Buckling of Scroll Waves

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A scroll wave in a sufficiently thin layer of an excitable medium with negative filament tension can be stable nevertheless due to filament rigidity. Above a certain critical thickness of the medium, such a scroll wave will have a tendency to deform into a buckled, precessing state. Experimentally this will be seen as meandering of the spiral wave on the surface, the amplitude of which grows with the thickness of the layer, until a breakup to scroll wave turbulence happens. We present a simplified theory for this phenomenon and illustrate it with numerical examples.

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Spiral waves in two dimensions, and scroll waves in three dimensions, are regimes of self-organization observed in physical, chemical, and biological dissipative systems, where wave propagation is supported by a source of energy stored in the medium [1,2]. Due to effective localization of the critical adjoint eigenfunctions, or *response functions* [3,4], the dynamics of a spiral wave can be asymptotically described as that of pointwise objects, in terms of its instant rotation center and phase [5]. The third dimension endows scrolls with extra degrees of freedom: the filaments, around which the scroll waves rotate, can bend, and the phase of rotation may vary along the filaments, giving scrolls a twist [6]. The localization of response functions allows description of scroll waves as string-like objects [3,7–11]. One manifestation of the extra degrees of freedom is the possibility of *scroll wave turbulence* due to negative tension of filaments [12]. It has been speculated that this scroll wave turbulence is in some respects similar to the hydrodynamic turbulence, and may provide insights into the mechanisms of cardiac fibrillation [3,12–14].

The motivation for the present study comes from the analogy with hydrodynamics. At intermediate Reynolds numbers, laminar flow can be unstable, leading to nonstationary regimes which are not turbulent [2]. The possibility of similar preturbulent regimes in scroll waves is interesting, e.g., in view of its possible relevance to cardiac arrhythmias. Cardiac muscle may be considered quasi-two-dimensional if it is very thin. Since scroll turbulence is essentially three dimensional, it bears no reflection on behavior of spiral waves in truly two-dimensional media. Hence, the behavior of scrolls in layers of a given thickness may be effectively two dimensional, unaffected by the negative tension, or truly three dimensional, with full blown turbulence, or in an intermediate regime. The understanding of possible intermediate regimes is thus vitally important for interpretation of experimental data and for possible medical implications.

Here we consider one such intermediate regime, which is illustrated in Fig. 1. This is a snapshot of a scroll wave solution of an excitable reaction-diffusion model

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

where $\mathbf{u}, \mathbf{f} \in \mathbb{R}^\ell$, $\mathbf{D} \in \mathbb{R}^{\ell \times \ell}$, $\mathbf{u}(\vec{r}, t)$ is the dynamic vector field, $\vec{r} \in \mathbb{R}^3$, $\mathbf{D}$ is the diffusion matrix, and $\mathbf{f}(\mathbf{u})$ are reaction kinetics that sustain rigidly rotating spiral waves, in a rectangular box $\vec{r} = (x, y, z) \in [0, L_x] \times [0, L_y] \times [0, L_z]$, with no-flux boundaries and initial conditions in the form of a slightly perturbed straight scroll. In boxes with L_z below a critical height L_* , the scrolls keep straight and rotate steadily. In large enough L_z , the scroll wave turbulence develops. In a range of L_z slightly above L_* as in Fig. 1, the straight scroll is unstable, and its filament, after an initial transient, assumes an S-like shape which remains constant and precesses with a constant angular velocity. In almost any $z = \text{const}$ section, including the upper and lower surfaces, one observes spiral waves with a circular core, whose instant rotation center, in turn, rotates with an angular speed Ω , which changes little with L_z , but

FIG. 1 (color online). Buckled scroll and filament, with the tip path on the top of the box. Barkley model with $a = 1.1$, $b = 0.19$, $c = 0.02$, $D_v = 0.10$, box size $20 \times 20 \times 6.9$ [19].

with a radius which is vanishingly small for $L_z \gtrsim L_*$ and grows with L_z . The resulting tip path, observed on the upper and lower surfaces, is similar to classical two-periodic meander [15]. A similar phenomenon was observed in a model of heart tissue [16].

In this Letter, we investigate the instability which leads to such buckled, precessing filaments, using linear and nonlinear theory and numerical simulations. The instability is akin to the Euler's buckling in elasticity, where a straight beam deflects under a compressive stress that is large enough compared to the material's rigidity [17].

