Persistent entanglement due to helicity conservation in excitable media

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(Dated: January 30, 2009)

Abstract

This work addresses the topic of knotted stable structures in excitable media. These structures appear in a wide variety of situations, such as cardiac fibrillation, chemical reactions, etc. Entangled curves have been found in numerical computations of the equations that describe excitable media. They present an unusual stability. An explanation for this behaviour has been an open question. In the present work we introduce for the first time the meaning of the helicity in an excitable media as a new tool to study the stability of these systems. The helicity is related to the total entanglement of the system. We have studied how the helicity is conserved or lost through the walls of the medium and shown that these behaviours are dominated by the boundary conditions, so the distortion of these conditions could lead to the disappearance of the structures.

PACS numbers: 82.40.Ck, 47.32.C, 47.32.cd
There has been experimental reports on stable structures (rotors) in cardiac muscle that appear in cardiac fibrillation [1], which may support the ideas of Arthur T. Winfree [2] on the relation between electrical wave propagation in the heart and some stable structures appeared in excitable media. One of the most interesting aspects of excitable media 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 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. The important fact of the phase singularities is that they are the focus or organizing centres of the excitation of the complete medium, and that their stability has been numerically proof for some particular cases [3]. The stability of phase singularities has been studied locally [4]. However, definitive conclusions on the behaviour of the singular filaments 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. Preliminary studies on topologically non-trivial field configurations have appeared [5, 6]. Examples are the work by Berry and Dennis [7] on phase singularities in the Helmholtz equation or studies on the stability of ball lightning [8, 9]. Here we use a new approach to the stability of phase singularities in excitable media. We define the helicity of the excitable medium and we study its meaning in relation to the total entanglement of the system. We consider the time behaviour of the FitzHugh-Nagumo model, showing that the persistence of entanglement depends strongly on the conservation of the helicity. This observation could be of some utility to develop new methods of controlling the appearance of rotors by acting on the system boundaries in experimental situations.

Excitable media describe in good approximation some properties of certain chemical reactions [10], cardiac arrhythmias [11], etc. The simplest mathematical models for propagation in three-dimensional excitable media include two state variables $u$ and $v$ that satisfy the equations

$$\frac{\partial u}{\partial t} = \frac{1}{\varepsilon} f(u, v) + D_u \nabla^2 u,$$

$$\frac{\partial v}{\partial t} = \varepsilon g(u, v) + D_v \nabla^2 v. \quad (1)$$

Here $u$ is the excitation variable, $v$ is the inhibition variable and $\varepsilon$ is a small parameter. At one particular point in the spatial domain $\mathcal{D}$ in which the variables $u$ 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 $D_v$. When the system parameters have specific range of values, the excitation of a point of the system propagates as a shockwave, with a propagation velocity given by the value of $\varepsilon$ and the diffusion coefficients [12].

In order to study the topology of singular filaments in excitable media, we define a vector field in which 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 medium around them. The linking number is a measure of the extent to which the field lines of a divergence-free vector field curl themselves around one another, i.e. of the helicity of the field as was defined by Moffatt [13] in 1969.

Consider the situation of an excitable media, given by a pair of real scalar fields $(u,v)$ defined in a three-dimensional spatial domain $D$, that satisfy the system of equations (1).

Our aim is to describe the unusual stability of certain configurations from a new global point of view, taking into account the linkage of the curves obtained from the intersections of level surfaces of $u$ with level surfaces of $v$. Suppose that we are interested in a physical situation in which $u$ takes values between $u_{\text{min}}$ and $u_{\text{max}}$, and $v$ takes values between $v_{\text{min}}$ and $v_{\text{max}}$. We define new variables $U$ and $V$ from $u$ and $v$ through linear scaling, in such a way that $U$ and $V$ satisfy $0 \leq U^2 + V^2 \leq 1$. 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 the variables $p = \sqrt{U^2 + V^2}$, $q = \text{ArcTan}(V/U)$. A complex scalar field that describes the excitable medium is then given by

$$\phi = \sqrt{\frac{1-p}{p}} e^{iq}. \quad (2)$$

The level curves of $\phi$ are the intersections of the surfaces of constant $u$ and the surfaces of constant $v$ at any time. We now define a vector field given by

$$\Omega = \frac{\nabla \phi \times \bar{\nabla} \phi}{2\pi i (1 + \bar{\phi}\phi)^2}. \quad (3)$$

