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Reorientation of scroll rings in an advective field

Chaiya Luengviriya,[1,2] Stefan C. Müller,[1] and Marcus J. B. Hauser[1]
[1]*Biophysics Group, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany*
[2]*Department of Physics, Kasetsart University, 50 Phaholyothin, Jatujak, Bangkok, 10900, Thailand*
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When scroll rings in the excitable Belousov-Zhabotinsky reaction are subjected to an applied electrical current, a reorientation of the scroll ring is induced which is accompanied by a linear drift towards the cathode. The findings can be explained using a modified theory of local filament dynamics under parameter gradients. Numerical simulations using the Oregonator model with an additional advective term accounting for the applied electric field reproduce the experimental results and provide insights into the deformation of the structure of the filament during the reorientation.

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Spiral waves of excitation have been observed in thin layers of excitable media [1]. Unlike the two-dimensional (2D) case, the dynamics of scroll waves [2] (i.e., the 3D analogs of the spiral waves) are determined not only by the system parameters [3] but also the topology [4] of the wave filament—i.e., the line around which the wave rotates. It is conjectured that scroll waves and their instabilities are involved in causing certain types of cardiac arrhythmia, such as ventricular tachycardia and fibrillation [5]. Consequently, various computational studies of 3D excitable media report on numerous forms of complex dynamics of scroll waves [6].

Scroll rings are a special structure of scroll waves where the filament forms a closed loop. To describe the orientation of the scroll ring, a unit vector **S** has been defined by Vinson *et al.* [7] as the normal vector of the filament plane with an orientation given by applying the right-hand rule to **T** along the ring-shaped filament. The unit tangent vector **T** points in the direction of the local angular wave velocity. So far, in the absence of external forcing, scroll rings in the Belosov-Zhabotinsky (BZ) reaction were observed always to shrink and eventually vanish [7–9]. In addition, they drift slowly in the direction of their unit vector.

Scroll rings in the BZ reaction have been manipulated by applying gradients of temperature [7] or light intensity [10]. The scroll rings reoriented under the gradients and their lifetime were prolonged or shortened depending on the alignment of the scroll rings with respect to the gradients. Both types of external control induce spatial changes in the chemistry of the underlying reaction-diffusion system, either by affecting the rate constants of the involved reactions (manipulation via temperature gradients) or by an additional photosensitive reaction term (manipulation by light gradients). This means that the perturbations applied so far cause changes in the reaction term $f(\mathbf{u},\mathbf{k})$ of the generic reaction-diffusion system:

$$\frac{\partial \mathbf{u}}{\partial t} = f(\mathbf{u},\mathbf{k}) + D_u \nabla^2 \mathbf{u}, \tag{1}$$

where **u** is the vector of chemical species, D_u the respective diffusion coefficients, and $f(\mathbf{u},\mathbf{k})$ the reaction terms which depend on the concentrations of the reactants **u** and the rate constants **k**.

Vinson *et al.* [7,11] have modified the local filament theory [4] for the dynamics of scroll rings under parameter gradients and shown that numerical calculations agree quantitatively with the experiments using temperature gradients.

In this Rapid Communication, we present a study on the dynamics of scroll rings in the BZ reaction under the influence of an external electrical current. The applied current causes the advective motion of ionic species in the electrical field. In this case, the external perturbation corresponds to an additional advective term, rather than a change in the chemistry. This yields a generic equation system of the form

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

where $\mathbf{c}_u$ is the advective velocity induced by the electric field. To provide support for the experimental findings, we performed numerical simulations using the two-variable Oregonator model [12–14] for the BZ reaction supplied with an additional advective term [15–17]. The compliance of the scroll ring reorientation with the local filament theory modified for parameter gradients [11] was tested.

Experiments were performed using the BZ reaction according to recipe II of Ref. [18], which in a 2D system exhibits rigidly rotating spiral waves. To prevent hydrodynamic perturbations, the BZ reaction was embedded in an agarose gel. We observed the dynamics of a scroll ring under an electrical current from two perpendicular projections of the wave structures as in Ref. [19]. To this purpose, the BZ reaction was placed in a rectangular reactor made from transparent Plexiglas of $12 \times 12 \times 60\ \text{mm}^3$ volume. The longitudinal ends of the reactor chamber were connected to electrolytic compartments, which were filled with the BZ reaction of the same compositions as that in the main compartment (however 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 ($10 \times 20\ \text{mm}^2$) such that the direction of the current was

