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Turbulized Rotating Chemical Waves

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From the numerical study of a simple nonlinear kinetics with scalar diffusion, it is shown that rotating waves easily transform to turbulence. The turbulence here is triggered by a single phaseless point, and spreads over the entire system through the endless production of phaseless points in pairs. A possible turbulence-inducing mechanism is interpreted.

Rotating spiral waves are an intriguing mode of spatio-temporal organization in nonlinear dissipative media with oscillatory or excitable local kinetics. The existence of such waves has most clearly been demonstrated[1] for the Belousov-Zhabotinskii reaction, where even the geometrical structure of their three-dimensional version, viz. scroll waves, has been analyzed in detail.[2] Similar wave phenomena are also met in life processes.[3] For instance, the circus movement of electrical activities was shown to occur in rabbit heart tissue,[4] and this kind of circulating activity has long been speculated to have a connection with some forms of high frequency irregularity of heart beat.[5] Another well-studied biological system associated with the spiral wave pattern is the aggregation of slime mold amoebae.[6]

Rotating spiral waves have a topologically interesting feature. The small pivotal region round which the waves circulate contains a phaseless point, and if one makes a tour along a closed path encircling this core region, the net phase increment experienced is $\pm 2\pi$. In this respect, such waves have much in common with the vortex excitations in two-component (or complex) fields such as superfluid helium and XY spin systems.

One of the most important questions about spiral wave patterns is their stability. As far as the experiments to date are concerned, they seem to rotate almost steadily round a spatially fixed core, whereas closer observations revealed that in some cases the core position is not really fixed but seems to rotate rather irregularly.[1] The analog-computer simulation by Gul'ko and Petrov,[7] and the digital-computer simulation by Rössler and Kahlert[8] seem to support the idea that such core meandering actually occurs especially for the kinetics with slow manifolds. There exists a view that the core meandering may be a form of chemical turbulence.

In the present short communication, we report some results of our numerical simulation, together with their qualitative interpretation, showing that the transition of spiral wave patterns to turbulence easily occurs and that the turbulent motion there is much more violent than the mere core meandering. All these conclusions are, however, restricted to the media with *smoothly oscillating* local kinetics. Although the possibility of "diffusion-induced chemical turbulence" has been pointed out for a number of cases,[9] the present type of chemical turbulence differs from the preceding types in the respect that the diffusion need not be non-scalar.

The kinetic model we will adopt is a simple two-component system known as the λ-ω system[10] including scalar diffusion. Let the field amplitudes be X and Y. In terms of the complex field W defined by $W=X+iY$, the model equation is conveniently expressed as

$$\partial_t W=(\lambda(R)+i\omega(R))W+\nabla^2 W\ , \qquad (1)$$

where λ and ω are some functions of the amplitude $R\equiv|W|$. Of particular importance is the case: $\lambda(R)=\varepsilon-aR^2$, $\omega(R)=\omega_0-bR^2$ $(\varepsilon,\ a>0)$, or

$$\partial_t W=(\varepsilon+i\omega_0)W-(a+ib)|W|^2W+\nabla^2W\ . \qquad (2)$$

In fact every n-component reaction-diffusion system with scalar diffusion is known to reduce to system (2) whenever each local system (viz. the system without diffusion) lies near and above the threshold of the supercritical Hopf bifurcation.[11] By suitably rescaling the field amplitude W and the space-time coordinates, Eq. (2) takes an even simpler form:

$$\partial_t W=W-(1+i\beta)|W|^2W+\nabla^2W\ , \qquad (3)$$

where $\beta=a^{-1}b$. We have put $\omega_0=0$ (or eliminated ω_0 from Eq. (2) by the transformation $W\to W\exp(i\omega_0 t)$). Except that β is non-vanishing, Eq. (3) is identical to the time-dependent Ginzburg-Landau equation. The existence of the β-term, which is crucial to the discussion below, retains a characteristic of nonequilibrium open systems even after a drastic contraction of the dynamical equations as the above has been made. Taking the complex conjugate of Eq. (3) and changing the sign before β together keep the equation of motion invariant. Thus the only essential parameter is the absolute value of β. One should also note that $|\beta|$ becomes indefinitely large if the system approaches the borderline between supercritical and subcritical bifurcations across which the parameter a changes sign. A number of kinetic models including the FitzHugh-Nagumo equation have a parameter region of this kind. The fact that assuming $|\beta|$ to be very large is not necessarily unphysical turns out important in connection with the discussion later.