The field lines of $\Omega$ coincide with the level curves of $\phi$ by definition. In equation (3), $i$ is the imaginary unit and $\bar{\phi}$ is the complex conjugate of $\phi$. The particular definition (3) 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 $\Omega$ defined by equation (3) is divergence-free, a vector potential $\Psi$ can be
found so that $\Omega = \nabla \times \Psi$. The Hopf index $H(\phi)$, that is a topological invariant of the map
$\phi : S^3 \rightarrow S^2$, can be then written as the integral

$$H(\phi) = \int (\Psi \cdot \Omega) \, d^3 r .$$

This integral is known in fluid and plasma physics to be the helicity of the vector field $\Omega$, a
global measure of the linkage of the force lines of $\Omega$. Consequently, if we define the helicity
of the configuration, at any time, as in equation (4), 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 $D$ 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 vector field defined from the $(u, v)$
configuration through equations (2, 3): it is parallel to the vector field $\nabla u \times \nabla v$, whose
maximum value is used by many authors to detect the vortex that organizes the medium
[6]. In terms of the global scheme described in this work, the explanation of this fact is
related with 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
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 (4), is
\[
\frac{dH(\phi)}{dt} = \int_S \mathbf{\Psi} \cdot \left( \mathbf{u}_N \times \frac{\partial \mathbf{\Psi}}{\partial t} \right) dS.
\]  
(5)

Here, \(S\) is the boundary of the three-dimensional domain \(D\) and \(\mathbf{u}_N\) is a unit vector orthogonal to the surface \(S\) at each point. The integral (5) has to be computed on the boundary of the domain. In equation (5) we have
\[
\frac{\partial \mathbf{\Psi}}{\partial t} = \frac{-1}{2\pi i (1 + \bar{\phi}\phi)^2} \left( \frac{\partial \bar{\phi}}{\partial t} \nabla \phi - \frac{\partial \phi}{\partial t} \nabla \bar{\phi} \right).
\]  
(6)

Expression (5) can be used to investigate in what cases the helicity is constant during the evolution of the system and how it changes in other cases. A common feature is that the conservation of the helicity depends almost only on the boundary conditions, so that the stability of the system can be perturbed numerically by acting only on the surfaces of the medium. This observation could be of some utility in experimental situations.

Now let us examine some typical boundary conditions. First, 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 (5). This is the case of the electromagnetic knots in vacuum [14, 15, 16, 17, 18, 19]. 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. However, in numerical computations of excitable media, Neumann (null flux) and periodic boundary conditions are mostly used. As an example, consider that the domain \(D\) is a grid in \(R^3\) in which the spatial coordinates \((x, y, z)\) are confined to the range \(-L \leq x, y, z \leq L\), \(L\) being a certain length, and suppose that Neumann boundary conditions are applied to the \(x\) and \(y\) directions, and periodic boundary conditions are applied to the \(z\) direction. In this example, 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 parameters of the model that one is computing. Writing \(\partial \mathbf{\Psi}/\partial t\) in terms of \(u\) and \(v\) through equations (2, 6), the term in equation (5) 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 depends on the parameters of the model because $\partial_t u$ and $\partial_t v$ depend on them through the evolution equations (1).

We will give an example of the 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 have been extensively studied and it was conjectured that persistent solutions called organizing centres might exist in three dimensions for excitable media 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. Finally to address the fundamental issue of the existence of stable knots, numerical investigations were performed. Here we will analyse again the FitzHugh-Nagumo model but at the light of the global stability provided by helicity conservation. The FitzHugh-Nagumo equations are given by

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

(7)

Here $u$ represents the electric potential and $v$ the recovery variable associated with membrane channel conductivity. We choose the constants appearing in equation (7) to have the values $\varepsilon = 0.3$, $\beta = 0.7$ and $\gamma = 0.5$. We discretized the equations (7) 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.

In order to test the conservation of helicity we enforce $u = -1.03279$, $v = -0.66558$ at the boundaries, which are the equilibrium values of the system. We take initial conditions with nonzero helicity,

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

(8)
Here, $\lambda_1 = \sqrt{2}$ and $\lambda_2 = 1/\sqrt{2}$ respectively, which are used to cover the range of the excitation-recovery loop in $(u,v)$ space \cite{6} for the ordinary differential equation part of equations \cite{7}. Now for testing the conservation of helicity, 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. If helicity is conserved and the initial conditions are chosen in such a way that intersection of level surfaces are knotted with entanglement or linking number different from zero, we can find as time evolves that there must be intersection curves linked all the time.

In Figure \ref{fig1} 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 \cite{21} to get the intersections. In Figure \ref{fig2} 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 eventually will decay to the equilibrium values fixed by the boundary conditions, but it will do that keeping the linking number constant. In conclusion, we have presented a new global approach to investigate how organizing centres in excitable media persist or disappear in three dimensions. In particular, we have defined the helicity of an excitable medium as a quantity that describes the global linkage of the intersections of the level surfaces of the scalar fields in the medium. We have studied how the helicity is conserved or lost through the walls of the medium and shown that these behaviours are dominated by the boundary conditions, so the distortion of these conditions could lead to the disappearance of the structures.

We thank S. Betelú for discussions on parts of this research. The authors thank support from the Spanish Ministerio de Educación y Ciencia under project ESP2007-66542-C04-03.

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FIG. 1: **Evolution of surface levels.** The figure shows the evolution of two level surfaces, $u = -0.7$ (red) and $v = -0.1$ (green). 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.

FIG. 2: **Conservation of entanglement.** The 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.