Theory of spike spiral waves in a reaction-diffusion system

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We discovered a type of spiral wave solutions in reaction-diffusion systems—spike spiral wave, which significantly differs from the spiral waves observed in the models of FitzHugh-Nagumo type. We present an asymptotic theory of these waves in the Gray-Scott model [Chem. Sci. Eng. **38**, 29 (1983)]. We derive the kinematic relations describing the shape of this spiral, and find the dependence of its main parameters on the control parameters. The theory does not rely on the specific features of the Gray-Scott model and thus is expected to be applicable to a broad range of reaction-diffusion systems. [S1063-651X(99)09507-0]

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Formation of rotating spiral waves (rotors) is one of the most vivid and ubiquitous phenomena of nonlinear physics [1–12]. These waves are observed in nonlinear optical media [13], chemical reactions of Belousov-Zhabotinsky type, catalytic reactions on crystal surfaces [6–8], and in a variety of biological systems: social amoebae *Dictyostelium discoideum* [14], *Xenopus* oocytes [15], chicken retina [16], and the hearts of animals and man, where the formation of the spiral waves is responsible for cardiac arrythmias and the life-threatening condition of ventricular fibrillation [1,2,12].

A generic model used to describe the spiral waves is a pair of reaction-diffusion equations of activator-inhibitor type [1–11],

$$\tau_\theta \frac{\partial \theta}{\partial t} = l^2 \Delta \theta - q(\theta, \eta, A), \tag{1}$$

$$\tau_\eta \frac{\partial \eta}{\partial t} = L^2 \Delta \eta - Q(\theta, \eta, A), \tag{2}$$

where θ is the activator, i.e., the variable with respect to which there is a positive feedback; η is the inhibitor, i.e., the variable with respect to which there is a negative feedback and which controls activator's growth; q and Q are certain nonlinear functions representing the activation and the inhibition processes; l and L are the characteristic length scales and τ_θ and τ_η are the characteristic time scales of the activator and the inhibitor, respectively; and A is the bifurcation parameter. A considerable amount of studies was done on the excitable systems with the FitzHugh-Nagumo-type kinetics (N systems) (see, for example, Refs. [1–9] and references therein). These systems are described by Eqs. (1) and (2) with $L=0$, and the nonlinearity in q such that the nullcline of Eq. (1) is N shaped or inverted N shaped. The asymptotic theory of the spiral waves in N systems with $\alpha = \tau_\theta / \tau_\eta \ll 1$ and $L=0$ was recently developed by Karma [17,18].

The existence of the spiral waves in excitable N systems is due to the ability of such systems to sustain traveling waves, the simplest of which is a solitary wave— the traveling autosoliton (AS) [1–11]. In N systems the equation $q(\theta, \eta, A)=0$ has three roots: θ_{i1}, θ_{i2}, and θ_{i3}, for fixed A and $\eta = \eta_i$. For $\alpha \ll 1$ an AS consists of a front, which is a wave of switching from the stable homogeneous state $\theta = \theta_h$ and $\eta = \eta_h$ to the state with $\theta = \theta_{\max}$ ($\theta_h = \theta_{i1}$ and $\theta_{\max} = \theta_{i3}$ for $\eta_i = \eta_h$) whose width is of order l, and a back of width of order l that follows the front some distance $w \gg l$ behind the front. Thus in the AS the distribution of θ is a broad pulse, while the value of η slowly varies from $\eta = \eta_h$ to some value $\eta = \eta_m$ in the back of the pulse, and then slowly recovers from η_m to η_h behind it. In the limit $\alpha \to 0$ the amplitude of the wave (the value of $\theta_{\max}$) becomes independent of α, and the speed c does not exceed the value of order l/τ_θ, with both $\theta_{\max}$ and c determined only by the nonlinearity in q.

At the same time, many excitable systems are described by Eqs. (1) and (2) in which the nullcline of Eq. (1) is Λ or V shaped. Examples of such Λ systems are the well-known Brusselator and the Gray-Scott models of autocatalytic reactions and an example of a V system is the Gierer-Meinhardt model of morphogenesis [10]. Recently, we showed for the excitable Brusselator [19] and the Gray-Scott model [20] that they are also capable of propagating traveling waves—traveling spike AS. The properties of these AS's are essentially different from those in N systems. The distribution of θ in an AS has the form of a narrow spike whose amplitude grows as α decreases and can become huge as $\alpha \to 0$. In contrast to N systems, in the spike η varies abruptly and then slowly recovers back to η_h far behind the spike. The speed of such an AS is always greater than l/τ_θ, and goes to infinity as $\alpha \to 0$. Also, it is important to emphasize that in an AS the front and the back are not separated by a large distance, as in N systems. In this paper we will show that in excitable Λ or V systems it may also be possible to excite steadily rotating spiral waves and develop a theory of such waves in the case $\alpha \ll 1$.

