Formation of shocks and breakup of wave patterns in anisotropic excitable media

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Strong state-dependent diffusion anisotropy in nonlinear excitable media leads to spontaneous formation of shocks representing sharp edges of curved propagating wave fronts. These shocks cause breaking of waves and destruction of wave patterns.

Realistic excitable media, such as cardial tissue or systems with catalytic surface reactions, are often anisotropic [1,2]. An interesting question is whether anisotropy could produce new dynamical phenomena or lead only to some elongation of spatiotemporal patterns which are already present in an isotropic medium. In the simplest case of a single diffusive species with a constant diffusion tensor, the anisotropy can easily be eliminated by rescaling the coordinates and, obviously, no new dynamical behavior could be found (except for some special effects related to wave propagation in nonstationary or inhomogeneous anisotropic media; see [3,4]). However, anisotropy in nonlinear reaction-diffusion systems cannot generally be removed by rescaling the coordinates: when several species diffuse and their directions of fast and slow diffusion do not coincide there is no scaling transformation which makes the system isotropic. Even in excitable media with a single diffusive component the anisotropy can be state dependent, so that the principal axes of the diffusion tensor rotate under the variation of state variables and have different orientations in different parts of a wave. In this paper, I show that sufficiently strong complex anisotropy leads to dynamical instabilities revealed by the appearance of shocks on the propagating wave fronts which can result in the breakup of target wave patterns.

In anisotropic media, the normal propagation velocity V_0 of flat fronts depends on the propagation direction. If anisotropy is so simple that it can be scaled out, the angular dependence of V_0 can be obtained by applying the stretching transformation and further taking a projection in the normal direction, since such a transformation does not conserve angles. In two-dimensional media this yields the following universal dependence:

$$V_0(\alpha) = V_{min}(q\sin^2\alpha + \cos^2\alpha)^{1/2} \tag{1}$$

where α is the angle between the tangent at the front and the direction at the fast propagation, while the parameter $q = (V_{max}/V_{min})^2$ is determined by the ratio of the maximal (at $\alpha = \pi/2$) and minimal (at $\alpha = 0$) propagation velocities. In excitable media with complex anisotropy, there is no universal angular dependence of the propagation velocity and, if we write $V_0(\alpha)$ in the form (1), the parameter q will be angle dependent. We consider the

evolution of wave patterns in a medium with *arbitrary* angular dependences $V_0(\alpha)$ and $q(\alpha)$.

Within the eikonal approximation [5,6] any propagating wave in a two-dimensional excitable medium is specified by its front curve. Each element of the curve moves in its normal direction with velocity $V = V(k,\alpha)$ depending on its curvature k and, in anisotropic media, on the angle α. The motion of curves can be described in terms of the natural equation $k = k(l,t)$ giving curvature k as a function of the arc length l of the curve measured from a certain fixed point on it. The dynamical equation for motion of closed fronts in excitable media is [6–8]

$$\partial k/\partial t + \partial/\partial l\left[k\int_0^l kVd\xi + \partial V/\partial l\right] = 0. \tag{2}$$

This equation has also been used in the problems of crystal growth [9], and has recently been investigated in connection with completely integrable equations of nonlinear waves [10]. According to the definition of curvature, it can be expressed as a derivative $k = \partial\alpha/\partial l$. Substituting this into (2) and integrating over l, we obtain

$$\partial\alpha/\partial t + \left[\int_0^l kVd\xi\right]\partial\alpha/\partial l + \partial V/\partial l = C(t). \tag{3}$$

If a curve has reflection symmetry, we can measure the internal coordinate on it, i.e., the arc length l, from the point of intersection of the curve with the symmetry axis. It can be shown that under this agreement the integration function $C(t)$ in equation (3) is equal to zero. In our notations the front which is orthogonal to the symmetry axis has $\alpha = 0$.

When curvature is small, the normal propagation velocity of a curved front is approximated by $V(\alpha,k) = V_0(\alpha) - Dk$, where $V_0(\alpha)$ is the velocity of the flat front moving in the same direction. Although the coefficient D can also depend on α, for simplicity we neglect such a dependence. Substituting this expression into (2), and taking into account that $\partial V_0/\partial l = (dV_0/d\alpha)(\partial\alpha/\partial l)$ and $kdl = d\alpha$, yields

$$\partial\alpha/\partial t + Q(\alpha)\partial\alpha/\partial l = D\partial^2\alpha/\partial l^2, \tag{4}$$

where

$$Q(\alpha) = dV_0/d\alpha + \int_0^\alpha V_0(\alpha)d\alpha. \tag{5}$$

Here we have neglected a small term proportional to curvature k.

