

Rotating Spirals without Phase Singularity in Reaction-Diffusion Systems

Yoshiki KURAMOTO and Shin-ichiro SHIMA

Department of Physics, Graduate School of Sciences, Kyoto University, Kyoto 606-8502, Japan

(Received)

Rotating spiral waves without phase singularity are found to arise in a certain class of three-component reaction-diffusion systems of biological relevance. It is argued that this phenomenon is universal when some chemical components involved are diffusion-free. Some more detailed mathematical and numerical analyses are carried out on a complex Ginzburg-Landau equation with non-local coupling to which the original system is reduced close to a codimension-two parameter set.

§1. Introduction

Rotating spiral waves represent a most universal class of patterns observed in extended fields composed of excitable or self-oscillatory local elements. Recent experimental and theoretical studies on rotating spirals have focused exclusively on their complex behavior such as core meandering in 2D,¹⁾ control of the spiral dynamics using photo-sensitive BZ reaction,²⁾ and the topology and dynamics of the singular filaments of 3D scroll waves.³⁾ In the present article, we argue that there must be yet another problem of fundamental importance associated with the spiral dynamics.⁴⁾ This is the occurrence of spatial discontinuity near the core, which also leads to the loss of phase singularity. In reaction-diffusion systems, occurrence of spatial discontinuity itself is not surprising when the system involves some components without diffusion. Thus, our main concern will be under what general conditions such behavior arises, why the core is the weakest region regarding the loss of spatial continuity, and how singular is the structure of the core after such breakdown.

In §2, we introduce a simple class of reaction-diffusion systems which can exhibit 2D spiral waves without phase singularity. The specific system studied is a field of continuously distributed FitzHugh-Nagumo oscillators without direct diffusive coupling supplemented with an extra chemical component which is the only diffusive component thus mediating the coupling among the local oscillators. Our numerical simulation suggests that the coupling strength K between the diffusive component and the local oscillators is the crucial parameter, and that weaker coupling implies core anomaly. In order to proceed to more detailed analysis of the core anomaly, we apply in §3 a method of reduction to our reaction-diffusion system near the Hopf bifurcation. It is known that such reduction generally leads to the complex Ginzburg-Landau (CGL) equation which by no means exhibits the type of core anomaly of our concern. However, there is an exceptional case in which K is comparable in magnitude with the bifurcation parameter, and in that particular case the diffusion

coupling in CGL must be replaced with a non-local coupling. We take advantage of this fact for the purpose of detailed analysis of the core anomaly using this simple and universal equation. In §4, some mathematical and numerical study of our non-local CGL will be presented. First, it is almost trivially concluded that there is a critical condition across which steadily rotating waves with vanishing amplitude at the center of rotation becomes impossible. We also present some numerical results on the core anomaly exhibited by the non-local CGL. Section 5 is devoted to a speculative argument concerning possible statistical natures of the turbulent fluctuations inside the core. The point of our argument is to note the fact that the system has no characteristic length scale inside the core so that the turbulent fluctuations there should be scale-free or their statistics should be characterized by some scaling laws. A few concluding remarks will be given in §6.

§2. Loss of spatial continuity in the spiral core

In some previous works on spatio-temporal chaos in self-oscillatory media,^{5),6),7)} a particular class of three-component reaction-diffusion systems of the following form was considered:

$$\dot{X} = f(X, Y) + KB, \quad (2.1)$$

$$\dot{Y} = g(X, Y), \quad (2.2)$$

$$\tau \dot{B} = -B + D\nabla^2 B + X, \quad (2.3)$$

where the set of equations $(\dot{X}, \dot{Y}) = (f, g)$ represents a local limit-cycle oscillator. The above model, possibly with various generalizations, may serve as a suitable model for a large assembly of oscillatory units (represented by the first two equations) without direct mutual coupling supplemented with an extra component (represented by the last equation) which behaves as a coupling agent among the local oscillators. Our system, possibly with various modifications, bears some resemblance to biological assemblies of oscillatory and excitable cells such as yeast cells under glycolysis and slime mold amoebae. It has also some similarity with the recently developed experimental system of the Belousov-Zhabotinsky reaction dispersed in water-in-oil AOT microemulsion.⁸⁾ For the sake of convenience, parameter τ has been inserted in the last equation to indicate the time scale of the diffusive component B . When τ is sufficiently small, adiabatic elimination of B , which can be done explicitly because the equation for B is linear, leads to a two-component non-locally coupled system of the form

