Linear Stability of Scroll Waves

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A full linear stability of a straight scroll wave in an excitable medium is presented. The five eigenmode branches which correspond to deformation in the third dimension of the five main modes of two-dimensional (2D) spiral dynamics are found to play a dominant role. Modulations in the third dimension have stabilizing or destabilizing effects on the different modes depending on the parameter regimes. For untwisted scroll waves, our numerical results confirm the relation between the long-wavelength behavior of the translation branches and 2D spiral drift in an external field but show no similar direct relation for the meander branches. The influence of twist on the different branches is investigated. In particular, the sproing instability is seen to arise from the twist induced deformation of the translation branches above a threshold twist.

Scroll waves are three-dimensional (3D) extensions of the familiar spirals of excitable media. They have been directly observed in three-dimensional chemical reactions in gels and are suspected to play a role in the slug phase of slime molds life cycle and most importantly in ventricular fibrillation. Numerous simulations of scroll waves have been performed, different instabilities have been noted and a somewhat similar phenomenology has been found for 3D complex Ginzburg-Landau vortices. However, even in the simplest case of an homogeneous and isotropic excitable medium, the mechanisms of the different instabilities, their systematics and the influence of scroll wave twist still appear poorly understood. We attempt here to bring some clarification by performing a full linear stability analysis of straight scroll waves in various parameter regimes. In contrast to earlier stability studies, this gives access not only to the most unstable eigenmode but also to the other, stable or unstable, modes. In particular, this enables us to follow the five branches of modes which emerge from the two translation modes, the rotation zero mode and the two Hopf bifurcation meander modes of 2D spiral motion. As for spirals, these are found to play the dominant role in scroll wave dynamics.

The excitable medium dynamics is described in a simplified but usual way by the two-variables reaction-diffusion system

\[ \partial_t u = \nabla^2 u + f(u,v)/\varepsilon \]
\[ \partial_t v = \delta \nabla^2 v + g(u,v) \]

We restrict ourselves to the singly diffusive case with \( \delta = 0 \) and choose for definiteness Barkley’s reaction terms \( f(u,v) = u(1-u)[u-(v+b)/a], g(u,v) = u-v \) which permits fast direct simulations and comparison with some previous results. Previous experience with 2D spirals lead us to expect that similar results would be obtained with a different choice of excitable kinetics. The results should also be, at least qualitatively, comparable to experiments using Belousov-Zhabotinsky reaction.

Our numerical method is analogous to the one used in a previous linear stability analysis of spiral waves. We introduce a rotating coordinate system twisted along the \( z \)-axis where the steady scroll solution is time independent. That is, we seek and as functions of \( r, \phi = \theta - \omega t - \tau_w z, t \) and \( z \) where \((r,\theta,z)\) are cylindrical coordinates and \( \tau_w \) is the imposed twist. In these coordinates, Eq. (2) reads

\[ (\partial_t + 2\tau_w \partial_{\phi}^2 - \partial_z^2)u = (\omega \partial_{\phi} + \tau_w^2 \partial_{\phi}^2z + \nabla_{2D}^2)u + f(u,v)/\varepsilon \]
\[ \partial_t v = \omega \partial_{\phi} v + g(u,v) \]

The Laplacian is two dimensional on the r.h.s of Eq. (3) in contrast to the three dimensional one in Eq. (1). The twist \( \tau_w \) can be chosen at will and is not constrained by the finite size of the simulation box in the \( z \)-direction as in usual direct simulations. Determining a steady scroll rotating at the frequency \( \omega = \omega_1 \) consists in finding \((u_0(r,\phi), v_0(r,\phi), \omega_1)\), that nullifies the r.h.s of Eq. (3). To solve this nonlinear eigenvalue problem, the r.h.s. of Eq. (3) is discretized on a \( N_r \times N_\phi \) finite, \( 2\pi \phi \)-periodic box of radius \( R \) using finite differences of 4th order in space for the differential operators with rotationally symmetric boundary conditions imposed at the box edge, \( \partial_{r}u_0|_{r=R} = 0 \). The non-uniqueness of \((u_0(r,\phi), v_0(r,\phi))\) brought by the rotational invariance of (3) is taken care of by arbitrarily setting the value of \( u_0(N_r, \phi_0) \) equal to 0.5. Therefore the discrete problem is reduced to finding the zero of a \( (2 \times N_r \times \phi_0) \) valued function of the \((2 \times N_r \times \phi_0-1) \) unknown values of \( u_0 \) and \( v_0 \) and \( \omega_1 \). This is solved by Newton’s method starting from an initial guess of the solution provided by a direct simulation of the evolution equations. In a box of size \( 60 \times 120 \), solutions of the discrete problem are obtained with an accuracy of \( 10^{-8} \) (in a \( L_2 \) norm).