Initial insight can be obtained through linearization about a straight scroll wave solution $\mathbf{U}$ stretched along the z axis, as in Ref. [18]. Small perturbations $\tilde{\mathbf{u}}$ with wave number k_z will evolve according to $\partial_t \tilde{\mathbf{u}} = \hat{\mathbf{L}}_{k_z} \tilde{\mathbf{u}}$, where

$$\hat{\mathbf{L}}_{k_z} = \mathbf{D}\nabla^2 - \mathbf{D}k_z^2 + \omega_0 \partial_\theta + \mathbf{f}'(\mathbf{u}_0). \quad (2)$$

The scroll will be stable if all the eigenvalues to $\hat{\mathbf{L}}_{k_z}$ have negative real part for all allowed wave numbers $k_z = nk_0 = n\pi/L_z$, $n \in \mathbb{Z}$. Analytically, the Taylor expansion in k_z for the critical eigenvalues λ_+ , λ_- , associated to translational symmetry,

$$\lambda_\pm(k_z) = \pm i\omega_0 - (\gamma_1 \pm i\gamma_2)k_z^2 - (e_1 \pm ie_2)k_z^4 + \mathcal{O}(k_z^6), \quad (3)$$

relates to overlap integrals of the translational Goldstone modes and response functions [3,5,9]; see the Supplemental Material [19]. With the notation of Refs. [19,20] and $\hat{\pi} = 1 - |\mathbf{V}_+\rangle\langle\mathbf{W}^+|$, we found

$$\gamma_1 + i\gamma_2 = \langle\mathbf{W}^+|\mathbf{D}|\mathbf{V}_+\rangle, \quad (4)$$

$$e_1 + ie_2 = -\langle\mathbf{W}^+|\mathbf{D}(\hat{\mathbf{L}} - i\omega_0)^{-1}\hat{\pi}\mathbf{D}|\mathbf{V}_+\rangle. \quad (5)$$

Thus, a filament with negative tension γ_1 [3,9,10], can nevertheless be stabilized by higher order terms. We call e_1 *filament rigidity*; it is an analogue of the stiffness of an elastic beam, and has the most important stabilizing effect. If $e_1 > 0$, then the leading-order stability condition is

$$k_0 > k_* = \sqrt{-\gamma_1/e_1} \Leftrightarrow L_z < L_* = \pi\sqrt{-e_1/\gamma_1}. \quad (6)$$

When L_z slightly exceeds L_* , a single unstable mode with spatial dependency $\sim \cos\pi z/L_z$ will grow, causing the filament to buckle and precess at a rate

$$\Omega_* = \gamma_1(\gamma_1 e_2 - \gamma_2 e_1)/e_1^2. \quad (7)$$

The amplitude at which the buckling filament will stabilize requires nonlinear analysis. Our full nonlinear treatment of this phenomenon based on the time-dependent evolution equation for the scroll filament is rather technical, and we defer it to another publication. Here we will consider

simplified scroll dynamics, with the equation of motion of the scroll filament in the form [11]

$$\begin{aligned} (\ddot{\tilde{\mathbf{R}}})_\perp = & (\gamma_1 + \gamma_2 \partial_\sigma \tilde{\mathbf{R}} \times) \partial_\sigma^2 \tilde{\mathbf{R}} - (e_1 + e_2 \partial_\sigma \tilde{\mathbf{R}} \times) (\partial_\sigma^4 \tilde{\mathbf{R}})_\perp \\ & + |\partial_\sigma^2 \tilde{\mathbf{R}}|^2 (b_1 + b_2 \partial_\sigma \tilde{\mathbf{R}} \times) \partial_\sigma^2 \tilde{\mathbf{R}}, \end{aligned} \quad (8)$$

where $\tilde{\mathbf{R}}(\sigma, t)$ is the filament position and σ is the arc-length. The coefficients b_1 , b_2 improve the phenomenological ribbon model proposed in Ref. [21]; they relate to the accelerated shrinking of collapsing scroll rings. Linearization of Eq. (8) agrees with Eqs. (6) and (7) above. A filament obeying Eq. (8) at $L_z \approx L_*$ can be represented, in a frame precessing with frequency Ω , by its Fourier expansion $[X', Y', Z'] = [A \cos(k_0 z), 0, z] + \dots$ with $k_0 = \pi/L_z$. Then collecting the terms $\sim \cos k_0 z$ gives

$$\dot{A} = -k_0^2 A [(\gamma_1 + e_1 k_0^2) + k_0^2 A^2 q(k_0)] = 0, \quad (9)$$

where $q(k_0) = -\gamma_1/2 + (3b_1/4 - e_1)k_0^2$, which describes a pitchfork bifurcation. By evaluating $q(k_*)$, one finds that the case $b_1 > 2e_1/3$ yields a supercritical bifurcation, with stable branch

$$A_* \approx \frac{L_*}{\pi} \sqrt{\frac{8e_1}{3b_1 - 2e_1}} \sqrt{\frac{L - L_*}{L_*}}, \quad L_z \rightarrow L_*. \quad (10)$$

In the opposite case, the bifurcation is subcritical.