$$\dot{X}(\mathbf{x}, t) = f(X, Y) + K \int G(|\mathbf{x} - \mathbf{x}'|) X(\mathbf{x}', t) d\mathbf{x}', \quad (2.4)$$

$$\dot{Y}(\mathbf{x}, t) = g(X, Y). \quad (2.5)$$

The spatial extension of our system is assumed to be sufficiently large, so that in two-dimensional systems to which our discussion below will exclusively be confined, $G(r)$ is given by a modified Bessel function $K_0(r/D^{1/2}) \cdot (2\pi D)^{-1}$. Note that the effective coupling range is of the order of $D^{1/2}$.

Diffusion-coupling approximation of the above non-local coupling is valid if the pattern obtained from Eqs. (2.4) and (2.5) is such that the characteristic wavelength of X , denoted by l_p , is sufficiently longer than the coupling range, i.e., if

$$l_p \gg D^{1/2}. \quad (2.6)$$

Under the above condition, our system behaves similarly to a two-component reaction-diffusion systems with effective diffusion constant of the order of KD , thus arousing no particular interest associated with the dynamics peculiar to non-locality in coupling. Since the result of the diffusion-coupling approximation made on Eq. (2.4) implies that the characteristic wavelength of the pattern scales like

$$l_p \sim (KD)^{1/2}, \quad (2.7)$$

this approximation is consistent only if $(KD)^{1/2} \gg D^{1/2}$ or only if the coupling strength K is sufficiently large. Thus, our main concern below is how our system behaves as K is made smaller by which something peculiar to non-locally coupled systems is expected to emerge. Among others, this article is particularly concerned with the dynamics of rotating spiral waves.

As a simple model for the local oscillators, let us choose the FitzHugh-Nagumo model

$$f = \epsilon^{-1}\{(X - X^3) - Y\}, \quad g = aX + b \quad (2.8)$$

under an oscillatory condition $a = 1.0$, $b = 0.2$ and $\epsilon = 0.1$. Numerical simulation of Eqs. (2.4) and (2.5) was carried out for different values of K . Figure 1a shows a typical case of large K for which the spiral pattern rotates steadily and there is nothing anomalous. The corresponding phase portrait at a given time projected onto the XY plane is shown in Fig. 1b. The phase portrait is a set of points in the phase space representing the current state of all local oscillators. In reaction-diffusion systems, we usually expect that this mapping between the physical space and the phase space is homeomorphic. Hence, the inner region of the phase portrait should be completely filled, or equivalently, this object is simply connected in the continuum limit. Figure 1b confirms this fact. The center of rotation of the spiral is mapped to a certain fixed point (X_0, Y_0, B_0) in the phase space. Under other parameter conditions the spiral core may exhibit meandering. No such fixed point could exist then, still the phase portrait should remain simply connected.

Let the coupling strength K become smaller. The overall spiral pattern shown in Fig. 1c does not seem very different from the strong coupling case except that the characteristic wavelength, which is comparable with the core radius, becomes smaller. However, the corresponding phase portrait (see Fig. 1d) changes qualitatively. This object (called \mathcal{O} hereafter) is no longer simply connected, and we clearly see a large central hole. What does a hole mean physically? Imagine that we moved along the frame of the spiral picture of Fig. 1c. The corresponding trajectory in the phase space will trace the periphery of \mathcal{O} . We now let the square along which we move in the physical space be shrunk a little. The corresponding phase trajectory will come a little inside the periphery of \mathcal{O} . Let the closed path in the physical space be made smaller and smaller, down to an infinitesimal size. It is clear that, in the presence of

