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A THREE-DIMENSIONAL AUTOWAVE TURBULENCE

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Autowave vortices are topological defects in autowave fields in nonlinear active media of various natures and serve as centers of self-organization in the medium. In three-dimensional media, the topological defects are lines, called vortex filaments. Evolution of three-dimensional vortices, in certain conditions, can be described in terms of evolution of their filaments, analogously to that of hydrodynamical vortices in LIA approximation. In the motion equation for the filament, a coefficient called filament tension, plays a principal role, and determines qualitative long-time behavior. While vortices with positive tension tend to shrink and so either collapse or stabilize to a straight shape, depending on boundary conditions, vortices with negative tension show internal instability of shape. This is an essentially three-dimensional effect, as two-dimensional media with the same parameters do not possess any peculiar properties. In large volumes, the instability of filaments can lead to propagating, nondecremental activity composed of curved vortex filaments that multiply and annihilate in an apparently chaotic manner. This may be related to a mechanism of cardiac fibrillation.

1. Introduction

The purpose of this paper is to describe basic features of the phenomenon of three-dimensional autowave (AW) turbulence. This interesting phenomenon provides an instructive example of spatiotemporal chaos, and may have useful applications. We believe that it deserves a peer study.

Turbulence is a term from hydrodynamics and so using it for autowave media is, of course, a metaphora. We use it to stress the essential properties of the phenomenon in question:

- It means complicated, apparently chaotic, spatiotemporal behavior.
- The complexity of behavior grows with the size of the system, with other parameters unchanged.
- It is related to vortex-like activity.
- It is essentially a three-dimensional behavior, qualitatively different from whatever may happen in the same system in two dimensions (hydrodynamists agree that "real" turbulence is essentially three-dimensional, unlike "weak" 2-D turbulence).

An AW medium is a 1 to 3-D continuum of points each exhibiting a special sort of nonlinear kinetics, and linked together via a diffusion-type process. These properties enable nondecaying propagation of nonlinear waves, called autowaves, which have their own inherent amplitude and form. At appropriate initial conditions, the autowaves may form "AW vortices" which have the form of spiral waves in two dimensions or scroll waves in three dimensions. These interesting classes of nonlinear waves were first observed in the Belousov–Zhabotinsky reaction [Zaikin & Zhabotinsky, 1970; Winfree, 1973], where the aforementioned nonlinear kinetics are autocatalytic oxidation of malonic acid. Since then, AW vortices were observed experimentally and predicted theoretically in a wide variety of systems of different physical natures [Swinney & Krinsky, 1991; Holden *et al.*, 1991; Brindley & Gray, 1994]. A very important example is cardiac tissue [Gray & Jalife, 1996], where the nonlinear kinetics are the excitation (electric depolarisation) and recovery of cardiocytes' membranes, and the diffusion-like process is inter-cellular electric conductivity. AW media are most often described in terms of "reaction–diffusion" equations,

$$\partial_t u = \mathbf{D}\nabla^2 u + f(u) \qquad (1)$$

where $u(\mathbf{r}, t) = (u_1, u_2, \ldots)^T \in \mathrm{R}^l$, $l \geq 2$, are concentrations of reagents, $\mathbf{r} = (x, y) \in \mathrm{R}^3$, $f(u)$ are reaction rates and $\mathbf{D}$ is the matrix of diffusion coefficients. One of the "basic" AW models is the FitzHugh–Nagumo system of equations (FHN). In the form proposed by Winfree [1991] it reads

$$\begin{aligned} \partial_t u &= \epsilon^{-1}(u - u^3/3 - v) + \nabla^2 u \\ \partial_t v &= \epsilon(u + \gamma - \beta v) \end{aligned} \qquad (2)$$

where $u(x, y, z, t)$ and $v(x, y, z, t)$ are the dynamic variables and ϵ, β and γ are constant parameters of the medium. Spiral wave solution for a biophysically detailed model of ventricular excitation is shown in Fig. 1.

The whole picture rotates counterclockwise around a region called core of the spiral. Far from the core, normal autowaves propagated form, approximately, the shape of an Archimedean spiral; within the core the behavior is more complicated. The core may be defined as the region circumscribed by the tip of the spiral. The tip may be defined as the point where the propagation wavefront ends meeting the "waveback", or as an intersection point of two isolines, as in Fig. 1. As it is seen in the figure, the behavior of the tip may be complicated — the so-called meander. FHN model is a rough caricature of the ventricular model shown in this picture, which, in turn is a simplification of the reality, as it ignores completely the nontrivial spatial structure of the tissue. Nevertheless, during the last 35 years, FHN model and its modifications were the most powerful heuristic tool for understanding the reentrant cardiac arrhythmias.

