Vortex rings in the ionization of atoms by positron impact

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Abstract. We uncovered the morphology of quantum vortex structures in positron-atom ionization collisions. By performing an exhaustive calculation of the position of vortices in the final momentum space of the problem with only one kinematic restriction, we could elucidate that quantum vortices form a closed structure, which is one of the two possible scenarios for their emergence in three dimensions. This is the first time that these structures are fully calculated for positron atom collisions.

1. Introduction

Quantum vortices have been the subject of both theoretical and experimental interest in the last decade for the ionization of atomic and molecular targets by the impact of proton, electron and positron projectiles [1, 2, 3]. They are zeroes on the Fully Differential Cross Section (FDCS) and exhibit structures which are submanifolds of co-dimension 2 on the phase space of the collision. This means that they appear as points in two dimensions, and as lines in three dimensions [4]. The velocity field associated with the transition matrix $T$, exhibits a solenoidal field similar to that of irrotational vortices in Fluid Dynamics. This velocity field, which comes from the hydrodynamical interpretation of quantum mechanics [5] as well as from the de-Broglie Bohm theory [6, 7], has proven to be a very useful tool for uncovering the emergence of quantum vortices in few body problems. It is worth to highlight the latter point, because these quantum vortices are sometimes confused with those which arise in superfluids, superconductors, or Bose-Einstein condensates, which are of a different nature.

A previous systematic study [3] of the ionization of atoms for different positron impact energies, contributed to the understanding of how these structures emerge in a collinear geometry as pairs of isolated points with velocity fields of opposite circulation. In a subsequent work [8] we analysed the same problem for a fixed collision energy in a coplanar geometry which proved that many structures that seemed isolated when studied in two dimensions where in fact part of a single vortex line. In the current study, we deepen the analysis of the aforementioned vortex line for the whole coplanar phase space.
2. Calculation method

We analyse the emergence of quantum vortices in the positron impact ionization of atoms, with the help of the hydrodynamic interpretation of quantum mechanics [5]. The three-body electron–positron–ion system is described by the wave function $\psi$, which evolves in time like an ensemble of trajectories of density $|\psi|^2$ and an associated velocity field defined as $\text{Im} \left( \nabla \psi / \psi \right)$ [9]. This velocity field is irrotational (because it is derived from the gradient of a scalar field) at every point of the ensemble, except at quantum vortices where the density vanishes, and around which it exhibits a solenoidal shape.

To understand how this phenomenon manifests itself in a collision process we make use of the imaging theorem [10, 11, 12], which relates the transition matrix $T$ [13] of the collision in momentum space, with the asymptotic behaviour of the wave function in configuration space for large times:

$$|T(k, K, K_R)| \propto \lim_{t \to \infty} t^{3/2} |\psi(kt, Kt, K_R t/MT, t)|,$$

where $k$, $K$ and $K_R$ are the final momenta of the electron, the positron and the recoil ion, respectively, and $MT$ is the mass of the ion (atomic units are used throughout the article unless otherwise stated). We can also define a generalized velocity field $u$ for $T$ in the following way [1, 9]:

$$u = \text{Im} \left[ \nabla k, K, K_R T \right].$$

Energy-momentum conservation properties and the azimuthal symmetry about the initial velocity $v$ of the positron, lessen the relevant scalar variables required to describe the collision from nine to four. In order to get more intelligible results, a further reduction of the dimensionality is mandatory. One way to achieve this is by integrating in some of the remaining variables, which in turn would blur the presence of zeros. Thus, we chose another option which consists in performing a cut to the $T$-matrix by taking into account more restrictive geometries. For instance, we found useful to work in a coplanar geometry, for which the final momenta of the three particles lie on the same plane, as can be seen in figure 1 on the left. Studying the process in a still more restrictive geometry like the collinear one, for which the electron and the positron escape with the same final momentum, as can be seen in figure 1 on the right, the ionization cross section depends only on two variables. Since, at vortices, both the real and imaginary parts of $T$ must vanish, these two conditions imply that for instance in a three

![Figure 1.](image_url)

(on the left) Coplanar geometry: the three particles’ momenta lie in the same plane.
(on the right) Collinear geometry: the positron and the electron escape in the same direction.
dimensional space, like that corresponding to the coplanar geometry, they will be isolated point like structures. Likewise, if $T$ depends of four variables, vortices will be found as lines on that space, either as unbounded lines or as closed structures [4].

3. Results

In order to fully describe the structure of vortex lines in positron-atom ionization collisions in a coplanar geometry, we traced their locations on the phase space of the final components of the electron momentum $k_{//}$ and $k_\perp$, parallel and perpendicular (respect to the initial direction of the projectile) and the relative angle between the final momentum of the positron and electron, $\Theta$ and $\theta$, respectively (see figure 1). The position of the zeroes was determined based on the method described in [9], and the T-matrix was calculated with a Continuum Distorted Wave (CDW) model that takes into account the correct Coulomb asymptotic conditions [14, 15]. In particular, we chose a positron impact energy of 275 eV because in a previous study [8] we observed that at that particular energy, a pair of vortices emerged on the transition matrix of the collision for collinear geometry, while a third one was already present. That study, which was performed in a coplanar geometry, allowed us to determine that those three vortices were part of a single vortex line. However, it was not possible to describe the overall structure of the line connecting the vortices, because it was performed for a reduced range of the relative angle $\Theta - \theta$ between the electron and the positron.