We will now be interested in the solution of Eq. (3) for a two-dimensional medium. It may easily be checked that the homogeneously oscillating state, $W=\exp(-i\beta t)$, is linearly *stable* irrespective of the value of β. The stability of rotating wave solutions, on the other hand, seems to depend crucially on β, although no analytic proofs for this exist.

A rotating wave may be initiated from the condition that the "concentration isobars" $X=0$ and $Y=0$ intersect deeply enough. Once a well isolated phaseless point (the point at which $X=Y=0$) has been established in this way, the system becomes unable to come back to the state of homogeneous oscillation. Instead, a rotating wave having the phaseless point at its end appears. For relatively small $|\beta|$, the wave then develops into a steadily rotating spiral pattern such as illustrated in Fig. 1. If the boundary effects are negligible, such a steady solution is expected to have a perfectly symmetric form

$$W(r,\theta)=R(r)\exp[i(\Omega t-\theta+S(r))] \qquad (4)$$

in polar coordinates (r,θ). It is known that the quantities R and S have the following properties:[12]

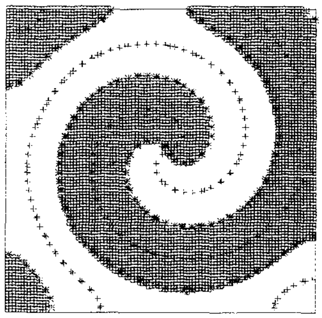

Fig. 1. Steadily and stably rotating spiral wave pattern. $\beta=1.0$. System size: 35.0×35.0. Mesh size: 0.35. Zero-flux boundary condition is assumed. The shaded part shows the region of positive X. The other two dotted contour lines indicate $Y=0$.

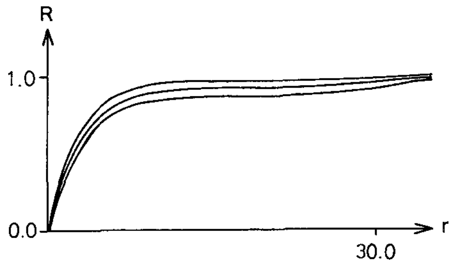

Fig. 2. Field amplitude R of steadily rotating waves as a function of the distance from the phaseless center. $\beta=0.5$, 1.0 and 1.5 for curves with the largest, middle and smallest amplitudes, respectively.

$$R(0)=0\,,\quad \left.\begin{array}{l} R(r)\to \mathrm{const}<1\,, \\ dS(r)/dr\to \mathrm{const} \end{array}\right\} \text{ as } r\to\infty\,. \tag{5}$$

Figure 2 shows numerically calculated $R(r)$ for different values of β, for each of which the steady solution (4) is stable. Note that the curve $R(r)$ is rather insensitive of β.

We have found numerically that the solution of the form (4) becomes unstable for larger $|\beta|$. The consequence of this instability is turbulence as far as the case of relatively large $|\beta|$ is concerned. Detailed analysis on the onset of turbulence has not been carried out yet, and the following results are only for $\beta=3.5$. Figure 3 shown how our turbulence develops from an initially perfect spiral wave. The starting wave pattern at $t=1.50$ is almost identical to that of Fig. 1 viz. a steadily rotating pattern appropriate for $\beta=1.0$. The initial position of the core had been displaced slightly from the center of symmetry so that axially asymmetric disturbances might be ready to grow whenever the pattern loses stability. We now increase β suddenly to the value 3.5, and the temporal development thereafter up to $t=12.00$ is shown in the same figure. The rotating pattern is apparently unable to adapt smoothly to the new parameter condition by readjusting its rotation period and wavelength. It becomes increasingly distorted until here and there the contour lines $X=0$ and $Y=0$ come into contact with each other tangentially, whereby new pairs of phaseless points are created. Some of such phaseless points may soon be pair-annihilated, while the others survive for a long time. Since the very existence of a single phaseless point at the initial time has turned out to be the cause of the instability, the newly born phaseless points could as well be the sources of subsequent instabilities, thus producing a number of phaseless points again. Repeated applications of the same reasoning ad infinitum lead to the picture that the turbulence here is not confined within a finite spatial region but spreads until it comes to dominate the entire system. Without initial phase singularity, in contrast, nothing would happen other than completely homogeneous oscillations.