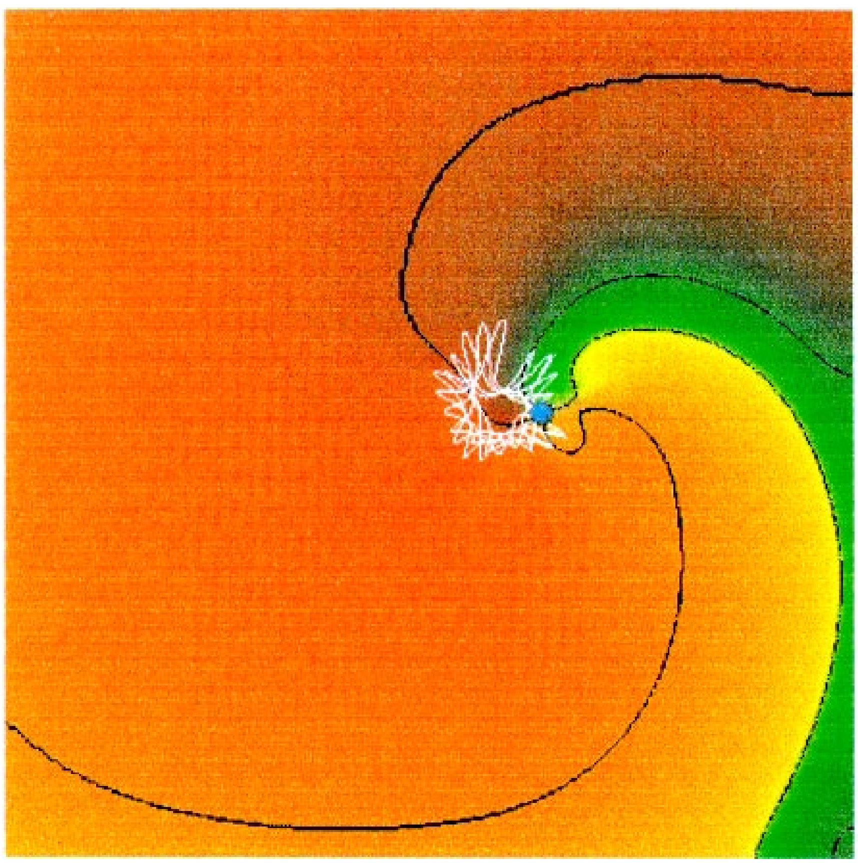


Fig. 1. Snapshot of the spiral wave in a model of ventricular tissue of guinea pig (details described in [Biktashev & Holden, 1996]). Red component of color coding shows the value of the transmembrane voltage, and green component that of one of the recovery variables. Two isolines of these two variables are shown in black. The blue ball at their intersection is the spiral tip. The white line shows its trajectory over last few rotations. The spiral rotates counterclockwise, the rotation is not stationary but "meandering".

