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Twist effects on quantum vortex defects

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Twist effects on quantum vortex defects

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Abstract. We demonstrate that on a quantum vortex in Bose-Einstein condensates can form a new, central phase singularity. We define the twist phase for isophase surfaces and show that if the injection of a twist phase is global this phenomenon is given by an analog of the Aharonov-Bohm effect. We show analytically that the injection of a twist phase makes the filament unstable, that is the GP equation is modified by a new term that makes the Hamiltonian non-Hermitian. Using Kleinert's theory for multi-valued fields we show that this instability is compensated by the creation of the second vortex, possibly linked with the first one.

1. Introduction

A Bose-Einstein condensate (BEC) is a diluted gas of bosons at very low temperature (see [1] and [2]) described by a unique scalar, complex-valued field $\psi = \psi(\boldsymbol{x}, t)$ called *order parameter*, that depends on position $\boldsymbol{x}$ and time t.
The equation that describes the dynamics of a BEC is the Gross-Pitaevskii equation (GPE) written here in a non-dimensional [3]:

$$\partial_t \psi = \frac{i}{2}\nabla^2\psi + \frac{i}{2}\left(1 - |\psi|^2\right)\psi. \tag{1}$$

This is a type of non-linear Scrhödinger equation in three-dimensional space.
The energy associated with a BEC is

$$E = \int \left(\frac{1}{2}\left|\boldsymbol{\nabla}\psi\right|^2 - \frac{1}{2}|\psi|^2 + \frac{1}{4}|\psi|^4\right) d^3\boldsymbol{x}. \tag{2}$$

In what follows we will describe a BEC at zero temperature, fulfilling the entire space and such that $\rho \to 1$ as $|\boldsymbol{x}| \to +\infty$.
A great advantage in describing BECs is provided by the *Madelung transform* of the order parameter,

$$\psi(\boldsymbol{x}, t) = \sqrt{\rho}(\boldsymbol{x}, t)e^{i\chi(\boldsymbol{x},t)}, \tag{3}$$

where χ is the phase of the condensate. Madelung transform has the advantage of interpreting the evolution of a condensate as an irrotational fluid with velocity $\boldsymbol{v} = \boldsymbol{\nabla}\chi$ and density ρ.

Indeed, if we substitute the Madelung transform into (1) we get

$$\partial_t \rho + \boldsymbol{\nabla} \cdot (\rho\, v) = 0; \tag{4}$$

$$\partial_t \chi = -\frac{1}{2}|\boldsymbol{v}|^2 - Q + \frac{1}{2}(1-\rho), \tag{5}$$

a continuity equation for the density ρ and a quantum version of the Hamilton-Jacobi equation for the phase χ, where Q is quantum potential. If we take the gradient of the second equation we get Navier-Stokes-like equations [3].
BECs can have non-trivial ground states with points where the order parameter vanishes: $\psi = 0$. Loci where $\rho = 0$ and phase undefined are lines in three-dimensions. These phase defects are empty, singular lines denoted by γ. These lines are called vortices because they are characterized by a quantized circulation along any path C encircling γ:

$$\Gamma(\gamma) = \int_C \boldsymbol{\nabla}\chi \cdot\, d\boldsymbol{x} = 2\pi\, n \qquad n \in \mathbb{Z}. \tag{6}$$

Thus, even though there is no vorticity (because $\boldsymbol{\nabla} \times \boldsymbol{\nabla}\chi = 0$), the presence of these topological defects produces circulation. One can treat a phase singularity as if vorticity $\boldsymbol{\omega} = \boldsymbol{\nabla} \times \boldsymbol{v}$ were concentrated on the line. Since these vortices have a core of the order of some Ångstroms it is reasonable and useful to think of this vorticity as a Dirac delta, singular field along γ and zero everywhere else:

$$\boldsymbol{\omega}(\gamma, t) = \Gamma\delta(\boldsymbol{x}, \gamma, t)\hat{t}, \tag{7}$$

