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Vortices in ionization collisions

F. Navarrete, R.O. Barrachina *

Centro Atómico Bariloche and Instituto Balseiro, Comisíon Nacional de Energía Atómica and Universidad Nacional de Cuyo, 8400 Bariloche, Río Negro, Argentina

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ABSTRACT

We review the concept of quantum vortices and their appearance in ionization collisions. By relaxing the usual geometrical restrictions on the momenta of the final-state, we study these vortices as submanifolds of codimension 2 in the space where the transition matrix element T is defined. In particular, we exemplify their main characteristics by studying the ionization of hydrogen by positron impact. Previous calculation under a collinear geometry for impact energies larger than 270 eV have shown the presence of three isolated vortices. Here we demonstrate that they are produced by a single vortex line intersecting three times the corresponding two-dimensional collinear plane.

1. Introduction

We have a basic knowledge about vortices steaming from our everyday experience. We see vortices while stirring a cup of coffee. They evidence in smoke rings, the whirlpool in the wake of a boat, or a dust devil crossing the road in front of our car. They can even have planetary dimensions, as in the red spot of Jupiter. Besides these macroscopic examples, vortices can also appear in Quantum Physics. Their existence was predicted by Lars Onsager [1] in connection with superfluid helium and by Alexei Abrikosov [2] in type-II superconductors. Quantum vortices were also observed experimentally in Bose–Einstein condensates [3].

In this article we discuss a completely different kind of quantum vortices that can be observed in atomic collisions. They are not the result of the interaction of a lot of particles as in a superfluid; they are not related to any magnetic field, as in a superconductor; and they do not require any external non-linear term to be added to the dynamical equation, as in a Bose–Einstein condensate. They appear in the Schrödinger equation for a few-body system with Coulomb interactions. Nothing else is required.

But, how can we talk about vortices in such a simple quantum system? In these previous cases we actually had a fluid flowing, or a current. But, what is flowing in a few-body system? These very valid questions will be addressed in Sections 4 and 5. But first, let us review some basic concepts about vortices.

* Corresponding author.
E-mail address: barra@cab.cnea.gov.ar (R.O. Barrachina).

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2. Vorticity and circulation

At a very basic level, a vortex is a region in a fluid where the flow rotates about an axis. Its study requires the introduction of some quantities that would help to define this rotation locally. One of this key quantities is the vorticity, defined as the curl of the velocity field $\mathbf{u}(\mathbf{r},t)$ of the fluid, namely

$$\vec{\omega}(\mathbf{r},t) = \nabla \times \mathbf{u}. \tag{1}$$

Using Stokes' theorem it can be easily demonstrated that $\vec{\omega}(\mathbf{r},t)$ *is proportional to the rate of rotation of a small fluid element about its own axes* [7]. Since, by its own definition as a curl, $\nabla \cdot \vec{\omega} = 0$, only two out of its three components are independent.

Another quantity of interest is the circulation Γ [8] which for any closed contour C around an arbitrary curved surface S in the fluid reads

$$\Gamma = \oint_C \mathbf{u} \cdot d\mathbf{l} = \int_S \vec{\omega} \cdot d\mathbf{s}, \tag{2}$$

where the circuit C is oriented counterclockwise with respect to the surface normal $\mathbf{s}$. Let us consider, for instance, a fluid rotating as a rigid body with angular speed Ω around an axis $\hat{z}$. In cylindrical coordinates (ρ, ϑ, z), its velocity field is $\mathbf{u} = \Omega\rho\hat{\vartheta}$, and the vorticity reads $\vec{\omega} = 2\Omega\hat{z}$, i.e. it is constant and equal to twice the angular velocity. Thus, the circulation about a surface S reads $\Gamma = 2S\Omega$.