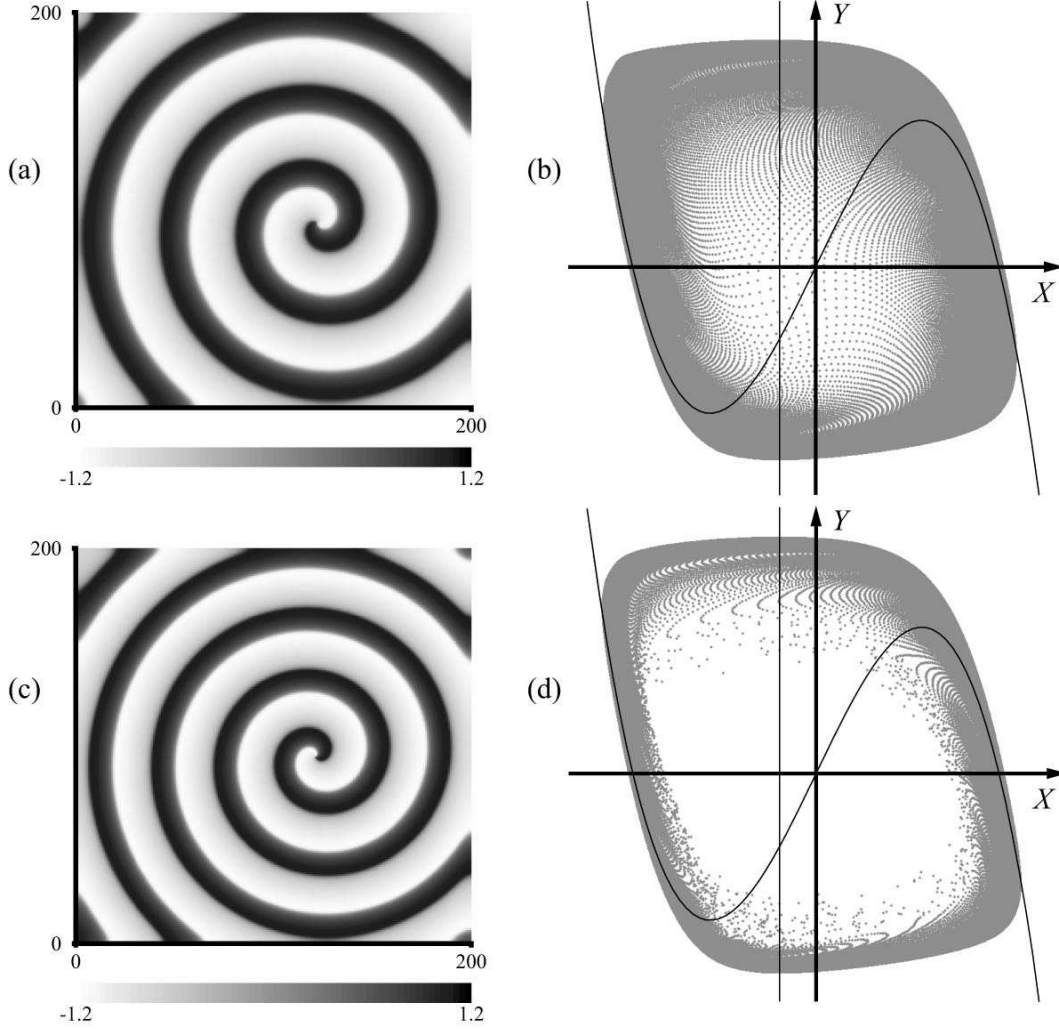


Fig. 1. Two-dimensional Spiral patterns for the component X in gray scale exhibited by the reaction-diffusion model given by Eqs. (2.1)~(2.3) in the oscillatory regime, and the corresponding phase portraits projected on the X - Y space. In the latter, the nullclines $f(Y, Y) = 0$ and $g(X, Y) = 0$ are also indicated. Parameter values are $K = 10.0$ for (a) and (b), and $K = 4.0$ for (c) and (d); $a = 1.0$, $b = 0.2$ and $\epsilon = 0.1$ are common.

a hole in the phase portrait, there is a limitation beyond which the phase trajectory can no longer be shrunk. This is apparently a contradiction as long as we adhere to a homeomorphism between the two objects in the physical space and the phase space. We are forced to abandon this property of the mapping, or we have to admit that a neighborhood in the physical space can no longer be mapped to a neighborhood in the phase space. This implies that the spatial continuity of the pattern has been lost which is likely to occur in the central core. If we look closely into the spiral core in the strong- and weak coupling cases (see Fig. 2), we actually find that there is nothing anomalous for the first case, while for the second case a small group of

oscillators near the core seem to be behaving individually rather than collectively. In