To be specific, we will consider the excitable ($L=0$) Gray-Scott model, which is described by the equations [21]

$$\frac{\partial \theta}{\partial t} = \Delta \theta + A \theta^2 \eta - \theta, \tag{3}$$

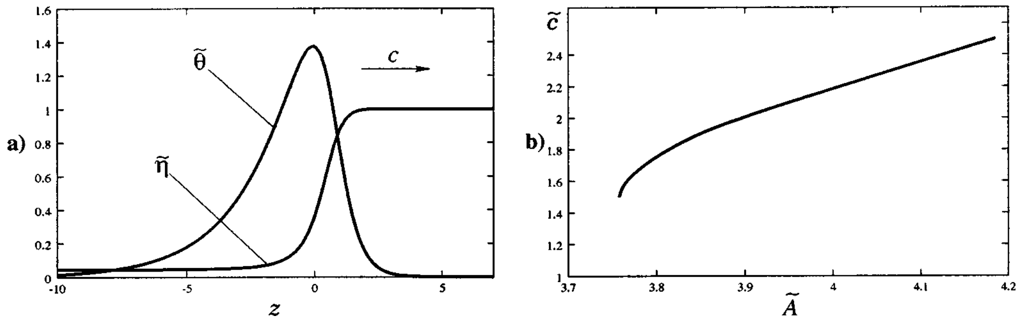

FIG. 1. (a) Distributions of $\tilde{\theta}$ and $\tilde{\eta}$ in the sharp front for a particular value of $\tilde{A}=3.76$; (b) dependence $\tilde{c}(\tilde{A})$. Results of the numerical solution of Eqs. (9) and (10).

$$\alpha^{-1}\frac{\partial\eta}{\partial t}=-\theta^2\eta+1-\eta, \tag{4}$$

where we chose l and τ_θ as the units of time and length, respectively. Recently, we showed numerically that steadily rotating spiral waves may be excited in this model at sufficiently small α [20]. From these simulations one can see that the spiral wave is a steadily rotating slightly curved sharp spike front of width of order 1 which in the cross section looks like a periodic traveling wave train (sufficiently far from the core). We would like to emphasize that it is this kind of concentration profile that is experimentally observed in the Belousov-Zhabotinsky reaction [22,23].

Let us derive the equation of motion for the traveling sharp front in the Gray-Scott model with $\alpha \ll 1$. Since η varies slowly outside the front, it can be replaced by a constant value $\eta=\eta_i$ ahead of the front. Let us introduce self-similar variable $z=\rho-ct$, where ρ is the coordinate along the normal direction to the front. For definiteness we will assume that $c>0$, which means that the front is moving in the $+z$ direction. In the sharp front the value of θ is large [20], so one can neglect the last two terms in Eq. (4). Therefore, in the presence of small curvature K, Eqs. (3) and (4) can be written as

$$\frac{d^2\theta}{dz^2}+(c+K)\frac{d\theta}{dz}+A\theta^2\eta-\theta=0, \tag{5}$$

$$\alpha^{-1}c\frac{d\eta}{dz}-\theta^2\eta=0. \tag{6}$$

These equations have to be supplemented by the boundary conditions $\theta(\pm\infty)=0$ and $\eta(+\infty)=\eta_i$, where the infinity actually means sufficiently far ahead of the front compared to the front thickness.

Let us introduce the new variables

$$\tilde{\theta}=\alpha^{1/2}\theta\left(\frac{c+K}{c}\right)^{1/2}, \quad \tilde{\eta}=\frac{\eta}{\eta_i}, \tag{7}$$

and the quantities

$$\tilde{A}=A\alpha^{-1/2}\eta_i\left(\frac{c}{c+K}\right)^{1/2}, \quad \tilde{c}=c+K. \tag{8}$$

In these variables Eqs. (5) and (6) become

$$\frac{d^2\tilde{\theta}}{dz^2}+\tilde{c}\frac{d\tilde{\theta}}{dz}+\tilde{A}\tilde{\theta}^2\tilde{\eta}-\tilde{\theta}=0, \tag{9}$$

$$\tilde{c}\frac{d\tilde{\eta}}{dz}-\tilde{\theta}^2\tilde{\eta}=0, \tag{10}$$

with the boundary condition $\tilde{\eta}(+\infty)=1$. Observe that all α, A, and η_i dependences now enter only via the parameter $\tilde{A}$.