We are not interested in this kind of rigid body rotating fluid though, but in one that would contain "irrotational vortices". This is apparently a *contradictio in terminis* since, how can a vortex exist in a fluid that is not rotating? To address this question, let us consider a velocity field that is inversely proportional to the distance ρ

from its axis, namely $\mathbf{u} \propto \hat{\vartheta}/\rho$. Then, the vorticity is zero everywhere (and so, the flow is said to be irrotational), except at the axis itself, where it diverges. But because this singularity is integrable, the circulation is zero for any contour not encircling the axis, and constant for a contour around the axis, independently of its size and shape. We'll come back to this example in a following section.

3. Irrotational vortices

We might have a quotidian understanding about vortices, but not a rigorous definition, or even a broadly accepted one. Many proposals have been made in the past [4–7], but none seems to be entirely satisfactory [7]. Fortunately, here we are not dealing with general vortices, but with irrotational ones, and so a precise definition is possible. We can define an irrotational vortex as any region of an irrotational fluid where the vorticity is different from zero (or more specifically, diverges).

As it was first proven by von Helmholtz in 1858 [9] and further developed by Lord Kelvin [10], the circulation around any point of a vortex is constant. This constancy means that vortices cannot terminate within a fluid, and therefore they must form loops or reach the fluid's boundary.

Since the seminal articles by Helmholtz and Kelvin, much work have been devoted to the study of the kinematics and dynamics of vortices, but the simple characterization provided here will be enough for the purpose of the present analysis. Thus, without any further delay, let us address the question stated in the introduction, on how a vortex can be defined in a simple quantum system.

4. Madelung's hydrodynamical interpretation

Some few months after the publication of the famous article by Schrödinger on wave mechanics [11], Erwin Madelung [12,13] noticed that if the wave function for a particle of mass m under the action of a potential $V(\mathbf{r},t)$ is written in terms of amplitude and phase

$$\Psi(\mathbf{r},t) = \mathcal{A}(\mathbf{r},t)\exp\left(\frac{i}{\hbar}\mathcal{S}(\mathbf{r},t)\right), \tag{3}$$

and replaced in Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(\mathbf{r}) - i\hbar\frac{\partial\Psi}{\partial t} = 0, \tag{4}$$

separating it in its real and imaginary parts, we get, after some simple maths, two coupled real equations

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\eta\mathbf{u}) = 0, \tag{5}$$

$$\frac{\partial u_j}{\partial t} + (\mathbf{u}\cdot\nabla)u_j = -\frac{1}{m}\nabla_j V - \frac{1}{m\eta}\sum_i \nabla_i \mathcal{P}_{ij}. \tag{6}$$

Here we have defined the following quantities,

$$\eta(\mathbf{r},t) = |\mathcal{A}|^2, \tag{7}$$

$$\mathbf{u}(\mathbf{r},t) = \nabla\mathcal{S}/m, \tag{8}$$

and

$$\mathcal{P}_{ij}(\mathbf{r},t) = -\left(\frac{\hbar^2}{4m}\right)\rho\,\frac{\partial^2 \ln\eta}{\partial x_i \partial x_j}. \tag{9}$$

Even though there has been some controversy regarding the equivalence between Schrödinger and Madelung equations [14,15], it is clear that a solution of Schrödinger equation is also a solution of the two coupled Eqs. (5) and (6). Thus, these equations represent a different way of addressing the same problem than Eq. (4). When we see the problem under this light, we notice that Eq. (5) is clearly a continuity equation, where the square of the amplitude is a density, and the gradient of the phase divided by the mass is a velocity. On the other hand, Eq. (6) is the very well known Euler equation for the movement of a fluid of non-interacting particles of mass m under a potential $V(\mathbf{r})$, except that now it is affected by a pressure tensor $\mathcal{P}_{ij}$ of quantum origin. So, here we have all the elementary entities for describing a vortex in a simple quantum system. Basically, a fluid and a velocity field.

