Motion of Scroll Wave Filaments in the Complex Ginzburg-Landau Equation

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Explicit asymptotic analytical results are derived for the motion of scroll wave filaments in the complex Ginzburg-Landau equation. Good agreement with numerical tests is obtained. The analysis highlights the necessity of allowing for previously ignored small wave-number shifts in the propagation of the waves away from the filament. [S0031-9007(97)02618-5]

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Rotating spiral waves are observed in a variety of physical, chemical, and biological settings including the Belousov-Zhabotinsky (BZ) reaction, thermal convection in a thin fluid layer, slime mold on a nutrient-supplied medium, and waves of electrical activity in heart tissue [1,2]. While much attention has been devoted to spiral waves in two dimensions, there has also been increasing interest in the study of spiral waves in three dimensions or "scroll waves" [2]. The simple point singularity or "defect" at the center of a two-dimensional (2D) spiral wave now becomes a line defect known as the scroll wave filament which can be straight, curved, closed to form a loop, knotted, or interlinked with other loops. The scroll wave can be given a "twist" by allowing for a relative phase difference of the spirals along the filament. Scroll waves have been observed experimentally in the BZ reaction [3], in slime mold [4], and they are also believed to occur in the heart [5]. For a large class of extended systems in the vicinity of a Hopf bifurcation, expansion of the relevant equations [6] leads to a universal equation called the complex Ginzburg-Landau equation (CGLE),

$$\partial A/\partial t = A - (1 + i\alpha)|A|^2 A + (1 + i\beta)\nabla^2 A, \quad (1)$$

where A is a complex scalar field, and α and β are real parameters. (For example, in a system of diffusing chemically reacting constituents, a nonzero β arises due to unequal diffusion coefficients of the chemicals.) Equation (1) exhibits spiral waves in two dimensions and scroll waves in three dimensions. In this paper, we shall study the fundamental problem of obtaining the dynamical behavior of a three-dimensional (3D) CGLE scroll wave filament [7].

In a pioneering work by Keener [8], analysis techniques and results for the evolution of scroll wave filaments for general systems of reaction-diffusion equations were formulated. The results are based on certain hypotheses concerning the asymptotic form of the solution and the number of solutions of an adjoint equation that results from the analysis. Quantitative tests of the theory against numerical or laboratory experiments have never been made in the generic case of unequal diffusion coefficients [analogous to $\beta \neq 0$ in (1)]. This is because coefficients in Keener's general theory are expressed in terms of inner products with solutions of the adjoint equation, which has never been solved. In our paper, by focusing on the simpler CGLE, we are able to derive *explicit* results and to quantitatively test them numerically. Our solution, while adopting some of Keener's techniques, also makes evident a defect in the hypotheses utilized in the previous theory. In particular, we find that it is necessary to include the possibility of wave-number shifts in the propagation of the spiral wave away from the filament.

Our result for the filament motion (derived subsequently) is $\mathbf{R}_t \cdot \mathbf{n} = (1 + \beta^2)\kappa$, $\mathbf{R}_t \cdot \mathbf{b} = 0$. Here $\mathbf{R}(s,t)$ denotes the position of the filament parametrized by the arclength s along the filament. The subscript t denotes differentiation with respect to time, κ is the curvature of the filament, $\mathbf{n}$ is a unit vector pointing towards the center of curvature, and $\mathbf{b}$ is a unit vector perpendicular to the filament and $\mathbf{n}$; $\mathbf{b} = \mathbf{t} \times \mathbf{n}$, where $\mathbf{t} = d\mathbf{R}/ds$ is the tangent vector; see Fig. 1. The quantities $\mathbf{n}, \mathbf{b}$, and κ depend on s and t. The above equation for $\mathbf{R}_t$ is valid when the radius of curvature of the filament is much larger than the filament core radius (the core is the region of rapid rise in the amplitude $|A|$ surrounding the defect). We denote the ratio of these lengths ε and regard it as a small parameter.