where with this notation we intend that the vorticity is different from zero only for points $\boldsymbol{x}$ on γ. We introduced here the unit tangent vector $\hat{t}$ to γ. From now on all the constants will be set to unity.
Nowadays there is a lot of work for searching for new methods of producing non-trivial topological defects, not only in BECs but also in optics, liquid crystals, nano-materials and other fields [4], [5]. Numerical simulations with vortices in BECs [6] show that closed, three-dimensional, quantum vortices reconnect, as in classical, viscous fluids, and may form very complicated bundles where vortices may knot and link together. A topological and geometric study of quantum turbulence might help to understand aspects of reconnection and classical turbulence from a structural point of view.
In managing closed, classical vortices we already use some topological and geometric tools, as topological invariants given by the *linking number* between two or more vortices and *self-linking* of a single vortex line [7]. The natural question is whether these tools can be applied also for the study of quantum vortices. In this paper we will focus particularly on the notion of twist of a singular vortex line and study what happens when twist is present in vortex states in BECs.

Let us consider closed vortex lines. Classical vortices have an internal structure given by many vorticity lines. This ensemble of vorticity lines around a central line leads to the following

Definition 1.1 (Ribbon)**.** Given a curve γ described by the vector $\boldsymbol{x}(s)$, a *ribbon* $\mathcal{R}(\gamma, \hat{N})$ relative to a frame $\hat{N} \perp \hat{t}$ is given by a couple $\gamma, \hat{N}$ such that the first edge of $\mathcal{R}$ is γ and the second edge is a curve γ^* defined by the vector $\boldsymbol{x}^*(s) := \boldsymbol{x}(s) + \epsilon\hat{N}(s)$, where ϵ is the ribbon spanwise width.

We can recall the definition of twist for a classical vortex [7]:

Definition 1.2 (Total twist)**.** Given a ribbon $\mathcal{R}(\gamma, \hat{N})$ the twist Tw of the ribbon relative to the frame $\hat{N}$ is

$$Tw(\gamma, \hat{N}) = \int_\gamma \left(\hat{N} \times \frac{d}{d\,s}\hat{N}\right) \cdot \hat{t}\; d\,s. \tag{8}$$

We note that, while for quantum singular vortices the linking number is well defined, twist is not, because a quantum vortex has no internal structure. We thus need to generalize the concept of twist for a quantum vortex.

2. Twist phase for quantum vortices

Since vortices in BECs are singularities of phase, they have no structure. It would seem impossible to define a twist for them. Anyway, they posses an internal, unobservable structure given by the phase of the condensate. Now we propose a generalization of twist for vortices in BECs.

Given a vortex γ we can define isophase surfaces, i.e. orientable surfaces of constant phase, that foliate the entire condensate domain. They are also called Seifert surfaces of γ. Since vortex lines are phase defects, in presence of a vortex γ any isophase surface is bounded by γ. Close to the vortex line any isophase surface S is approximated by a plane that is spanned by the tangent $\hat{t}$ and by a (normalized) vector $\hat{N}$, that is orthogonal to $\hat{t}$ and tangent to S at every point of γ. We call $\hat{N}$ a *natural frame* of γ. Any different isophase defines a different natural frame $\hat{N}$.

Now, imagine an isophase surface as a fabric surface with γ the boundary of this surface. If it is unperturbed it remains flat, also along the boundary. Any perturbation bends locally or globally the fabric surface, creating creases. Moreover, a perturbation can have a privileged direction. Now imagine to perturb the whole fabric in such a way there are creases throughout the surface and that, at least near the boundary, the perturbation is sufficiently large that a portion of the fabric twirls around it going along the boundary. A twist associated with γ produces a very similar situation: it is just a phase perturbation [8], with distortion of the isophase surface, that, close to the vortex grows along the vortex [9]. Close to the vortex line, the amount of the perturbation is indicated by a rotation of the frame $\hat{N}$ that now measures the local rotation of the isophase surface around $\hat{t}$ going along γ with respect to the unperturbed situation. When there is a twist perturbation, $\hat{N}$ is no more parallel transported along the curve. Therefore, close to the curve we get the classical definition of twist, so that now we can define twist even far from the vortex. Since a rotation of the isophase changes the phase along the vortex line, then the perturbed total phase χ has a non-zero component of $\nabla\chi$ along γ. We call the phase field that perturbs any isophase surface a *twist phase* $\theta_{tw}(\boldsymbol{x}, t)$. The total (perturbed) phase of the condensate is the sum of the unperturbed phase and the twist phase. Let us call the perturbed phase χ and the unperturbed phase θ. We have:

