012, Sanz and Miret-Artés 2012).

In a recent article (Navarrete *et al* 2013) we addressed for the first time the theoretical study of vortices in positron impact ionization collisions. Their presence was recently shown to be quite ubiquitous in the ionization of atoms by intense electric pulses (Ovchinnikov *et al* 2010) and by the impact of electrons (Macek *et al* 2010, Colgan and Pindzola 2011, Ward and Macek 2014) and ions (Macek *et al* 2009, Ovchinnikov *et al* 2011, Schmidt *et al* 2014), but not by positrons. In our previous study we observed the presence of a vortex at an electron velocity that corresponds to the saddle-point of the potential produced by the positron and the residual target ion potentials (Della Picca *et al* 2004, 2005). Furthermore, we demonstrated that this vortex persists at impact energies as small as 60 eV, thus being amenable to experimental investigation.

In view of these background and motivations, the purpose of this article is to perform a systematic and thoughtful study of deep minima in the differential cross section for $e^+ + \mathrm{H}$ ionization collisions. For instance, we demonstrate that the minimum uncovered by Brauner and Briggs in 1991 actually represents a vortex on the transition matrix element T, and we also investigate its precise location as a function of the impact energy E. Brauner and Briggs (1991) have demonstrated that this structure exists for $E \geqslant 10$ keV, but that it was no longer present for $E = 250$ eV. Here we explore the possibility that it would still persist at energies not too large compared with this lower limit, so as to make its experimental observation feasible. Finally, taking into account that vortices emerge either as closed submanifolds or in pairs of opposite circulation (Bialynicki-Birula *et al* 2000), we investigate if this particular vortex has a companion that was unnoticed by Brauner and Briggs (1991) and, if that turns out to be the case, we search for its precise location and circulation.

2. Theoretical description of vortices in the ionization of hydrogenic atoms by positron impact

Let us consider the positron impact ionization of a hydrogenic atom. In the framework of Madelung's hydrodynamic interpretation (Madelung 1926, Ghosh and Deb 1982), the electron–positron–ion system, which is described by a wave function Ψ, evolves like a fluid of density $|\Psi|^2$ and velocity field $\boldsymbol{u} = \mathrm{Im}\,(\nabla \ln \Psi)$ (Navarrete *et al* 2013). This flow is irrotational everywhere except at vortices where the density $|\Psi|^2$ vanishes. These vortices might emerge as closed submanifolds or in pairs of opposite circulation (Bialynicki-Birula *et al* 2000). According to the imaging theorem (Dollard 1971, Macek *et al* 2010), those vortices that survive up to the asymptotic regime would show up as zeros on the FDCS for the ionization collision (Brauner and Briggs 1991).

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E_-\,\mathrm{d}\Omega_-\,\mathrm{d}\Omega_+} = (2\pi)^4\,\frac{k_-\,k_+}{v}\,\left|T\left(\boldsymbol{k}_-, \boldsymbol{k}_+\right)\right|^2 .$$

Here, we are describing the three-body kinematics of the system by means of ion-centered coordinates given by the relative positions $\boldsymbol{r}_\pm$ and momenta $\boldsymbol{k}_\pm$ of the electron (−) and the positron (+), with respect to the residual target ion. $E_\pm = k_\pm^2/2$ and $\Omega_\pm$ are the corresponding emission energy and solid angle. Atomic units are employed throughout this article.

Note that energy–momentum conservation and the rotation symmetry about the initial velocity $\boldsymbol{v}$ of the positron reduce the number N of relevant scalar variables of the FDCS from six to four. Since, at an exact zero, both the real and imaginary parts of the corresponding transition matrix element $T\,(\boldsymbol{k}_-, \boldsymbol{k}_+)$ have to vanish, this zero spans an (N-2)D surface into an ND space. By employing a 'symmetric geometry' (Gottschalk *et al* 1965),which lowers the dimension of the problem to $N = 2$, where $\boldsymbol{k}_+$ and $\boldsymbol{k}_-$ have equal magnitude and polar angles about $\boldsymbol{v}$, Brauner and Briggs (1991) forced this structure to show up as a point, an isolated zero. Since the deep minimum observed by them occurs when the electron and the positron emerge in the same direction, we decided to achieve the same dimension reduction by employing a 'collinear geometry' such that $\boldsymbol{k}_+ \cdot \boldsymbol{k}_- = k_+\,k_-$ (Navarrete *et al* 2013).

