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# Vorticity field, helicity integral and persistence of entanglement in reaction-diffusion systems

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**Abstract**

We show that a global description of the stability of entangled structures in reaction-diffusion systems can be made by means of a helicity integral. A vorticity vector field is defined for these systems, as in electromagnetism or fluid dynamics. We have found under which conditions the helicity is conserved or lost through the boundaries of the medium, so the entanglement of structures observed is preserved or disappears during time evolution. We illustrate the theory with an example of knotted entanglement in a FitzHugh–Nagumo model. For this model, we introduce new non-trivial initial conditions using the Hopf fibration and follow the time evolution of the entanglement.

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(Some figures in this article are in colour only in the electronic version)

Many physical phenomena giving rise to natural patterns can be understood in terms of a short-range self-enhancing reaction between two species (or reactions) coupled with transport [1]. A reaction-diffusion (RD) system combines Fick's law of diffusion with a kinetic reaction rate term. Examples of such systems arise in the phenomenological theory of superconductivity known as Ginzburg–Landau equations [2], chemical reaction waves [3], optics [4], models of cardiac fibrillation [5, 6], etc. One of the most interesting aspects of RD systems in a three-dimensional space is that they support vortices, called spiral or scroll waves. Spiral waves are characterized by the fact that they rotate around a topological point defect called a phase singularity or rotor. Since spiral waves are the cross sections of a scroll wave, the phase singularity can be interpreted as the cross section of a filament in three dimensions. These curves can be linked or constitute knots. In numerical experiments, it was found that there are configurations which present an unusual stability for these phase singularities [7]. The stability of phase singularities has been analysed locally [8]; however, definitive conclusions on its global behaviour have not been obtained. An alternative approach to this problem could come from the study of non-local mechanisms that allow certain topological invariants of the organizing centres to be conserved. There are preliminary studies on topologically non-trivial field configurations in the literature [9, 10]. Examples are the work by Berry and Dennis [11] on phase singularities in the Helmholtz equation or studies on the stability of ball lightning [12, 13].

In this work, we introduce a vorticity vector field for any reaction-diffusion system that includes all the information about the global entanglement. We define a helicity integral of the vorticity vector field in analogy to Moffatt's vortex helicity [14]. We then prove that the persistence of entanglement in the RD system depends on the conservation of the helicity. We give the conditions to be fulfilled for the conservation of the helicity that depend on the boundary conditions in a non-trivial way. In order to illustrate how this mechanism works, a new case of knotted entanglement in the FitzHugh–Nagumo model is provided.

A simple archetypical example of an RD system includes two scalar fields $u(\mathbf{r}, t)$ and $v(\mathbf{r}, t)$, which satisfy the equations

$$\frac{\partial u}{\partial t} = f(u, v) + D_u \nabla^2 u, \qquad \frac{\partial v}{\partial t} = g(u, v) + D_v \nabla^2 v. \tag{1}$$

At one particular point in the spatial domain $\mathcal{D}$ in which the fields $u$ and $v$ are defined, both quantities evolve in time according to (in general, nonlinear) functions $f(u, v)$ and $g(u, v)$, respectively. The coupling between close points in the medium occurs due to diffusion terms with coefficients $D_u$ and $D_v$.

In order to study the topology of singular filaments, we will define a vorticity vector field in such a way that the field lines coincide with the intersections of level surfaces of $u$ with level surfaces of $v$, since these intersections include the phase singularities that organize the complete dynamics around them. The unusual stability of certain configurations will be described by taking into account the linkage of the curves obtained from the intersection curves. A measure of the extent to which the field lines of a divergence-free vector field curl themselves around one another is the helicity of the field as was defined by Moffatt [14] in 1969.

In a physical situation, generally $u$ takes values between $u_{\min}$ and $u_{\max}$, and $v$ takes values between $v_{\min}$ and $v_{\max}$. We take new variables $U$ and $V$ from $u$ and $v$ through linear scaling:

$$U(\mathbf{r}, t) = \frac{2u - (u_{\max} + u_{\min})}{\sqrt{2}(u_{\max} - u_{\min})}, \qquad V(\mathbf{r}, t) = \frac{2v - (v_{\max} + v_{\min})}{\sqrt{2}(v_{\max} - v_{\min})}, \tag{2}$$

in such a way that $U$ and $V$ satisfy $0 \leqslant U^2 + V^2 \leqslant 1$. Note that the level surfaces of $u$ and $v$ coincide with the level surfaces of $U$ and $V$, respectively, since the change is linear. Now we define