Definition 2.1 (Twist phase)**.** Given a vortex γ, a *twist phase* is a phase field $\theta_{tw}(\boldsymbol{x}, t)$ such that:

(i) the new, perturbed phase χ can be written as the sum of the unperturbed phase θ and θ_{tw}: $\chi(\boldsymbol{x}, t) = \theta(\boldsymbol{x}, t) + \theta_{tw}(\boldsymbol{x}, t)$;

(ii) close to γ there must be a non-zero, longitudinal, gradient component of the phase $\nabla\chi \cdot \hat{t}$ such that $\nabla\chi \cdot \hat{t} = \nabla\theta_{tw} \cdot \hat{t} \neq 0$.

Thus, a twist perturbation produces an extra velocity of the condensate $\nabla\theta_{tw}$ that near the vortex is longitudinal to the defect line γ. An experiment to inject twist phase onto a vortex ring using Gauss-Laguerre beams and geometric phase has been proposed in [8].

The main aspect of injecting twist on a quantum vortex is that immediately after the perturbation, a second, central vortex can form by changing the linking number of the system (as shown numerically in [10] and demonstrated theoretically in [8], and discussed in [11]). This is a new, quantum effect, not observable for classical vortices. In a context of quantum turbulence it is of high interest to study the dynamics of twisted quantum vortices to see the implications of that on the system and on the cascade of reconnections [12]. Since any phase of a closed defect is multi-valued, to demonstrate theoretically this secondary vortex production we need to apply a mathematical theory to easily manage global, multi-valued fields.

3. Application of Kleinert's theory to multi-valued fields

Consider for the moment, a BEC vortex without twist, i.e. $\chi = \theta$. The gradient $\nabla\chi$ is the vector normal to any unperturbed isophase surface, orthogonal to both $\hat{t}$ and $\hat{N}$ for any given natural frame. This is a velocity field. Now, in [13] it is demonstrated that the gradient of a multi-valued function produces a singular vorticity field, despite the fact that the gradient field is curl-free. This fact was clear to Maxwell [14]: the vector potential produced at a point by a singular, closed magnetic field line can be written as the gradient of the multi-valued solid angle Ω subtended by the field line. Since the phase χ of the condensate at a point $\boldsymbol{x}$ is multi-valued, it plays the role of the solid angle. Since we have that the velocity produced by the vortex is (fixing time) $\boldsymbol{v} = \nabla\chi(\boldsymbol{x})$, it is the gradient of a multi-valued phase, because the values of χ jump by an integer multiple of 2π at any turn around the singularity. To easily manage multi-valued phases we must fix a cut surface S, which is itself an isophase surface hinged to the vortex line. By Biot-Savart law it is possible to demonstrate (see [13], page 113 and foll., where the demonstration is given using solid angle) that:

$$\boldsymbol{v}(\boldsymbol{x}, S) = \nabla\chi(\boldsymbol{x}, S). \tag{9}$$

Note, however, that the velocity does not depend on the choice of the particular discontinuity surface S, but only on the presence of the vortex line γ. Thus, if we want to compute $\boldsymbol{v}$ correctly, we have to take care of the contribution of the cut surface to the velocity, that Kleinert demonstrates to be proportional to a delta function on S. Hence the correct formula for the velocity becomes

$$\boldsymbol{v}(\boldsymbol{x}) = \nabla\chi(\boldsymbol{x}) = \nabla\chi(\boldsymbol{x}, S) + \boldsymbol{\delta}(\boldsymbol{x}, S), \tag{10}$$

where we have defined a delta field on the cut surfaces as

$$\boldsymbol{\delta}(\boldsymbol{x}, S) := \int_S \delta^{(3)}(\boldsymbol{x} - \boldsymbol{x}')\, d\boldsymbol{S}'. \tag{11}$$

The value of $\boldsymbol{v}$ is still that due to Biot-Savart, but re-arranged to take care of the multi-valuedness of the phase.

Now the velocity, as the gradient of a multi-valued phase, is decomposed into the sum of a gradient of a single-valued, discontinuous, function dependent of the cut surface, and of a Dirac delta function defined only on the cut surface. The adding of a delta function on the cut surface is necessary in order to make the expression for the velocity independent of the choice of the cut S.