The initial state Ψ_i in the transition matrix element $T = \langle \Psi_f^- | V | \Psi_i \rangle$ accounts for the free motion of the positron and the bound state of the target. The potential is given by $V = Z/r_+ - 1/|r_+ - r_-|$, where Z is the effective charge of the residual target ion. For the description of the final continuum state Ψ_f^- we relay on the same approximation developed by Berakdar and Briggs (1994) and successfully employed by Macek *et al* (2010) in their study of vortices in (e, 2e) collisions in a symmetric geometry. Note that in the collinear geometry employed in this article, the latter reduces to the

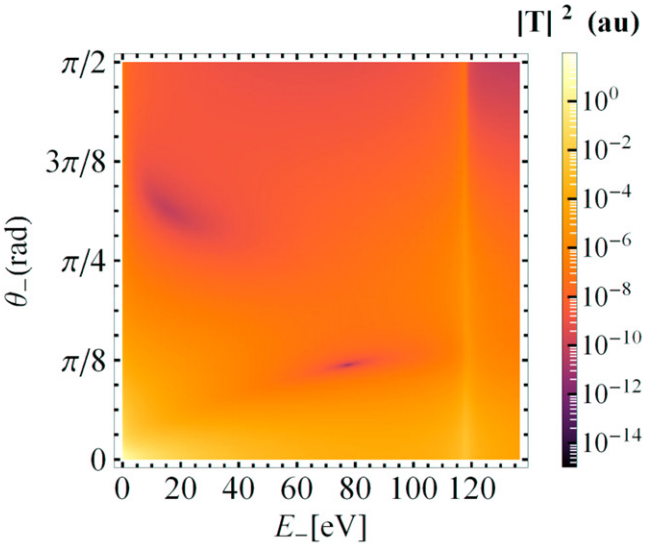

Figure 1. Square modulus of the transition matrix element, $|T|^2$, for the ionization of a hydrogen atom by the impact of a 250 eV positron. Conditions are set to a collinear geometry configuration (see text). E_- and θ_- are the electron's energy and emission angle (with respect to the direction of the initial velocity of the positron), respectively. The logarithmic scale in atomic units sets the lowest and highest values of $|T|^2$ in dark and light tones, respectively (dark red and light yellow in the on-line version).

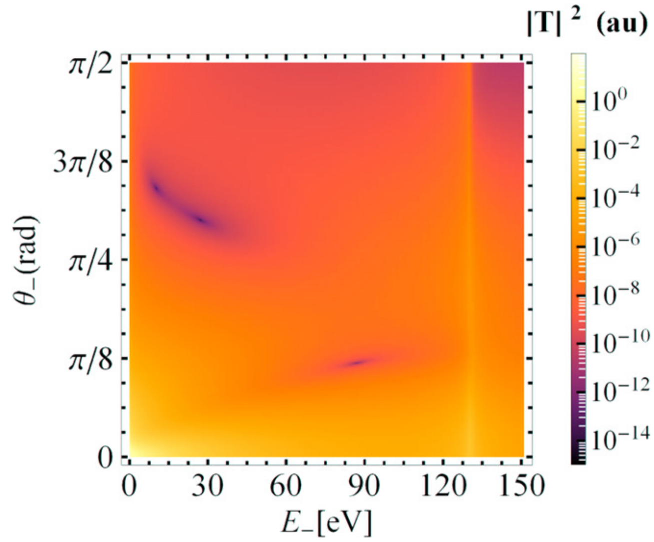

Figure 2. As figure 1 but for E = 275 eV.

correlated wavefunction employed by us in our previous study of vortices (Navarrete *et al* 2013), namely

$$\Psi_f = \psi_{-Z}(\boldsymbol{k}_+, \boldsymbol{r}_+) \times \psi_Z(\boldsymbol{k}_-, \boldsymbol{r}_-) \times \frac{\psi_{1/2}(\boldsymbol{k}_- - \boldsymbol{k}_+, \boldsymbol{r}_- - \boldsymbol{r}_+)}{\psi_0(\boldsymbol{k}_- - \boldsymbol{k}_+, \boldsymbol{r}_- - \boldsymbol{r}_+)},$$

where

$$\psi_\alpha(\boldsymbol{p}, \boldsymbol{q}) = (2\pi)^{-3/2}\, \Gamma(1 + \mathrm{i}\alpha/p) \exp(\pi\alpha/2p)\, {}_1F_1 \times (-\mathrm{i}\alpha/p, 1; -\mathrm{i}(pq + \boldsymbol{p} \cdot \boldsymbol{q}))\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{q}},$$

is the continuum state for a two-body system of relative position $\boldsymbol{q}$, momentum $\boldsymbol{p}$ and unity reduced mass, interacting via a Coulomb potential $V(q) = -\alpha/q$. The main characteristics, scopes and limitations of this model are described in our previous article (Navarrete *et al* 2013).

