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Evidence for Burgers' equation describing the untwisting of scroll rings

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Abstract – We study the dynamics of rotating scroll waves in three-dimensional excitable systems. Experiments are carried out with the 1,4-cyclohexanedione Belousov-Zhabotinsky reaction and wave patterns are measured using optical tomography. We create twisted scroll rings for which the rotation phase varies along their circular rotation backbone and measure the untwisting dynamics of the collapsing structures. Experimental data reveal the formation of an asymmetric, plateau-like phase profile with a growing region of leading phase and a shrinking region of lagging phase. The experimental data support a quantitative description in terms of a nonlinear diffusion equation.

In three-dimensional excitable media, most wave patterns are organized by scroll waves. They are the dominant self-sustaining wave source and analogous to rotating spirals in two dimensions. These rotors have been observed in numerous biological systems such as the cellular slime mold *Dictyostelium discoideum* [1,2], cardiac tissue [2,3], and retinal neurons [4]. Moreover, scroll waves have been linked to ventricular arrhythmias [5] and sudden cardiac death in humans. Fully understanding these systems clearly requires the characterization of the dynamics of scroll waves.

Scroll waves rotate around one-dimensional curves, called filaments, and the system is adequately described by the spatio-temporal behavior of these lines [6]. The reduction of a complex three-dimensional pattern to a one-dimensional curve has allowed beautiful theoretical descriptions [7]. Recent experimental work has tested some of these results for curved, but untwisted, filaments [8,9], including the collapse of scroll rings. The influence of gradients in rotation phase along the filament, called twist, has been described theoretically by Burgers' equation [10,11] and studied qualitatively in experiments [12]. A measurement of the average twist was made earlier [13]; however, the local twist dynamics have yet to be quantified in experiments.

The nonlinear diffusion equation, or Burgers' equation, is

$$u_t + uu_x = du_{xx}, \qquad (1)$$

where u is a one-dimensional field, the subscripts t and x denote partial differentiation with respect to time and space, respectively, and d is a constant diffusion parameter. This equation was originally proposed in hopes of modeling turbulence in fluid flow [14]. While ultimately unsuccessful in the field of fluid turbulence, Burgers' equation has more recently been applied to a number of other systems including interface growth [15], cosmology [16], and traffic flow [17,18]. For excitable media, a form of eq. (1) was derived to describe the spatial coupling of the oscillation phase along the filament of a scroll wave [10,11]. Here we report experiments in an excitable medium that can be explained by the effects of the nonlinear term in eq. (1) on the untwisting dynamics of a twisted scroll wave filament.

Experiment and analysis. – Experiments employ the autocatalytic 1,4-cyclohexanedione Belousov-Zhabotinsky (CHD-BZ) reaction [19]. Initial concentrations of reagents are as follows: $[H_2SO_4] = 0.6$ M, $[NaBrO_3] = 0.18$ M, $[CHD] = 0.19$ M, and $Fe[batho(SO_3)_2]_3^{-4} = 0.475$ mM. The reaction is carried out in a viscous polyacyrlamide solution.

Scroll rings are generated using a technique that exploits the system's anomalous dispersion and specifically the "merging" of trailing wave pulses within the wake of a slower leading pulse [8,9]. This procedure involves the initiation of three half-spherical waves from small silver wires. The first two waves collide and create an hourglass-shaped wavefront with an equatorial hole. The

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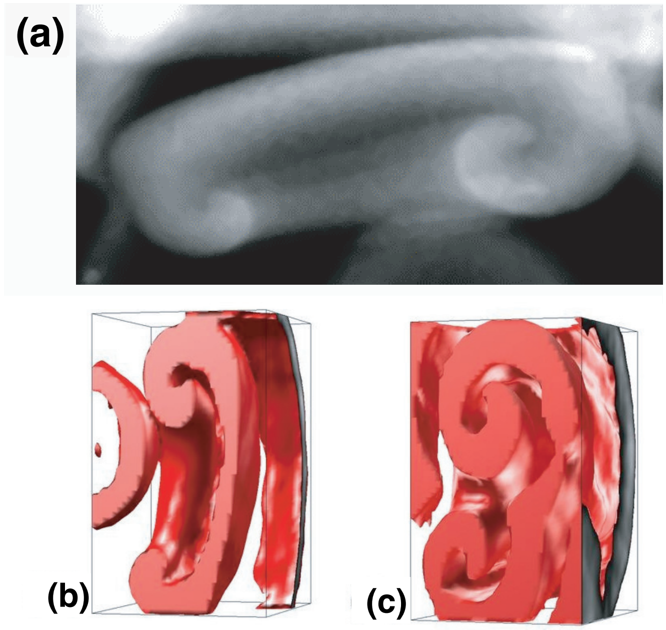

