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Diffusive boundary layers in the free-surface excitable medium spiral

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Spiral waves are a ubiquitous feature of the nonequilibrium dynamics of a great variety of excitable systems. In the limit of a large separation in time scale between fast excitation and slow recovery, one can reduce the spiral problem to one involving the motion of a free surface separating the excited and quiescent phases. In this work, we study the free-surface problem in the limit of small diffusivity for the slow field variable. Specifically, we show that a previously found spiral solution in the diffusionless limit can be extended to finite diffusivity, without significant alteration. This extension involves the creation of a variety of boundary layers which cure all the undesirable singularities of the aforementioned solution. The implications of our results for the study of spiral stability are briefly discussed. [S1063-651X(97)50604-0]

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Understanding the behavior of spiral waves in excitable media remains an important and challenging problem [1]. From the perspective of numerical simulation, two component reaction-diffusion models [2,3] have been shown to capture the important features of spiral patterns, in particular, the transition from rigid rotation to meandering and the phenomenology of the nonlinear meandering state [4,5]. More recently, simulations [6], and a numerical stability analysis [7] based on the free boundary limit [8] (see below) have confirmed that the finite thickness of the front (separating the excited region from the quiescent one) is not crucial for the meandering behavior. It is therefore of interest to pursue analytical techniques (which make use of this free boundary limit) in the hope of gaining a more fundamental understanding of the nature of this instability.

This work reports progress towards the aforementioned goal of having an analytic theory of spiral waves. Specifically, we revisit an approach due to Pelce and Sun [9] who derived a spiral solution in the case of zero diffusion for the ''controller'' variable. Their solution exhibits singular behavior near the spiral ''tip'' (for example, the front curvature has a discontinuous derivative across the tip point) which raises questions regarding the validity of the solution and to date has precluded a full stability analysis. Here, we show how the inclusion of small but finite diffusivity provides, via the introduction of boundary layers, for a regularization of the singular behaviors. This therefore confirms the physical validity of their construction. The implications of our results for a (future) calculation of spiral stability are discussed at the end.

The free boundary approach starts from the equations coupling a concentration field $v(\vec{x},t)$ to an interface between an excited state of the medium (+) and the quiescent state (−). In so-called ''Fife''-scaled units [wherein lengths, time and the v field have been rescaled to bring the eikonal equation (2) into the simple form shown—see Ref. [10]],

$$\partial v_{\pm}/\partial t = g_{\pm} - \mu v_{\pm} + D\nabla^2 v, \tag{1}$$

where μ is a positive constant (and where for simplicity we have assumed equal values of the linear coefficient in the two states), g_+, g_- are positive, negative constants and $v_{\pm}$ refers to the field in the +,− regions, respectively. The field obeys the boundary conditions at the interface [11]

$$c_n + \kappa = -v_{int}, \tag{2}$$

where c_n is the normal velocity, κ the curvature, and the value of v (as well as its normal derivative) is continuous across the interface.

This system of equations is not rigorously derivable from the original reaction diffusion system

$$\partial u/\partial t = \nabla^2 u + \frac{f(u,v)}{\epsilon}, \tag{3}$$

$$\partial v/\partial t = D\nabla^2 v + g(u,v). \tag{4}$$

The reason for this is that replacing the ''propagator'' field equation for $u(x,t)$ by an interfacial boundary condition is only valid asymptotically as $\epsilon \to 0$. The coefficient μ of the linear term in Eq. (1) is formally small, of order $\epsilon^{1/3}$. Hence, we cannot rigorously keep this linear term without keeping additional terms of the same order as well. As we have already mentioned, however, simulations show that Eqs. (1) and (2) do capture the spiral phenomenology of interest, at least for finite diffusivity D. Furthermore, an exact numerical steady-state solution [12] and subsequent stability analysis [7] directly supports this conclusion. On the other hand, results obtained by dropping the linear term and working at small D seem, at present, to be rather unphysical [13,7]; this is presumably due to the need to have the spiral tip remain a finite distance away from the origin, which occurs at small D only if μ is finite. We will therefore adopt Eqs. (1), (2) as our fundamental model and proceed to consider the small D limit.