Once a steady scroll wave \((u_0, v_0, \omega_1)\) is found, the time evolution equations (3) are linearized around \((u_0, v_0)\) in the twisted rotating frame. Setting \( u = u_0 + \exp[\sigma(k_z)t - ik_z z]u_1(r,\phi), v = v_0 + \exp[\sigma(k_z)t - ik_z z]v_1(r,\phi) \), leads to
a linear eigenvalue problem for the growth rates $\sigma(k_z)$ as a function of the wave-vector $k_z$:
\[
\sigma(k_z) u_1 = (-k_z^2 + 2i\tau \partial u_z \partial_\phi) u_1 + (\omega_1 \partial_\phi + \tau_\omega \partial^2_\phi + \nabla_{2D}^2) u_1 + [\partial_u f(u_0, v_0) u_1 + \partial_v f(u_0, v_0)]/\varepsilon
\]
\[
\sigma(k_z) v_1 = \omega_1 \partial_\phi v_1 + [\partial_u g(u_0, v_0) u_1 + \partial_v g(u_0, v_0)]
\]

These linear equations are discretized in the same manner as Eq. (3). We denote by $L_{k_z}$ the discrete version of the linear operator appearing on the r.h.s. of Eq. (4). Being interested in the stability of the scroll wave and in its modes of destabilization, we focus on determining the eigenvalues of $L_{k_z}$ of largest real parts. This can be accurately done by using an iterative method fully described in [4]. Firstly, the contributions of eigenvalues with very negative real parts are effectively suppressed by computing by iterations $x_1 = (1 + dtL_{k_z})t_0/dt x_0$, for an arbitrary vector $x_0$ and a sufficiently large integer $t_0/dt$ and a sufficiently small $dt$ (in the following calculations, typical values are $t_0 = 5$ and $dt \approx 10^{-5}$). One then builds an orthonormal set of vectors that spans $\{x_1, x_2 = (1 + dtL_{k_z})t_1/dt x_0, \ldots, x_m = (1 + dtL_{k_z})t_1/dt x_0\}$ and evaluates the restriction $L_{k_z}^{(m)}$ of $L_{k_z}$ to this subspace. The integer $t_1/dt$ should be chosen large enough to make $(1 + L_{k_z} dt)^{t_1/dt}$ significantly different from the identity but small enough to limit computation time (as a typical value, $t_1 \approx 0.5$ is used here). One finally computes the $n$ eigenvalues $\{\sigma_j, 1 \leq j \leq n\}$ of largest real part $(\Re(\sigma_j) > \Re(\sigma_k), j < k)$ and the corresponding eigenvectors of $L_{k_z}^{(m)}$. They approximate the corresponding n eigenvectors of $L_{k_z}$ with an accuracy of order $\exp[-(\sigma_n^r - \sigma_m^r)(m-n)t_0]$. With $m = 50$, we reach a precision of more than $10^{-6}$, in computing eigenvalues of $L_{k_z}$ (in $L_2$ norm $|||L_{k_z} - \sigma(k_z)|||(u_1, v_1)|| < 10^{-6}$).

We have determined steady rotating scroll waves and computed their stability spectrum for several different parameters of Eq. (3) where steady spiral waves exist and are stable. We now summarize these results beginning with the case of untwisted scroll waves.