Fig. 1: (a) Single projection through the three-dimensional BZ medium. The spirals on the right and left edge of the scroll ring are out of phase with each other. (b) Cutaway of a three-dimensional reconstruction of the BZ system shortly after initiation of a twisted scroll ring. The spirals at the top and bottom are at different phases. (c) The same scroll ring at a later time. The ring is smaller and the spirals at the top and bottom nearly oscillate in phase. The volume of the three-dimensional plot is $7.3 \times 8.2 \times 11.7\,\text{mm}^3$.

third, trailing wave vanishes in the wake of its predecessor but a small segment survives within the hole. Subsequently, the rim of this wave cap begins to curl, thus, nucleating the desired scroll ring with a period of approximately 30 s.

In this study the third wave is initiated off-center from the wave it merges with creating a time delay in spiral initiation along the ring. This time delay induces a gradient in the rotation phase and the result is a twisted scroll ring with a leading phase at the earliest and a lagging phase at the latest points of vortex initiation. In most of our experiments, the phase difference between the leading and lagging phase is just over 180°. The phase increases along the filament backbone until it comes to a maximum and then decreases and returns to its starting value as one revolution around the ring is completed. This scenario must be clearly distinguished from Möbius-like filaments for which the phase would complete a full 2π increase around the ring.

A representative snapshot through such a pattern and three-dimensional reconstructions are shown in fig. 1. The two latter figures are generated by taking 62 snapshots through the cylindrical sample at equally spaced angles over the course of 5 seconds. The images are then back-projected with an inverse radon transform and filtered [9]. This process follows an approach pioneered by Winfree [20] and yields three-dimensional reconstructions of light absorption patterns (figs. 1b and c).

Two-dimensional slices normal to a scroll wave filament contain a spiral rotating around a quiescent core with some rotation phase, ϕ. In our experiments, the core region is small enough that we can estimate the location of the filament by the tip of a spiral at a particular instant. The rotation phase may vary for different slices and its gradient along the filament defines the twist, $\tau = \phi_s$, where the subscript s denotes differentiation with respect to the filament arc length. The phase is measured in a coordinate system defined by the tangent, normal, and bi-normal vectors of the filament so that the curvature and torsion of the filament do not contribute an effective twist. We can then think of the system as a continuous one-dimensional chain of coupled oscillators where the form of the coupling will determine how the phase gradients evolve.

Measurements of the filament's rotation angle, ϕ, are made at 40 points around the scroll ring. For each point a two-dimensional slice is taken normal to the filament and the spiral core is located. One of the slices is taken as a reference slice with $\phi = 0$. Each of the remaining slices is rotated by an angle that results in the best correlation with the reference slice. This angle of maximum correlation is taken to be the phase, ϕ, of the spiral at that slice. This procedure is repeated for 13 equally spaced reference slices and the results are averaged.

Burgers' equation for filament twist. – Keener and Tyson derived from the FitzHugh-Nagumo equations a form of eq. (1) for the twist, $\tau = \phi_s$, assuming small values of τ [10],

$$\tau_t = c(\tau^2)_s + D\tau_{ss}. \tag{2}$$

Barkley and Margerit derived directly an equation for the phase, ϕ,

$$\phi_t = \omega_0 + c(\phi_s)^2 + D\phi_{ss} \tag{3}$$

and demonstrated that it is an expansion in orders of the twist [11]. Equations (2) and (3) are equivalent as can be seen by integrating eq. (2) once with respect to s. Since we directly measure ϕ and are generally concerned with the coupling of the phase of the oscillators, we focus on eq. (3).

Each of the terms in eq. (3) can be interpreted physically. The first term indicates that in the absence of twist, the scroll wave rotates with frequency ω_0. The last term, $D\phi_{ss}$, indicates a diffusive coupling of the phase along the filament, which attracts the phase at each point to the mean local phase. The second term is the most intriguing as it induces an asymmetry in the phase coupling, but does not contribute to the change in the average twist. Since $(\phi_s)^2$ is always positive, the typical case where $c > 0$ implies that the phase at each point is attracted to its leading neighbors. This feature results in a phase profile with a flat plateau-like region of leading phase and a kink of lagging phase. In the case $c < 0$ the behavior is identical but the role of leading and lagging phases is reversed.