5. Quantum vortices

Since the velocity field of a quantum system, as defined in Eq. (8), is the gradient of a scalar function, namely the action S, then the corresponding vorticity, defined as the curl of this velocity, is equal to zero. In other words, the velocity field of a quantum system is irrotational. Therefore, the only vortices that can appear in a quantum system are irrotational.

Going back to the example of an irrotational vortex, as described at the end of Section 2, it is easy to demonstrate that it can be achieved by a quantum system whose action $\mathcal{S}$ is linear with the angle ϑ around a certain axis. In cylindrical coordinates (ρ,ϑ,z) we write $S = \hbar \mathrm{m}\vartheta$. Note that, since the wave function is single valued, the quantity m has to be a whole number. This action produces a velocity field that diverges on the line $\rho = 0$, namely $\mathbf{u} = \hbar\mathrm{m}\,\hat{\vartheta}/m\rho$. The circulation is zero everywhere, except if the circuit encircles the line $\rho = 0$, where it reads $\Gamma = 2\pi\hbar\mathrm{m}/m$. The vorticity diverges at $\rho = 0$ and is zero everywhere else. Therefore, the line $\rho = 0$ corresponds to an irrotational vortex. Thus, we see that a simple quantum system with "magnetic quantum number" m provides a trivial example of an irrotational vortex.

The vortex in this simple example is located upon a straight line. But in general, quantum vortices can have complex shapes. Furthermore, in Section 8 we will demonstrate that vortices can even have different dimensions, depending on the configuration space of the problem at hand. Finally, as we will explain in the following section, a vortex can evolve in time, stretching and twisting, and even collapse onto itself or with another vortex of opposite circulation.

Thus we can generalize the result obtained for the simple example described previously, and write for a set of canonical coordinates and a circuit C encircling the vortex

$$\Gamma = \oint_C \mathbf{p}\cdot d\mathbf{q} = 2\pi\hbar\,\mathrm{m}, \tag{10}$$

where $\mathrm{m}\in\mathbb{Z}$ represents a "magnetic quantum number" associated to the angular momentum carried by the vortex. Let us note that the main controversy regarding the equivalence between the Schrödinger and Madelung equations is related to this quantization condition [14,15].

Finally it is very important to stress that the action $\mathcal{S}$ is undefined at a quantum vortex. And this is possible only if the wave function is zero on this same locus. This can also be demonstrated by means of the continuity Eq. (5), by taking into account that the velocity diverges at the vortex. Thus quantum vortices are nodes of the wave function.

6. Vortices in ionization collisions

By numerically solving the Schrödinger equation, Macek and co-workers [16] exemplified the appearance and evolution of quantum vortices in the ionization of hydrogen atoms by the impact of protons of 5 keV. In particular, their example shows some different scenarios for the creation and destruction of quantum vortices [8]. For instance, they showed how a vortex line reaches a vortex ring and partially collapses with one of its sides of opposite circulation in order to form a single structure, as shown in Fig. 1. Interesting as it is, this example does not represent a practical way of experimentally observing quantum vortices in ionization collisions, since it does not seem very easy (even when it might not be impossible) to measure the time evolution of such a process. But it is right here where we can rely on the "Imaging Theorem" demonstrated by John Dollard in 1971 [17–19]. For the case at hand, the final electron momentum distribution $\mathcal{P}(\mathbf{k})$ is shown to be proportional to the probability density $\eta(\mathbf{r},t)$ evaluated at the ballistic trajectory $\mathbf{r}=\mathbf{k}t/m$

$$\mathcal{P}(\mathbf{k})\,d^3\mathbf{k}=\eta\left(\frac{t}{m}\mathbf{k},t\right)\left(\frac{m}{t}\right)^3 d^3\mathbf{r}, \tag{11}$$

for $t\to\infty$. Thus, in the limit of very large times, the spatial distribution of the electrons emitted in the ionization process leads to the corresponding momentum distribution, where the impulse is related to position and time in a ballistic way. This result tells us that if a vortex appears during the collision, and if this vortex does not collapse during the evolution of the system, then we might be able to observe it as a zero of the transition matrix element, with a non-zero circulation around it.