$$p = \sqrt{U^2 + V^2}, \qquad q = \arctan(V/U) \tag{3}$$

and a complex scalar field,

$$\phi = \sqrt{\frac{1-p}{p}}\, \mathrm{e}^{\mathrm{i}q}. \tag{4}$$

The level curves of $\phi$ are the intersections of the surfaces of constant $u$ and the surfaces of constant $v$ at any time. Finally, we introduce the vorticity vector field associated with the RD system as

$$\mathbf{\Omega} = \frac{\nabla\phi \times \nabla\bar{\phi}}{2\pi\, \mathrm{i}(1 + \bar{\phi}\phi)^2}, \tag{5}$$

whose field lines coincide with the level curves of $\phi$ by definition. In equation (5), i is the imaginary unit, and $\bar{\phi}$ is the complex conjugate of $\phi$. The particular definition (5) has an interesting bonus. If the scalar is a map, $\phi : S^3 \to S^2$, these maps yield knots and can be classified in homotopy classes characterized by the integer value of the Hopf index, $H(\phi)$, which gives a measure of the linkage or entanglement of the level curves of the map. Since the vector field $\mathbf{\Omega}$ defined by equation (5) is divergence free, a vector potential $\mathbf{\Psi}$ can be found so that $\mathbf{\Omega} = \nabla \times \mathbf{\Psi}$. The Hopf index, $H(\phi)$, that is a topological invariant of the map, $\phi : S^3 \to S^2$, can then be written as the integral

$$H(\phi) = \int (\mathbf{\Psi} \cdot \mathbf{\Omega})\, \mathrm{d}^3 r. \tag{6}$$

This integral is known in fluid and plasma physics to be the helicity of the vector field $\mathbf{\Omega}$, a global measure of the linkage of the force lines of $\mathbf{\Omega}$. Consequently, if we define the helicity of the configuration, at any time, as in equation (6), this quantity will inform us about the global linkage of the intersections of the level surfaces of $u$ and $v$ at any time, and, more important, if this quantity is conserved during the evolution of the system given by equations (1), then the *global* topology of the initial configuration is preserved, constituting a strong source of stability of the system. In general, $\phi$ will not correspond to a real map from $S^3$ to $S^2$, so its helicity will not be equal to a Hopf index. This may happen if, for example, the domain $\mathcal{D}$ is not infinite but a box with finite edges. Then the value of the helicity will be a real number instead an integer one, but its meaning is always related to the global linkage of the intersections of the level surfaces of $u$ and $v$.

An interesting observation can be noted here on the vorticity vector field: it is parallel to the cross product $\nabla u \times \nabla v$, whose maximum value is used by many authors to detect the vortex that organizes the medium [10]. In terms of the global scheme described in this work, the explanation of this fact is related to high values of the helicity density in regions where the density of linked lines is also high.

Suppose that a particular initial configuration has been given, in which the initial helicity given by equation (6), at $t = 0$, has a non-zero value. When the system evolves in time according to equations (1), due to the presence of diffusion there will be reconnections of the lines given by intersections of level surfaces, and the value of the helicity will change in general. However, as we will see, there are situations in which the helicity remains constant, or it changes very slowly with time compared to the characteristic time of the system. In these situations, the non-zero value of the helicity reflexes an unusual stability of the configuration that can explain important numerical, or even experimental, observations. The time variation of the helicity, from equation (6), is

$$\frac{\mathrm{d}H(\phi)}{\mathrm{d}t} = \int_S \mathbf{\Psi} \cdot \left( \mathbf{u}_N \times \frac{\partial \mathbf{\Psi}}{\partial t} \right) \mathrm{d}S. \tag{7}$$

Here $S$ is the boundary of the three-dimensional domain $\mathcal{D}$, and $\mathbf{u}_N$ is a unit vector orthogonal to the surface $S$ at each point. The integral (7) has to be computed on the boundary of the domain. In equation (7), we have

$$\frac{\partial \mathbf{\Psi}}{\partial t} = \frac{-1}{2\pi\, \mathrm{i}(1 + \bar{\phi}\phi)^2} \left( \frac{\partial \bar{\phi}}{\partial t} \nabla \phi - \frac{\partial \phi}{\partial t} \nabla \bar{\phi} \right). \tag{8}$$

Expression (7) shows that the helicity conservation depends on the boundary conditions, so that the stability of the system can be perturbed by acting only on the boundaries of the medium.