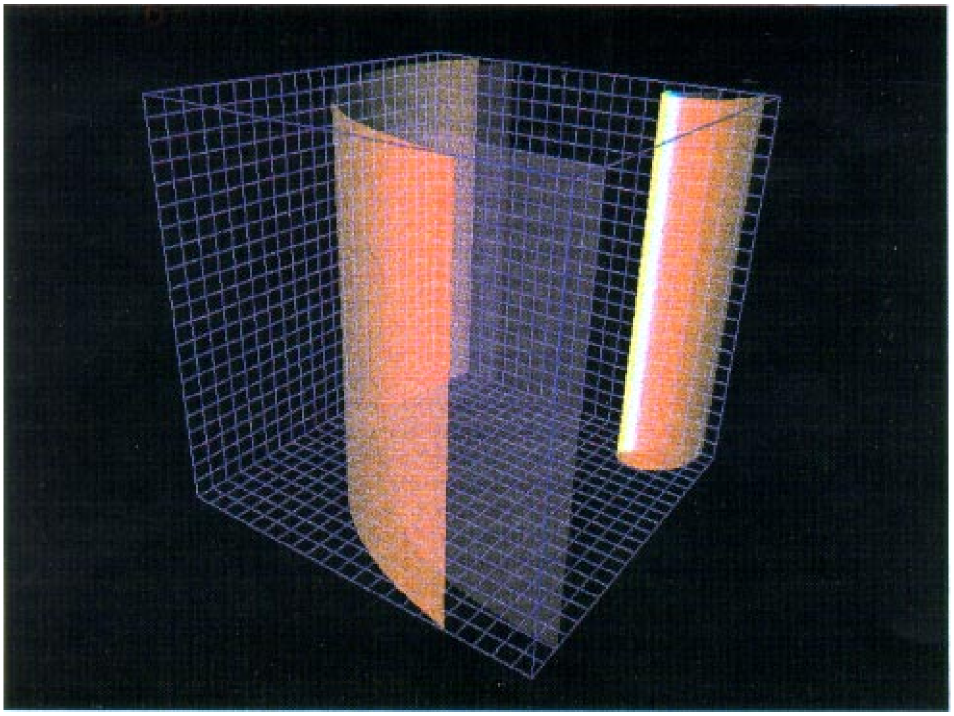


Fig. 2. Simple scroll wave, in the FHN medium 85^3 s.s. large. Shown is a snapshot of the excitation wave front, defined as the surface $u = 0$, colored depending on the value of the other dynamic variable, v. Fore-front (smaller v) is red and semi-transparent, back-front (higher v) is completely transparent and invisible. Surface near the edge of the excitaion wave, for intermediate values of v, is greenish and solid. This edge region is a visualization of the scroll filament. The solution is virtually independent on the vertical coordinate.

2. Scroll Waves and Their Dynamics

Dynamics of 3-D AW vortices are much more complicated than that in two dimensions. The front of the excitation wave is now a surface not a line, and so its break is now not a point, but a line, called scroll filament. A simple scroll wave is depicted in Fig. 2.

Topological classification of possible three-dimensional AW patterns has been considered by Winfree and Strogatz [1983, 1984], and numerical experiments have revealed a rich variety of different scroll wave behaviors (see e.g. the review by Panfilov [1991]). An analytical approach for the description of scroll wave dynamics was proposed by Keener [1989]. It was an asymptotics assuming that the characteristic spatial scale of the filament is much greater than the characteristic scale of a spiral wave, and in any cross-section orthogonal to the filament, the scroll wave is close to the 2-D spiral wave. The result of the singular perturbation theory, valid for generic reaction–diffusion system not only the FHN system, are equations for slow evolution of the filament and of the distribution of spiral wave rotation phase along the filament. Subsequent analysis of these equations [Biktashev *et al.*, 1994] has shown that in the main order of magnitude, the equation of the filament motion is independent on the phase distribution, and has the form

$$\partial_t R = b_2 \mathcal{D}_s^2 R + c_3 [\mathcal{D}_s R \times \mathcal{D}_s^2 R] , \qquad (3)$$

where $R = R(\sigma, t)$ describes the period-averaged position of the filament at the time moment t with parameter σ chosen so that points with equal σ move orthogonally to the filament, and arbitrary in other respects (note that the arc length s may not obey this property). Then the arc length differentiation operator $\mathcal{D}_s$ is defined as

$$\mathcal{D}_s f(\sigma, t) \equiv \partial_\sigma f(\sigma, t) / |\partial_\sigma R(\sigma, t)| . \qquad (4)$$

A simple fact from differential geometry is that the rate of change of total length of a moving curve is equal (disregarding fringe effects) to the integral over the curve of the scalar product of the curve motion velocity $\partial_t R$ and the vector of curvature $\mathcal{D}_s^2 R$. Thus, an elementary but important property of Eq. (3) is that the evolution of the total length is monotonic decreasing if b_2 is positive, and monotonic increasing if b_2 is negative. Biktashev *et al.* [1994] suggested the term "filament tension" for this important medium characteristic. Its heuristical value is that it predicts qualitatively different behaviors for 3-D AW media with positive and negative filament tensions. If the tension is positive, then a straight filament (simple scroll) should be stable, and the vortex ring should shrink and collapse. On the contrary, if the tension is negative, the vortex ring should expand rather than collapse, and straight filaments are unstable. Despite obvious limitations of the asymptotical theory, numerical experiments described in [Biktashev *et al.*, 1994] have shown that these predictions do catch the main qualitative features of the 3-D vortex dynamics.