We now consider the reason for the occurrence of the instability for larger $|\beta|$. Equation (3) written in the form of Eq. (1) with $\lambda=1-R^2$ and $\omega=-\beta R^2$ permits us to interpret β as the measure of how strongly the local frequency ω depends on the local amplitude R. For the steadily rotating waves, one may understand qualitatively how ω depends on the radial coordinate r with the help of Fig. 2 showing the r-dependence of R. Thus our system looks something like an array of radially coupled oscillators with a nonuniform distribution of the native frequency $\omega(r)$. It is obvious that increasing $|\beta|$ makes the spatial gradient of $\omega(r)$ steeper in some region near the core, so that the oscillators will find it increasingly difficult to maintain synchrony among themselves over the entire system. The resulting breakdown of the synchronized motion will accompany the creation of pairs of phaseless points, and the rotating waves induced round such points will also be bound to experience a similar kind of instabilities.

The present study has been confined to perfectly smooth oscillatory kinetics. It would be of great interest to explore the possibility of obtaining turbulence for relaxa-

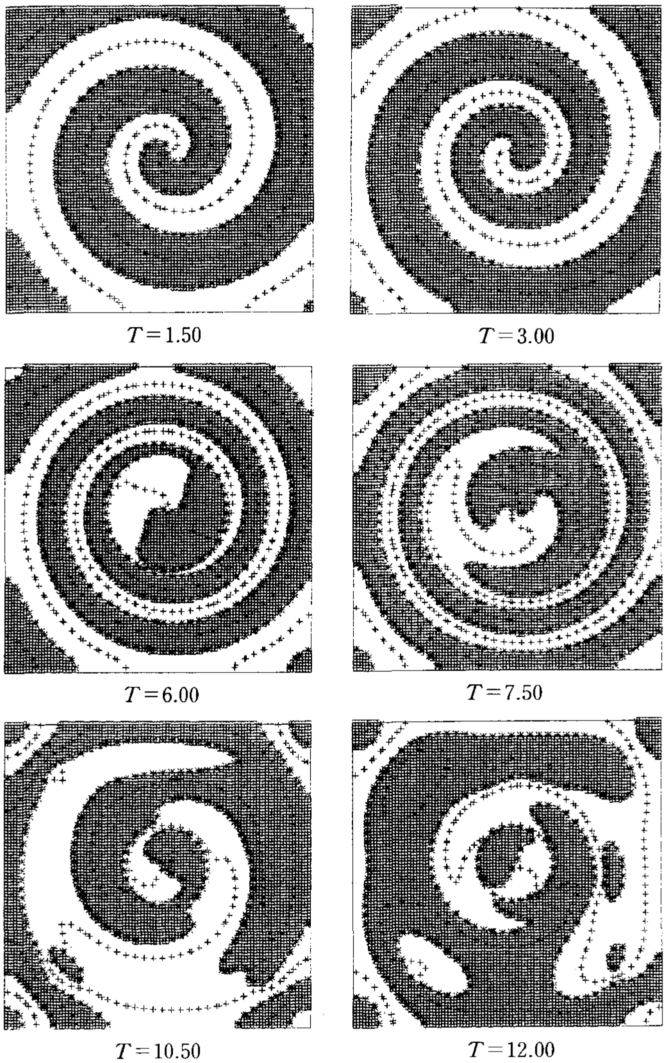

Fig. 3. Temporal development of "spiral wave turbulence". $\beta=3.5$. System size, mesh size and boundary condition are the same as for Fig. 1.

tion oscillations and excitable kinetics due to the mechanisms similar to the above. Such a study seems important because unsmooth kinetics rather than smooth one is much more commonly met in physiological, chemical and biochemical contexts. A turbulized excitable medium with spontaneously excited many rotors might possibly be realized, and such a system would look much like a fibrillating heart tissue. In this connection, a possible desynchronization mechanism as proposed by Rössler and Kahlert[7] for systems of stiff oscillators seems quite suggestive.

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