Equations (9) and (10) can be solved numerically (see also Ref. [20]). This numerical solution shows that the distribution of $\tilde{\theta}$ indeed has the form of a spike [Fig. 1(a)]. In the spike, $\tilde{\eta}$ varies from $\tilde{\eta}=1$ at $z=+\infty$ (ahead of the front) to some $\tilde{\eta}=\tilde{\eta}_{\rm min}$ at $z=-\infty$ (behind the front); see Fig. 1(a). The value of $\tilde{\theta}\sim 1$ in the spike, so in the original variables we indeed have $\theta\sim\alpha^{-1/2}\gg 1$ [see Eq. (7)]. The speed of the front $\tilde{c}$ as a function of $\tilde{A}$ obtained from the numerical solution of Eqs. (9) and (10) is presented in Fig. 1(b). One can see that this solution exists only at $\tilde{A}>\tilde{A}_b$, and its speed is always greater than $c=c_{\rm min}$, where

$$\tilde{A}_b=3.76, \quad c_{\rm min}=1.5 \tag{11}$$

The numerical analysis of Eqs. (9) and (10) also shows that $\tilde{\eta}_{\rm min}=\tilde{\eta}^{\,b}_{\rm min}=0.05$ at $\tilde{A}=\tilde{A}_b$, and rapidly decreases as $\tilde{A}$ increases.

From Eq. (8), it immediately follows that for small K the correction δc to the velocity c due to curvature is

$$\delta c=-K\left(1+\frac{\tilde{A}}{2\tilde{c}}\frac{d\tilde{c}}{d\tilde{A}}\right), \tag{12}$$

where on the right-hand side $\tilde{A}$, $\tilde{c}$, and $d\tilde{c}/d\tilde{A}$ are evaluated at $K=0$. Also, as we showed in Ref. [20], for $\tilde{A}$ not in the immediate vicinity of $\tilde{A}_b$ with good accuracy $\tilde{c}=0.86\tilde{A}$ and $\tilde{\eta}_{\rm min}=0$. Then, going back to the original variables, we may write

$$c=c_\infty-aK, \tag{13}$$

where

$$c_\infty=0.86A\alpha^{-1/2}\eta_i, \quad a=\tfrac{3}{2}. \tag{14}$$

Note the anomalous coefficient multiplying the curvature in Eqs. (12) and (13). Observe that this effect was recently studied numerically in N systems with imperfect time scale separation [24,25].

Behind the sharp front the value of η drops from η_i to $\eta_{\min}$, and θ goes exponentially to zero [20]. On the much longer time scale α^{-1} the value of η recovers from $\eta_{\min}$ according to Eq. (4), in which outside of the front the term $-\theta^2\eta$ can be neglected. From this we obtain that, after the front passes a point x at time $t_i = t_i(x)$ we have

$$\eta(x,t) = 1 - [1 - \eta_{\min}(t_i)]e^{-\alpha(t-t_i)}, \tag{15}$$

where $\eta_{\min} = \eta_i \tilde{\eta}_{\min}$. In a steadily rotating spiral wave we must have $\eta(x, t_i + T) = \eta_i(t_i) = \text{const}$, where $T = 2\pi/\omega$ and ω is the angular frequency of the rotation of the spiral. Therefore, the spiral should be described by Eq. (13) with $c_\infty = \text{const}$, which is in turn related to ω. This equation was first analyzed by Burton, Cabrera, and Frank (BCF) for growth of screw dislocations on crystal surfaces [26] (see also Ref. [9]). They calculated the shape of the spiral and its frequency in the case where the tip of the spiral is at rest. Applying their results to Eq. (14), we obtain $\omega = 0.16\alpha^{-1}A^2\eta_i^2$, where for simplicity we used the expressions in Eq. (14) and put $\eta_{\min} = 0$. Since $A\eta_i \gtrsim \alpha^{1/2}$ in order for the front to be able to propagate, we must have $\omega \gtrsim 1$, so one can expand the exponential in Eq. (15), and obtain $\eta_i = 3.4\alpha^{2/3}A^{-2/3}$ and $\omega = 1.8\alpha^{1/3}A^{2/3}$. The spatial step h of the spiral far from the core will be $h = 10\alpha^{-1/6}A^{-1/3}$. Notice that a similar method was recently used to analyze asymptotically the spiral waves in N systems [17,18].

