Nonlocal Boundary Dynamics of Traveling Spots in a Reaction-Diffusion System

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The boundary integral method is extended to derive a closed integro-differential equation applicable to computation of the shape and propagation speed of a steadily moving spot and to the analysis of dynamic instabilities in the sharp boundary limit. Expansion of the boundary integral near the locus of traveling instability in a standard reaction-diffusion model proves that the bifurcation is supercritical whenever the spot is stable to splitting. Thus, stable propagating spots do already exist in the basic activator-inhibitor model, without additional long-range variables.

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Localized structures in nonequlibrium systems (dissipative solitons) have been studied both in experiments and computations in various applications, including chemical patterns in solutions [1] and on surfaces [2], gas discharges [3], liquid crystal convection [4], and nonlinear optics [5]. The interest in dynamic solitary structures, in particular, in optical [5] and gas discharge systems [6], has been recently driven by their possible role in information transmission and processing.

A variety of observed phenomena can be reproduced qualitatively with the help of simple reaction-diffusion models with separated scales [7–11]. Extended models of this type included nonlocal interactions due to gas transport [10,12], Marangoni flow [13], or optical feedback [5,14]. A great advantage of scale separation is a possibility to construct analytically strongly nonlinear structures in the sharp interface limit. An alternative approach, based on Ginzburg-Landau models supplemented by quintic and/or fourth-order differential (Swift-Hohenberg) terms [15], has to rely on numerics in more than one dimension.

Dynamic solitary structures, observed experimentally in different applications [2–4,16,17], are most interesting from the point of view of both theory and potential applications. Existence of traveling spots in sharp-interface models is indicated by translational instability of a stationary spot [12]. This instability is a manifestation of a general phenomenon of parity breaking (Ising-Bloch) bifurcation [18,19] which takes a single stable front into a pair of counterpropagating fronts forming the front and back of a traveling pulse. Numerical simulations, however, failed to produce stable traveling spots in the basic activator-inhibitor model, and the tendency toward moving spots to spread out laterally had to be suppressed either by global interaction in a finite region [12] or by adding an extra inhibitor with specially designed properties [20].

The dynamical problem is difficult for theoretical study, since a moving spot loses its circular shape, and a free-boundary problem is formidable even for the simplest kinetic models. Numerical simulation is also problematic, due to the need to use fine grid to catch sharp gradients of the activator; therefore actual computations were carried out for moderate scale ratios. A large amount of numerical data, such as the inhibitor field far from the spot contour, is superfluous. This could be overcome if it was possible to reduce the partial differential equation (PDE) solution to local dynamics of a sharp boundary. Unfortunately, a purely local equation of front motion [19] is applicable only when the curvature radius far exceeds the diffusion scale of the long-range variable, whereas a spot typically suffers splitting instability [7] before growing so large. On the other hand, the nonlocal boundary integral method [21] is applicable only when the inhibitor dynamics is fast compared to the characteristic propagation scale of the front motion, i.e., under conditions when no dynamic instabilities arise and traveling spots do not exist.

It is the aim of this Letter to extend the nonlocal boundary integral method to dynamical problems, and to find out with its help the conditions of supercritical bifurcation for steadily moving spots. We consider the standard FitzHugh-Nagumo model including two variables—a short-range activator u and a long-range inhibitor v:

$$\epsilon^2 \tau u_t = \epsilon^2 \nabla^2 u + V'(u) - \epsilon v , \tag{1}$$

$$v_t = \nabla^2 v - v - \nu + \mu u . \tag{2}$$

Here $V(u)$ is a symmetric double-well potential with minima at $u = \pm 1$; $\epsilon \ll 1$ is a scale ratio, and other parameters are scaled in such a way that the effects of bias and curvature on the motion of the front separating the up and down states of the short-range variable are of the same order of magnitude. The local *normal* velocity of the front is, in the leading order,

$$c_n = \tau^{-1}(bv - \kappa) + O(\epsilon), \tag{3}$$

where κ is a curvature and b is a numerical factor dependent on the form of $V(u)$; for example, $b = 3/\sqrt{2}$ for the quartic potential $V(u) = -\frac{1}{4}(1 - u^2)^2$. By definition, the velocity is positive when the down state $u < 0$ advances.