Equation (3) is analogous to Da Rios equations of motion of vortex lines in fluids [Ricca, 1991, 1992], obtained in so-called localized-induction approximation (LIA); in fact, these equations are a partial case of (3) for $b_2 = 0$. The specifics of hydrodynamical vortices is that the LIA procedure involves logarithmic divergence (this problem does not exist for the AW vortices), and that their filament tension b_2 is always exactly zero, so that this term is sometimes used for the other parameter, c_3, which is not a medium constant but a characteristic of the vortex magnitude.

The assumptions of the asymptotic theory require that the filaments are smooth and far from each other and from medium boundaries. Naturally, evolution of filaments with negative tension will lead to violation of all these assumptions, as lengthening of the curve will increase both its curvature and "concentration" within the medium. Thus, this asymptotical theory only predicts that the behavior of such AW media will be unusual and complicated, but fails to predict the details. These details can be revealed by numeric experiments.

3. Dynamics of Vortex Filaments with Negative Tension

We simulated PDE system (2) in cubic domains with impermeable boundaries, for sufficiently long-time intervals. We have chosen medium parameters $\epsilon = 0.3$, $\beta = 0.75$ and $\gamma = 0.5$. 2-D spirals at these parameter values are stationary (not meandering), and 3-D scrolls have negative but relatively small filament tension. In different experiments, we kept the parameters fixed and varied only the size of the medium. We used explicit Euler (first-order forward time) differencing, with the simplest 7-point approximation of the 3-D Laplacian operator. Time step (t.s.) was fixed to be 0.03 time units (t.u.), i.e. math units of time in Eq. (2), and space step (s.s.) was fixed to be 0.5 space units (s.u.).

If the size of the medium is just large enough to contain the scroll wave but too small to let the

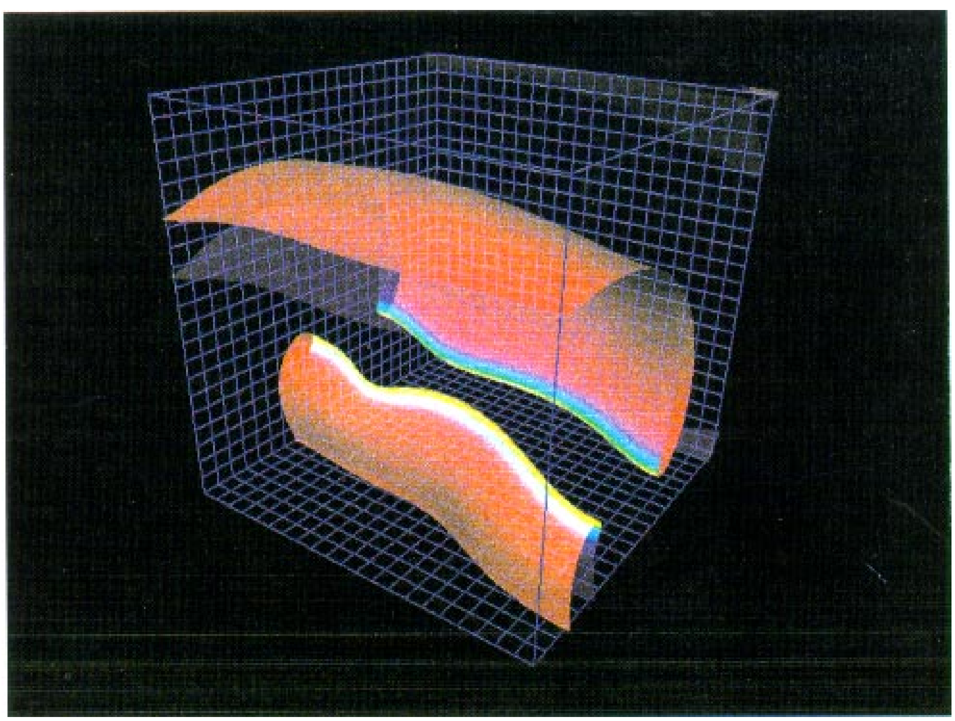


Fig. 3. Double scroll wave, in the medium of 86^3 s.s. large. Notations are the same as in Fig. 2. The two filaments exhibit irregular dynamics but always remain only two, i.e. do not split, annihilate or join.