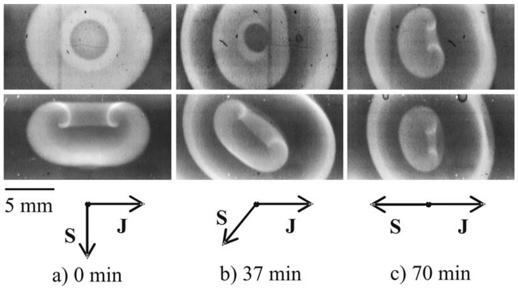

FIG. 1. Projections of a scroll ring in the BZ reaction under an applied electrical currrent. Top row: top projection. Bottom row: lateral projection. The applied current density $J=40\ \mathrm{mA\ cm^{-2}}$ pointed to the right. (a) At the beginning, the unit vector **S** was perpendicular to **J**. The projections of the scroll ring appeared as circles (top view) and two counterrotating spirals (lateral view). (b) The applied current caused a continuous reorientation of the scroll ring, until (c) **S** was antiparallel to **J**. The dimensions of the images are $17\times 8.8\ \mathrm{mm^2}$.

horizontal—i.e., pointing from one vertical planar electrode to the other.

The reactor was mounted onto a support and placed into a Plexiglas thermostating bath at $22.0\pm 0.1\ °\mathrm{C}$. A 45° tilted mirror fitted underneath the reactor allows for the illumination from the side and a simultaneous observation of the lateral and vertical views of the reactor.

Scroll rings were initiated by using a two-layer strategy [8,18], which implies filling the reactor with a first layer of reaction medium, initiating a wave front with a free edge at the top surface of the first layer, and subsequently filling a second layer of the medium on top of the first layer.

Figure 1 shows a scroll ring subjected to electrical current density value $J=40\ \mathrm{mA\ cm^{-2}}$ as observed from two perpendicular projections, the top and lateral views. The direction of the applied current points to the right of the figure. The filament initially lies in a horizontal plane and its unit vector **S** points downwards, forming a right angle with the current density vector **J** [Fig. 1(a)]. Hence, the scroll ring appears as circular wave fronts and two counterrotating spirals in the top and lateral projections, respectively. Due to the effect of the applied current, the filament plane rotated [Figs. 1(b) and 1(c)]. During this reorientation, the scroll ring both drifted towards the cathode and also contracted. At the end of the experiment, **S** was antiparallel to **J** [Fig. 1(c)] before the scroll ring disappeared due to contraction and subsequent self-annihilation.

To evaluate the dynamics of scroll rings in detail, we estimated the angle θ of **S** with respect to **J**, as well as the radius r and the center (x,z) of the scroll ring. The lateral projection was used for evaluation purposes, since in this view the shape of the scroll ring projection remains a pair of counterrotating spirals during the reorientation of the scroll ring (Fig. 1).

Figure 2 shows the position of core centers of two counterrotating spirals in the lateral projection. The spiral cores were determined by superposition of an image series taken during one rotation period. The center of the area never visited by the spiral wave was taken as the center of the core.

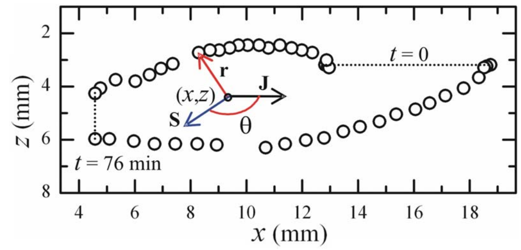

FIG. 2. (Color online) Dynamics of the scroll ring in the BZ reaction under an applied electrical current density $J=40\ \mathrm{mA\ cm^{-2}}$. Circles show core centers of two counterrotating spirals in the lateral projection at $t=0-76$ min. The radius r (i.e., $r=|\mathbf{r}|$) and center (x,z) of the scroll ring were estimated as half of the distance and the center of mass of a pair of the core centers, respectively. The unit vector **S** is perpendicular to **r** and accounts for the spiral rotating direction. The orientation θ is the angle between **S** and **J**.

We define a straight line connecting the two core centers as the diameter of the ring filament. This allows the determination of the radius r (i.e., $r=|\mathbf{r}|$), the orientation θ, and the center (x,z) of the scroll ring as shown in Fig. 3.