Kleinert ([13], pag. 115) demonstrates that, being

$$\boldsymbol{\delta}(\boldsymbol{x}, \gamma) := \int_\gamma \delta^{(3)}(\boldsymbol{x} - \boldsymbol{x}')\, d\boldsymbol{x}', \tag{12}$$

then

$$\boldsymbol{\delta}(\boldsymbol{x}, \gamma) = \nabla \times \boldsymbol{\delta}(\boldsymbol{x}, S), \tag{13}$$

where now the vortex γ is seen as the boundary of S. This delta vector field $\boldsymbol{\delta}(\boldsymbol{x}, \gamma)$ points along the tangent vector $\hat{t}$ of γ. Therefore, the gradient of a multi-valued function is not curl-free and its curl is exactly the phase defect line:

$$\nabla \times \nabla\theta(\boldsymbol{x}) = \boldsymbol{\delta}(\boldsymbol{x}, \gamma). \tag{14}$$

This means that any isophase surface meets in γ, where the phase is undefined, and rotates around it generating a circulation. We note that, beside being invariant under added gradients of single-valued functions to the velocity field, equation (14) is also independent on the choice of the cut surface S. Indeed, Kleinert shows that if we changed the cut surface $S \to S'$ the delta function (11) would change by a gradient of the delta of the volume V swept by S when changes to become S':

$$\boldsymbol{\delta}(\boldsymbol{x}, S') = \boldsymbol{\delta}(\boldsymbol{x}, S) + \boldsymbol{\nabla}\delta(\boldsymbol{x}, V). \tag{15}$$

Hence

$$\boldsymbol{\nabla} \times \boldsymbol{\delta}(\boldsymbol{x}, S') = \boldsymbol{\nabla} \times \boldsymbol{\delta}(\boldsymbol{x}, S). \tag{16}$$

Therefore, equation (14) can be seen as a double gauge theory.
The production of curl by a gradient is due to the cut surface, present only if the phase is globally defined and multi-valued. Kleinert's theory has a clear, natural explanation. To understand this physically let us think of BEC as a classical fluid, that at time $t = 0$ is stationary and irrotational (without vortices). In this case all the streamlines are orthogonal to infinite, parallel surfaces at each point of space for which the normal vector is the velocity field $\boldsymbol{v}$. This parallel surfaces are iso-potential surfaces. Indeed, without vorticity we have $\boldsymbol{v} = \boldsymbol{\nabla}\chi$, where χ is the velocity potential. In this case it is a single-valued potential and thus it is curl free. Imagine now that at a certain instant of time, abruptly, we put an infinitesimally thin, bi-dimensional boundary layer in the fluid, parallel to the streamlines. Then, under a shear force on that surface, the speed will change producing rotation of the stream lines and thus an almost singular vorticity field. Vice versa, given a singular vorticity field, we can always think of it as due to a very thin surface layer present in the fluid. The presence of the vortex is independent on the choice of the surface layer. In this case the role of the boundary layer is played by the the cut surface S and the delta function indicates the extra velocity acquired by fluid particles to close the curved streamlines once we remove the layer. In the next sections we will apply Kelinert's theory for twisted vortices in BECs.

4. Instability of a twisted vortex line

In the paper [15] we demonstrate that a twisted vortex is unstable. We first consider a twisted vortex state of the BEC written by the Madelung transform (3):

$$\psi_{tw} = \sqrt{\rho}e^{i\chi} = \sqrt{\rho}e^{i(\theta+\theta_{tw})}. \tag{17}$$

Then, imposing that the unperturbed vortex state ($\theta_{tw} = 0$) satisfies the GPE, we find what is the evolution equation for the twisted state. Since the GPE is not symmetric under a local change of phase, the twisted state satisfies a modified GPE. From this equation we compute the new energy functional and find

$$E = \int \left[\frac{1}{2}|\tilde{\boldsymbol{\nabla}}\psi_{tw}|^2 - \frac{1}{2}|\psi_{tw}|^2 + \frac{1}{4}|\psi_{tw}|^4 + \left(-\partial_t\theta_{tw}|\psi_{tw}|^2 + \frac{i}{2}\,\psi^*_{tw}\,\boldsymbol{\nabla}\theta_{tw}\cdot\boldsymbol{\nabla}\psi_{tw}\right)\right] d^3\,\boldsymbol{x}, \tag{18}$$