So, in absence of other instabilities (say two- or three-dimensional meander), and subject to the inequalities $\gamma_1 < 0$, $e_1 > 0$ and the limits of small $|\gamma_1|$ and small $|L_z - L_*|$, we have an approximate solution Eqs. (6), (7), and (10). The condition of negative tension, $\gamma_1 < 0$, is the key cause of the buckling instability. The condition $e_1 > 0$ ensures that fourth-order arclength derivatives are sufficient to suppress high wave number perturbations and so is important only for particular formulas but not for the phenomenon itself. Violation of the supercriticality condition $b_1 > 2e_1/3$ does not preclude the unstable branch from becoming stable at larger A , as will be seen in Fig. 3(c) below. Finally, the conditions $|\gamma_1| \ll 1$, $|L_* - L_z| \ll 1$ are only required for the asymptotics; in reality, one would expect some finite, interdependent ranges for γ_1 and L_z to support buckled scrolls. Hence, we expect that buckled scrolls are fairly typical and have *finite chances* to be observed in some range of L_z , if only $\gamma_1 < 0$.

In our numerical simulations [19] below, the asymptotics for $\lambda_+(k_z)$ are evaluated using Eqs. (4) and (5), after numerically obtaining the modes $|\mathbf{V}_+\rangle$ and $\langle\mathbf{W}^+|$ using DXSPIRAL [20,22]. These asymptotics are compared to the numerical continuation of $\hat{\mathbf{L}}(k_z)\mathbf{V}(k_z) = \lambda_+(k_z)\mathbf{V}(k_z)$ by the parameter k_z [19].

We used the reaction-diffusion system (1) with Barkley [23] kinetics, $\ell = 2$, $\mathbf{u} = (u, v)$, $\mathbf{f} = (f, g)^T$, $f = c^{-1}u(1-u)[u - (v+b)/a]$, $g = u - v$, and $\mathbf{D} = \text{diag}(1, D_v)$. We mostly use kinetic parameters a , b , c as in Ref. [24], which give negative filament tension $\gamma_1 < 0$,

FIG. 2 (color online). (a) Bifurcation diagram ($a = 1.1$, $b = 0.19$, $c = 0.02$, $D_v = 0.1$): the amplitude (upper panel) and precessing frequency (lower panel) of the straight and buckled scrolls. (b) The corresponding translational branch: real part (upper panel) and imaginary part (lower panel). For the meandering mode, $\text{Re}(\lambda) < -0.24$ [19].

and consider also $D_v > 0$ so as to make $|\gamma_1|$ smaller; note that $D_v = 1$ guarantees $\gamma_1 = 1 > 0$.

Figure 2(a) shows how the buckling amplitude and precession frequency depend on the thickness of the layer, L_z , for the same set of parameters as used to generate Fig. 1. We see that just above the bifurcation point, $L_z \geq L_*$, there is good agreement with Eq. (10). Linear fitting of the $A^2(L_z)$ dependence for the weakest buckled scrolls gives a bifurcation point $L_* \approx 6.310$, and a linear extrapolation of the precessing frequency from the same set gives $\Omega(L_*) \approx 0.2789$. Panel (b) shows the results of the linear analysis, both asymptotic as given by Eq. (3) and obtained by numerical continuation of the eigenvalue problem. The latter gives the $k_* \approx 0.497$, i.e., $L_* = \pi/k_* \approx 6.33$, in agreement with the direct simulations shown in panel (a). The DXSPIRAL calculations using Eqs. (4) and (5) give $\gamma_1 = -0.353$, $e_1 \approx 2.49$, resulting in $k_* \approx 0.376$. The nearly 25% difference between the continuation and asymptotic predictions is consistent with k_z being not very small, and should decrease for smaller $|\gamma_1|$. This is indeed true, as seen below. The precessing frequency predicted by continuation is $\Omega_* = \text{Im}[\lambda(k_*)] - \omega_0 \approx 1.4188 - 1.1408 = 0.2780$, in agreement with simulations.