As a test, consider the case of a circular filament of radius R for which our equation for $\mathbf{R}_t$ yields

$$dR/dt = -(1 + \beta^2)/R. \quad (2)$$

We have tested (2) for untwisted scroll rings using a numerical simulation of the 3D CGLE. The numerical scheme uses a splitting technique whereby the CGLE is evolved in two steps. The first step involves integrating forward the equation $\partial A/\partial t = A - (1 + i\alpha)|A|^2 A$,

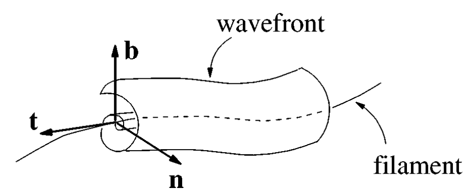

FIG. 1. Axes for the filament-based coordinate system.

which can be solved exactly. The second step involves integrating forward $\partial A/\partial t = (1 + i\beta)\nabla^2 A$. Using periodic boundary conditions in rectangular coordinate space, this is done by Fourier transforming to wave-number space, doing the integration, and then transforming back to real space. Equation (2) predicts that $R^2(t) = R^2(0) - 2\nu t$ with $\nu = 1 + \beta^2$. Figure 2 shows R^2 versus t for $\alpha = 0.5$ and $\beta = -2.0$. The measured value for the collapse rate coefficient, $\nu = 5.2 \pm 0.1$, agrees very well with the predicted value of $\nu = 5$. We have measured ν for other values of α and β and have obtained excellent agreement with the theory [9]. The simulations also agree with the theoretical result that, to first order in the curvature, there is no motion of an untwisted scroll ring parallel to its axis.

We now outline the theory used to derive the equations of motion for a slowly varying CGLE scroll wave filament. The specific quantities of interest are the "collapse" rate ($\mathbf{R}_t \cdot \mathbf{n}$), "drift" rate ($\mathbf{R}_t \cdot \mathbf{b}$), frequency shift, and wave-number shifts. The perturbation method we employ follows the framework of [8] in which the scroll wave problem is treated as a small correction to the 2D spiral wave solution. The single-armed spiral wave solution of the 2D CGLE is of the form

$$A_0(r, \theta, t) = F(r) \exp\{i[-\omega_0 t \pm \theta + \psi(r)]\}. \quad (3)$$

Looking at the $\pm\theta$ term, one sees that the phase change of A_0 around the origin is $\pm 2\pi$. The plus or minus sign is the "topological charge" of the defect at the origin. Since the phase is undetermined at the defect, continuity requires that A_0 vanish at the origin. The real functions $F(r)$ and $\psi(r)$ have the following asymptotic behavior: $F \sim r, \psi' \sim r$ as $r \to 0$ and $F \to \sqrt{1 - k_0^2}, \psi' \to k_0$ as $r \to \infty$. The prime signifies differentiation with respect to r. The frequency ω_0 is determined uniquely by the parameters α and β [10,11]. This, in turn, uniquely

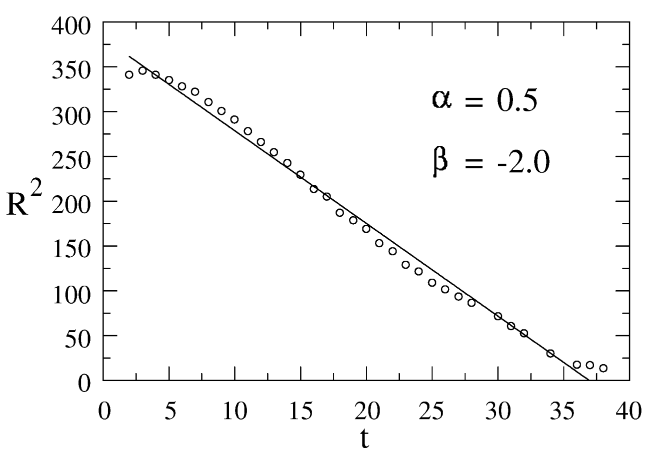

FIG. 2. R^2 vs time for $\alpha = 0.5$, $\beta = -2.0$, $R(0) = 6\pi$, side length $= 40\pi$, grid size $= 128^3$, time step $= 0.1$. The line is a fit to the data.

specifies the asymptotic wave number k_0 via the plane wave dispersion relation $\omega = \alpha + (\beta - \alpha)k^2$.