where the integral is over all the three-dimensional space occupied by the BEC and $\tilde{\boldsymbol{\nabla}} := \boldsymbol{\nabla} - \boldsymbol{\nabla}\theta_{tw}$. We immediately see that the energy functional changes with respect to that of the ground state. First of all, it is evident the imaginary part, associated with the non-Hermitian Hamiltonian ([15],[16], [17]), that makes the probability to be no more locally conserved and the system subject to some sort of loss and gain process during its dynamics. Moreover, in [15] we demonstrate that the energy for a vortex ring in a twisted state is greater than that of the untwisted one. This means that the twisted state is unstable. In the paper mentioned above we apply Kleinert's theory and find a system of integro-differential equations that describes the dynamics of this transient, from a twisted vortex to a more stable state. We also look for the linear stability for ψ_{tw} and we demonstrate that a small perturbation of a twisted vortex creates Kelvin waves whose amplitude grows exponentially in time if and only if $\nabla^2\theta_{tw} > 0$. Twist phase seems to be an extra energy source. Studying the stability of the complex conjugate ψ^*_{tw}, as in Bogoliubov's analysis, we would have that Kelvin waves would grow their amplitudes if and only if $\nabla^2\theta_{tw} < 0$. Therefore the more general statement is that the amplitude of a linear perturbation near the vortex that is a superposition of propagating and counter-propagating Kelvin waves grows exponentially in time if and only if $\nabla^2\theta_{tw} \neq 0$. We can see this condition also if we write (18) as

$$E = E_0 + \frac{i}{2}\int \psi_{tw}^* \, \boldsymbol{\nabla}\theta_{tw} \cdot \boldsymbol{\nabla}\psi_{tw} \; d^3\boldsymbol{x} \tag{19}$$

and write the integrand in (19) as $\boldsymbol{\nabla}\cdot(|\psi_{tw}|^2\boldsymbol{\nabla}\theta_{tw}) - |\psi_{tw}|^2\nabla^2\theta_{tw}$. Since the first term is a divergence integrated over the entire space it cancels out and it remains a term proportional to the Laplacian of the twist phase. Apart from the vortex itself, where $|\psi_{tw}|^2 = 0$, the condition for the stability and for the conservation of the probability is that $\nabla^2\theta_{tw}$ becomes zero.

5. Stabilization by the formation of a secondary vortex: an analog of the AB effect

To fix ideas we can consider a vortex ring in a BEC. Let us imagine to perturb isophases globally with a twist phase, giving a uniform perturbation such that every isophase is perturbed in the same way throughout the region, and not just close to the defect. This cannot be done in a classical vortex since twist is only locally defined in a tubular neighborhood. In this case, fixed an isophase surface, at every point s of γ we can define an *isotwist phase surface* which, close to γ, is normal to $\hat{t}$ and contains $\hat{N}$, for any possible choice of frame $\hat{N}$. This surface is the locus of constant twist phase at a fixed s independently of the choice of the frame. If we imagine to inject the same twist phase everywhere (and on γ), then any isotwist surface is consequently globally defined along γ. If the twist phase is global, then any of these isotwist surfaces will intersect in a central line where all the possible values of the twist phase coexist, leaving the twist undefined on that line. The only possibility for such a scenario to be physically possible is that the density ρ of the BEC goes to zero on that line. This explains why a global twist phase must produce a secondary vortex. For the vortex ring the second vortex is straight and produced at the center of the ring. The linking-number between the two defects is different from zero (see [10] again).

Since the twist phase is multi-valued, when it comes back to the initial point all the surfaces associated with an integer multiple of 2π coincide. We introduce a cut surface Σ at the origin with $\hat{t}$ as normal vector, in a very similar way as we have defined the cut surface S for isophase surfaces. In this case, since the twist is also global in our hypothesis, we can apply Kleinert's theory also for the perturbed phase $\chi = \theta + \theta_{tw}$. Introducing an unperturbed and a twist velocity, $\boldsymbol{v}_{unp.} = \boldsymbol{\nabla}\theta$ and $\boldsymbol{v}_{tw} = \boldsymbol{\nabla}\theta_{tw}$ respectively, we have:

$$\boldsymbol{v}(\boldsymbol{x}) = \boldsymbol{v}_{unp.}(\boldsymbol{x}) + \boldsymbol{v}_{tw}(\boldsymbol{x}) = \boldsymbol{\nabla}\theta(\boldsymbol{x}, S) + \boldsymbol{\delta}(\boldsymbol{x}, S) + \boldsymbol{\nabla}\theta_{tw}(\boldsymbol{x}, \Sigma) + \boldsymbol{\delta}(\boldsymbol{x}, \Sigma). \tag{20}$$