Equation (4) belongs to a well-known class of equations describing the formation of shock waves [11]. If we entirely neglect the curvature effects by setting $D = 0$ in this equation, it can easily be integrated. It has a family of characteristics $l = l(\xi, t)$ such that the angle α remains constant along any of them. These characteristics satisfy equation $dl/dt = Q(\alpha)$, and represent straight lines on the plane (α, l). The general solution of (4) with the initial condition $\alpha = f(l)$ at $t = 0$ is given by $l = \xi + Q(f(\xi))t$ and $\alpha = f(\xi)$. If the initial curve is a circle of radius R, then $f(l) = l/R$, and the solution takes the form

$$l = \alpha R + Q(\alpha)t . \tag{6}$$

If characteristics of Eq. (4) intersect, its solution is multivalued. The solution ceases to be single valued and develops a caustic when the derivative $\partial \alpha / \partial l$ becomes infinite at some point l_0 on the curve or, respectively, when the derivative $\partial l / \partial \alpha$ vanishes at a certain angle α_0. Using (6) we obtain

$$\partial l / \partial \alpha = R + tQ'(\alpha) . \tag{7}$$

Therefore, $\partial l / \partial \alpha$ may become zero only if $Q'(\alpha) = dQ/d\alpha$ is negative at some angle α. The singularity of the front first appears at time moment $t_0 = R/c$, where $c = -\min Q'(\alpha)$.

When the dependence of l on the angle α along the curve, given by solution (6), is known, the coordinates (x, y) of the curve on the plane can be found to be

$$x(\alpha, t) = \int_0^\alpha (\partial l / \partial \alpha)\cos \alpha \, d\alpha,$$
$$y(\alpha, t) = V_0(0)t - \int_0^\alpha (\partial l / \partial \alpha)\sin \alpha \, d\alpha . \tag{8}$$

Note that the characteristics, which represent straight lines in the plane (α, l), are curved on the coordinate plane (x, y). Moreover, they are not orthogonal to the fronts and hence are not tangent to the velocity vectors $\mathbf{V}$. This is a particular case of the general property that the vectors of phase and group velocities are directed differently in anisotropic media [11]. Since characteristics are not straight lines, they can cross and thus produce shocks.

We see that function

$$Q'(\alpha) = V_0(\alpha) + d^2 V_0 / d\alpha^2 \tag{9}$$

plays an important role in the evolution of curved fronts. Substituting (1) into (9), it can be shown that $Q'(\alpha)$ is always positive if $q = \text{const}$. Hence caustics do not develop in the media where anisotropy can be scaled out. On the other hand, if anisotropy is complex and the deviation of the function $q(\alpha)$ from a constant is strong enough to
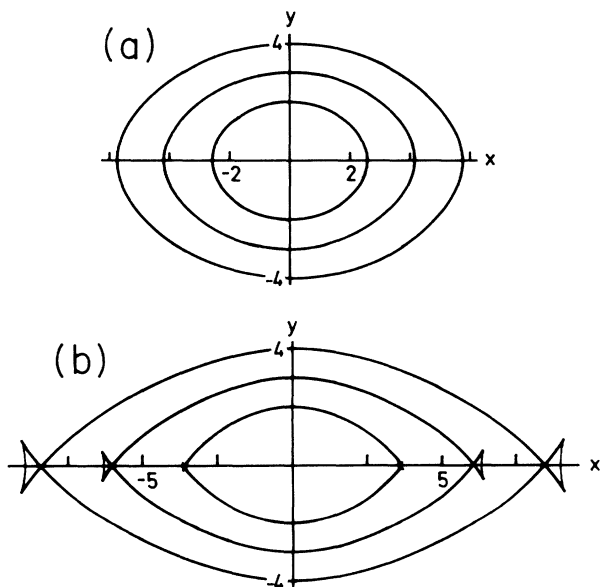

FIG. 1. (a) and (b) Expanding concentric wave fronts (target patterns) in the medium with complex anisotropy: $q = a + b\sin^2\alpha$, with (a) $b = 0.5$ and (b) $b = 5$; other parameters are chosen as $a = 2$, $V_{\min} = 1$, and $D = 0$. The initial shape of the wave front at $t = 0$ is a circle of radius $R = 1$; the wave fronts at time moments $t = 1$, 2, and 3 are shown. The outer loops ("swallow tails") of the fronts are unphysical and should be cut off.
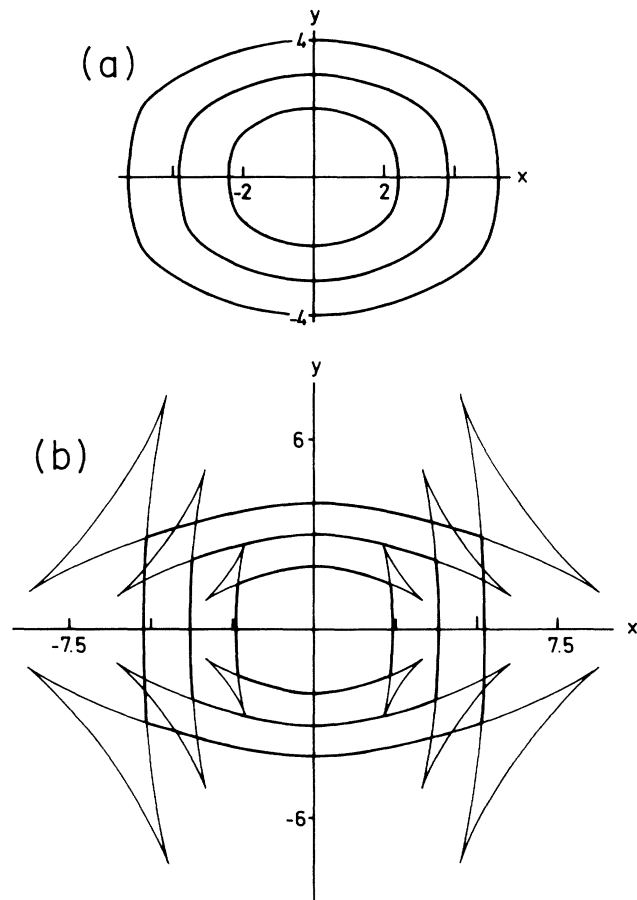
FIG. 2. (a) and (b) "Square-shaped" target patterns in a medium with complex anisotropy given by $q = a + b\sin^2 2\alpha$, with (a) $b = 0.4$ and (b) $b = 5$, other parameters the same as in Fig. 1. The outer loops ("swallow tails") shown by thin lines in (b) are unphysical and should be cut off.