We now introduce the filament-based coordinate system [8]. A position in space is represented using the coordinates $s, \tilde{x}$, and $\tilde{y}$ as $\mathbf{X} = \mathbf{R}(s) + \tilde{x}\mathbf{n}(s) + \tilde{y}\mathbf{b}(s)$ (see Fig. 1). The vectors $\mathbf{t}, \mathbf{n}$, and $\mathbf{b}$ are related through the Frenet-Serret equations,

$$\frac{d\mathbf{R}}{ds} = \mathbf{t}, \quad \frac{d\mathbf{t}}{ds} = \kappa\mathbf{n}, \quad \frac{d\mathbf{n}}{ds} = -\kappa\mathbf{t} + \tau\mathbf{b}, \quad \frac{d\mathbf{b}}{ds} = -\tau\mathbf{n}. \quad (4)$$

The torsion τ measures the degree to which the filament is nonplanar, with a circular loop, for instance, having zero torsion while a helix will have nonzero torsion. The Frenet-Serret equations can be used to express the gradient as

$$\nabla A = (HA)\mathbf{t} + (\partial A/\partial \tilde{x})\mathbf{n} + (\partial A/\partial \tilde{y})\mathbf{b}, \quad (5)$$

and the Laplacian as

$$\nabla^2 A = H(HA) - \frac{\kappa}{1 - \kappa\tilde{x}} \frac{\partial A}{\partial \tilde{x}} + \frac{\partial^2 A}{\partial \tilde{x}^2} + \frac{\partial^2 A}{\partial \tilde{y}^2}. \quad (6)$$

The operator H is given by $HA = (1 - \kappa\tilde{x})^{-1}(\partial A/\partial s - \tau\partial A/\partial\theta)$, where θ is the polar angular coordinate in the $\tilde{x}$-$\tilde{y}$ plane. [The $1/(1 - \kappa\tilde{x})$ term in the above equations is singular at $\tilde{x} = 1/\kappa$ reflecting the fact that the coordinate system is only valid locally.] Allowing the coordinate system to move with the filament means replacing $\partial A/\partial t$ with

$$\frac{\partial A}{\partial t} - \mathbf{X}_t \cdot \mathbf{t}HA - \mathbf{R}_t \cdot \mathbf{n}\frac{\partial A}{\partial \tilde{x}} - \mathbf{R}_t \cdot \mathbf{b}\frac{\partial A}{\partial \tilde{y}} - \mathbf{n}_t \cdot \mathbf{b}\frac{\partial A}{\partial \theta},$$

where the subscripts denote time derivatives of slowly changing quantities, and $\mathbf{X}_t = \mathbf{R}_t + \tilde{x}\mathbf{n}_t + \tilde{y}\mathbf{b}_t$.

We write the perturbed solution in the form,

$$A = [a_0(r) + u(r, \theta)] \times \exp\{i[-\omega_0 t + \theta + \Phi(\tilde{x}, \tilde{y}, s, t)]\}. \quad (7)$$

Here, the radial dependence of A_0 in the $\tilde{x}$-$\tilde{y}$ plane has been written as $a_0(r) = Fe^{i\psi}$, and for simplicity we have chosen the positive sign in Eq. (3). The complex function u is a correction to the 2D solution which we take to be of the order of the smallness parameter ε. The real function Φ depends slowly on s, t, and the transverse coordinates, $\tilde{x} = r\cos\theta, \tilde{y} = r\sin\theta$, and corresponds to the fact that the basic 2D spiral solution is invariant to a change of phase. As will become clear upon our subsequent expansion of (1), the function Φ can be split into three pieces: one constant in θ, one varying as $\cos\theta$, and one varying as $\sin\theta$. To linear order in r, we write $\Phi = -\varphi(s,t) + \delta k_r(s,t) r + \delta k_x(s,t) r\cos\theta + \delta k_y(s,t) r\sin\theta$, where the wave-number shifts $\delta k_{r,x,y}$ depend slowly on s and t, $\delta k_{r,x,y} = \delta k_{r,x,y}(s,t)$. [In contrast with (7), the ansatz for the perturbed solution used in Ref. [8] omits the dependence of Φ on the transverse coordinates $\tilde{x}$ and $\tilde{y}$.] We find that the inclusion of the wave-number shifts $\delta k_{r,x,y}$ is necessary because small changes in the phase gradient will, for large enough r, cause large changes in A that cannot be absorbed by the small correction u. The derivative of φ with respect to arclength, φ_s, is the twist, and the time derivative, φ_t, represents a frequency shift.