Starting with an initial angle $\theta_0=90°$, the scroll ring reoriented under the applied current leading to an increase of θ from 90° to 180° (circles in Fig. 3). The reorientation is accompanied by a linear drift towards the cathode with a rate of $0.17\ \mathrm{mm\ min^{-1}}$ and a slight downward drift (rate $=0.03\ \mathrm{mm\ min^{-1}}$). Due to intrinsic contraction, the radius of the scroll ring diminished and the scroll ring eventually vanished (circles in Fig. 3). The lifetime of the scroll ring was $\approx$80 min. A comparison with the experiment in the absence of the external electrical current shows that the external forcing also prolonged the lifetime of the scroll ring, since in

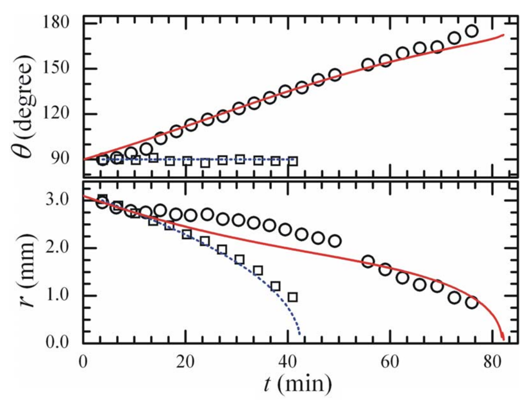

FIG. 3. (Color online) Reorientation of the scroll ring under an electrical current density $J=40\ \mathrm{mA\ cm^{-2}}$. Top and bottom graphs show the dynamics of the orientation (θ) and the radius (r) of the scroll ring, respectively. Circles and squares indicate results from experiments with and without applied current, respectively. During the reorientation under $J=40\ \mathrm{mA\ cm^{-2}}$, the angle θ increased from 90° to 180° and the radius r decreased, however, slower than in the case of $J=0$. Solid and dotted lines show numerical calculations using the theory of local filament dynamics under parameter gradients with $J=32\ \mathrm{mA\ cm^{-2}}$ and $J=0$, respectively.

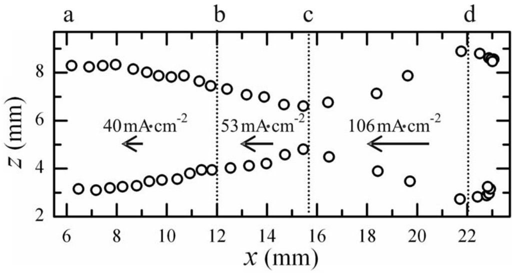

FIG. 4. Manipulation of a scroll ring by a stepwise variation of the electrical current. Circles show the position of core centers of two counterrotating spirals in the lateral projection at 200-s intervals. The current density **J** was antiparallel to the unit vector **S** of the scroll ring (**J** pointed to the left), causing the scroll ring to drift to the right without reorientation. For $0<t<37$ min (*a* to *b*), J was kept constant at 40 mA cm^{-2} and the scroll ring drifted to the right with decreasing radius. At $t=37$ min (*b*), J was increased to 53 mA cm^{-2}; however, the radius of the scroll ring still contracted. Shortly before self-annihilatition occurred, J was increased to 106 mA cm^{-2} ($t=54$ min, at *c*). Under this strong applied field, the scroll ring expanded. At $t=67$ min (*d*), the external field was switched off and the scroll ring contracted again at an approximately fixed position.

experiments without applied current, the scroll ring of the same initial radius r_0 (≈ 3 mm) vanished within 45 min (squares in Fig. 3).

Experimental observations follow the theory of local filament dynamics [4] subjected to the influence of parameter gradients [see Fig. 2 and Eq. (5) in [11]]. In the case where the electrical current acts as a gradient, the changes in radius r and in the angle θ read

$$\frac{dr}{dt} = -\frac{\alpha}{r} - \beta J \cos\theta, \tag{3}$$

$$\frac{d\theta}{dt} = \frac{\beta J}{r}\sin\theta, \tag{4}$$

where α is the intrinsic contraction constant of the scroll ring that was measured in the absence of external forcing (squares in Fig. 3) as $\alpha=0.12\pm0.01$ mm^2 min^{-1}. This agrees well with the value measured in Refs. [7,8]. The coefficient $\beta=0.17\pm0.01$ mm^3 min^{-1} mA^{-1} was obtained from the experiments of scroll waves with a straight filament under applied electrical current ($J=40$ mA cm^{-2}). The calculations of the orientation and radius of the scroll ring with $J=32$ mA cm^{-2} (solid lines in Fig. 3) are in good agreement with the experimental data.

Control of the scroll ring using electrical current can be performed efficiently. The strength and direction of the applied current can be changed within seconds, which is very short compared to the wave dynamics (period of spiral rotation ≈ 200 s). Figure 4 shows the evolution of a scroll ring under a stepwise variation of the electrical current at an antiparallel orientation ($\theta=180°$). The plots show the positions of the scroll ring (i.e., the core centers of a counterrotating spiral pair at 200-s intervals) which drifted to the right of the figure while **J** pointed to the left. Starting with $J=40$ mA cm^{-2} (at *a*), the scroll ring contracted slowly. At $t=37$ min (*b*), J was increased to 53 mA cm^{-2} and the ring radius still decreased. When the radius was ≈ 1 mm (at $t=54$ min, *c*), J was increased drastically to 106 mA cm^{-2}. This strong forcing led to an expansion of the scroll ring. Note that under a weaker field—e.g., $J=40$ mA cm^{-2}—the scroll ring with $r\approx 1$ mm would self-annihilate very soon (after about one period). Finally, the current was switched off ($J=0$ mA cm^{-2}) at $t=67$ min (*d*), thus causing the scroll ring to shrink again.