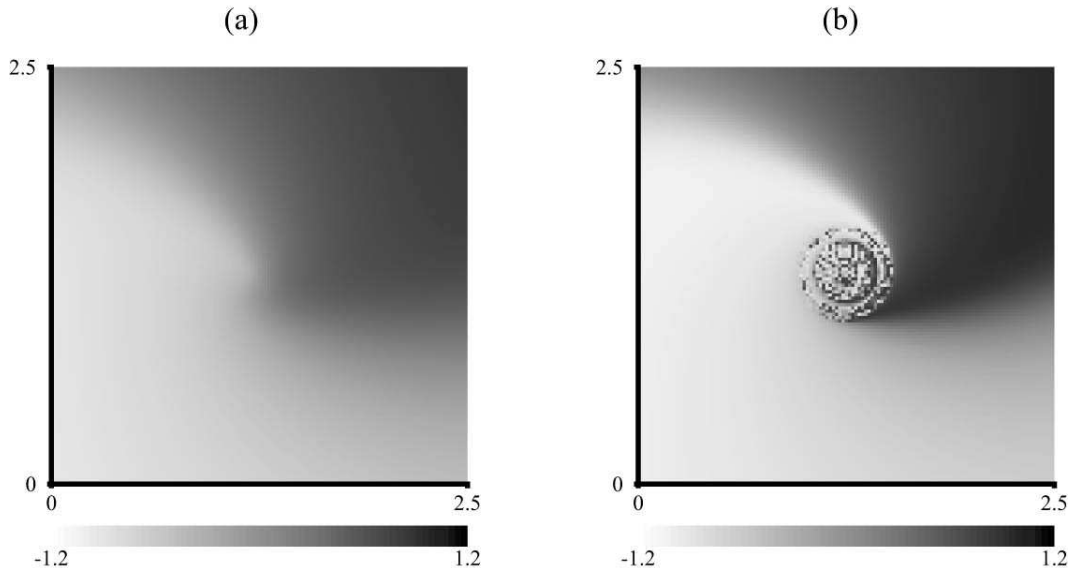


Fig. 2. Structures near the core of the spiral patterns in Fig. 1 (a) and (c). $K = 10.0$ for (a) and 4.0 for (b).

the next section, we develop an efficient way of uncovering the origin of this anomaly by means of a reduction of our evolution equations.

§3. Case of non-locally coupled complex Ginzburg-Landau equation

As a well-known fact, reaction-diffusion systems are generally reduced to a complex Ginzburg-Landau equation near the Hopf bifurcation point of the local oscillators.⁹⁾ The same is true of our reaction-diffusion system Eqs. (2.1)–(2.3) or their approximate form given by Eqs. (2.4) and (2.5). Since spatial continuity can never be broken in the complex Ginzburg-Landau equation, the reduction method near the bifurcation is useless for our purposes. As anticipated in the preceding section, the present type of anomaly arises as a result of effective non-locality in coupling, particularly when the effective radius of coupling becomes comparable with the characteristic scale of the pattern (typically the core radius). The failure of the reduction method applied to the present problem comes from the loss of effective non-locality near the bifurcation point. The reason is clear: Near the bifurcation point, the characteristic wavelength of patterns becomes as large as $\mu^{-1/2}$ in terms of the bifurcation parameter μ , so that the effective non-locality such as given by the last term in Eq. (2.4) disappears and can well be replaced with a diffusion term.

From the above reasoning, we may notice that there is still a way of retaining effective non-locality near a bifurcation point if the coupling K is made as weak as $O(\mu)$.¹⁰⁾ Thus, applying an idea similar to the one underlying the multiple bifurcation theory, we now try to reduce our reaction-diffusion system near the codimension-two point $(\mu, K) = (0, 0)$ by which effective non-locality may be recovered. The same

idea was used previously in the study of multi-affine chemical turbulence⁶⁾ for which effective non-locality was also crucial.

For the sake of simplicity, the third variable B is assumed to change very rapidly, and we take the limit $\tau \rightarrow 0$. Thus, the set of equations to be reduced is Eqs. (2.4) and (2.5). As usual, the reduced equation is obtained in the form of an equation governing a complex variable $A(\mathbf{x}, t)$. Under suitable rescaling of A and the space-time coordinates, it takes the form

$$\dot{A} = (1 + i\omega_0)A - (1 + ib)|A|^2 A + K \cdot (1 + ia)(Z - A), \quad (3.1)$$

where

$$Z(\mathbf{x}, t) = \int d\mathbf{x}' G(|\mathbf{x} - \mathbf{x}'|) A(\mathbf{x}'). \quad (3.2)$$

The coupling parameter K in Eq. (3.1) is not the original K but the scaled K with the factor μ^{-1} , so that, by assumption, the latter K has an ordinary magnitude. We call Eq. (3.1) non-locally coupled complex Ginzburg-Landau equation (or simply the non-local CGL). It reduces to the ordinary CGL when K is sufficiently large, under the condition of which A becomes so long-waved that the diffusion-coupling approximation of the last term in Eq. (3.1) would be valid.