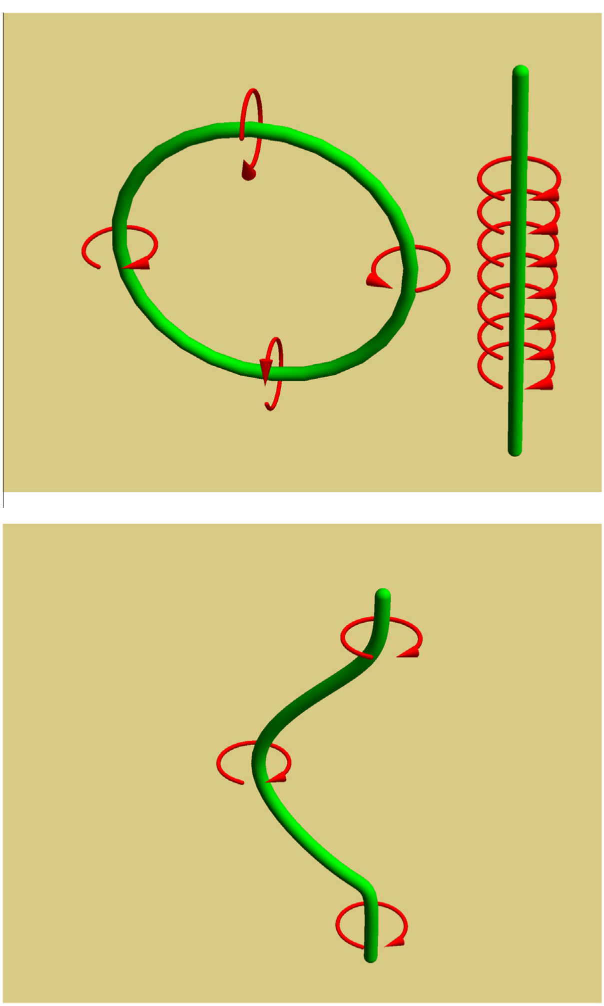

Fig. 1. A vortex line merges with a vortex ring along their sides of opposite circulation, becoming a single structure.

7. Evidence of quantum vortices in ionization collisions

In 1991 Brauner and Briggs [20] employed a three Coulomb (3C) approximation [21,22] to evaluate the differential cross section for the ionization of hydrogen by the impact of positrons. At an impact energy of 10 keV, they found a deep minimum in the electron momentum distribution in a collinear geometry, i.e. with the electron and positron traveling in the same direction. This sharp minimum was observed on the low-energy side of the electron capture to the continuum (ECC) peak and at an emission angle of 45°. Because of this, it was attributed to an interference effect between two double-binary (Thomas) collision amplitudes. More that two decades later, it was demonstrated that this minimum was actually a vortex, and that it could be also observed at more realistic impact energies in the range of 270 eV [23].

In 1993 Murray and Read [24] experimentally found a very pronounced minimum in the differential cross section for a (e, 2e) process in Helium at incident energies from 44.6 to 74.6 eV. They employed the symmetric geometry introduced in 1965 by Gottschalk it et al. [25], where both electrons emerge with the same energy and polar angle ψ. For $\psi=67.5^\circ$ the differential cross section showed a deep minimum when the angle between the electrons' momenta was approximately 140° within the range of energies studied. At that time, the minimum was attributed to an interference between the forward- and backward-scattering amplitudes. By means of a Dynamically screened three Coulomb (DS3C) approximation [26], Macek and co-workers [27] managed to reproduce this deep minimum, and recognized it as a quantum vortex.