Now let us examine some typical boundary conditions. If the domain is the complete $R^3$ space and the fields are taken initially so that they are zero at infinity, then the vector field, $\partial \mathbf{\Psi}/\partial t$, will always be zero at the boundaries and the helicity will be conserved in time according to equation (7), as in [15–20]. A similar situation happens if Dirichlet boundary conditions are imposed in all the boundaries of a finite box provided the scalars $u$ and $v$ are smooth functions of space and the time evolution is also smooth. A non-trivial situation appears when considering Neumann (null flux) and periodic boundary conditions. Suppose that the domain $\mathcal{D}$ is a grid in $R^3$ in which the spatial coordinates $(x, y, z)$ are confined to the range $-L \leqslant x, y, z \leqslant L$, $L$ being a certain length, Neumann boundary conditions are applied to the $x$- and $y$-directions, and periodic boundary conditions are applied to the $z$-direction. In this case, there will not be loss of helicity through the $z$-direction but helicity will be lost through the $x$- and $y$-directions in an amount that depends on the specific system considered (1). Writing $\partial\boldsymbol{\Psi}/\partial t$ in terms of $u$ and $v$ through equations (4) and (8), the term in equation (7) is proportional to $\mathbf{u}_N \times (\partial_t v \nabla u - \partial_t u \nabla v)$. Taking into account the contributions of both the faces $z = -L$ and $z = L$ in which the field is periodic, this is equal to zero, so that the helicity is conserved in the directions in which periodic boundary conditions are applied. In the faces in which Neumann boundary conditions are applied, the term $\mathbf{u}_N \times (\partial_t v \nabla u - \partial_t u \nabla v)$ is not zero but it will depend on the terms of the RHS of equation (1).

Next we will provide a completely new case of knotted entanglement with helicity conservation in the FitzHugh–Nagumo model. This model set a paradigm which allows a geometrical explanation of important biological phenomena related to neuronal excitability and spike-generating mechanism. It has extensively been studied [10], and it was conjectured that persistent solutions called organizing centres might exist in three dimensions in which two-dimensional vortices are embedded into three-dimensional space forming knotted vortex rings. In order to prove the existence of these solutions, a theoretical framework based on local analysis involving effective models of short-range repulsive forces between vortex cores was proposed, but only certain limiting cases of slight curvature and twist of vortex lines had partial results [8, 21]. Here we will analyse the FitzHugh–Nagumo model at the light of the global stability provided by helicity conservation. The FitzHugh–Nagumo equations are given by

$$\frac{\partial u}{\partial t} = \frac{1}{\varepsilon}(u - u^3/3 - v) + \nabla^2 u, \qquad \frac{\partial v}{\partial t} = \varepsilon(u + \beta - \gamma v). \tag{9}$$

Here $u$ represents the electric potential and $v$ the recovery variable associated with membrane channel conductivity. We choose the constants appearing in equation (9) to have the values [10] $\varepsilon = 0.3$, $\beta = 0.7$ and $\gamma = 0.5$. We discretized equations (9) with finite differences on a cubic domain of size $2L$ with a uniform cubic grid of spacing $h$. For the Laplacian operator, we use a second-order accurate finite difference approximation which is symmetrical up to third order. We have to keep in mind the stability criteria about $t < h^2/2D$ when setting the spatial mesh.

Enforcing $u = -1.03279$, $v = -0.66558$ at the boundaries, which are the equilibrium values of the system, helicity will be conserved. We take initial conditions with non-zero helicity:

$$\begin{aligned} u(x, y, z, 0) &= \lambda_1 \frac{2xz + y(x^2 + y^2 + z^2 - 1)}{(x^2 + y^2 + z^2 + 1)^2} - 0.4, \\ v(x, y, z, 0) &= \lambda_2 \frac{2yz - x(x^2 + y^2 + z^2 - 1)}{(x^2 + y^2 + z^2 + 1)^2} - 0.4. \end{aligned} \tag{10}$$

This configuration corresponds to fibres of the Hopf map [18]. In equations (10), $\lambda_1 = \sqrt{2}$ and $\lambda_2 = 1/\sqrt{2}$, respectively, which are used to cover the range of the excitation-recovery loop in $(u, v)$ space [10] for the ordinary differential equation part of equations (9). We will solve the system and plot the intersection of level surfaces. Each level surface of constant $u$ can intersect another surface of constant $v$ in a curve, few curves or an empty set. Since helicity is conserved, we expect to find that there must linked curves all the time.

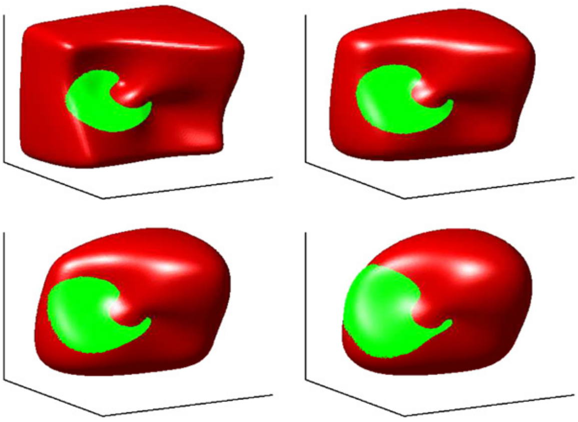

**Figure 1.** This figure shows the evolution of two level surfaces, $u = -0.7$ (red/dark) and $v = -0.1$ (green/light). From left to right and top to bottom, the snapshots correspond to 0.2, 0.4, 0.6 and 0.8 instants of simulation time.