In the sharp boundary approximation valid at $\epsilon \ll 1$, a closed equation of motion for a solitary spot propagating with a constant speed can be written by expressing the local

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curvature in Eq. (3) with the help of a suitable parametrization of the spot boundary and resolving Eq. (2), rewritten in a coordinate frame propagating with a speed c (as yet unknown). It is convenient to shift the long-range variable $v = w - \nu + \mu$, so that $w(\infty) = 0$ when the up state $u = 1 - O(\epsilon)$ prevails at infinity. The stationary equation of w in the coordinate frame translating with the speed $\mathbf{c}$ is

$$\mathbf{c} \cdot \nabla w + \nabla^2 w - w = 2\mu H, \tag{4}$$

where, neglecting $O(\epsilon)$ corrections, $H = 1$ inside and $H = 0$ outside the spot. The solution can be presented in the form of an integral over the spot area S:

$$w(\mathbf{x}) = -\frac{\mu}{\pi} \int_S \mathcal{G}(\mathbf{x} - \boldsymbol{\xi})\, d^2\boldsymbol{\xi}, \tag{5}$$

where the kernel $\mathcal{G}$ contains a modified Bessel function K_0:

$$\mathcal{G}(\mathbf{r}) = \tfrac{1}{2} e^{-(1/2)\mathbf{c}\cdot\mathbf{r}} K_0(|\mathbf{r}|\sqrt{1 + \tfrac{1}{4}c^2}). \tag{6}$$

This integral can be transformed into a contour integral with the help of the Gauss theorem. To avoid divergent expressions, the contour should exclude the point $\mathbf{x} = \boldsymbol{\xi}$. Clearly, excluding an infinitesimal circle around this point does not affect the integral (5), since the kernel (6) is only logarithmically divergent. Replacing $\mathcal{G}(\mathbf{r}) = \nabla^2\mathcal{G}(\mathbf{r}) + \mathbf{c} \cdot \nabla\mathcal{G}(\mathbf{r})$ ($\mathbf{r} \neq 0$), we transform the integral in Eq. (5) as

$$\begin{aligned} -\int_S \mathcal{G}(\mathbf{x} - \boldsymbol{\xi})\, d^2\boldsymbol{\xi} &= \int_S \nabla_{\xi} \cdot \mathbf{H}(\mathbf{x} - \boldsymbol{\xi})\, d^2\boldsymbol{\xi} \\ &= \oint_{\Gamma'} \mathbf{n}(s) \cdot \mathbf{H}(\mathbf{x} - \boldsymbol{\xi}(s))\, ds, \end{aligned} \tag{7}$$

where $\mathbf{H}(\mathbf{r}) = \nabla\mathcal{G}(\mathbf{r}) + \mathbf{c}\mathcal{G}(\mathbf{r})$ and $\mathbf{n}$ is the normal to the contour Γ'. The vector Green's function $\mathbf{H}$ corresponding to the kernel in Eq. (5) is computed as

$$\begin{aligned} \mathbf{H}(\mathbf{r}) = e^{-(1/2)\mathbf{c}\cdot\mathbf{r}} \Bigg[&\frac{1}{2}\, \mathbf{c} K_0\left(|\mathbf{r}|\sqrt{1 + \frac{1}{4}c^2}\right) \\ &- \sqrt{1 + \frac{1}{4}c^2}\, \frac{\mathbf{r}}{|\mathbf{r}|} \\ &\times K_1\left(|\mathbf{r}|\sqrt{1 + \frac{1}{4}c^2}\right)\Bigg]. \end{aligned} \tag{8}$$

When $\mathbf{x}$ is a boundary point, Γ' consists of the spot boundary Γ cut at this point and closed by an infinitesimally small semicircle about $\mathbf{x}$. The integral over the semicircle equals to π. Defining the external normal to Γ as the tangent $\mathbf{t} = \mathbf{x}'(s)$ rotated clockwise by $\pi/2$, the required value of the long-range variable on the spot boundary (parametrized by the arc length s or σ) is expressed, using the 2D cross product $\times$, as

$$v(s) = -\nu + \frac{\mu}{\pi} \oint_{\Gamma} \mathbf{H}(\mathbf{x}(s) - \mathbf{x}(\sigma)) \times \mathbf{x}'(\sigma)\, d\sigma. \tag{9}$$