Since these early evidences by Brauner and Briggs [20] and Murray and Read [24], vortices have also been observed in the photoionization of atoms, and in ionization collisions by the impact of ions and antiprotons (see [28,30] and references therein). These examples show that quantum vortices might be more ubiquitous than originally thought but, as it is explained in the following sections, not necessarily easy to find.

8. Quantum vortices as submanifolds of codimension 2

When considering single ionization collisions, we are dealing with a transition matrix element which depends on the momenta of the three particles in the final state. By energy and momentum conservation, the number of relevant scalar variables of T is reduced from nine to five. Furthermore, since the collision is symmetrical about the initial velocity $\mathbf{v}$; the number of relevant variables is further reduced to four. Thus vortices are regions in this multidimensional space where the wave function vanishes and the vorticity diverges. But, what is the dimensionality of these submanifolds?

As we have already seen, the transition matrix element T is zero at a vortex. Now, since T is complex, we end up with two real conditions; i.e. both the real and imaginary parts of T have to be zero simultaneously. The loci of these conditions are submanifolds of codimension 1, and the region where they intersect, i.e. the vortex, would be a submanifold of codimension 2. In other words, the dimensionality of a vortex is lower by two than that of the space where T is defined.

When we consider a restrictive geometry, as the symmetric and collinear ones described in the previous section, we are arbitrarily reducing the dimensionality of the problem in order to solve the conundrum of picturing a multidimensional object in our three dimensional space. However, a given vortex will go unnoticed unless the subspace defined by any of these geometries intersects the corresponding submanifold in the configuration space of T. On the other hand, if both submanifolds intersect, the vortex would appear as an isolated zero of T, as explained in the following section.

9. Quantum vortices in ionization collisions with collinear geometry

Fig. 2 shows a 3C calculation of the velocity field associated to the transition matrix element T in the ionization of hydrogen by 275 eV positrons. We compute T in terms of the components of the electron final momentum $\mathbf{k}$, parallel ($k_{\parallel}$) and perpendicular ($k_{\perp}$) to the positrons' initial direction. Details of the theoretical model are provided in previous articles, together with a description of its scopes and limitations [23,28]. We are employing an energy sharing or collinear geometry, where the electron and the positron are traveling in the same direction.

The representation in Fig. 2 shows all the information we can seek from the transition matrix element. Its modulus is represented by the density plot and its phase is related to the velocity field. We observe three isolated zeroes. The velocity field around them clearly shows that they correspond to quantum vortices. Besides, it can be shown that the circulation around each one of these three vortices is equal to $\pm 2\pi\hbar$, in accordance with the quantization rule for the magnetic quantum number.

As we explain in a previous section, quantum vortices might be ubiquitous, but not easy to find. Thus we need a better strategy than plotting the modulus of the transition matrix element and looking for zeroes. Thus we plot the conditions Real $(T) = 0$ and Im $(T) = 0$ separately, as shown in Fig. 3. Each of these conditions defines a line in the plane, and the vortices would be located where these two lines intersect each other.

At an impact energy of 255 eV, the nodal lines intersect only at one point. But when this energy is increased to 270 eV, these lines intersect at two further points. This means that a pair of vortices of opposite circulation has appeared. If we increase the energy even further [23], one vortex will migrate towards the origin, while the other will approach the electron capture to the continuum (ECC) line at an angle of 45°. Thus, we demonstrate that the minimum found by Brauner and Briggs in 1991 [20], as explained in the previous section, did actually represent a quantum vortex. Furthermore, the reason why they did not observe it at the lower