Comparing the results obtained above with Eq. (11), one can see that in order for the solution in the form of the traveling front to exist, one should have $A \gtrsim \alpha^{-1/2} \gg 1$. On the other hand, for $A \gg \alpha^{-1/2}$, we have $\omega \gg 1$, so θ will not have enough time to decay behind the wave front. This means that this kind of the spiral wave may exist only at $A \sim \alpha^{-1/2}$. Notice that according to Eq. (14) we have $c_\infty \sim 1$ and $h \sim 1$ for these values of A, so the formulas obtained above for the frequency of the spiral should only be correct qualitatively.

When $A_{bT} < A \ll \alpha^{-1/2}$, where $A_{bT} = 3.76\alpha^{1/2}$ is the excitability threshold which is obtained from Eq. (11) for $\eta_i = \eta_h = 1$ [20], the structure of the spiral wave solution changes. For these values of A the spiral acquires a core of radius $R \gg 1$. Obviously, we have $\eta = \eta_h = 1$ in the core. The reason the front will not propagate inside the core is that the spiral tip which moves along the core boundary is right at the propagation threshold. If this were not true, a small increase of the front curvature near the tip would allow its motion inside the core where $\eta > \eta_i$ [see Eq. (15)], which would in turn increase the front's speed [see Eq. (14)], making the circular motion of the tip unstable. For cores of radius $R \gg 1$ one can neglect the curvature at the tip and assume that $\eta_i = \eta_i^b = 3.76\alpha^{1/2}A^{-1}$ in the limit $\alpha \to 0$. The frequency ω is then determined by Eq. (15), with $\eta_i = \eta_i^b$. In particular, for $\alpha^{1/2} \ll A \ll \alpha^{-1/2}$, we can expand the exponential and asymptotically obtain

$$\omega = 1.76\alpha^{1/2}A. \tag{16}$$

This equation shows that the value of ω lies in the range $\alpha \lesssim \omega \lesssim 1$, as should be expected.

Far away from the core the speed c should only slightly exceed $c_{\min}$, so the step of the spiral will be $h = 5.4\alpha^{-1/2}A^{-1}$. Note, however, that because of the closeness to the threshold point $\tilde{A} = \tilde{A}_b$ the expansion in Eq. (12) is no longer justified, and therefore the BCF theory, as well as Eq. (13), is not applicable to the spiral waves in this parameter range. This theory can be modified by noting that close to $\tilde{A}_b$ we have, approximately,

$$c = c_{\min} + b\left(\tilde{A} - \tilde{A}_b - \frac{\tilde{A}_b}{2c_{\min}}K\right)^{1/2}, \tag{17}$$

where b is a constant and the tilde quantities in the right-hand side are evaluated at $K = 0$. The analysis of Eqs. (9) and (10) shows that $b = 1.4$. Note that this equation reduces to

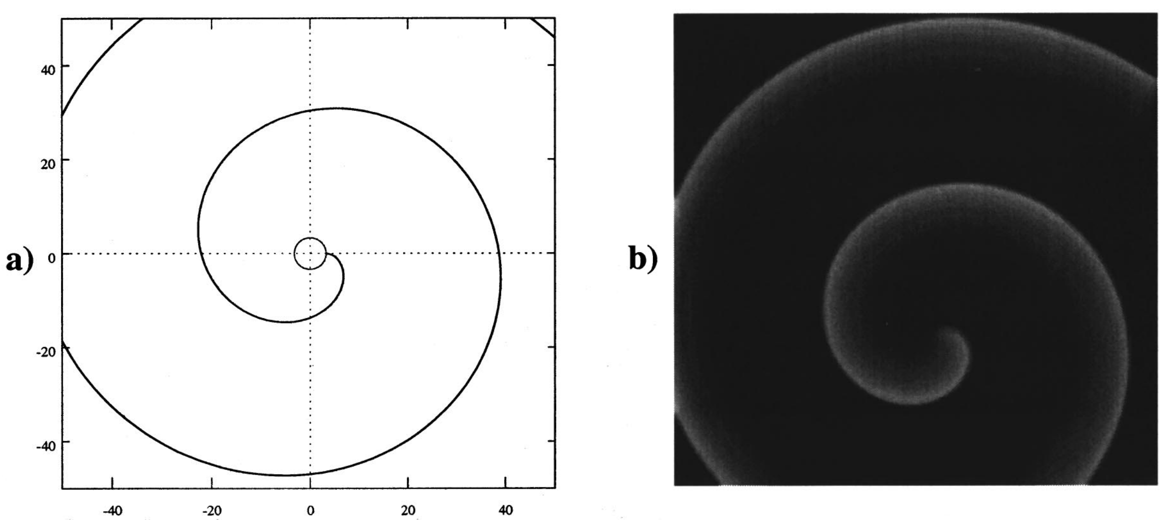

FIG. 2. Steadily rotating spiral wave: (a) Result of the numerical solution of Eq. (18) with $\omega = 0.47$ and $\tilde{A} - \tilde{A}_b = 0.49$ (the circle shows the core of the spiral); (b) Result of the numerical solution of Eqs. (3) and (4) with $A = 2$ and $\alpha = 0.1$ (distribution of θ). The system is 100 $\times$100.

the form of Eq. (13) only very far from the core. Also note that an equation of this kind was introduced by Zykov for N systems without strong separation of time scales [2].