For 2D-spiral waves, the linear stability operator has three marginally stable modes coming from the symmetries of the dynamics: the rotation eigenmode with an eigenvalue equal to zero and the two translation eigenmodes with purely imaginary eigenvalues equal to $\pm i\omega_1$, the spiral rotation frequency. For untwisted scroll waves, these correspond to eigenmodes of the linearized operator at $k_z = 0$. The computations reported in Figs. 1,2,3 show good agreement with these expectations. For $k_z = 0$, we find an eigenvalue of magnitude smaller than $10^{-9}$ which we identify with the rotation eigenmode and two eigenvalues equal to $\pm i\omega_1$ with an error of $10^{-4}$ which we identify with the translation eigenmodes.

For 2D-spiral waves, in addition to these three marginal eigenvalues, two complex conjugate eigenvalues cross the imaginary axis on the 2D meander instability line. The corresponding meander eigenmodes play an important role in spiral dynamics and belong to the untwisted scroll wave spectrum at $k_z = 0$. The results of our computations show that in general, the eigenvalues with the largest real parts in the untwisted scroll wave spectrum belong to the five finite-$k_z$ branches of modes originating from the translation, rotation or meander eigenmodes at $k_z = 0$. The rotation mode appear to be stabilized by finite $k_z$ values. On the contrary, we have observed three different behaviors of the translation and meander branches as a function of $k_z$ for different choices of the parameters $a, b, \varepsilon$ characterizing the reaction term $f(u,v)/\varepsilon$ in Eq. (4):

- In the first case, both the translations and the meander modes are stabilized when $k_z$ becomes non-zero, as shown in Fig. 4.

The second case is shown in Fig. 5. The translation modes now become unstable for low $k_z$ while the meander modes are stabilized. This corresponds to the "negative filament tension" instability previously described in [4].

- A third case opposite to the previous one is also observed as shown in Fig. 6. The translations modes are here stabilized when $k_z$ becomes non-zero. On the contrary, the real part of the meander modes grows proportionally to $k_z^2$ at low $k_z$ before decreasing for higher wave numbers. This qualitatively corresponds to the phenomenon reported in [4]: the scroll waves can be unstable with respect to meander at finite $k_z$ in a parameter regime where 2D spirals are stable, as shown in Fig. 7.

The fourth logical possibility consisting of a destabilization of both the translation and meander modes was
not observed in the present limited search.

We have performed some direct numerical simulations of Eq. (12) to observe the nonlinear development of the different instabilities [2]. When the translation modes are destabilized at low $k_z$ (Fig. 3), the filament grows and no restabilization is observed. On the contrary, a restabilization at finite amplitude is observed when the meander modes are destabilized at finite $k_z$. This 3D instability thus inherits the direct character of the 2D meander bifurcation. These observations corroborates previous findings [2,8]. However, a detailed characterization of the nonlinear dynamics is beyond the scope of the present letter.

We now proceed and study the effect of a finite twist ($\tau_w \neq 0$) [14]. At a general level, we note that the spectra obey $\sigma(-k_z) = \sigma^*(k_z)$ where the star denotes complex conjugation, since $L_{-k_z} = L^*_{k_z}$. As in the untwisted case, the symmetries of the dynamics provide three known eigenvalues, one zero eigenvalue at $k_z = 0$ for the rotation eigenmode and two complex conjugate eigenvalues for the translation eigenmodes: $\imath \omega_1$ at $k_z = -\tau_w$ corresponding to the eigenvector $\exp(i\phi) (\partial_t w_0 + i\partial_\phi w_0/r, \partial_r v_0 + i\partial_\phi v_0/r)$ and $-\omega_1$ at $k_z = +\tau_w$ for the complex conjugate eigenvector. These exact results provide sensitive checks on the numerics.