To obtain a closed integral equation of a steadily moving spot, it remains for one to define a shift of parametrization accompanying shape-preserving translation. Recall that Eq. (3) determines the propagation velocity c_n along the *normal* to the boundary. In addition, one can introduce arbitrary *tangential* velocity c_t which has no physical meaning but might be necessary to account for the fact that each point on a translated contour is, generally, mapped onto a point with a different parametrization even when the shape remains unchanged. The tangential velocity can be defined by requiring that each point on the surface be translated strictly parallel to the direction of motion, i.e., $c_n\mathbf{n} + c_t\mathbf{t} = \mathbf{c}$. Taking the cross product with $\mathbf{c}$ yields $c_t = c_n(\mathbf{c} \times \mathbf{t})/(\mathbf{c} \cdot \mathbf{t})$. Then, eliminating c_t gives the normal velocity $c_n = \mathbf{c} \times \mathbf{t}$ necessary for translating the contour along the x axis with the velocity c. Using this in Eq. (3) yields the condition of stationary propagation,

$$\mathbf{c} \times \mathbf{x}'(s) = \tau^{-1}[b v(s) - \kappa(s)]. \tag{10}$$

This equation, combined with Eq. (9), is the basis for further analysis.

The form and the propagation speed of a slowly moving and weakly distorted circular contour can be obtained by expanding Eq. (10) in $c = |\mathbf{c}|$ near the point of traveling bifurcation $\tau = \tau_0$, which is also determined in the course of the expansion. For a circular contour with a radius a, Eq. (9) takes the form

$$\begin{aligned} v(\phi) = -\nu + \frac{\mu a}{\pi} \int_0^{2\pi} e^{-(1/2)ca(\cos\phi - \cos\varphi)} \Bigg[&\frac{1}{2}\, c \cos\varphi K_0\left(2a\sqrt{1 + \frac{1}{4}c^2}\, \sin\frac{1}{2}|\phi - \varphi|\right) \\ &+ \sin\frac{1}{2}|\phi - \varphi| \sqrt{1 + \frac{1}{4}c^2}\, K_1\left(2a\sqrt{1 + \frac{1}{4}c^2}\, \sin\frac{1}{2}|\phi - \varphi|\right)\Bigg] d\varphi, \end{aligned} \tag{11}$$

where ϕ or φ is the polar angle counted from the direction of motion. The angular integrals that appear in the successive terms of the expansion are evaluated iteratively, starting from $\Phi_0(a) = \pi I_0(a)K_0(a)$ and using the relations

$$\begin{aligned} \Psi_k(a) &= \int_0^{\pi} \sin^{2k+1}\frac{\phi}{2}\, K_1\left(2a \sin\frac{\phi}{2}\right) d\phi \\ &= -\frac{1}{2}\, \frac{d\Phi_k}{da}, \end{aligned}$$

$$\begin{aligned} \Phi_k(a) &= \int_0^{\pi} \sin^{2k}\frac{\phi}{2}\, K_0\left(2a \sin\frac{\phi}{2}\right) d\phi \\ &= -\frac{1}{2a}\, \frac{d(a\Psi_{k-1})}{da}. \end{aligned}$$

The effect of small boundary distortions on v can be computed directly with the help of Eq. (5), where the integration should be carried out only over a small area swept by the displaced spot boundary. This approach is most useful for stability analysis with respect to small perturbations of a known static shape, and is easier than using the expansion of Eq. (9) with a perturbed boundary. For a nearly circular spot, we expand the perturbations of both v and the local radius $\rho(\phi)$ in the Fourier series

$$\tilde{\rho}(\phi,t) = \rho(\phi) - a = \sum_{n\geq 2} c^n a_n e^{\lambda_n t}\cos n\phi\,, \qquad \tilde{v}(\phi,t) = \sum_{n\geq 2} \hat{v}_n e^{\lambda_n t}\cos n\phi\,. \tag{12}$$

The curvature is expressed as

$$\kappa(\phi) = \frac{\rho^2 - 2\rho_\phi^2 - \rho\rho_{\phi\phi}}{(\rho^2 + \rho_\phi^2)^{3/2}} = a^{-1} + 3(c/a)^2 a_2 e^{\lambda_2 t}\cos 2\phi + O(c^3)\,. \tag{13}$$

Since the displaced point should remain on the boundary, the distortion $\tilde{\rho}(\varphi)$ should be compensated by rigid displacement of the spot by an increment $\tilde{\rho}(\phi)$ when $\tilde{v}(\phi)$ is computed (see the inset of Fig. 1). The resulting equation for eigenvalues λ_n following from Eq. (3) is

$$\tau\lambda_n = \frac{n^2-1}{a^2} - \frac{4ab\mu}{\pi^2}\int_0^\pi \cos n\phi\, d\phi \int_0^\pi [\tilde{\rho}(\varphi) - \tilde{\rho}(\phi)\cos(\varphi - \phi)] e^{-(1/2)ca(\cos\phi - \cos\varphi)} \times K_0\left(2a\sqrt{1 + \lambda_n + \frac{1}{4}c^2}\sin\frac{1}{2}|\phi - \varphi|\right) d\varphi\,. \tag{14}$$