Following Ref. [26], we rewrite Eq. (17) for the steadily rotating spiral in terms of the angle ϕ between the tangent vector to the front and the radius vector as a function of the distance r to the origin. A straightforward calculation shows that in these variables Eq. (17) becomes

$$\frac{d\phi}{dr} = -\frac{1}{r}\tan\phi + \frac{2c_{\min}}{\tilde{A}_b b^2 \cos\phi}[b^2(\tilde{A}-\tilde{A}_b) - (c_{\min} - \omega r \cos\phi)^2], \tag{18}$$

with the boundary conditions $\phi(+\infty) = \pi/2$ [26] and $\phi(R) = 0$. The latter condition shows that at its tip the front is normal to the circle along which it rotates, which also follows from the stability considerations for the tip. Since the front at $r = R$ is at the propagation threshold, its normal velocity there should be equal to $c_{\min}$, so $R = c_{\min}/\omega$. Knowing the value of R, one can then calculate $\tilde{A} - \tilde{A}_b$ as a function of ω. The numerical solution of Eq. (18) shows that for $\omega \ll 1$ we have $\tilde{A} - \tilde{A}_b = 0.93\omega^{4/5}$. Note that with good accuracy this formula is valid even for $\omega \gtrsim 1$. Knowing the value of $\tilde{A}$ and hence $\eta_i = \tilde{A}\alpha^{1/2}A^{-1}$, one can then find a unique value of ω for which it agrees with Eq. (15). Since for $\omega \ll 1$ we have $\tilde{A} - \tilde{A}_b \ll 1$, Eq. (16) should indeed be recovered in the limit $\alpha \to 0$ with $\alpha^{1/2} \ll A \ll \alpha^{-1/2}$, with the spiral wave solution close to an involute of a circle of radius R [3]. For a particular value of $\omega = 0.29$ we find $\eta_i = 0.86$, within 4% agreement with Eq. (15). Comparing these quantities with the results of the numerical simulations of Eqs. (3) and (4) for $\alpha = 0.1$ and $A = 1.5$, in which this value of ω was observed, we find that the value of η_i agrees with the predicted one within 3% accuracy. The speed $c_\infty = 2.3$ obtained from Eq. (17) also agrees with that observed numerically within a few percent accuracy. The comparison of the shapes of the spiral obtained from the solution of Eq. (18) and from the numerical simulations (for slightly different parameters) is presented in Fig. 2. This agreement is quite remarkable considering the fact that at these parameters the spiral wave already underwent meandering instability. In fact, according to our analysis, a steady rotation of the spiral requires a fine tuning of the value of η_i at the tip of the spiral. Note that the tip of the spiral is not described by the interfacial equations derived above, and thus is a rather singular object capable of sudden movements on the smallest length scale. Thus it is natural to expect that the tip trajectory in a meandering spiral may be rather abrupt. Notice that a similar situation is observed in the simulations of models of cardiac tissue (see, for example, Ref. [27]).

In conclusion, we developed a theory of spike spiral waves in the Gray-Scott model. Spike traveling waves are observed in a variety of excitable systems including nerve and cardiac tissue. Even though we performed an analysis of a concrete system, Eqs. (17) and (18) have a general character and thus are expected to apply to other Λ and V systems (see also Refs. [10, 11]) and other excitable systems of different nature in which spike traveling waves are observed. Also, such waves can be expected in combustion systems and the Belousov-Zhabotinsky reaction in continuous flow reactors. Indeed, although in Eqs. (1) and (2) describing these systems, the activator nullcline may formally be N shaped, for typical parameters the value of $\theta_{\max}$ may be several orders of magnitude greater than θ_h, so the system effectively behaves as a Λ or V system. In particular, this is true for models of systems with uniformly generated combustion material [10,11] and the two-parameter version of the Oregonator [28]. Recent numerical simulations of the Oregonator showed that it has the same curvature-velocity relationship as in Eq. (17) [25].

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