3. Results and discussion

Employing a technique described in a previous article (Navarrete *et al* 2013), we conduct a systematic search of vortices in the ionization of atomic hydrogen by positrons at different impact energies $E = v^2/2$. In figure 1 we show the square modulus of the transition matrix element $|T|^2$, at an impact energy of 250 eV, i.e. the minimum energy analyzed by Brauner and Briggs in 1991. Note that only the zero studied by us in a previous article (Navarrete *et al* 2013) is visible at this impact energy. In this collinear geometry, this particular zero appears at an emission angle of $\theta_- \approx \pi/8$ and an electron energy $E_- \approx E_{\max}/3$ (with $E_{\max}$ the maximum emission energy allowed by energy conservation), i.e. in the vicinity of the condition for an electron to ride on the saddle point potential produced by the positron and the target ion (Della Picca *et al* 2004, 2005, 2006).

The cusp-shaped divergence corresponding to the well-known electron excitation to the continuum (EEC), is clearly visible in figure 1 as a large increase of $|T|^2$ at $E_- = 0$. On the other hand, the electron capture to the continuum (ECC) cusp that occurs when $E_- = E_{\max}/2$ in a collinear geometry (Kövér and Laricchia 1998, Fiol *et al* 2001, 2002, 2011) is also clearly visible. Besides them, and even though the zero at $\theta_- \approx \pi/8$ and $E_- \approx E_{\max}/3$ is the only such a structure present at an impact energy of 250 eV, the presence of a deep minimum is evident at $\theta_- \approx \pi/3$. When the impact energy E is further increased slightly above 265 eV (while Brauner and Briggs in 1991 considered an energy E = 250 eV), this disturbance gives rise to a pair of zeros, as shown in figure 2.

By applying the imaging theorem in the asymptotic regime, i.e. $|\Psi|^2 \mathrm{d}\boldsymbol{r}_+\, \mathrm{d}\boldsymbol{r}_- \propto |T|^2 \mathrm{d}\boldsymbol{k}_+\, \mathrm{d}\boldsymbol{k}_-$, with $\boldsymbol{r}_\pm = \boldsymbol{k}_\pm t$ (Dollard 1971, Macek *et al* 2010), we introduce the generalized velocity field $\boldsymbol{u} = \mathrm{Im}\,(\nabla_{\boldsymbol{k}_+, \boldsymbol{k}_-} \ln T)$ in order to analyze the zeros in figure 2 (Navarrete *et al* 2013). In figure 3, this field is superimposed onto the square modulus of T. We clearly see that the velocity field around the zeros of T corresponds to that of vortices in the framework of Madelung's hydrodynamic interpretation of quantum mechanics (Madelung 1926, Ghosh and Deb 1982). We evaluate the circulation around each vortex and confirm that one is opposite in sign to the other, and that both are quantized to 2π so as to assure the single valuation of the transition matrix element. These two vortices appear (and, in fact, coalesce) at an impact energy of $E \approx 265$ eV, which is small enough to make the cross section measurable. It is remarkable how close Brauner and Briggs (1991) were to actually observe the emergence of this pair of vortices, had the calculated angle being increased to $\theta_- \approx \pi/3$, as it is shown in figure 4. Furthermore, the zero at $\theta_- \approx \pi/8$ was already observable at this impact energy.