Using the constant zero-order term in the expansion of Eq. (11), together with $\kappa = a^{-1}$ in Eq. (3), yields the stationarity condition

$$\nu = -(ba)^{-1} + \mu a[K_1(a)I_0(a) - K_0(a)I_1(a)]\,. \tag{15}$$

A stationary solution stable against collapse or uniform swelling exists in the region in the parametric plane μ, ν (Fig. 1) bounded by the cusped curve C joined by the line $\nu = 0$, $\mu > 2/b = \frac{2}{3}\sqrt{2}$. This curve is drawn as a parametric plot with $\nu(a)$ given by Eq. (15) and $\mu(a)$ by Eq. (14) with c, n, and λ_0 set to zero [or, equivalently, by the condition $F_0'(a) = 0$, where $F_0(a)$ is the right-hand side of Eq. (15)].

The first-order term in the expansion of Eq. (11) is proportional to $\cos\phi$, and should compensate at the traveling bifurcation point the left-hand side of Eq. (10). This yields

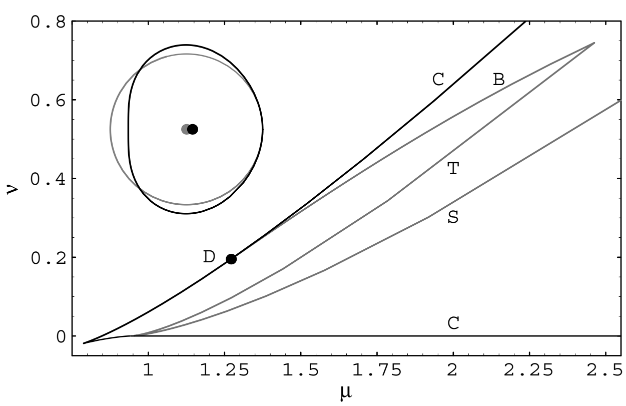

FIG. 1. The bifurcation diagram for stationary spots at $\tau = 1$. C—existence boundary, S—locus of splitting instability. The stability region is bounded by the locus of breathing instability B, branching off at the point of double zero eigenvalue D, and the locus of traveling instability T. Inset: a circular spot distorted by second and third harmonics with amplitudes proportional to c^n. The shape is characteristic of a spot propagating to the right, and the amplitudes are chosen in such a way that the curvature on the back side vanishes. The center of the gray circle is shifted from the black to the gray spot to compensate the distortion at $\phi = 0$, so that the integral is taken over the area between the black contour and the gray circle when the effect of small distortions on the v field at this point is computed.

the bifurcation condition

$$\tau_0 = b\mu a[a(I_1(a)K_0(a) - I_0(a)K_1(a)) + 2I_1(a)K_1(a)]\,, \tag{16}$$

which coincides with the known result obtained by other means [12]. The curve T in Fig. 1 shows the traveling instability threshold for $\tau_0 = 1$. The static spot is unstable below this curve; the locus shifts up (to smaller radii) as τ decreases, and exits the existence domain at $\tau < \frac{1}{4}$. At $\tau > 1$, the dominant instability at large radii is a static splitting instability. Its locus, determined by Eq. (14) with $n = 2$ and $c = \lambda_2 = 0$, is the curve S in Fig. 1.

Another possible dynamic instability is breathing instability [3,7,17]. Its locus is given by Eq. (14) with $c = n = 0$ and $\lambda_0 = i\omega$. The frequency ω as a function of the spot radius a [related to ν and μ by Eq. (15)] is computed by solving the equation $\tau\omega = a^{-2}\,\mathrm{Im}F(a,\omega)/\mathrm{Re}F(a,\omega)$, where $F(a,\omega)$ is the right-hand side of Eq. (14) computed as

$$F(a,\omega) = 2\mu a[I_1(a\sqrt{1+i\omega})K_1(a\sqrt{1+i\omega}) - I_0(a\sqrt{1+i\omega})K_0(a\sqrt{1+i\omega})]\,. \tag{17}$$

The curve B in Fig. 1 shows the bifurcation locus at $\tau = 1$. The instability region retreats to small radii (large ν) at large τ and spreads downwards as τ decreases. The balloon of stable solutions disappears at $\tau < 0.5$ after the tips of both dynamic loci meet on the existence boundary.