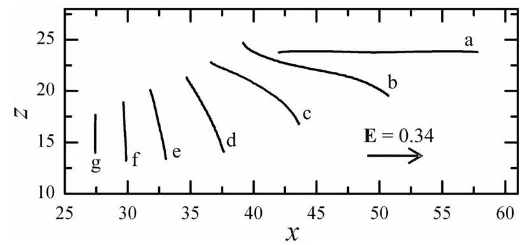

FIG. 5. The *xz* projection of scroll ring filaments in the Oregonator model under an applied electric field $E=0.34$ at $t=0$, 9.2, 18.4, 27.6, 32.9, 38.9, and 42.3 (a–g). Their shape and orientation changed with time. During the reorientation, the pattern of filament projection changed from an almost straight (*a*) to wavy (*b*), and curved line (*c*, *d*). Towards the end of the simulations (e–g), the projection pattern returned to a straight line before the scroll ring self-annihilated.

In our numerical simulations, we used the two-variable Oregonator model with advection terms of both u and v accounting for the electric field strength E in the x direction:

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

$$\frac{\partial v}{\partial t} = u - v + D_v\nabla^2 v - M_v E\frac{\partial v}{\partial x}. \tag{5}$$

The parameters were chosen as in Refs. [13,16]: $q=0.002$, $f=1.4$, $\epsilon=0.01$, 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 [20] and centered-space approximation of the gradient term. The grid space $\Delta x=0.2$ and time step $\Delta t=0.012$. The size of the system is $350\times200\times200$ grid points.

A scroll ring is initiated using a procedure similar to that described in the experimental part. First, a spherical wave front is created by a local perturbation. When the sphere has a desired size, one hemisphere is erased by setting $u=0$, creating an open edge of the remaining wave front, which curls in to form a scroll ring. The wave filament is defined as the intersection line of the surfaces $u=0.15$ and $v=0.0935$, which ensures that $\partial u/\partial t=0$ on the filament [14].

Figure 5 shows the dynamics of a scroll ring filament in the simulations using $E=0.34$ and the initial angle $\theta_0=90°$. As found in the experiments, the scroll ring reoriented, contracted, drifted linearly antiparallel to the electric filed (rate =0.53) and downwards (rate=0.21), and eventually self-annihilated.

The projection of the filament on the *xz* plane shows the orientation of the filament with respect to the electric field **E**. During the reorientation, the filament plane deformed from a flat (*a*) to wavy (*b*) and curved (*c*, *d*) plane. Later, the curved plane straightened to a flat plane again (*e*–*g*). The *xz* projection of the closed-loop filament has a straight or a curved line shape, implying that the reorientation and the modulation of the filament plane never occurred in the *y* direction.

In summary, we have studied the influence of an applied direct electrical current on scroll rings in the BZ reaction. The applied field caused a scroll ring reoriention from perpendicular to antiparallel with respect to the direction of the applied current. Even though the scroll rings still contracted intrinsically and eventually self-annihilated, the applied current prolonged the lifetime of the scroll rings.

Numerical calculations using the kinematic theory of the local filament dynamics under parameter gradients [7,11] agreed well with the experimental results presented here. Similar behavior has also been reported for a system subjected to temperature gradients, thus showing common influences of the electrical current and the gradient of temperature [7] on the dynamics of scroll ring in the BZ reaction.

The experimentally observed effects of the applied electrical current are reproduced to a good agreement by 3D numerical simulations using the Oregonator model with an additional advective migration term. The advective term in Eq. (2) may be viewed as a perturbation term, which in the present case models the applied electrical field; however, more complex types of external forcing can be conveniently implemented by a simple modification of this perturbation, leaving the reaction and diffusion parts untouched. Thus, the effects of different kinds of perturbations may be easily compared to each other.

Finally, we demonstrated that a manipulation of scroll rings by using electrical current can be done effectively in experiments. Unlike the case of temperature gradients, a desired current is applied precisely in a short time. As an example, the strength of applied current density was increased substantially within a short time to cause a small contracting scroll ring, which otherwise would soon be self-annihilated, to survive and expand.

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