This free boundary problem with $D=0$ was first tackled by Pelce and Sun [9]. If one assumes a uniformly rotating field $v(\vec{x},t) \to v(r,\theta-\omega t)$ one obtains

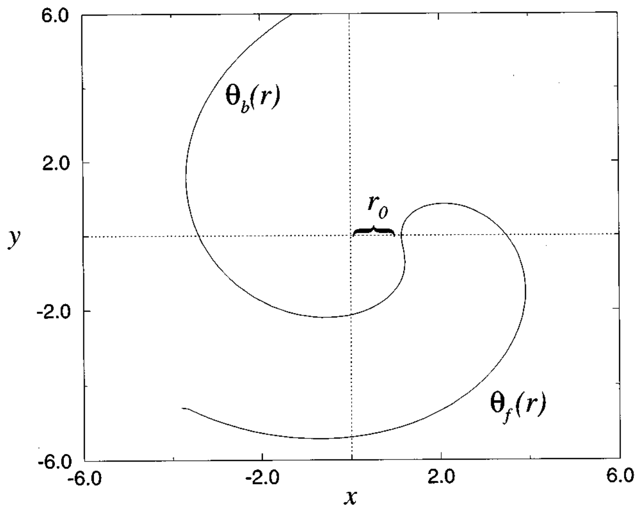

FIG. 1. A typical spiral, with r_0, $\theta_f(r)$, $\theta_b(r)$ indicated.

$$-\omega(\partial v_\pm/\partial\theta)=g_\pm-\mu v\,. \tag{5}$$

This can be solved by imposing the matching conditions $v_+(\theta_f)=v_-(\theta_f)$ and $v_+(\theta_b)=v_-(2\pi+\theta_b)$ where $\theta_f(r)$ and $\theta_b(r)$ are the positions of the interface from quiescent to excited and back to quiescent, as a function of the radius r (see Fig. 1). Defining $\tilde{\omega}\equiv\omega/\mu$, $\tilde{g}_\pm\equiv g_\pm/\mu$, the solution can be written as

$$v_\pm(r,\theta)=\tilde{g}_\pm+A_\pm(r)e^{\theta/\tilde{\omega}}, \tag{6}$$

where

$$A_-(r)=(\tilde{g}_+-\tilde{g}_-)\frac{(e^{-\theta_f/\tilde{\omega}}-e^{-\theta_b/\tilde{\omega}})}{1-e^{2\pi/\tilde{\omega}}},$$

$$A_+(r)=A_-(r)-(\tilde{g}_+-\tilde{g}_-)e^{-\theta_f/\tilde{\omega}}.$$

This can then be substituted into the "eikonal" equation (2) to find the interfaces $\theta_f(r),\theta_b(r)$. Near the tip $(\theta=0,\ r=r_0)$, smoothness requires $-\theta_b(r)=\theta_f(r)=\alpha\sqrt{r-r_0}$, for some positive α. This condition allows for the determination of the rotation frequency ω. It is easy to check that the field value v takes the value $\tilde{g}_-$ at the tip and for all $r<r_0$.

This solution has several unattractive features. Since the interface positions $\theta_{f,b}$ vary as $\sqrt{r-r_0}$,

$$\partial v/\partial r\sim 1/\sqrt{r-r_0} \tag{7}$$

for all θ when r is close to but above the tip radius r_0. Also, $\partial v/\partial\theta$ has a finite jump discontinuity at $r=r_0$, $\theta=0$, so that the derivative of v along the interface has a jump discontinuity at the tip where the front and back meet; this leads via the relation (2) to a similar jump for the derivative of the curvature. In addition, the normal derivative of v has a finite jump discontinuity across the interface. These difficulties have had the practical effect of making it impossible to do a full stability analysis of the spiral solution [14] and, in general, raise questions concerning whether the introduction of finite diffusivity dramatically alters the conclusions one derives via this construction. We now show that, in fact, finite diffusivity smoothes out this singularities without making any quantitatively significant change in the interface shape and selected rotation frequency.

To proceed, we use an integral equation formulation of the problem [8]. The field $v-\tilde{g}_\pm$ obeys a homogeneous, linear field equation with a fixed discontinuity across the interface. Following standard manipulations, we can, therefore, express v in the rotating frame as

$$v_\pm(r,\theta)=\tilde{g}_\pm+(\tilde{g}_+-\tilde{g}_-)D\int ds'\left(\hat{n}'\cdot\vec{\nabla}'G-\frac{\omega r'}{D}\hat{n}'_\theta G\right), \tag{8}$$

where G is the Green's function for the equation

$$\left(D\vec{\nabla}^2+\omega\frac{\partial}{\partial\theta}-\mu\right)G(r,\theta;r',\theta')=\frac{-\delta(r-r')\,\delta(\theta-\theta')}{r'}. \tag{9}$$