In this work, we continued to trace the points constituting the vortex line for 275 eV positron impact ionization of hydrogen, for the whole range of relative angles, as can be seen in figure 2. In the figure, together with the vortex line, we show a density plot which represents the FDCS for a collinear geometry. The dark blue semicircle which can be seen in the density plot is the so called Electron Capture to the Continuum (ECC) cusp [16, 17, 18]. It comprises the region of the phase space corresponding to a situation where both the electron and the positron escape from the collision region with the same final velocity. A relation between vortices and the ECC cusp have not been established yet, but there has been a previous study where the presence of the ECC cusp could help to determine experimentally the presence of vortices [19].

It is intriguing that, for a collinear geometry, at energies smaller than 275 eV, there is only one quantum vortex present [9, 3], which led to the assumption that it did not have any companion. If that was true, it should emerge as an unbounded vortex line, which is one of the possible structures that a vortex line can exhibit [4] (the other one is a closed structure named vortex ring). Nevertheless, figure 2 seems to contradict this. The vortex line reaches the kinetic limit (the boundary where the T-matrix is null because of energy-momentum conservation) at two finite points. We could resolve this apparent contradiction by representing the vortex line in cartesian coordinates for all variables, replacing the relative angle for the perpendicular momentum of the positron $K_\perp$, as it is shown in figure 3. We can arrive to the conclusion that the vortex line is clearly a closed structure, a vortex ring.

4. Conclusions

We have tracked vortex structures in a coplanar geometry. From choosing the appropriate set of axis to study this structure we could uncover that among the possible ways this type of structure can emerge on quantum mechanics, they form closed structures named vortex rings.

Vortex rings had been predicted mathematically [4], but they had never been calculated for a collision problem before. Their geometry and the conditions for their emergence are not only of interest for positron-atom collisions, but for the three-body quantum problem in general. The full understanding of these structures could give us more insight on the angular momentum transfer in a collision, as suggested previously [12].
Figure 2. Vortex line on the $T$-matrix element for the ionization of hydrogen by positron impact at an energy of 275 eV in coplanar geometry. It is represented in the phase space of the final momenta of the electron ($k_\parallel$ and $k_\perp$, parallel and perpendicular to the initial direction of the projectile) and the relative angle between the positron and the electron ($\Theta - \theta$). On the ($k_\parallel$, $k_\perp$) plane we plot $|T|^2$ for a collinear geometry.

Figure 3. Vortex ring on the $T$-matrix element for the ionization of hydrogen by positron impact at an energy of 275 eV in coplanar geometry. It is represented in the phase space of the final momenta of the electron ($k_\parallel$ and $k_\perp$, parallel and perpendicular) and the positron ($K_\perp$).
References

[1] Macek J H et al. 2010 Phys. Rev. Lett. 104 033201
[2] Schmidt LâPhâH et al. 2010 Phys. Rev. Lett. 112 083201
[3] Navarrete F and Barrachina R O 2015 J. Phys. B: At. Mol. Phys. 48 055201
[4] Bialynicki-Birula I et al. Phys. Rev. A 61 032110
[5] Madelung E 1926 Z. Phys. 40 332-6
[6] Dür D and Teufel S 2009 Bohmian Mechanics: The Physics and Mathematics of Quantum Theory. Berlin: Springer-Verlag
[7] Holland P R 1993 Quantum Theory of Motion. Cambridge: Cambridge University Press
[8] Navarrete F and Barrachina R O 2016 Nucl. Instrum. Meth. B 379 72
[9] Navarrete F, Della Picca R, Fiol J and Barrachina R O 2013 J. Phys. B: At. Mol. Opt. Phys. 46 115203
[10] Dollard J D 1971 Rocky Mountain J. Math., 1, 5488
[11] Macek J H, Sternberg J B, Ovchinikov S Y, Lee T G and Briggs J S 2009 Phys. Rev. Lett. 102 143201
[12] Macek J 2012 Dynamical Processes In Atomic And Molecular Physics. Beijing: Bentham Science Publishers
[13] Taylor J R 1972 Scattering Theory: The Quantum Theory on Nonrelativistic Collisions. Hoboken, New Jersey: John Wiley & Sons, Inc.
[14] Brauner M and Briggs J S 1986 J. Phys. B: At. Mol. Phys. 19 L325
[15] Garibotti C R and Miraglia J E 1980 Phys. Rev. A 21 572
[16] Kövér Á and Laricchia G 1998 Phys. Rev. Lett. 80 5309
[17] Fiol J and Barrachina R O 2011 J. Phys. B: At. Mol. Opt. Phys. 44 075205
[18] Barrachina R O and Fiol J 2012 J. Phys. B: At. Mol. Opt. Phys. 45 065202
[19] Navarrete F, Feole M, Kövér Á and Barrachina R O 2015 J. Phys. Conf. Ser. 583 012026