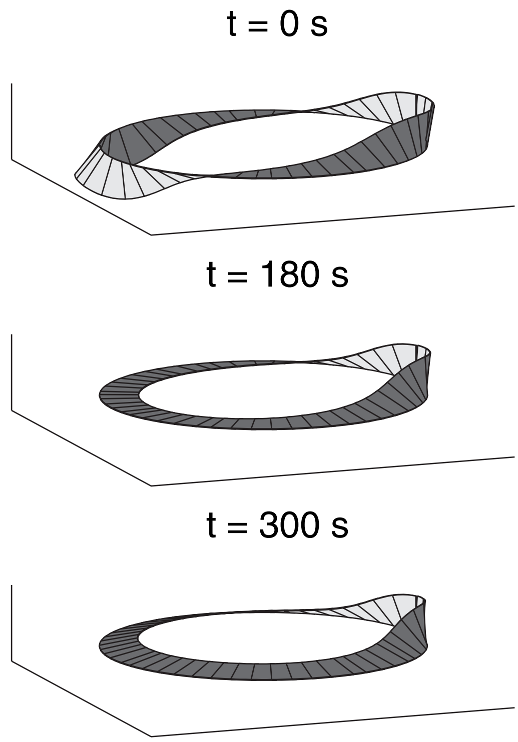

Fig. 2: Three-dimensional representation of an untwisting filament. The initial filament ($t = 0$) has a total phase difference of just over 180°. As the total phase difference decreases, we observe an asymmetric evolution of the phase with a kink developing at the lagging phase (right-hand side) and a flat plateau at the leading phase (left side).

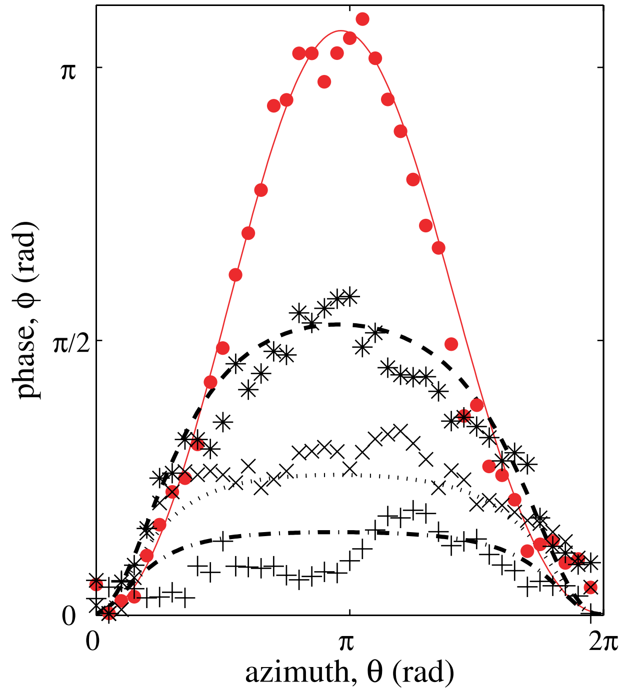

Fig. 3: Rotation phase along a shrinking filament measured at times 0, 180, 300, 360 s (•, ∗, ×, +, respectively). The solid curve is a fit to the data at $t = 0$. The dashed, dotted, and dash-dotted lines are from a simulation of eq. (4) using the curve at 0 s as the initial condition. The parameters of the simulation are $c = 2.66 \times 10^{-4}$ cm^2/s and $D = 1.89 \times 10^{-4}$ cm^2/s.

Results. – The twisted scroll rings described earlier can be represented as a ribbon where one edge of the ribbon is the filament backbone and the other edge is at the end of a vector pointing in the direction of the rotation phase. The ribbon representation of the experimental initial condition is shown in the top panel ($t = 0$) of fig. 2. In this figure, smooth curves are drawn through the data points in the following way: first the scroll ring filament is drawn as a circle; then the phase at 40 points around the circle is measured as described in the previous section and approximated by a smooth curve with a single maximum and single minimum. Note that this feature is consistent with the initiation technique that creates a leading phase at one end of the ring and a lagging phase at the other.