An explicit representation of G which will be used below is

$$G(r,\theta;r',\theta')=\int_{-\infty}^{t}\frac{dt'}{4\pi D(t-t')}\exp\left\{\frac{-(r^2+r'^2-2rr'\cos[\theta-\theta'+\omega(t-t')])}{4D(t-t')}-\mu(t-t')\right\}. \tag{10}$$

The integral in Eq. (8) is over the entire interface with arclength variable s' and $\hat{n}'$ is the unit normal which points outward from the excited region; $\hat{n}'_\theta$ is the component of $\hat{n}$ in the direction of the $\hat{\theta}'$ vector. For a given interface, this construction gives a field which obeys the field equation and the continuity condition; a full solution can then be found in principle by substituting the field value at the interface into the eikonal condition and iterating the interface shape until the equation is satisfied. What we will do instead is evaluate this integral for the Pelce-Sun (PS) interface obtained at $D=0$. We will show that this field is completely free from singularities but differs from the Pelce-Sun field solution only by terms which are small in the small D limit.

Let us first focus on some point away from either the interface or $r=r_0$. In this region, we will show how our formulation reproduces the known results of Pelce and Sun. Since G will never be singular, the $\hat{n}'\cdot\nabla'G$ in Eq. (8) is order D and can be neglected. The integral $\hat{n}'_\theta ds'$ can be replaced by $\pm dr'$ (for front and back, respectively). Now, the integrals over r' [in Eq. (8)] and t' (in the definition of G) are dominated by the saddle point contributions coming from

$$r'=r+O(\sqrt{D})$$

$$t_n'=t+(\theta-\theta'-2\pi n)/\omega+O(\sqrt{D}).$$

If $\theta>\theta'$, n runs from 1 to ∞; otherwise n goes from 0 to ∞. Doing the Gaussian integrals around these saddle points leads after some algebra to

$$v_{\pm}=\tilde{g}_{\pm}-(\tilde{g}_{+}-\tilde{g}_{-})\left(\sum_n \exp(\theta-\theta_f-2\pi n)/\tilde{\omega} - \sum_n \exp(\theta-\theta_b-2\pi n)/\tilde{\omega}\right) \tag{11}$$

where the n values in each sum obey the aforementioned rule. In the excited region, for example, $\theta_f>\theta>\theta_b$, yielding

$$v_{+}(\theta)=\tilde{g}_{+}-(\tilde{g}_{+}-\tilde{g}_{-})e^{\theta/\tilde{\omega}}\left[e^{-\theta_f/\tilde{\omega}}\sum_{n=0}^{\infty} e^{-2\pi n/\tilde{\omega}} - e^{-\theta_b/\tilde{\omega}}\sum_{n=1}^{\infty} e^{-2\pi n/\tilde{\omega}}\right] \tag{12}$$

with a similar expression obtainable for $v_-(\theta)$. Doing the sums, we directly recover the result of Eq. (6) above. For $r<r_0$, there are no saddle points and the integral is exponentially small.

We now wish to understand the departure from the Pelce-Sun solution due to finite diffusivity. As we have seen, there are a number of different regions where the Pelce-Sun solution breaks downs and exhibits singular behavior. These breakdowns are all cured by boundary layers whose width vanishes with D. Interestingly enough, as we shall see, the scaling of the boundary-layer width differs in each region. We first examine the region $r\simeq r_0$, but still away from the interface, i.e., θ is not close to 0. We saw in Eq. (8) that dv/dr was singular in this region. Examining our integral representation for v we see that the saddle point contribution from the t' integration is unchanged; however, the Gaussian integral with $r'\simeq r+0(\sqrt{D})$ cannot be blithely extended to infinity since the lower limit of the r' integration range is r_0. Also, we must use the fact that the integral of the Green's function along the front and back have opposite signs and cancel to lowest order for $r'\simeq r_0$. Those considerations lead to the expression

$$v_-(\theta)$$

$$=\tilde{g}_- -(\tilde{g}_+-\tilde{g}_-)\omega r_0\sqrt{D}\int_0^\infty d\tilde{r}'\,\frac{\partial G}{\partial\theta'}(\tilde{r},\tilde{r}';\theta,\theta')|_{\theta'=0}\times[\theta_f(\tilde{r}')-\theta_b(\tilde{r}')], \tag{13}$$