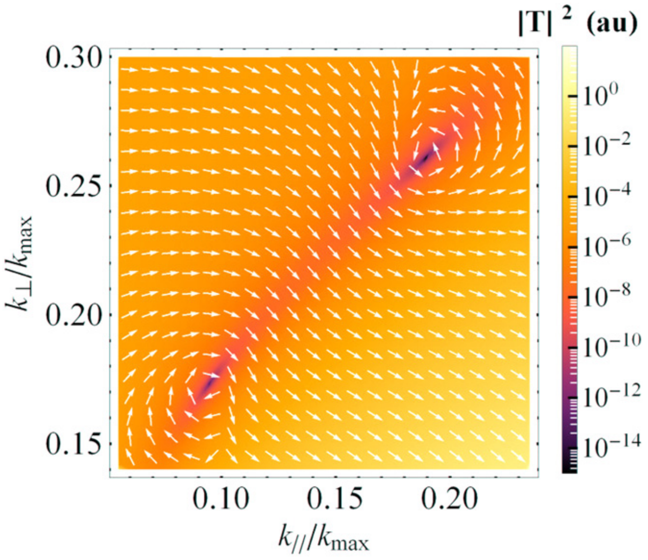

Figure 3. Detailed plot of the square modulus of the transition matrix element, $|T|^2$, for the 275 eV e^+ + H ionization collision in the vicinity of the pair of zeros shown in figure 2. The axes represent components of the electron momentum ($\boldsymbol{k}_-$) parallel ($k_\parallel$) and perpendicular ($k_\perp$) to the initial velocity of the positron, respectively; and are normalized to the maximum momentum $k_{\max} = \sqrt{2E_{\max}}$ allowed by energy conservation. The directions of the generalized velocity field (see text) are shown superimposed onto $|T|^2$, as white unitary vectors.

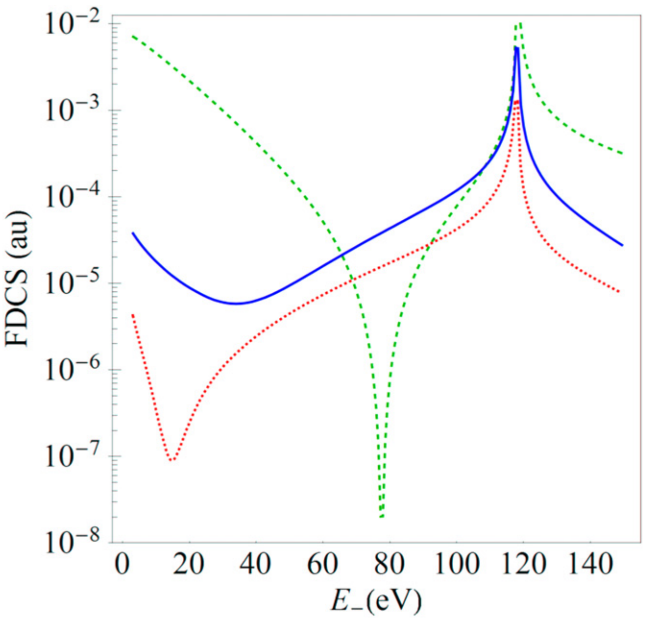

Figure 4. Fully differential cross section (FDCS) for the 250 eV e^+ + H ionization collision, as a function of the electrons energy E_- for fixed values of the emission angle $\theta_- = \pi/8$ (red dotted curve), $\pi/4$ (blue solid curve) and $\pi/3$ (green dashed curve). Conditions are set to a collinear geometry configuration (see text). The curve for $\theta_- = \pi/4$ exactly matches the result in figure 2 of Brauner and Briggs (1991).

As it was explained in the previous section, a vortex is a two-dimensional manifold in the four-dimensional (4D) space spanned by the variables of the FDCS. By choosing a particular geometry, as the collinear one employed in this article,