We can now derive the perturbation equation. The following ordering is chosen: $\tau, \varphi_s \sim \mathcal{O}(\varepsilon^{1/2})$ and κ, τ_s, φ_{ss}, u, $\mathbf{X}_t$, φ_t, δk_x, δk_y, $\delta k_r \sim \mathcal{O}(\varepsilon)$. When (7) is substituted into the CGLE (cast in the filament coordinate system), the $\mathcal{O}(\varepsilon)$ equation can be decomposed into two independent systems of ordinary differential equations by writing $u = u_0 + u_+ e^{i\theta} + u_- e^{-i\theta}$ ($u_{0,+,-}$ depend only on r). One set of equations, which we call the rotational perturbation equation, contains u_0, the twist, torsion, frequency shift, and radial wave-number shift, and is

$$\begin{pmatrix} l_0 & m \\ \overline{m} & \overline{l}_0 \end{pmatrix}\begin{pmatrix} u_0 \\ \overline{u}_0 \end{pmatrix} = \begin{pmatrix} iC_\theta a_0 + i(1+i\beta)\delta k_r v_0 \\ -i\overline{C}_\theta \overline{a}_0 - i(1-i\beta)\delta k_r \overline{v}_0 \end{pmatrix}, \tag{8}$$

$$C_\theta = \varphi_t + (1+i\beta)[i(\varphi_s+\tau)^2 - (\varphi_{ss}+\tau_s)] - \mathbf{R}_t\cdot\mathbf{t}(\varphi_s+\tau) + \mathbf{n}_t\cdot\mathbf{b},$$

where $\overline{C}_\theta$ is the complex conjugate of C_θ, $v_0 = 2a_0' + a_0/r$, $m = (1+i\alpha)a_0^2$, $l_0 = -(1+i\beta)(\nabla_r^2 - 1/r^2) - (i\omega_0+1) + 2(1+i\alpha)|a_0|^2$, and $\nabla_r^2 = d^2/dr^2 + r^{-1}d/dr$. The second system, which we call the translational perturbation equation, contains u_+, $\overline{u}_-$, the curvature, the collapse and drift rates, and the x and y wave-number shifts. It is

$$\begin{pmatrix} l_+ & m \\ \overline{m} & \overline{l}_- \end{pmatrix}\begin{pmatrix} u_+ \\ \overline{u}_- \end{pmatrix} = \begin{pmatrix} C_+ v_+ \\ C_- v_- \end{pmatrix}, \tag{9}$$

where $v_+ = a_0' - a_0/r$, $v_- = \overline{a}_0' + \overline{a}_0/r$, $l_+ = -(1+i\beta)(\nabla_r^2 - 4/r^2) - (i\omega_0+1) + 2(1+i\alpha)|a_0|^2$, and $l_- = -(1+i\beta)\nabla_r^2 - (i\omega_0+1) + 2(1+i\alpha)|a_0|^2$. The coefficients on the left side of (9) are $C_+ = (C_x - iC_y)/2$ and $C_- = (\overline{C}_x - i\overline{C}_y)/2$ with

$$C_x = \mathbf{R}_t\cdot\mathbf{n} + (1+i\beta)(2i\delta k_x - \kappa),$$
$$C_y = \mathbf{R}_t\cdot\mathbf{b} + 2i(1+i\beta)\delta k_y.$$

We can write (9) more succinctly as $L_T\mathbf{u}_T = \mathbf{v}_T$, where $\mathbf{u}_T = (u_+\overline{u}_-)^T$.

