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Stability of scroll ring orientation in an advective field

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The stability of the orientation of scroll rings in the excitable Belousov-Zhabotinsky reaction under an applied electrical current was investigated in experiments and simulations. The parallel and antiparallel orientations of the scroll ring unit vector with respect to the current are two stationary states, the first one unstable, the latter stable. For any other orientation, the scroll rings were forced to rotate by the current. At the stable stationary orientation, the scroll rings may contract or expand under the same applied current depending on the radius of the scroll rings. In simulations, delicate adjustments caused a scroll ring to propagate with a constant radius in an advective field.

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Excitable media including biological and chemical systems generally exhibit excitation waves known as spiral waves [1–6] in two dimensions (2D) and scroll waves [7,8] in three dimensions (3D). Scroll waves and their instabilities [9–12] are involved in the generation of certain types of cardiac arrhythmias, such as ventricular tachycardia and fibrillation [13]. Consequently, many computational studies of 3D excitable media report on numerous forms of complex dynamics of scroll waves [14–23].

Among the scroll waves, scroll rings are a special structure where the filament [24–27]—i.e., the line around which the wave rotates—forms a closed loop. To describe the orientation of the scroll ring, a unit vector $\mathbf{S}$ has been defined by Vinson *et al.* [28] as the normal vector of the filament plane with an orientation given by applying the right-hand rule to $\mathbf{T}$ along the ring-shaped filament. The unit tangent vector $\mathbf{T}$ points in the direction of the local angular wave velocity. In the absence of external forcing, scroll rings in the Belousov-Zhabotinsky (BZ) reaction were observed to contract and eventually vanish [28–31]; however, recent experiments showed that scroll rings may also expand [31,32]. In addition to contraction and expansion, persistent scroll rings propagating with a constant radius have been obtained in numerical simulations [33,34] using the parameters at the boundary between the contraction and the expansion regimes.

External forcing by gradients of temperature [28] or light intensity [35] and by electrical current [36] have been studied. The scroll rings reoriented under the gradients and their lifetimes were prolonged or shortened depending on the alignment of the scroll rings with respect to the gradients. External forcing by temperature or light gradients induces spatial changes in the chemistry [in the reaction term $f(\mathbf{u},\mathbf{k})$ in Eq. (1)] of the reaction-diffusion system, by affecting either the rate constants of the involved reactions in the case of temperature gradients or an additional photosensitive reaction term in the case of light gradients. The situation is different for an applied electrical current, which causes an advective motion of ionic species and a corresponding gradient term in the equation system

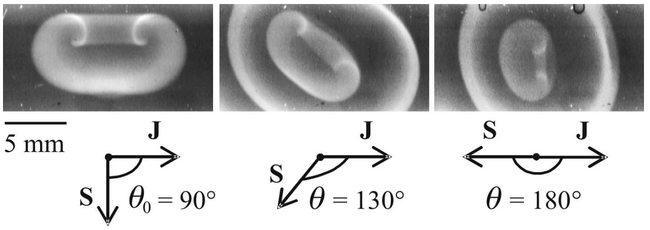
$$\frac{\partial \mathbf{u}}{\partial t} = f(\mathbf{u},\mathbf{k}) + D_u \nabla^2 \mathbf{u} - \mathbf{c}_u \cdot \nabla \mathbf{u}. \quad (1)$$

Here $\mathbf{u}$ is the vector of chemical species, $f(\mathbf{u},\mathbf{k})$ the reaction terms which depend on the concentrations of the reactants $\mathbf{u}$ and the rate constants $\mathbf{k}$, D_u the respective diffusion coefficients, and $\mathbf{c}_u$ the advective velocity induced by the electrical forcing.

In this paper, we present a study of the stability of both the scroll ring orientation and the scroll ring radius in the BZ reaction under the influence of an electrical current. Under these conditions, the scroll rings are subjected to two simultaneous processes, namely, an intrinsic contraction and a possible reorientation with respect to the direction of the applied current. When the orientational stability of scroll rings was studied, two stationary orientations were found and their stabilities were determined. While the orientation of a scroll ring parallel to the current was unstable, an antiparallel orientation was found to be stable. By preparing scroll rings that were aligned antiparallel to the current, we investigated the influence of the initial radius on the fate of the scroll rings. At a given electrical current, a critical radius r_c was found, which separates contracting $(r_0 < r_c)$ from expanding $(r_0 > r_c)$ scroll rings. Finally, all scroll rings drifted toward the anode, i.e., in the opposite direction to the applied current.