For the purpose of gaining a qualitative understanding of how the solution of Eq. (3.1) behaves, it is sometimes useful to regard this equation as describing a single oscillator driven by a forcing Z . Similarly, the system as a whole may be regarded as an assembly of oscillators without direct mutual coupling, but under the influence of a common forcing field Z which may depend on space as well as on time. The characteristic wavelength of Z cannot be shorter than the decay length of G which is chosen to be 1. The forcing Z is actually of *internal* rather than external origin, and thus should be related to the totality of the individual motion of the oscillators in a self-consistent manner. In the statistical-mechanical language, this may be called a mean-field picture which works exactly in the present system because, in the continuum limit, infinitely many oscillators fall within the coupling range.

§4. Core anomaly in the non-local CGL

We want to know if a spiral-core anomaly similar to the one observed for our reaction-diffusion model also arises in the non-local CGL, especially when K is small. It is well known that even the spiral waves in the ordinary CGL can exhibit complex behavior. Therefore, in order to separate the type of anomaly to be caused by the non-locality in coupling from the conventional one, we will work with in the parameter region in which the diffusion-coupling approximation of Eq. (3.1) admits a steadily rotating spiral solution. Under the same condition, Eq. (3.1) itself should exhibit steadily rotating spiral waves provided K is sufficiently large. It is easy to show that such a solution is bound to lose stability for sufficiently small K . The reason is the following. From the system's symmetry, the center of rotation of such a solution has a vanishing value of A . From the same symmetry, Z should also vanish there. This means that, if we work with the forced-oscillator picture mentioned in

§3, and apply it to the central oscillator, then this oscillator is free of forcing and simply obeys the equation

$$\dot{A} = (1 - K + i\omega'_0)A - (1 + ib)|A|^2 A, \quad (4.1)$$

where $\omega'_0 = \omega_0 - Ka$. It is clear that if $K > 1$, vanishing value of A is stable, while if $K < 1$ it is unstable contradicting the existence of steadily rotating solution with vanishing central amplitude. Note that the above argument does not guarantee the stability of the steadily rotating solution for K larger than 1.

Some results of our numerical simulation on Eq. (3.1) for K less than 1 are displayed in Fig. 3 to Fig. 5. A typical case is shown in Fig. 3 from which a