Figure 3 illustrates variations in the buckling bifurcation caused by change of parameter D_v . In panels (a), (b), parameters are as in Ref. [24] and the filament tension is strongly negative. The DXSPIRAL predictions are $\gamma_1 \approx -2.18$, $e_1 \approx 48.2$ so the asymptotic $k_* \approx 0.213$ is vastly different from the continuation prediction $k_* \approx 0.890$, and this discrepancy is clearly visible in panel (b). Yet, panel (a) shows that the bifurcation still takes place, and the critical thickness $L_* \approx 3.60$ is in agreement with the prediction of the continuation, $L_* = \pi/k_* \approx 3.53$. This confirms that the

FIG. 3 (color online). (a) Bifurcation diagram (buckling amplitude) and (b) translational branch (real part), for $a = 1.1$, $b = 0.19$, $c = 0.02$, $D_v = 0$. (c, d) Same, for $a = 1.1$, $b = 0.19$, $c = 0.02$, $D_v = 0.25$. For the meandering modes, $\text{Re}(\lambda) < -0.098$ and -0.32 , respectively [19].

assumption of smallness of the negative tension is only technical and does not preclude buckled scroll solutions, which still occur via a supercritical bifurcation as the medium thickness varies.

Panels (c), (d) present a variation where the negative filament tension is much smaller. Panel (d) shows much better agreement between the asymptotics: $\gamma_1 \approx -0.0362$,

FIG. 4 (color online). Development of (a) autowave turbulence ($a = 1.1$, $b = 0.19$, $c = 0.02$, $D_v = 0$) and (b) wrinkled scroll as restabilized solution after 3D meandering bifurcation ($a = 0.66$, $b = 0.01$, $c = 0.025$, $D_v = 0$, which corresponds to the leftmost point of Fig. 10(a) in Ref. [18]). Wave fronts are cut out by clipping planes halfway through the volume, to reveal the filaments. Curves on the right are real parts of rotational, translational and meandering eigenvalue branches of $\hat{\mathbf{L}}_{k_z}$ from Eq. (2).

$e_1 \approx 1.65$, such that $k_* = 0.148$ ($L_* = 21.23$), whereas continuation gives $k_* = 0.152$ ($L_* = 20.66$). However, the bifurcation in this case is subcritical with a hysteresis; see panel (c), which shows that the assumption of supercriticality is not absolute, and that a subcritical bifurcation can likewise lead to buckled scroll solutions.

Finally, we illustrate the difference of the buckling bifurcation we have described here, from the 3D meander bifurcation described previously [18,25]. On the formal level, the restabilized scrolls following a 3D meandering instability look similar: at any moment, the filament has a flat sinusoidal shape (given Neumann boundary conditions), and the top and bottom surfaces, as well as almost every $z = \text{const}$ cross section, show meandering spiral wave pictures. However, the behavior is completely different as L_z grows, as illustrated in Fig. 4. Row (a) shows that in the negative tension case, at sufficiently large L_z the scroll buckles so much it breaks up and a scroll turbulence develops, in agreement with previous results. Row (b) shows that in the case of 3D meander, the amplitude remains bounded, and even when L_z is large enough to hold several wavelengths of the curved filament, the restabilized *wrinkled scroll* can persist for a long time (compare these with *zigzag shaped filaments* described in Ref. [26]). Moreover, these two bifurcations occur in different parametric regions via different mechanisms. The key difference is, apparently, the availability or not of infinitely small unstable wave numbers [19].

To summarize, we predict that in an excitable medium with negative nominal filament tension γ_1 , a sufficiently thin quasi-two-dimensional layer will nonetheless support transmural filaments which are straight and stabilized by filament rigidity. When the medium thickness L_z is increased beyond a critical thickness L_* , scroll waves may buckle and exhibit an S shaped, precessing filament. On the surface of the layer, this will look like a classical flower-pattern meander. If the system parameters yield a bifurcation of the supercritical type, a stationary buckling amplitude proportional to $\sqrt{L_z - L_*}$ will be reached, at which nonlinear filament dynamics compensates for the negative tension γ_1 . In the subcritical case, loss of stability of straight scrolls will be abrupt, but it still may lead to restabilized buckled scrolls. The knowledge about the buckling transition and its properties is important for the planning and interpretation of experiments where the medium thickness is comparable to the typical length scale of the spiral wave. In particular, it can be expected that stability of transmural scroll waves in atrial and right ventricular cardiac tissue may in some cases depend on filament rigidity.

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