The BZ reaction was prepared according to recipe II of Ref. [37], which in a 2D system exhibits rigidly rotating spiral waves. The BZ medium contained 0.050 mol l^{-1} malonic acid, 0.200 mol l^{-1} H_2SO_4, 0.050 mol l^{-1} $NaBrO_3$, 0.5 mmol l^{-1} ferroin, 0.05 mmol l^{-1} sodium dodecyl sulfate (SDS), and 1.0 wt % agarose. The surfactant SDS and the agarose gel were employed to suppress the generation of CO_2 bubbles and to prevent hydrodynamic effects, respectively.

The dynamics of the scroll rings under an electrical current were observed from two perpendicular projections of the wave structures as in Refs. [36,38]. For this purpose, the BZ reaction was placed in a rectangular reactor made from transparent Plexiglas of $12 \times 12 \times 60$ mm^3 volume. The longitudinal ends of the reactor chamber were connected to electrolytic compartments, which were filled with BZ reactants of the same concentration as that in the main compartment (but without the gel). The electrolytic compartments were separated from the main part by porous glass filters to prevent any perturbation of the scroll ring by gas bubbles formed during electrolysis. A constant electrical current was applied via two planar platinum plate electrodes (10×20 mm^2) such that the direction of the current was horizontal. The reactor



(a) 0 min (b) 37 min (c) 70 min

FIG. 1. Lateral projections of a scroll ring in the BZ reaction under an electrical current. The applied current density **J** ($J=|\mathbf{J}|=40$ mA cm^{-2}) pointed to the right. (a) At the beginning, the unit vector **S** was perpendicular to **J**. The projections of the scroll ring showed up as two counter-rotating spirals for the entire experiment. (b) The applied current induced a continuous reorientation of the scroll ring, until (c) **S** was antiparallel to **J**. The dimensions of the images are 17×8.8 mm^2.

was mounted onto a support and placed into a Plexiglas thermostatting bath at 22.0 ± 0.1 °C.

Scroll rings with different initial orientations θ_0 with respect to the applied current density **J** (Fig. 1) were initiated by using a two-layer strategy [29,37], which consists of filling the reactor with a first layer of reaction medium, initiating a wave front with a free edge at its top surface, and subsequently adding a second layer of the medium on top of the first layer. The initial orientation θ_0 can be adjusted by setting the reactor with a tilt angle with respect to the ground during the initiation. The top surface of the first layer aligns horizontally, but at a desired tilt angle with respect to the bottom of the reactor which, in turn, yields a filament plane of the scroll ring that has a desired angle with respect to the applied electrical current. Typical lateral projections of a scroll ring in the BZ reaction appear as two counter-rotating spirals (Fig. 1).

The scroll ring dynamics were evaluated as described in Ref. [36]. The cores of the counter-rotating spirals (Fig. 1) were determined by superposition of a series of images taken during one rotation period. The center of the area never visited by wave fronts was taken as the center of the core. The radius r of the scroll ring was estimated as half of the straight line connecting the two core centers. The unit vector **S** of the scroll ring was perpendicular to this connecting line. The orientation θ is the angle between **S** and the applied current density **J**.

Figure 1 shows a series of projections during a reorientation of a scroll ring. An electrical current density $J=40$ mA cm^{-2} pointing to the right was applied to the system. The filament initially laid in a horizontal plane and its unit vector **S** pointed downward, leading to an initial orientation $\theta_0=90°$ [Fig. 1(a)]. Under the applied current, the filament plane rotated [Figs. 1(b) and 1(c)] and the angle θ increased to 180°. During this reorientation, the scroll ring both drifted toward the anode and also contracted, which led to a self-annihilation of the scroll ring at the end of the experiment. In experiments with a smaller field strength (e.g., $J=30$ mA cm^{-2}, $\theta_0=90°$) scroll rings also reoriented in a similar way. However, they self-annihilated at $\theta < 180°$ since the reorientation rate is proportional to the electrical current [28,36].