where

$$r=r_0+\sqrt{D}\tilde{r},\quad r'=r_0+\sqrt{D}\tilde{r}'. \tag{14}$$

Plugging in the expression of the Green's function and performing the t' integral, we obtain

$$v_-(\theta)=\tilde{g}_-+2(\tilde{g}_+-\tilde{g}_-)\alpha D^{3/4}(\partial F/\partial\theta),$$

with

$$F(\theta)=\sum_n\int_0^\infty \frac{d\tilde{r}'\sqrt{\tilde{r}'}}{\sqrt{4\pi D(2\pi n-\theta)/\omega}}\times\exp\left[\frac{-(\tilde{r}^2+\tilde{r}'^2-2\tilde{r}\tilde{r}')}{4(2\pi n-\theta)/\omega}+(\theta-2\pi n)/\tilde{\omega}\right]. \tag{15}$$

F can be expressed in terms of the parabolic cylinder function [15] $\mathcal{D}_\nu$ for index $\nu=-3/2$

$$v_-(\theta)=\tilde{g}_-+\frac{\tilde{g}_+-\tilde{g}_-}{\sqrt{2}}D^{1/4}\frac{\partial}{\partial\theta}\left[\sum_n \frac{\delta_n}{\mu}{}^{1/4}\exp(\mu\delta_n/2)\times\exp\left(\frac{-\tilde{r}^2}{4\delta_n}\right)\mathcal{D}_{-3/2}(-\tilde{r}/\sqrt{\delta_n})\right] \tag{16}$$

with $\delta_n=2(2\pi n-\theta)/\omega$. This structure represents a boundary layer of (minimum) width $(2D|\theta|/\omega)^{1/2}$. For negative $\tilde{r}$, the parabolic cylinder function decays as a Gaussian and $v_-(0)$ approaches $\tilde{g}_-$; for large positive $\tilde{r}$, $\mathcal{D}$ grows and cancels the exponential factor, leading to the expected behavior $v_-(\theta)-\tilde{g}_-\sim\sqrt{\tilde{r}}\,D^{1/4}\sim\sqrt{r-r_0}$. Note that the change in the field itself is negligible as it vanishes in the small D limit as $D^{1/4}$, even though the derivative is of order $D^{-1/4}$ and approaches infinity.

So, we have shown how integrating over the Pelce-Sun interface with the finite D Green's function leads to a regularization of the infinite slope discontinuity at $r=r_0$, without modifying the field. In fact, this lack of field modification is true everywhere including the interface. This follows from the fact that we have already shown that our field construction agrees with the PS field everywhere that is a distance $O(1)$ away from the interface and the PS fields are continuous across the interface. Field derivatives near the interfaces, on the other hand, are significantly modified due to the presence of diffusion-induced interfacial boundary layers. We now turn to a discussion of the form of these layers.

Let us consider first the interface *away* from the tip. Expressed in terms of our discussion so far, the only necessary modification is to the $n=0$ saddle point in the t' integral. Specifically, if $\theta-\theta_f(r)=\tilde{\theta}$ is small (i.e., we are close to the front), we need to keep an extra term in the argument of the cosine appearing in the Green's function

$$\theta-\theta_f(r')+\omega(t-t')\simeq\tilde{\theta}+\frac{\partial\theta_f}{\partial r'}(r-r')+\omega(t-t'). \tag{17}$$

The modified t' saddle point occurs at

$$\omega(t-t')=-\tilde{\theta}-\frac{\partial\theta_f}{\partial r'}(r-r'), \tag{18}$$

(which must of course be positive). Doing the t' integral leaves us with an expression of the form

$$\int \frac{dr'}{\left[\frac{4\pi D}{\omega}\left|\tilde{\theta}+\frac{\partial\theta_f}{\partial r}(r-r')\right|\right]^{1/2}}\exp\left[\frac{-(r-r')^2}{\left[\frac{4D}{\omega}\left|\frac{\partial\theta_f}{\partial r}(r-r')+\tilde{\theta}\right|\right]}+\left(\tilde{\theta}+\frac{\partial\theta_f}{\partial r'}(r-r')\right)\Big/\tilde{\omega}\right], \tag{19}$$

where the integral ranges over those values of r' consistent with the aforementioned positivity constraint on $t-t'$. This expression implies there is a crossover in behavior from the previous off-interface structure when $\tilde{\theta}$ is order D and that the range of relevant r' variation is also of order D. The overall structure of the v field can be shown to be [16]

$$v=v_{ps}+D\hat{v}(\tilde{\theta}/D) \tag{20}$$

and $\hat{v}$ is constant on one side, exponentially decaying on the other side, of the interface. This form is necessary to cure the finite slope discontinuity across the PS interface.