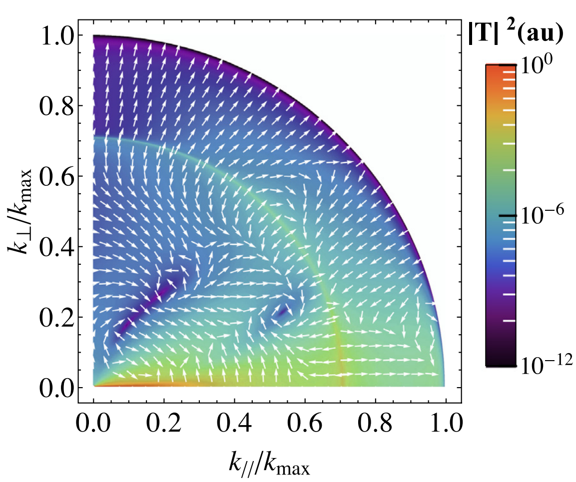

Fig. 2. Transition matrix element T in atomic units (au) for the ionization of H by the impact of 275 eV positrons in a collinear geometry. $k_{\parallel}$ and $k_{\perp}$ are the components of the electron momentum $\mathbf{k}$ parallel and perpendicular to the initial velocity $\mathbf{v}$ of the positron, respectively. These components are normalized to the maximum momentum $k_{\max} = m\sqrt{|\mathbf{v}|^2 - 2\epsilon/m}$, where ϵ is the first ionization energy of the hydrogen atom. The density plot displays the modulus of T, while the arrows represent the directions of the generalized velocity field $\mathbf{u} = \mathrm{Im}\nabla_{\mathbf{k}} \ln T$.

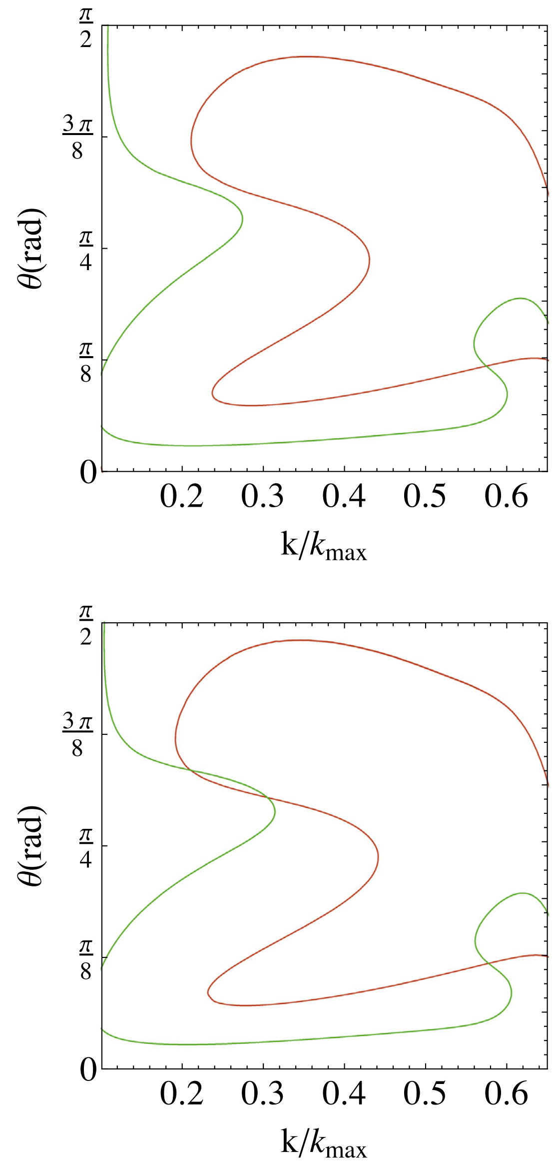

Fig. 3. Lines of zero real (red) and imaginary (green) parts of the transition matrix element T for the ionization of H by positron impact in a collinear geometry. k and θ are the electron's momentum and emission angle (with respect to the initial velocity $\mathbf{v}$ of the positron), respectively. The figures correspond to impact energies of 255 eV (upper figure) and 270 eV (lower figure). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

energy analyzed at that time, is that it collapses with a twin vortex below 270 eV. But, as we can see in Fig. 3, one vortex is still present at this impact energy, and it remains at impact energies as low as 30 eV, making it a prime candidate to be experimentally observed [28].