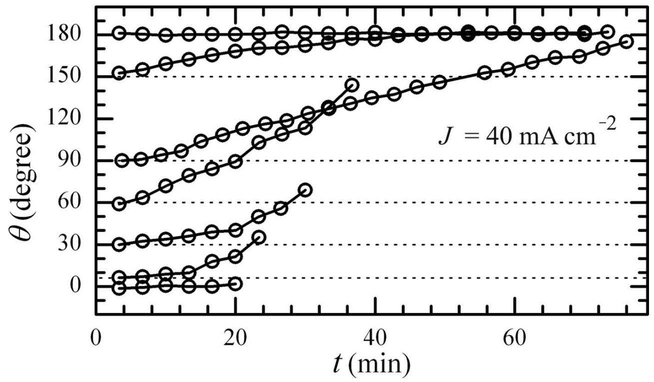


FIG. 2. Orientation of scroll rings in the BZ reaction under an electrical current. The scroll rings were initiated with different initial orientations $\theta_0=0°$, 6°, 30°, 60°, 90°, 150°, and 180° while a constant electrical current density of $J=40$ mA cm^{-2} was applied during the entire experiments. Except for the experiments starting with $\theta_0=0°$ and 180°, the external field caused a scroll ring reorientation and the angle always increased toward 180°. During the experiments, the scroll rings contracted and eventually self-annihilated.

To study the stability of the scroll ring orientation under an electrical current, experiments were performed using different initial angles θ_0. Figure 2 shows the scroll ring orientation in the experiments with initial angles $\theta_0=0°$, 6°, 30°, 60°, 90°, 150°, and 180°. In many of these experiments, the scroll rings contracted and self-annihilated while the reorientation was still in progress. By varying θ_0, we have investigated the dynamics of the scroll rings in overlapping ranges of orientation (6°–35°, 30°–70°, 60°–144°, 90°–180°, and 150°–180°). For $6° \leq \theta < 180°$, the scroll rings were found to change their orientation. In fact, θ increased toward 180°. When $\theta=0°$ or 180°, the orientation of the scroll rings remained unchanged. The results indicate that both parallel and antiparallel orientations ($\theta=0°$ and 180°) are stationary states. As every angle $\theta \geq 6°$ leads to an increase of θ toward 180°, the antiparallel orientation of the scroll ring unit vector **S** with respect to the current **J** is a stable solution of the system. By contrast, the parallel orientation is also a stationary solution; however, it represents an unstable stationary state, since small derivations will induce a reorientation of the scroll ring.

As we have shown recently [36], the electrical forcing can extend the lifetime of a self-contracting scroll ring with an initial angle $\theta_0=90°$. In the following, we investigate the stability of scroll rings in dependence on their radii. To eliminate any effects of the reorientation, the experiments were performed at the stable stationary orientation $\theta=180°$. The initial radius r_0 of the scroll ring was varied while θ and J were kept constant (Fig. 3). At $J=40$ mA cm^{-2}, a small scroll ring with $r_0=2.6$ mm still contracted; however, it lasted for a longer time (>50 min) than that in the free running case (no forcing) whose lifetime ≈30 min for the same r_0. By contrast, a larger scroll ring with $r_0=3.3$ mm expanded. This implies that there must exist an initial radius ($2.6 < r_0 < 3.3$ mm) where the self-contraction of the scroll ring and the expanding effect of electrical forcing are balanced, leading to a persistent scroll ring of invariant radius.

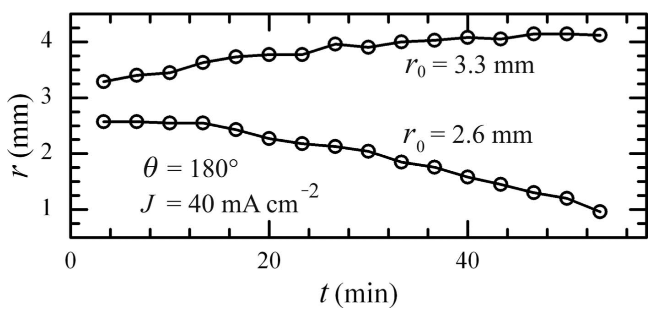


FIG. 3. Mean radius of scroll rings in the BZ reaction under an applied electrical current. The orientation of the scroll rings was constant at $\theta = 180°$. In the presence of an electrical current density of $J = 40$ mA cm^{-2}, a scroll ring with an initial radius $r_0 = 3.3$ mm expanded, while a smaller ring of $r_0 = 2.6$ mm contracted.