make the minimum of $Q'(\alpha)$ negative, the caustics (or shocks) will appear on the expanding fronts.

The actual form of $q(\alpha)$ depends on the particular excitable reaction-diffusion system, and no general expression for it can be given. As an example, we take $q = a + b \sin^2\alpha$, so that parameter b characterizes the deviation from the simple constant anisotropy. The above analysis predicts that in this case the minimum of $Q'(\alpha)$ becomes negative and hence the caustics develop when $b > b_{cr}$, where $b_{cr} = [1 + (1 + a^2)^{1/2}]/2$. Figure 1 shows the evolution of expanding concentric wave fronts, computed using (6) and (8) with this choice of $q(\alpha)$. We see that for the smaller value of the parameter b the pattern is elongated but the fronts remain smooth [Fig. 1(a)]. However, when a larger value of b is chosen, two caustics, looking like "swallow tails" in Fig. 1(b), appear after some time on the expanding front.

The multivalued parts of solution $\alpha(l, t)$ are not physically meaningful. Whenever they appear, they should be replaced by a *discontinuous* single-valued solution. It is constructed by cutting off the outer loops of the front curve [i.e., the swallow tails in Fig. 1(b)]. The edges where the tangent direction changes by a finite angle $\Delta\alpha$ represent shocks of the wave front. The magnitude of the angle jump increases for stronger deviations from the simple anisotropy.

Until now we neglected the term $D(\partial^2\alpha/\partial l^2)$ in Eq. (4). Although this term is indeed small for the main part of the spreading front (provided that $R \gg D/V_0$), it becomes important inside the shock regions where the solution is discontinuous if $D = 0$. Its principal effect consists of smoothing the jump (as in the theory of hydrodynamical shock waves [12]). The width of a shock can then be estimated as $\delta l \sim D/c\Delta\alpha$; the curvature $k = \partial\alpha/\partial l$ of the front in the shock region is about $k_0 \sim c\Delta\alpha^2/D$. Hence this curvature grows when the deviation from the simple anisotropy is stronger and both $\Delta\alpha$ and $c = -\min Q'(\alpha)$ increase.

Equation (4) is based on the linear approximation $V = V - Dk$, which is valid only when $Dk \ll V_0$. For larger curvatures, the normal propagation velocity V decreases faster with k and, when a certain critical curvature k_{cr} is reached, wave propagation becomes impossible [13]. If the curvature of the wave front locally exceeds the critical curvature k_c about D/V_c, it breaks up in this region and two free tips appear. This means that the front shocks in the excitable media with strong state-dependent anisotropy should break up at the locations of the shocks.

In a recent experiment with a surface chemical reaction, "square-shaped" target patterns were observed, and this geometrical property has been attributed to the presence of state-dependent anisotropy [14]. When the reaction parameters were changed, the waves started to break at the edges. Each of the closed wave fronts, forming a target pattern, disintegrated into segments, some of which later collapsed while the others moved away from the observation window. To reproduce this behavior qualitatively, the evolution of concentrical expanding wave fronts was computed using (6) and (8) with $q = a + b \sin^2 2\alpha$. Under this choice, function $q(\alpha)$ has four maxima at different angles α. We see that when the deviation from the simple anisotropy is still small [Fig. 2(a)], the target pattern approaches a rectangular shape but the fronts remain smooth. When the deviation is larger [Fig. 2(b)] shocks appear on the expanding fronts which can lead to their breakup.

Thus it can be concluded that the strong complex anisotropy of diffusion can essentially influence the properties of patterns and the course of pattern formation in excitable media.

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