(a)

(b)

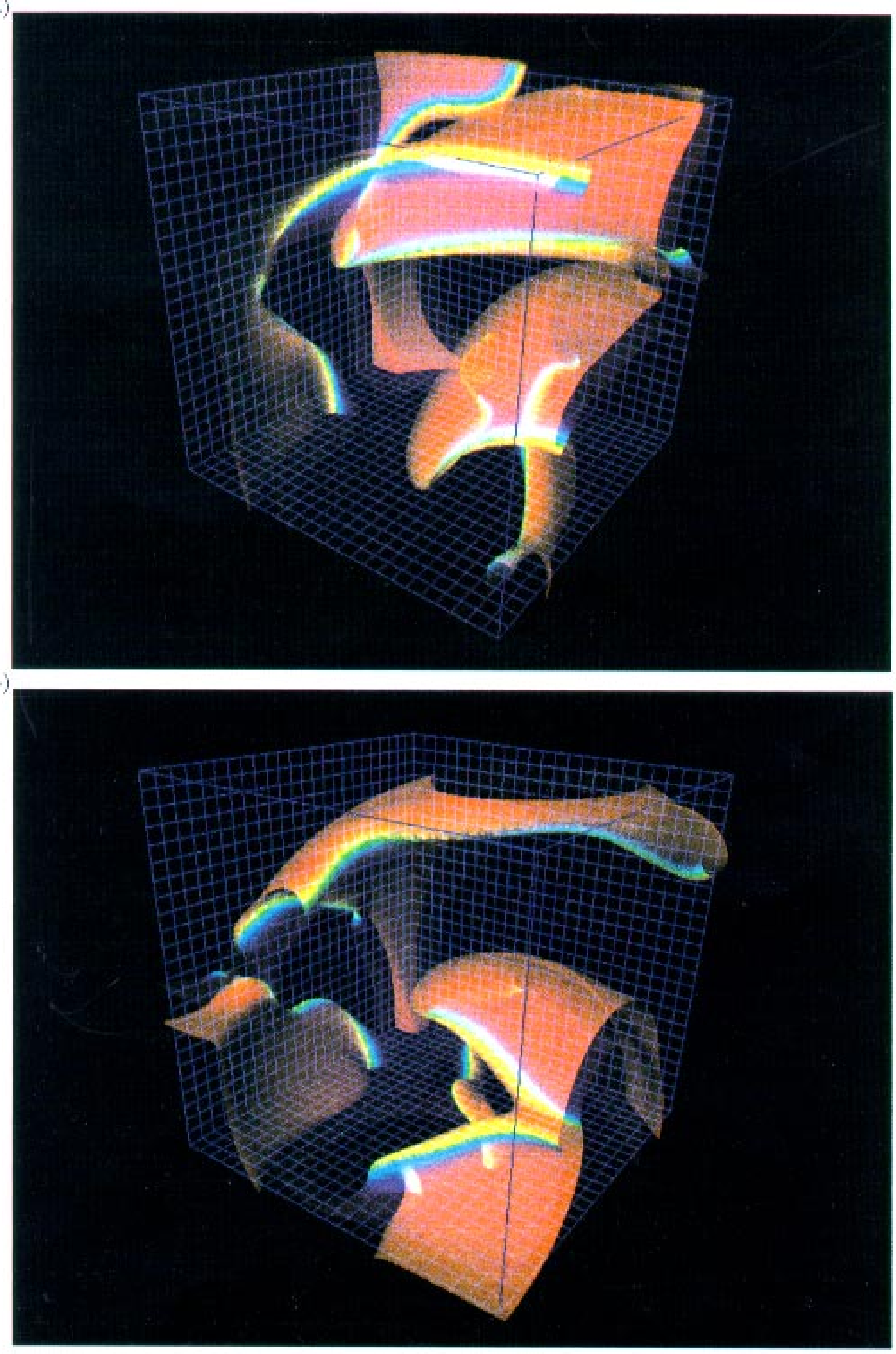
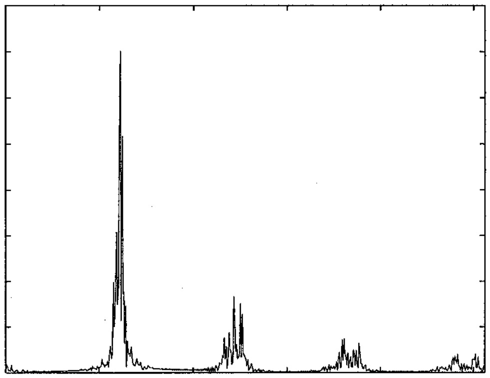
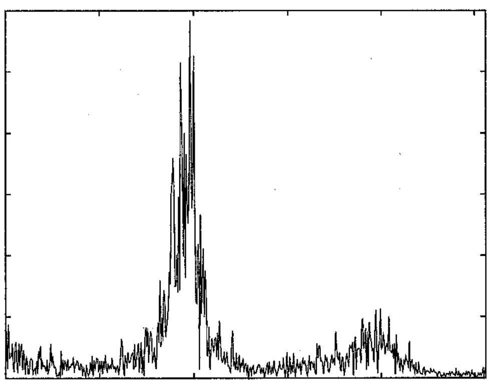