In fact, the width of this interfacial boundary layer is proportional to $|\partial\theta_f/\partial r|$. Since this derivative diverges near the tip, the boundary layer is much wider than order D in this region. To analyze this region, we modify Eq. (17) above, making explicit the square root dependence of θ_f with r' near the tip

$$\theta-\theta_f(r')+\omega(t-t')\simeq\tilde{\theta}-\alpha\sqrt{r'-r_0}+\omega(t-t'), \tag{21}$$

(where $\tilde{\theta}$ is measured from zero angle). Letting $r=r_0+\tilde{r}, r'=r_0+\tilde{r}'$, we obtain for the G term

$$\frac{-\partial}{\partial\theta}\int\frac{d\tilde{r}'\,2\alpha\sqrt{\tilde{r}'}}{\sqrt{4\pi D(-\tilde{\theta}+\alpha\sqrt{\tilde{r}'})}}\times\exp\left[\frac{-(\tilde{r}-\tilde{r}')^2}{4D(-\tilde{\theta}+\alpha\sqrt{\tilde{r}'})}+(\tilde{\theta}-\alpha\sqrt{\tilde{r}'})\Big/\tilde{\omega}\right]. \tag{22}$$

The crossover from the previous $r\sim r_0$ behavior at finite $\tilde{\theta}$ occurs at

$$\tilde{\theta}\sim\sqrt{\tilde{r}}\sim D^{1/3}, \tag{23}$$

so that the boundary-layer size in $\tilde{r}$ is $\tilde{r}'\sim D^{2/3}$.

Hence, the leading boundary-layer structure near the tip is [17]

$$v=g_-+D^{1/3}\hat{v}\left(\frac{r-r_0}{D^{2/3}},\frac{\theta}{D^{1/3}}\right). \tag{24}$$

Note that this is exactly the type of relationship that we need. The tangential derivative discontinuity of v_{PS} can be explicitly canceled by the θ derivative of the second term; if we iterate the equation perturbatively, we will find that the curvature of the PS solution needs to be corrected by an amount of the form $D^{1/3}f(s/D^{1/3})$ for small arclengths and this boundary layer will compensate for the jump in $\partial\kappa/\partial s$ across the tip. On the other hand, the normal derivative $\partial v/\partial r|_{r_0}$ is actually of order $D^{-1/3}$ and, hence, appears to diverge in the Pelce-Sun solution.

To summarize, we have shown how to construct a singularity-free spiral field, starting from the Pelce-Sun solution, by including the effects of a small diffusion constant. The fact that this construction goes through without difficulty proves that the Pelce-Sun solution gives the correct interface shape and concomitant rotation frequency in the $D\to 0$ limit. However, the demonstration that the normal derivative of the field near the tip is actually divergent means that the stability problem is subtle; since a perturbation to the interface will in general move the tip in the radial direction, this induces large field changes which must be explicitly balanced by interfacial structure on the boundary layer length scale $D^{1/3}$. Work on this stability problem is in progress.

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[14] There is one (unsuccessful) attempt to carry out such an analysis; see P. Pelce and J. Sun, Physica D **63**, 273 (1993). More recently [M. Falcke and H. Levine (unpublished)], it has been shown that the stability calculation can in fact be done if one makes certain assumptions regarding the correct boundary conditions on the perturbed interface near the tip. These assumptions can only be checked by a regularized theory of the type we are constructing in this paper.
[15] See, e.g., I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1965).
[16] One can easily show that Eq. (20) gives rise to a one-sided exponential boundary layer by changing variables of integration. We should note that for this boundary layer, the other term $\hat{n}'\cdot\nabla' G$ in Eq. (8) is also relevant, since the derivative acting on the inner variable (of order D) exactly compensates for the explicit extra factor of D.
[17] Again a quantitative treatment must include the $\hat{n}'\cdot\nabla' G$, since there is no $D^{1/3}$ factor and the normal derivative pulls down a factor of $D^{-2/3}$, which thus compensates for the explicit extra factor of D in Eq. (8).