3D numerical simulations using the two-variable Oregonator model [39–41] together with an advective term accounting for the applied electric field [42–45] reproduced well the experimental results presented above. An electric field $\mathbf{E}$ (field strength $E = |\mathbf{E}|$) was applied in the x direction so that the model equations read

$$\frac{\partial u}{\partial t} = \frac{1}{\epsilon}\left(u - u^2 - fv\frac{u-q}{u+q}\right) + D_u\nabla^2 u - M_u E\frac{\partial u}{\partial x},$$

$$\frac{\partial v}{\partial t} = u - v + D_v\nabla^2 v - M_v E\frac{\partial v}{\partial x}. \tag{2}$$

The parameters were chosen as in Refs. [40,44]: $q = 0.002$, $f = 1.4$, $\epsilon = 0.01$, the diffusion coefficients $D_u = 1$ and $D_v = 0.6$, and the ionic mobilities $M_u = -1.0$ and $M_v = 2.0$. The simulations were performed using an explicit Euler method with a 19-point approximation of the 3D Laplacian [46] and centered-space approximation of the gradient term. The grid space $\Delta x = 0.2$ and time step $\Delta t = 0.012$ as required for numerical stability $\Delta t_{\max} = (3/8)(\Delta x)^2$ [46]. The size of the system is $350 \times 200 \times 200$ grid points as used in Ref. [36].

Scroll rings with different initial orientations θ_0 were initiated using a similar procedure as in the experimental part: First, a spherical wave front was created by a local perturbation. When the sphere reached a desired size, one hemisphere was erased by setting $u = 0$, creating an open edge of the remaining wave front, which curled in to form a scroll ring. The initial orientation θ_0 depends on the angle of the open edge with respect to the x axis, i.e., to the vector $\mathbf{E}$.

For the simulations, the filament, the radius r, and the orientation θ can be measured at any time. The filament of the scroll ring is defined as the intersection line of surfaces $u = 0.15$ and $v = 0.0935$, which ensures that $\partial u / \partial t = 0$ on the filament [41]. After the filament was detected, the radius r and the orientation θ were calculated.

The scroll ring reorientation for simulations starting with $\theta_0 = 0°$, 6°, 20°, 40°, 90°, and 180° is shown in Fig. 4(a). Except for $\theta_0 = 0°$ and 180°, the angle θ increased, as also found in the experiments. Furthermore, the scroll rings contracted and self-annihilated so that the reorientation can be studied in a limited range of angles for a specific value of θ_0.

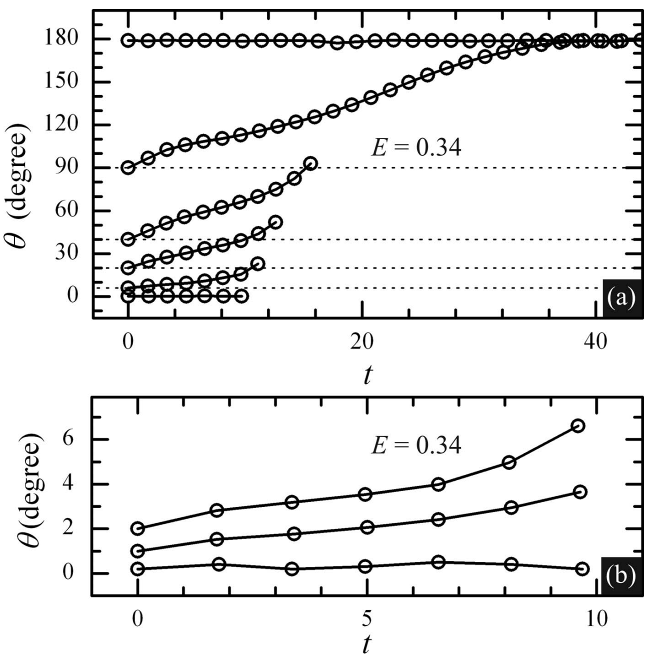


FIG. 4. Orientation of scroll rings in the Oregonator model under an advective field. The scroll rings were initiated with different initial orientations (a) $\theta_0 = 0°$, 6°, 20°, 40°, 90°, and 180°; and (b) $\theta_0 = 0°$, 1°, and 2°. A constant electric field ($E = 0.34$) was applied during the entire simulations. Except for the simulations starting with $\theta_0 = 0°$ and 180°, the external field caused scroll ring reorientation. For $\theta \neq 0°$, the angle always increases toward 180°. During the simulations, the scroll rings contracted and eventually self-annihilated.