Our two sets of perturbation equations are combined with boundary conditions by noting that the perturbation u is bounded as $r\to\infty$, and that u vanishes at the origin because the phase singularity at the filament requires that A be zero there. For both the rotational and translational equations we require that the solution obtained by integrating out from the origin can be matched with that obtained by integrating in from infinity.

We first consider the translational perturbation equation. To begin we examine the asymptotic forms of the solutions of the homogeneous equation $L_T\mathbf{U} = 0$ as $r\to 0$ and as $r\to\infty$, where $\mathbf{U} = (U_+\overline{U}_-)^T$. For small r, $a_0 \sim r$ and so the dominant terms in U_+ and $\overline{U}_-$ can be found from $(\nabla_r^2 - 4/r^2)U_+ = 0$ and $\nabla_r^2\overline{U}_- = 0$. This yields four independent solutions to the homogeneous equation near the origin whose leading order components are $U_+\sim r^2, U_+\sim 1/r^2, \overline{U}_-\sim$ const, and $\overline{U}_-\sim \ln r$, respectively. Only the solution with $U_+\sim r^2$, which we denote as $\mathbf{U}_<^{(1)}$, satisfies the boundary condition at the origin.

As $r\to\infty$, $a_0 \sim e^{ik_0 r}$. Substituting $U_+\sim e^{(ik_0+\lambda)r}$ and $\overline{U}_-\sim e^{(-ik_0+\lambda)r}$ into the large r homogeneous equation, one finds that the resulting characteristic equation gives four roots: a $\lambda = 0$ root corresponding to a solution with an asymptotically constant magnitude which we denote by $\mathbf{U}_>^{(1)}$, and either three real roots or one real root and a pair of complex conjugates, which in either case correspond to two exponentially growing solutions and one exponentially decaying solution. Only the latter, denoted by $\mathbf{U}_>^{(2)}$, is acceptable.

We can now construct the general forms of the solutions to Eq. (9) that are to be matched at some distance $r = r^*$. One solution, $\mathbf{u}_{T<}$, is obtained by integrating the equation $L_T\mathbf{U}_T = \mathbf{v}_T$ out in r, starting at $r = 0$. The integration is not actually performed, as it will suffice for our purposes that it can be done in principle. The condition that $\mathbf{u}_{T<}$ vanish at the origin means that it will be a linear combination of the homogeneous solution, $\mathbf{U}_<^{(1)}$, and the particular solutions, $\mathbf{U}_<^{(+)}$ and $\mathbf{U}_<^{(-)}$, satisfying $L_T\mathbf{U}_<^{(+)} = (v_+0)^T$, and $L_T\mathbf{U}_<^{(-)} = (0v_-)^T$, with $\mathbf{U}_<^{(+)}(0) = \mathbf{U}_<^{(-)}(0) = 0$. The most general form of the solution for $r < r^*$ is, therefore,

$$\mathbf{u}_{T<} = B_1\mathbf{U}_<^{(1)} + C_+\mathbf{U}_<^{(+)} + C_-\mathbf{U}_<^{(-)}, \tag{10}$$

where B_1 is an as yet undetermined complex constant.

The solution obtained by integrating the translational perturbation equation in from $r=\infty$, $\mathbf{u}_{T>}$, must remain finite as $r\to\infty$, and is written most generally as

$$\mathbf{u}_{T>} = D_1\mathbf{U}_>^{(1)} + D_2\mathbf{U}_>^{(2)} + C_+\mathbf{U}_>^{(+)} + C_-\mathbf{U}_>^{(-)}, \tag{11}$$

where D_1 and D_2 are unknown complex constants. The particular solutions $\mathbf{U}_>^{(+)}$ and $\mathbf{U}_>^{(-)}$ are defined in a manner analogous to $\mathbf{U}_<^{(+)}$ and $\mathbf{U}_<^{(-)}$ except that we require that they be bounded at infinity. This requirement is enforced through the imposition of a solvability condition. Taking the large r asymptotic form of $\mathbf{u}_T$ to be $u_+ \sim p_+ e^{ik_0 r}$ and $\overline{u}_- \sim \overline{p}_- e^{-ik_0 r}$, we find from (9) as $r \to \infty$ that there will be no nontrivial solutions for the constants p_+ and $\overline{p}_-$ unless the inhomogeneous terms satisfy