Fig. 4. Multiple scroll waves, in the medium of 100^3 s.s. large. Notations are the same as in Fig. 2. (a) Four filaments can be seen. (b) 2460 t.s. (73.8 t.u. or about two periods) later, six filaments can be seen.

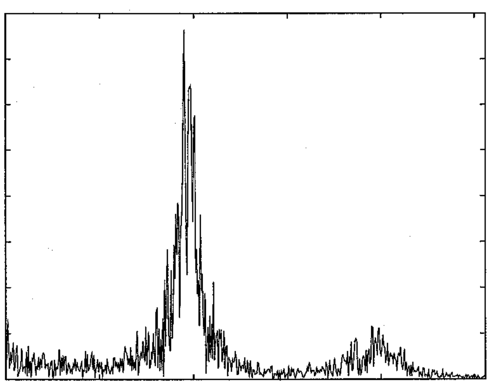
filament instability to evolve, then the simple scroll wave persists, purely independent on one of the spatial variables. Figure 2 shows such a scroll wave in the medium 85^3 s.s. large. Its straight form is stabilized by its short length and also by interaction with boundary, the farther one in the figure. Due to this interaction, the rotation is not rigid but modulated by a rather slow motion, as it is seen in Fig. 5 below, the drift along the boundary. As this solution does not depend on the



(a)



(b)



(c)

Fig. 5. (a–c): Magnitude spectra of time series recorded in the numerics illustrated by Figs. 2–4, respectively. Time series were 8192 values of $\int u(x, y, z, t)dxdydz$ over a half of the medium, recorded in every 10 t.s. = 0.3 t.u. The horizontal scale in all three graphs is 1024 harmonics, which corresponds to 4.17 t.u.$^{-1}$. Spectrum (a) shows nearly periodic dynamics; higher harmonics are slightly split due to the slow motion of the scroll along the boundary. Spectra (b, c) are qualitatively the same and show irregular dynamics, with the main peak corresponding to the rotation frequency. The main frequency in (b, c) is different from that of (a); this reveals strong interaction of vortices with each other and hence inapplicability of the asymptotic theory.

vertical coordinate, it is the well-known purely 2-D phenomenon, described by Ermakova and Pertsov [1986].

Increasing the size of the medium just by one space step in each direction, up to 86^3 s.s., makes the simple scroll wave unstable. Its intermediate evolution involves curving the filament, touching the boundaries and the annihilation of a piece of it, leading to its doubling, which eventually leads to the pattern shown in Fig. 3.

It is a double scroll, in each orthogonal cross-section looking as a pair of likewise rotating spirals, or a two-armed spiral. This rotation is by no means stationary, and is clearly different in different cross-sections. The evolution looks like a competition between inherent instability of the shape of each filament, and their stabilization by mutual attraction. This attraction is, apparently, of the same nature as that observed in 2-D experiments by Ermakova *et al.* [1989]. Its dynamics are apparently chaotic rather than biperiodic (see Fig. 5 below). However, after this double-scroll configuration has been reached, the dynamics lead only to curving of the two filaments, but not multiplications or annihilations.

Further increase in medium size makes any persistent structures unstable very soon, and the dynamics become highly complicated and visually disordered. Figure 4 shows two snapshots of wavefronts in a medium 100^3 s.s. large, made at different time moments. One of the snapshots shows four vortex filaments, the other shows six; in general, their number "oscillates" between two and seven. The careful visual analysis of the "movie" of pictures like Fig. 4 shows relatively long-living (actually, just a few rotations) structures like pairs of twisted helicoidal filaments; one of them can be seen in Fig. 4(a). This is, however, just a visual observation, and has not been tested by any objective method.