10. Vortex lines

Quantum vortices in ionization processes have been primarily studied as isolated points on 2D constrained regions of the phase space of a multidimensional transition matrix element T. These reductions are customarily achieved through restrictive geometries, as for instance the collinear arrangement that we have used to study the positron impact case in the previous section.

However, since vortices are submanifolds of codimension 2, the isolated points revealed by restrictive 2D geometries are only

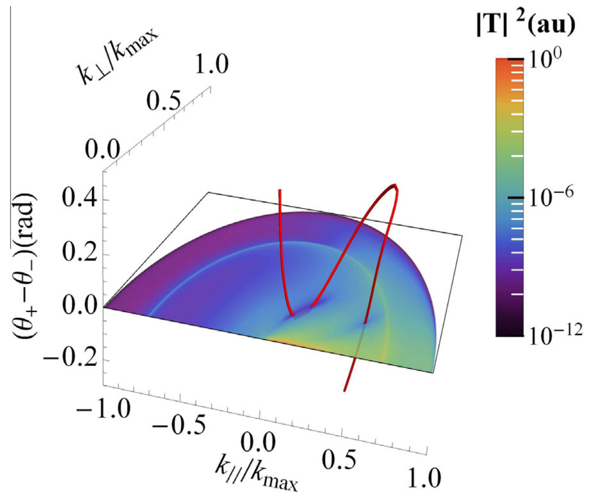

Fig. 4. Vortex line of T for the ionization of H by the impact of 275 eV positrons. $k_\parallel$ and $k_\perp$ are the components of the momentum $\mathbf{k}$ of the electron parallel and perpendicular to the initial velocity $\mathbf{v}$ of the positron, respectively. θ_- and θ_+ are the emission angles of the electron and the positron, respectively. The density plot shows $|T|^2$ in the collinear geometry ($\theta_- = \theta_+$).

providing a limited glimpse of a much more complex structure. Thus, in Fig. 4 we have tracked the vortices out of the collinear arrangement. We still keep a coplanar geometry, i.e. with the final momenta of the electron and the positron in the same plane with the initial velocity $\mathbf{v}$, but we do not keep the relative emission angle between the positron and the electron equal to zero any longer. Note how the isolated vortices observed for the collinear geometry are in fact part of a single vortex line [29]. They just appear or disappear depending on how the vortex line turns back and forth in the configuration space. In other words, the vortices that we were observing in a collinear geometry turned out to correspond to a planar cut of a single vortex line. In a recent article, Ward and Macek [30] also evaluated a segment of a vortex line for the K-shell ionization of carbon by electron impact by employing a Coulomb-Born approximation.

11. Summary and conclusions

In this article we have analyzed the appearance of quantum vortices in simple few-body systems. We employed Madelung's hydrodynamic formulation of quantum mechanics in order to explain their main characteristics. Furthermore, by means of the Imaging theorem it can be shown that a vortex that appears during the evolution of an ionization collision, might leave its fingerprint in the corresponding transition matrix element. We briefly reviewed some previous experimental and theoretical evidences of quantum vortices in ionization collisions and exemplified their main characteristics by studying the ionization of an atom by positron impact. Finally, by avoiding the standard restrictions on the final-state variables, we demonstrated that three isolated vortices previously observed under a collinear geometry, actually correspond to a single vortex line that is intersected three times by the surface defined by the collinear geometry.

The next obvious step in this effort to fully understand the topology of these quantum structures would be to trace the vortices in the full multidimensional space of the transition matrix element. Some basic and straightforward generalizations would be needed in order to study vortices in this multidimensional space. For instance, since we would no longer be dealing with a single particle, the concept of velocity field, as employed in previous sections, should be reviewed. Instead, it could be more straightforward to define trajectories (pathline) of the quantum system in a space of generalized coordinates. This analysis would finally allow to get the first look ever of a vortex surface in ionization collisions.

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