As the scroll ring rotates we observe a decrease in the overall twist. However, a kink persists on the right-hand side of the ribbon and a flat plateu-like region develops on the left. This is shown in the bottom two plots of fig. 2 at $t = 180$ s and $t = 300$ s. The phase of the kink lags behind the phase of the plateau region on the left. This phase relation is consistent with our interpretation of the nonlinear term in eq. (3) for $c > 0$. The shrinking and translation of the ring as reported for untwisted rings [8] are not measurably affected by the twist and the ring fully collapses in roughly 500 seconds.

To test the applicability of eq. (3) as a quantitative model for our observations, we perform numerical simulations. First, we reformulate eq. (3) for the specific case of a scroll ring. We carry out the substitution for the arc length, $s = R\theta$, where R is the ring radius and θ is the azimuth. The differential arc length is then $\partial s = R\partial\theta$ and eq. (3) becomes

$$\phi_t = \frac{c}{R^2}(\phi_\theta)^2 + \frac{D}{R^2}\phi_{\theta\theta}. \tag{4}$$

Due to the curvature of the filament, its radius decreases according to $R(t) = \sqrt{R(0)^2 - 2\alpha t}$, where α is the filament tension [8]. This square-root rate law was first measured for untwisted filaments and was confirmed in experiments with twisted filaments by demonstrating a linear relation between R^2 and t with slope 2α. For the purposes of the simulation, α is measured independently for each experiment we fit to. For the experiment presented, we obtain $\alpha = 7.6 \times 10^{-5}$ cm^2/s.

We take the data at $t = 0$ as the initial condition for a numerical integration of eq. (4). A typical result of the simulations is shown in fig. 3. We find that for $c = 2.66 \times 10^{-4}$ cm^2/s and $D = 1.89 \times 10^{-4}$ cm^2/s, eq. (4) describes both the rate of untwisting and the kink and plateau features observed in our data at the lagging and leading phases, respectively.

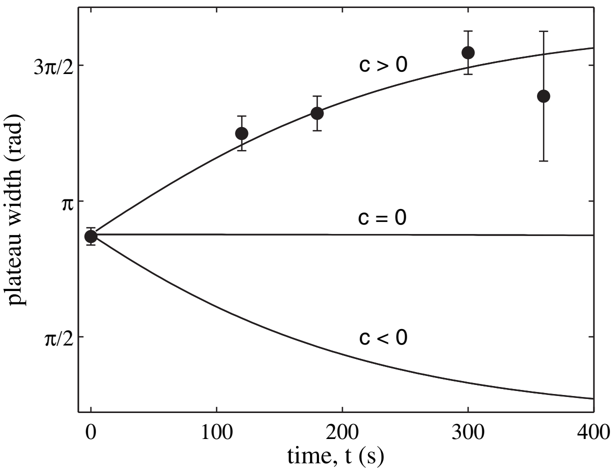

Fig. 4: Temporal evolution of the plateau width. Points are plotted from the experiment and solid lines are the results of simulations. The simulation parameters are as in fig. 3 (top curve), $c = 0$ (flat line), and c equal in magnitude but with opposite sign of the top curve (bottom curve).

To further evaluate the plateau phenomenon, we plot in fig. 4 the width of the plateau at half-maximum. The width is calculated in radians so that we do not see narrowing due to the collapsing of the ring. In the initial condition, the peak and the valley are nearly symmetric and the width of the peak is just below π. As the filament untwists, the plateau becomes wider. Along with the measured data, we plot the plateau width from the simulation of eq. (4). The effect of the nonlinear term is demonstrated by also plotting the peak width from the simulation when the coefficient of the nonlinear term is set to zero and when the sign is reversed. There is no plateau effect when the nonlinearity is removed, and the plateau occurs at the phase minimum instead of the maximum when the sign is reversed.

Conclusions. – We have presented quantitative evidence in a chemical experiment in favor of Burgers' equation, eq. (2), as the mathematical description for twist dynamics. In addition to the expected reduction of average twist by diffusion of phase, we observe the formation of a plateau-like interval of leading phase. This is the result of the nonlinear term in Burgers' equation for $c > 0$. We note that Burgers' equation also supports shock solutions for certain regimes of the parameters c and D, but we have not observed this phenomenon in our experiments.

We find no measurable effect of the filament twist on the collapse or translation of scroll rings reported for untwisted filaments [8]. However, we do believe that a more complex filament geometry, for example one with positive and negative curvature, will lead to structures where the coupling between twist and filament motion is more important.

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