In the second order, Eq. (11) yields a constant term

$$v^{(2,0)} = -\mu a^2[a(I_1(a)K_0(a) - I_0(a)K_1(a)) + I_1(a)K_1(a)] \tag{18}$$

and a dipole term $v^{(2,2)} = q^{(2,2)}\cos 2\phi$, where

$$q^{(2,2)} = \tfrac{1}{4}\mu a^2[a(I_0(a)K_1(a) - I_1(a)K_0(a)) - 3I_1(a)K_1(a) + 2I_2(a)K_2(a)]\,. \tag{19}$$

The constant term is positive and causes contraction of the average radius of the moving spot by an increment $\tilde{a} = -a^2c^2bv^{(2,0)}$.

The second-order dipolar term in the right-hand side of Eq. (10), $\tilde{v}^{(2,2)} = \tilde{q}^{(2,2)} a_2 \cos 2\phi$, as well as the third-order first harmonic term, $\tilde{v}^{(3,1)} = \tilde{q}^{(3,1)} a_2 \cos\phi$, needed for the solvability condition to follow, are read from Eq. (14) with $n = 2$ and $\lambda_2 = 0$, respectively, in zero and first order in c:

$$\tilde{q}^{(2,2)} = -3a^{-2} + 2b\mu[I_1(a)K_1(a) - I_2(a)K_2(a)], \tag{20}$$

$$\tilde{q}^{(3,1)} = b\mu a^2 I_1(a)K_1(a). \tag{21}$$

The coefficient $\tilde{q}^{(2,2)}$ vanishes at the splitting instability threshold (curve S in Fig. 1), and must be negative when the circular spot is stable. Consequently, the distortion amplitude is $a_2 = -q^{(2,2)}/\tilde{q}^{(2,2)} < 0$, so that the dipole term causes the contraction of the moving spot in the direction of motion and expansion in the normal direction.

Continuing the expansion to the third order, we compute the first harmonic term contributing to the solvability condition. The latter has the form $\tilde{\tau} c = kc^3$, where $\tilde{\tau} = \tau - \tau_0$ and the coefficient k determining the character of the bifurcation is computed as

$$k = b\mu\big(q^{(3,1)} - \tau_0'(a)a^2 v^{(2,0)} - \tilde{q}^{(3,1)} q^{(2,2)}/\tilde{q}^{(2,2)}\big). \tag{22}$$

The first term is the coefficient at the first harmonic in the third order of the expansion of Eq. (11). The second term takes into account the second-order radius correction to the first-order first harmonic term. The last term gives the effect of dipolar shape distortion; it becomes dominant when the locus of splitting instability is approached. Stable traveling solution should be observed beyond the traveling instability threshold, i.e., at $\tilde{\tau} < 0$; hence, the condition of supercritical bifurcation is $k < 0$. The numerical check of the symbolically computed expression shows that the traveling bifurcation is always supercritical when the spot is stable to splitting. The traveling solution bifurcating supercritically must be stable, at least close to the bifurcation point, where it inherits stability of the stationary spot to other types of perturbations.

The third harmonic term that appears in the third order of the expansion delineates, together with the second-order dipolar term, the characteristic shape of a translating spot, pointed in the direction of motion and spread sidewise, as in the inset of Fig. 1, which has also been observed in numerical simulations [20]. Beyond the range of the bifurcation expansion, the shape, as well as the propagation speed, can be determined by solving numerically Eq. (10) with $v(s)$ given by Eq. (9) and curvature computed using the fully nonlinear expression in Eq. (13). Although the boundary integral method reduces a PDE to a 1D integro-differential equation, the equation is rather difficult. An iterative numerical solution tends to break down rather close to the bifurcation point, as soon as the shape distortion becomes strong enough to flatten the spot at the back side. Since the boundary integral equation is nonevolutionary, there is no way to distinguish between a purely numerical failure of convergence and a physical instability that would lead to lateral spreading observed in PDE simulations [12].

The above bifurcation expansion proves that a stable traveling solution does exist in the basic model [(1) and (2)] in the sharp boundary limit. The result is applicable at $1 \gg c \gg \sqrt{\epsilon}$. It can be extended straightforward to models with more than one long-range variable, provided all long-range equations are linear. Stable traveling spot solutions should be, indeed, more robust in an extended model, where they have been obtained in PDE simulations [20], whereas in the basic model they require fine-parametric-tuning aided by the analytical theory.

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