$$0 = (1 - i\alpha)C_+ + (1 + i\alpha)C_- . \qquad (12)$$

This is the solvability condition. The real and imaginary parts of (12) yield one relationship between the collapse rate and the x wave-number shift,

$$\mathbf{R}_t \cdot \mathbf{n} = (1 + \alpha\beta)\kappa + 2(\beta - \alpha)\delta k_x , \qquad (13)$$

and one between the drift rate and the y wave-number shift, $\mathbf{R}_t \cdot \mathbf{b} = 2(\beta - \alpha)\delta k_y$.

We now impose the requirement that our solutions for $r < r^*$ and $r > r^*$ match at $r = r^*$. Since we are dealing with a second order differential equation, we have

$$\mathbf{u}_{T<} = \mathbf{u}_{T>} , \quad d\mathbf{u}_{T<}/dr = d\mathbf{u}_{T>}/dr \qquad (14)$$

at $r = r^*$ Recalling that $\mathbf{u}_T$ is a two-component complex vector, conditions (12) and (14) constitute a system of five homogeneous equations for the five complex unknowns B_1, D_1, D_2, C_+, and C_-. We can write these unknowns as a column vector and their coefficients as a 5×5 matrix. Generically, we expect the determinant of this matrix to be nonzero. A zero determinant would represent an exceptional case. Accordingly, we assume the determinant of the matrix to be nonzero which implies that $B_1 = D_1 = D_2 = C_+ = C_- = 0$ and hence $\mathbf{u}_T = 0$. From $C_+ = C_- = 0$, the collapse rate and the wave-number shift δk_x are found to be

$$\mathbf{R}_t \cdot \mathbf{n} = (1 + \beta^2)\kappa, \quad \delta k_x = \frac{\beta\kappa}{2} , \qquad (15)$$

and the drift rate $\mathrm{R}_t \cdot \mathbf{b}$ and y wave-number shift δk_y are both zero. The fact that our numerical results are in excellent agreement with Eq. (2) supports our hypothesis of nonzero determinant.

We omit the analysis for the rotational perturbation equation (8), and only state its result. The solution of (8) is $u_0 = k_0^{-1}\delta k_r r(a_0' - ik_0 a_0 + a_0/r)$, and the frequency and radial wave-number shifts are given by

$$\varphi_t = (\beta - \alpha)(1 - k_0^2)(\varphi_s + \tau)^2 + \mathbf{R}_t \cdot \mathbf{t}(\varphi_s + \tau) - \mathbf{n}_t \cdot \mathbf{b} + [1 + \alpha\beta + (\beta - \alpha)\beta k_0^2](\varphi_{ss} + \tau_s) , \qquad (16)$$

$$\delta k_r = -\frac{k_0}{2}[(\varphi_s + \tau)^2 - \beta(\varphi_{ss} + \tau_s)] . \qquad (17)$$

We have checked (16) and (17) for the case of a straight filament against numerical solutions of Eq. (1) and obtained very good agreement.

Equations (15)–(17) are our main results.

We note that if the wave-number shift is not included in the theory (as in [8]) then one can obtain an expression for the collapse rate directly from the solvability condition that imposes boundedness on the perturbation at infinity, without consideration of the boundary condition at the origin. If one were to (erroneously) set $\delta k_x = 0$, Eq. (13) would imply that the rate of change for the radius of a circular ring is $dR/dt = -(1 + \alpha\beta)/R$; a result that would allow for expanding (when $\alpha\beta < -1$) as well as collapsing rings. The same result was obtained using a different theoretical approach in [12]. Our data clearly contradict this result (for example, for the parameters of Fig. 2, $(1 + \beta^2) = 5$ while $(1 + \alpha\beta) = 0$).

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