Scalar time series were recorded for all the three cases illustrated above; the Fourier spectra of the series are shown in Fig. 5. There is a clear distinction in spectra of the nearly periodic activity in the 85^3 medium and apparently chaotic one in bigger media. It is interesting, however, that spectra of 86^3 and 100^3 media look similar, despite the evolution of the filaments being drastically different. This shows that the scalar time series are not an adequate tool for the analysis of this complex spatio-temporal activity. Attempts to estimate correlation dimension of the attractors in 86^3 and 100^3

media with the method of Rosenstein *et al.* [1993] showed no saturation in embedding dimensions of up to 9.

Low-dimensional chaotic attractors may be possible in smaller media. However, as the example in Fig. 2 shows, such an attractor would not be the only one in the system, and so studying it will require the choice of appropriate initial conditions, which we failed to find so far. Perhaps, double scroll would be a helpful heuristics here.

4. Discussion

Results presented in this paper put forward more questions than give answers. FitzHugh–Nagumo system is only one example of AW media where scroll filaments may have negative tension, and in this model we have considered only one set of parameter values, and, perhaps, other media with this property can demonstrate different behavior. We believe, that however little we have learned about this phenomenon, it demonstrates significant interest for general nonlinear science and, possibly, for applications, and further extensive research of this phenomenon is required.

The apparently chaotic behavior shown in Fig. 3 looks similar to the well-known chaos in Kuramoto–Sivashinsky equation. This is not a coincidence. If $c_3 = 0$ in Eq. (3), then the initially planar curve will remain planar. And if we supply this equation with fourth-order spatial derivative for regularization and rewrite it for function, say, $Y(X, t)$, it will lead to Kuramoto–Sivashinsky equation, which is quite natural, since the origin of the latter, the short-wave instability of the shape of propagating front, is similar to that of (3). Note however, that the analogy is not exact since Eq. (3) is for the period-averaged position of the filament, while the actual evolution for the filament is more complicated even in this simplest case $c_3 = 0$.

In the more general case, $c_3 \neq 0$, the behavior is more complicated still and is essentially three-dimensional. In hydrodynamics, the 3-D turbulence is a significantly more complicated phenomenon than the 2-D one. For AW media, as we have mentioned above, some types of instabilities are possible in 2-D. It would be interesting to compare properties of these different instabilities and chaos generated by them, to see if the 3-D AW turbulence is also much more complicated than the 2-D one. An indirect evidence for that is in the fact that the 3-D turbulence may arise in media which reveal no special properties in two dimensions (i.e. spiral wave rotate rigidly).

Another interesting analogy with hydrodynamic turbulence is the presence of coherent structures. It has been mentioned that in large media and developed AW turbulence, there are repeating motives in the vortices dynamics, like pairs of helical vortices. The existence of coherent structures, including those composed of vortices, is well-known in hydrodynamics [Monin, 1994].

The most interesting possible realization of the 3-D AW turbulence described here is the ventricular fibrillation, a severe life-threatening pathology which occurs as a terminal stage of various cardiac diseases. Despite the long history of the question, phenomenon of fibrillation is not fully understood as yet (which is also true for the hydrodynamic turbulence). The most popular view of the fibrillation is that it involves permanent creation, evolution, multiplication and annihilation of multiple excitation wavelets and micro-reentries, which is the electrophysiological term for the AW vortices. However, the detailed mechanisms of these elementary processes remain unclear. Attempts to explain these in terms of spiral wave evolution in excitable media have been made since the work of Moe *et al.*, [1964], where the immediate cause of the unordered behavior was random scattering of cellular properties, and [Krinsky, 1968], where the key process was interaction of excitation waves with sharp stepwise tissue inhomogeneities. A more recent discovery possibly relevant to this phenomenon is a 2-D instability of spiral waves, seen in a variant of the FHN model [Panfilov & Holden, 1990, 1991], in a model of myocardium [Winfree, 1989; Courtemanche & Winfree, 1991] and in a model of Pt-catalyzed oxidation of CO [Bär *et al.*, 1994], where intensive meander of the spiral leads to breakup of the radiated wavefronts and thus to generation of new spirals. The 3-D AW turbulence described here suggests another mechanism of fibrillation, different from those described so far in two main points, that it is not stipulated by medium inhomogeneities, and it is essentially three-dimensional. Negative filament tensions have been observed so far in excitable media with relatively low excitability, and this correlates with the increased likeliness of fibrillation in "fatigued" tissue.

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