Taking the curl of both sides and calling γ_{tw} the intersection line of the isotwist surfaces boundary of Σ, we have

$$\boldsymbol{\nabla}\times\boldsymbol{v}_{unp.} + \boldsymbol{\nabla}\times\boldsymbol{v}_{tw} = \boldsymbol{\delta}(\boldsymbol{x}, \gamma) + \boldsymbol{\delta}(\boldsymbol{x}, \gamma_{tw}) = \boldsymbol{\omega} + \boldsymbol{\omega}_{tw}, \tag{21}$$

where we have defined $\boldsymbol{\omega}_{tw}$ the tangent vector of the new singularity. When the secondary vortex line is produced the phase front of any quasi-particle becomes discontinuous passing across the phase defect, similarly to what happens for the wave fronts of a charged particle in the Aharonov-Bohm effect (AB effect) [18]. To be more precise, the secondary vortex formation is a sort of inverse AB effect. Indeed, in the AB effect a straight magnetic field generates a vector potential whose domain is multi-valued at the position of the singular magnetic line. This vector potential can be seen as the gradient of a multi-valued phase acquired going around the singularity field. Any charged particle does not feel the magnetic field directly because the field is zero outside, but its phase will shift going through the singularity by a quantity proportional to the magnetic flux. Hence, the presence of a singular field produces a measurable effect, a phase

difference, observed in a shift of the interference pattern on a screen behind the magnetic field. The phase shift acquired has a topological nature because does not depend on the particular path around the singular magnetic field line. In our case we start by a global, multi-valued phase which produces rotation around a central point, no matter how far from the curve. This means that also in this case the global twist phase is a topological phase. Moreover, the twist velocity $\boldsymbol{\nabla}\theta_{tw}$ has a non-zero circulation along γ and around γ_{tw} where it is not defined, exactly as for the vector potential in the AB effect. Hence, the second vorticity production can be seen as the inverse of an AB effect. The global twist phase is a topological phase producing a non-zero linking number between the two vortices.
The extra energy injected by the twist under the form of the new longitudinal velocity serves to create the new singularity field, by stabilizing the system. There is a instantaneously transition from a system with a single twisted vortex to a more stable system of two linked vortices (a vortex ring and a central straight vortex line following the example in [8]).
It is worth noting that there would be no secondary vortex production if the twist phase were local. It would be multi-valued only in an infinitesimal portion near the vortex line. Instead, outside this portion the phase should go smoothly to zero. In this case the twisted vortex would not be stabilized by any secondary vortex production and would continue in its transient, unstable evolution.

6. Conclusions

In order to deal with quantum turbulence it is useful to exploit some topological and geometric properties of quantum vortices. One of these is twist which has no simple analogue for quantum vortices. In this paper we have generalized the concept of twist as a twist phase. Therefore it is useful to study what happens to a twisted vortex state. In this case we have mentioned that this state is unstable if the Laplacian of the twist phase is different from zero. We have shown by using Kleinert's theory that if the twist phase is global there is a mechanisms that stabilizes the system in analogy with the AB effect, produced by the presence of a topological phase. A second, central phase defect linked with the first one will be produced changing the linking number of the system.
However, we think that this should not be the only mechanism. If the twist phase is injected only near the vortex the twist phase should be only local and this should not change the linking number of the system. Thus the twisted vortex should remain unstable and evolve following the system of equations given in [15]. If the Laplacian is different from zero, due to non-Hermiticity of the Hamiltonian, Kelvin waves will grow in amplitude by gaining energy from the injected twist changing the vortex configuration in space until some other mechanism will take place to dissipate the twist phase, stabilizing the system. We think this mechanism would coil the vortex giving writhe. The spontaneous formation of a second singularity in twisted vortices opens a new scenario on the possible relations between the dynamics of quantum vortices and their topological and geometric properties.

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