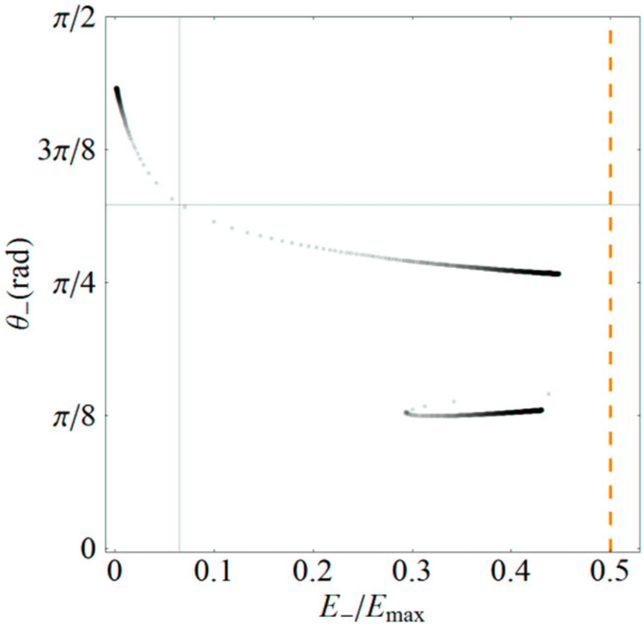

Figure 5. Stroboscopic images of the location of the vortices on the transition matrix element T for the ionization of a hydrogen atom by the impact of a positron of energy E in a collinear geometry configuration. As in figure 1, E_- and θ_- are the electron's energy and emission angle, respectively. $E_{\max}$ is the maximum electron energy allowed by energy conservation. Starting at an impact energy E = 60 eV for the vortex at $\theta_- \approx \pi/8$ and 270 eV for the other two vortices, the successive points correspond to increases of 10 eV up to 3 keV. The dashed line indicates the location of the ECC cusp, and the crossing of the black thin lines indicates the origin of the pair of vortices.

we are attempting to make a cut of this manifold. In this case, it might show up as an isolated point, but it can also be missed by this cut, i.e. its manifold and the collinear geometry do not intersect. This is probably the cause why the vortices are not observed for an impact energy of 250 eV. They are already present, but the geometry does not 'illuminate' them. When the energy is increased, the vortices are deformed and intersect the portion of the configuration space observed by the collinear geometry. In this sense, the emergence of the vortices at a particular impact energy is fortuitous, and only depends on the arbitrary choice of a particular geometry.

The question still remained if any of these two vortices is related to the deep minimum observed at E = 10 and 100 keV by Brauner and Briggs in 1991. In order to clear this doubt, we conduct a systematic analysis of their precise location for impact energies up to 3 keV. It is clearly seen in the stroboscopic image depicted in figure 5 that one of the vortices moves towards the ECC cusp. Furthermore, it rapidly approaches the critical angle of 45°. Thus, we clearly see that this vortex does actually correspond to the deep minimum observed by Brauner and Briggs two decades ago, as further calculations at 10 and 100 keV (not shown here) help to confirm.

But now we see that this vortex is related to a second one that approaches $E_- = 0$ at a critical angle of about $\theta_- > 3\pi/8$ for increasing impact energies. Naturally, independently of the impact energy considered, this vortex is out of the angular

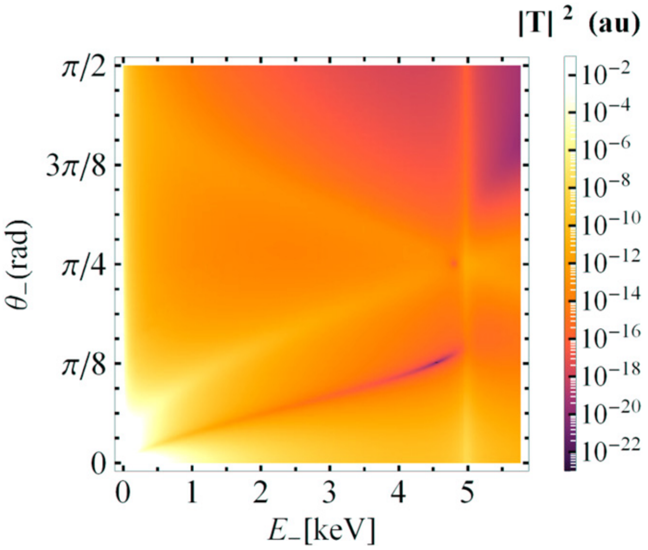

Figure 6. As figure 1 but for an impact energy of $E = 10$ keV.

range studied by Brauner and Briggs (1991) and thus remained hidden for more than two decades.

Let us mention that, contrary to the evolution exhibited by these two vortices, the one observed at a critical angle of $\theta_- \approx \pi/8$ and discussed in a previous article (Navarrete *et al* 2013) does not change its position appreciably as a function of the impact energy. In fact it remains near the angle corresponding to the electron sitting at the saddle point of its interaction with the positron and the residual ion. No presence of a companion vortex was observed in the range of impact energies studied in this article. Forcing the theory beyond its range of validity (Navarrete *et al* 2013), this vortex is still present at impact energies as low as 100 eV. Therefore, its coalescence with a companion vortex at a smaller impact energy, or even the presence and whereabouts of this second vortex, could not be studied or even confirmed within the validity limits of the present model.

