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Vortices in ionization collisions

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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.

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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