We generally find that increasing the twist $\tau_w$ from zero reduces the stability of the translation branches, destabilize them or amplify the instability when they are already unstable. The effect of twist increase appears much less pronounced on the meander modes. We focus here on the most interesting parameter regimes such as those of Fig. 3a for which the untwisted scroll waves are stable. A representative case is shown on Fig. 3b. The kinetics parameter are those of Fig. 3a. When twist is increased from zero, the zeroes of $\text{Re}[\sigma(k_z)]$ which correspond to the translation eigenmodes, move away from $k_z = 0$ and stand at $k_z = \pm \tau_w$ as they should. Most importantly, the translation eigenmodes remain local maxima of $\text{Re}[\sigma(k_z)]$. Beyond a threshold twist ($\tau_w \approx 0.20$) a secondary maximum appears for $k_z$ close to zero. One of the translation branch is shown on Fig. 3a for $\tau_w = 0.26$ when $\text{Re}[\sigma(k_z)]$ is still negative at this secondary maximum (the other translation branch can be deduced from the one shown by reflection with respect to the $k_z = 0$ axis). When the twist is increased further (past $\tau_w \approx 0.30$), $\text{Re}[\sigma(k_z)]$ becomes positive at this secondary maximum. The twisted scroll waves then become unstable for a finite range of wave numbers as shown on Fig. 3b for $\tau_w = 0.4$. The rotation and meander branches are also shown for this value of twist. One sees that the real parts of the two meander branches which are superimposed on Fig. 3a for $\tau_w = 0$ have been split by the twist. The maxima around $k_z = \pm 0.48$ for $\tau_w = 0$ have shifted around $\pm (0.48 + \tau_w)$ but their stability has not been significantly modified.

Direct numerical simulations show that this twist-induced instability leads to a restabilized state in which the scroll core itself acquires a helical shape. We can thus safely identify the present instability with the ‘sproing’ instability of [3] but again a detailed study of the nonlinear state is best deferred to another publication.

Our results can be partially rationalized on the basis of previous works but also show the limitations of some previous theoretical suggestions. In the untwisted case,
it was noted [17] that a weak scroll curvature $\kappa$ can be transformed away by adding a term $-E.\nabla u$ on the r.h.s of Eq. (1). This relates the curvature-induced motion of a weakly curved scroll wave [18] to 2D spiral drift in an external field $E$ and gives for the small $k_z$ behavior of the translation branches,

$$\sigma_{\pm}(k_z) = \pm i\omega_1 + (-\alpha_{\parallel} \pm i\alpha_{\perp})k_z^2$$  

This relation between the translation modes small $k_z$ curvature and the independently measured drift coefficients $\alpha_{\parallel}$ and $\alpha_{\perp}$ is very well satisfied by our numerics (see the captions of Fig. 2, 3). In the untwisted case, whether translation modes are stabilized or destabilized by the introduction of a third dimension is thus precisely related to a property of 2D spirals namely, their known change of drift direction as kinetics parameters vary [2].

The analogous question for meander modes is more complex than anticipated. A simple formal form proposed in [19] extends Eq. (1) to the low $k_z$ behavior of the two complex conjugate meander branches $\sigma_{m,\pm}(k_z) = \sigma_{m,\pm}(0) + (\alpha_{\parallel} \pm i\alpha_{\perp})k_z^2$. In contrast to Eq. (3), this relation is not obeyed by the data of Fig. 3. It even qualitatively disagrees with the data of Fig. 4, since it predicts that the low $k_z$ curvature of the translation and meander branches real parts are of opposite signs contrary to what we find. Thus, a simple two-dimensional account of the long-wavelength dependence of the meander branch remains to be developed.

For twisted scroll waves, we have found that the mechanism of the 'sproing' instability is a twist-induced deformation of the translation branches. This coupling of twist to the translation modes is not present in analytical calculations using averaging techniques [18, 20]. We will show elsewhere [21] that it can be analytically captured in the weakly excitable limit using the techniques of [17]. Nevertheless, the shape of the resulting translation branches and specially their double-peak structure shown on Fig.4a remains to be better understood. More generally, the precise knowledge of the important linear modes and their behavior, should allow the development of controlled reduced descriptions of scroll wave nonlinear dynamics. We also hope that our results and others will encourage further experimental studies of scroll wave instabilities.

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