We see in figure 5 that the vortices at $\theta_- \approx \pi/8$ and $\theta_- \approx \pi/4$ approach the ECC cusp at high impact energies, while maintaining the orientation and magnitude of their circulation. These vortices are shown in figure 6 for an impact energy of 10 keV. Naturally, at these asymptotic energies the magnitude of the FDCS would be too small to be measurable. However, the vortex at $\theta_- \approx \pi/8$ does also approach the threshold for positronium formation at small values of E, before disappearing for energies below those shown in figure 5. In particular, the vortex would produce a sharp distortion of the cusp that might be measured by standard electron spectroscopy techniques (Navarrete *et al* 2015). This would represent a unique opportunity for the first experimental observation of a vortex in positron-atom ionization collisions.

4. Conclusions

In this article we have studied afresh a deep minimum on the differential cross section for $e^+ + H$ ionization collisions theoretically uncovered by Brauner and Briggs (1991) more than two decades ago. At that time, it was only observed at extremely large impact energies, above 10 keV, where the differential cross section was too small to be experimentally accessible. Here we demonstrated that it might still be present at an impact energy as low as 275 eV, certainly prone to experimental observation by means of coincident electron–positron spectroscopy techniques. Furthermore, we showed that this minimum is actually related to a vortex structure. Let us recall that in such an extremely simple system, as the three-body problem with Coulomb interactions studied here, the origin and evolution of the vortices are governed by nothing more than the Schrödinger equation, with no need of including ad hoc potential models or a nonlinear term, as occurs in the study of superfluidity, superconductivity or Bose–Einstein condensation.

We discovered that this vortex is paired with a second one of opposite circulation, in accordance with one of the scenarios described by Bialynicki-Birula *et al* (2000). While for increasing impact energies the vortex studied by Brauner and Briggs (1991) approaches the ECC cusp at a critical angle of $\theta_- = \pi/4$, this other one moves towards the EEC cusp at $E_- = 0$, with $\theta_- > 3\pi/8$. On the contrary, the vortex discovered by us in a previous article (Navarrete *et al* 2013) practically remains fixed in angle over all the span of impact energies studied here. Let us mention that all these vortices seem to be located at, emerge from, or move towards specific points related to particular collision mechanisms, as the EEC, ECC, saddle-point and Thomas processes. More research is needed to assert whether there is more in this observation than a striking coincidence. For instance, as it is shown in figure 5, the zero observed by Brauner and Briggs (1991) varies its angular location by more than 10° before approaching $\theta_- = 45°$ at very high energies; a result which appears to weaken a possible link between the Thomas mechanism and the formation of vortices.

The vortices studied in this article persist at energies that are technically accessible with present-day equipments, and therefore prone to experimental observation. Even the study of their circulation might be at reach by means of weak pre- and post-selected measurements (Kofman *et al* 2012). However it is fair to say that until present, this novel technique has been mainly applied to optical systems, with some few exceptions (eg. Suter *et al* 1993); even though the original example discussed in the seminal paper by Aharonov *et al* (1988) corresponds to a weak PPS measurement performed on an electron beam.

We hope that the results presented in this article might stimulate both theoretical and experimental studies of positron-induced vortices. First of all, and even though the present model has successfully demonstrated its ability to describe the main characteristics of ionization collisions by the impact of charged particles within its range of validity, only an experimental confirmation might validate the present findings. On the other hand, a deeper theoretical study might shed light on the correct topology and dynamics of these vortex structures. In particular, it might help to explore a range of low impact energies that perturbative models as the one employed by us can not reach. In particular it might explain how the vortex located at the saddle-point appears, i.e. whether it emerges as a closed submanifold or as one of a pair of vortices of opposite circulation.

Finally, let us remember that prompted by the observation made by Brauner and Briggs (1991) that the deep minimum occurs when the electron and the positron emerge in the same direction, we have restricted our study to a collinear geometry. However, we have to keep in mind that the vortices observed here as isolated zeros of the transition matrix element are in fact only the fingerprints onto a two-dimensional plane of much more complex submanifolds of codimension 2 in a 4D space defined by the scalar variables of T. In any case, much is still to be done in order to grasp a clearer understanding about these new, complex and intriguing quantum structures.

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