An advantage of the simulations is that a small initial angle θ_0 can be set precisely. As shown in Fig. 4(b), the simulations were performed with θ_0 as small as 1° and 2° and θ still increased in both cases. The reorientation of scroll rings in the entire interval of angles between 0° and 180° has been determined in overlapping subset ranges (1°–4°, 2°–7°, 6°–23°, 20°–52°, 40°–93°, and 90°–180°). The simulations show

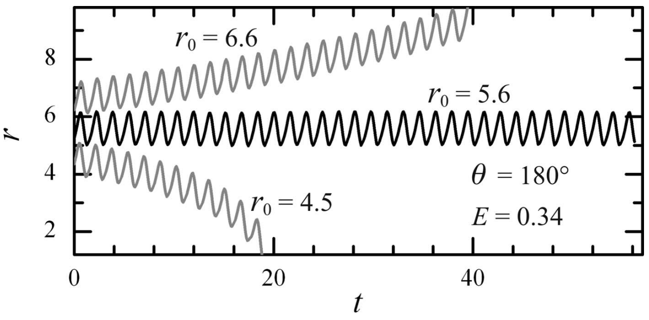


FIG. 5. Radius of scroll rings in the Oregonator model under an advective field. A constant electric field $E = 0.34$ was applied antiparallel to the unit vector of the scroll rings ($\theta = 180°$). Depending on their initial mean radius r_0, large scroll rings expanded ($r_0 = 6.6$) while small ones contracted ($r_0 = 4.5$). Furthermore, a balance of self-contraction of the scroll ring and the effect of the electric field led to a persistent scroll ring ($r_0 = 5.6$) whose mean radius was constant. The curves show the instantaneous radii of the scroll rings.

that the angle θ increased toward 180° if $\theta_0 \geq 1°$, thus reproducing the existence of two stationary orientations at $\theta = 0°$ and 180°. As in the experiments, the parallel orientation ($\theta = 0°$) is an unstable stationary state while the antiparallel alignment ($\theta = 180°$) is stable.

A persistent scroll ring in an advective field could be realized in our simulations. Figure 5 shows the instantaneous radii of scroll rings in the simulations starting with different r_0 while $\theta = 180°$ and $\mathbf{E}$ was kept constant. At $E = 0.34$, small scroll rings ($r_0 = 4.5$) contracted while large scroll rings ($r_0 = 6.5$) expanded. For $r_0 = 5.6$, the scroll ring traveled with a constant mean radius. Note that the plotted radii oscillate around local extrema since the instantaneous filament rotated around a small tube composed of 2D spiral cores.

In summary, we have presented a study on the stability of scroll ring dynamics under the influence of an electrical current. Unless the scroll rings were aligned parallel ($\theta = 0°$) or antiparallel ($\theta = 180°$) to the applied current, they reoriented toward the antiparallel orientation. Hence, the parallel orientation is an unstable stationary state while the antiparallel alignment is a stable orientational stationary state. At the stable orientation ($\theta = 180°$), the lifetime of the scroll rings, which intrinsically contract, was prolonged when an electrical current was applied. Because the self-contraction rate is inversely proportional to the radius and the expanding effect is linear with respect to the applied current at $\theta = 180°$ ($dr/dt = -\alpha/r + \beta J$, where α and β are constant [28,36]), an expansion of sufficiently large scroll rings was observed in the presence of electrical forcing.

The simulations using the Oregonator model with an advective field reproduced well all of aspects found in the experiments, namely, the angles of the unstable and stable stationary orientations with respect to the applied field, as well as the shrinkage and growth of the scroll rings as a function of their initial radii in case of the stable stationary orientation. Furthermore, some situations which are difficult to realize in experiments were accomplished by the simulations. First, a scroll ring with an initial angle θ_0 as small as 1° can be initiated precisely in the simulations, thus supporting the conclusion that the stationary orientation at 0° is unstable toward perturbations. Second, a persistent scroll ring subjected to electrical forcing at the stable stationary orientation $\theta = 180°$ requires an exact balance of the intrinsic contraction and the electrical expansion. By keeping the electric field constant and performing a fine adjustment of the scroll ring radius, the balance condition was satisfied in the simulations, leading to a persistent scroll ring traveling in the reaction-diffusion-advection system.

The exact conditions required for obtaining persistent scroll rings, i.e., rings of constant mean radius, in experiments are currently under investigation. With this purpose, we have started a systematic study of the scroll ring dynamics at stable stationary orientation as a function of the initial radius and the applied electrical current in both experiments and simulations. The results will be presented in a further publication.

Finally, it is worthwhile to note that the advective term in Eq. (1) represents a convenient target for manipulating scroll rings without affecting the reaction and diffusion parts. This flexibility can be readily exploited in implementations of more complex electrical currents (either in the form of the electrical current or in the geometrical orientation of the electrodes) and even feedback manipulations as typically used for control experiments. These types of manipulation can be easily realized in experiments and in calculations, thus providing the possibility of an elaborate manipulation and control of scroll rings.

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