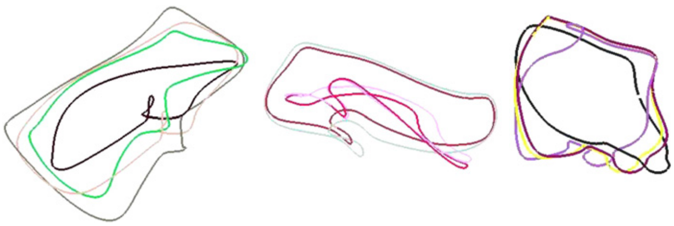

**Figure 2.** This figure shows the entanglement due to helicity conservation. Each curve results from the intersection of $u$ and $v$ level surfaces. It displays few curves at times equal 0.3, 0.5 and 0.8 from left to right. The values of the level surfaces are different, but at any instant of time there is the same number of linked curves.

In figure 1, we plot the evolution of two level surfaces for a domain size $L = 5$, and we have used 100 grid points in each direction. They correspond to the values $u = -0.7$ and $v = -0.1$. Those surfaces like them have a non-trivial intersection. One can use a marching cubes algorithm [22] to get these intersections. In figure 2, we have plotted the intersection of few pairs of $(u, v)$ level surfaces at different times. We can see that, as we have shown theoretically, they are linked. It is possible to find linked curves in all the instant of times as far we have enough numerical precision. The system will eventually decay to the equilibrium values fixed by the boundary conditions, but it will do that keeping the linking number constant.

In conclusion, in this paper we have introduced a vorticity vector field for any reaction-diffusion system given by two scalar fields. We have defined a helicity integral associated with the vorticity vector field which takes into account the total entanglement of the system. We have found the time evolution of the helicity and showed that this evolution (7) is dominated by the boundary conditions. We have introduced new non-trivial initial conditions in a FitzHugh–Nagumo model using the Hopf fibration. We have followed the time evolution of this system as an example of knotted entanglement with helicity conservation.

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## References

[1] Satnoianu R 2005 in *Encyclopedia of Nonlinear Science* ed A Scott (New York: Routledge) pp 783–9
[2] Ginzburg V L and Landau L D 1950 *Zh. Eksp. Teor. Fiz.* **20** 1064–82
[3] Ipsen M, Kramer L and Sorensen P G 2000 *Phys. Rep.* **337** 193–235
[4] Arecchi F T, Bocaletti S and Ramazza P 1999 *Phys. Rep.* **318** 1–83
[5] Gray R A, Jalife J, Panfilov A V, Baxter W T, Cabo C, Davidenko J M and Pertsov A M 1995 *Science* **270** 1222–3
[6] Winfree A T 1994 *Science* **266** 1003–6
[7] Winfree A T 1995 *Physica* D **84** 126–47
[8] Keener J P 1988 *Physica* D **31** 269–76
[9] Nye J F 1998 *J. Opt. Soc. Am.* A **15** 1132–8
[10] Sutcliffe P M and Winfree A T 2003 *Phys. Rev.* E **68** 016218
[11] Berry M W and Dennis M R 2001 *J. Phys. A: Math. Gen.* **34** 8877–88
[12] Rañada A F and Trueba J L 1996 *Nature* **383** 32
[13] Rañada A F, Soler M and Trueba J L 2000 *Phys. Rev.* E **62** 7181–90
[14] Moffatt H K 1969 *J. Fluid Mech.* **35** 117–29
[15] Rañada A F 1989 *Lett. Math. Phys.* **18** 97–106
[16] Rañada A F 1990 *J. Phys. A: Math. Gen.* **23** L815–20
[17] Rañada A F and Trueba J L 1995 *Phys. Lett.* A **202** 337–42
[18] Rañada A F and Trueba J L 1997 *Phys. Lett.* A **232** 25–33
[19] Rañada A F and Trueba J L 1998 *Phys. Lett.* B **422** 196–200
[20] Irvine W T M and Bouwmeester D 2008 *Nat. Phys.* **4** 716–20
[21] Biktashev V N, Holden A V and Zhang H 1994 *Phil. Trans. R. Soc.* A **347** 611–30
[22] Lorensen W E and Cline H E 1987 *Comput. Graph.* **21** 163–9