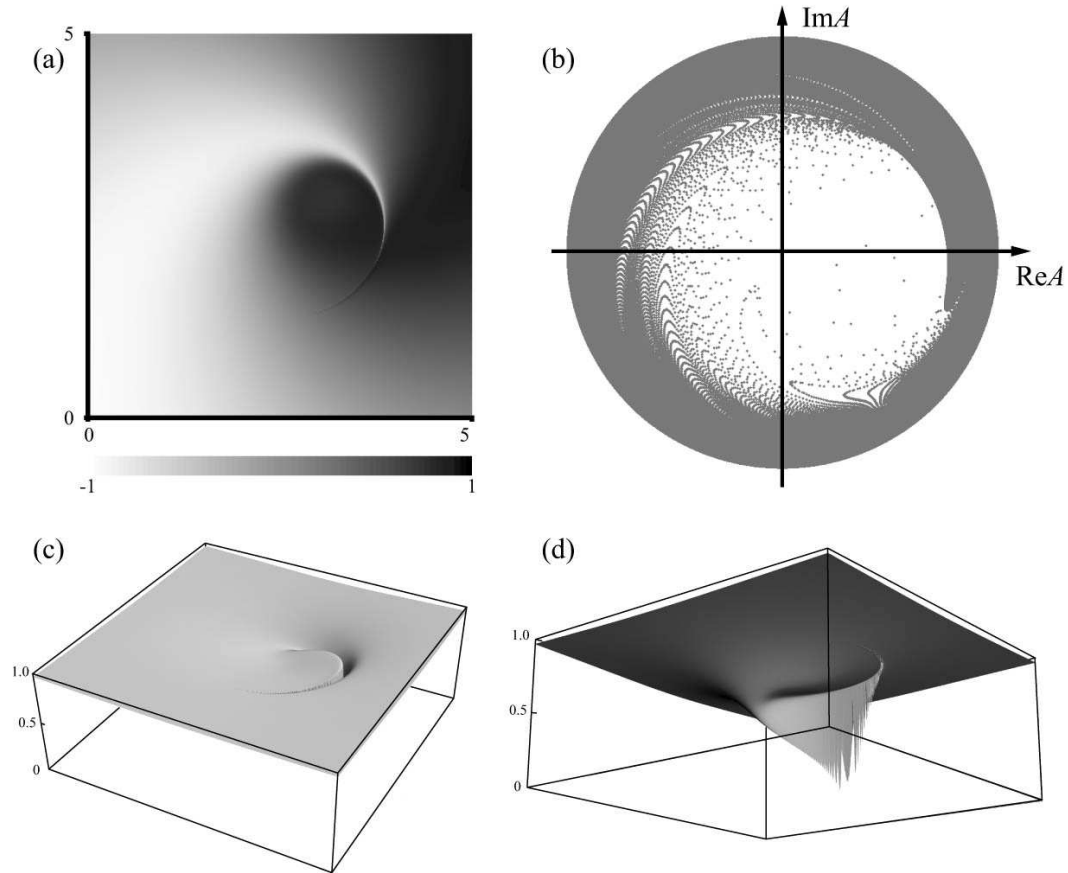


Fig. 3. Structure of the spiral core exhibited by the non-local CGL given by Eq. (3.1) with parameter values $K = 0.5$, $a = 0$ and $b = 0.5$. (a) Phase pattern in gray scale; (b) the corresponding phase portrait; (c) and (d) 3D views of $|A|$ from the top and the bottom, respectively.

large hole is seen in the phase portrait. The 3D views of the distribution of $|A|$ shows the appearance of a cut along which the oscillators behave incoherently with relatively small amplitude. The corresponding corrugated pattern never shows a sign of smoothening as the minimum spacing of the oscillators used in the numerical simulation is made smaller. This implies genuine spatial discontinuity distributed

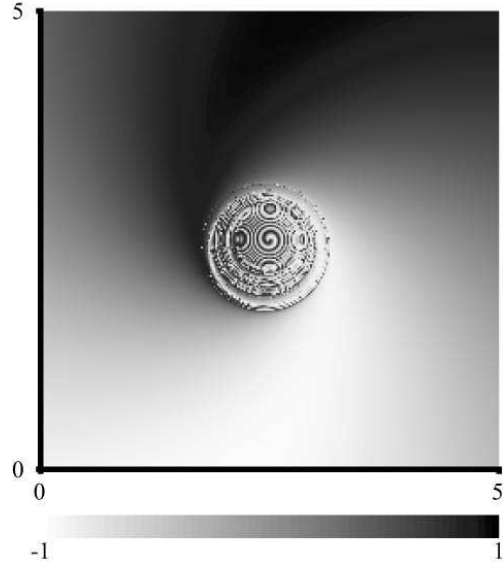


Fig. 4. Similar to Fig.3 (a) but for different parameter condition, i.e., $K = 0.3$, $a = 0$ and $b = 0.4$.

densely along the cut. The cut may not be a true one-dimensional object, still this makes a sharp contrast with the simulation on the original reaction-diffusion system displayed in Fig.1 where the incoherence seems to have a two-dimensional extension. The origin of such a difference may be understood from Fig. 4 showing a simulation result under a different parameter condition. The incoherent structure in that figure forms practically an extended object quite similar to Fig. 1.

It is interesting to observe that rotating spiral can persist when the coupling K is so small (as small as 0.1) that the phase portrait looks like a ring leaving only a very thin periphery (see Fig. 5). This means that the amplitude degree of freedom is almost dead. All oscillators are now oscillating with almost full amplitude, i.e. $|A| \simeq 1$, so that the pattern of $|A|$ would not be interesting. Instead, a meaningful pattern is exhibited by the real part of A from which the spatial discontinuity can well be seen. The absence of amplitude degree of freedom implies that the so-called phase oscillator model can well describe the same dynamics as the above, while our general view is that rotating spirals exhibited by phase oscillators are bound to lead to a topological contradiction.¹¹⁾ The last statement does not apply, however, in the absence of spatial continuity.

§5. Origin of spatial discontinuity and loss of smoothness

In the preceding sections, we have contrasted the spiral dynamics between the two cases of strong and weak couplings. In one case, the spiral core behaves normally while in the other case the dynamics is anomalous in the sense that there is a group of oscillators inside the core which are behaving individually. Although it would be interesting to know some more details of how one type of behavior changes to the other as the coupling constant K is made smaller, numerical data showing a detailed

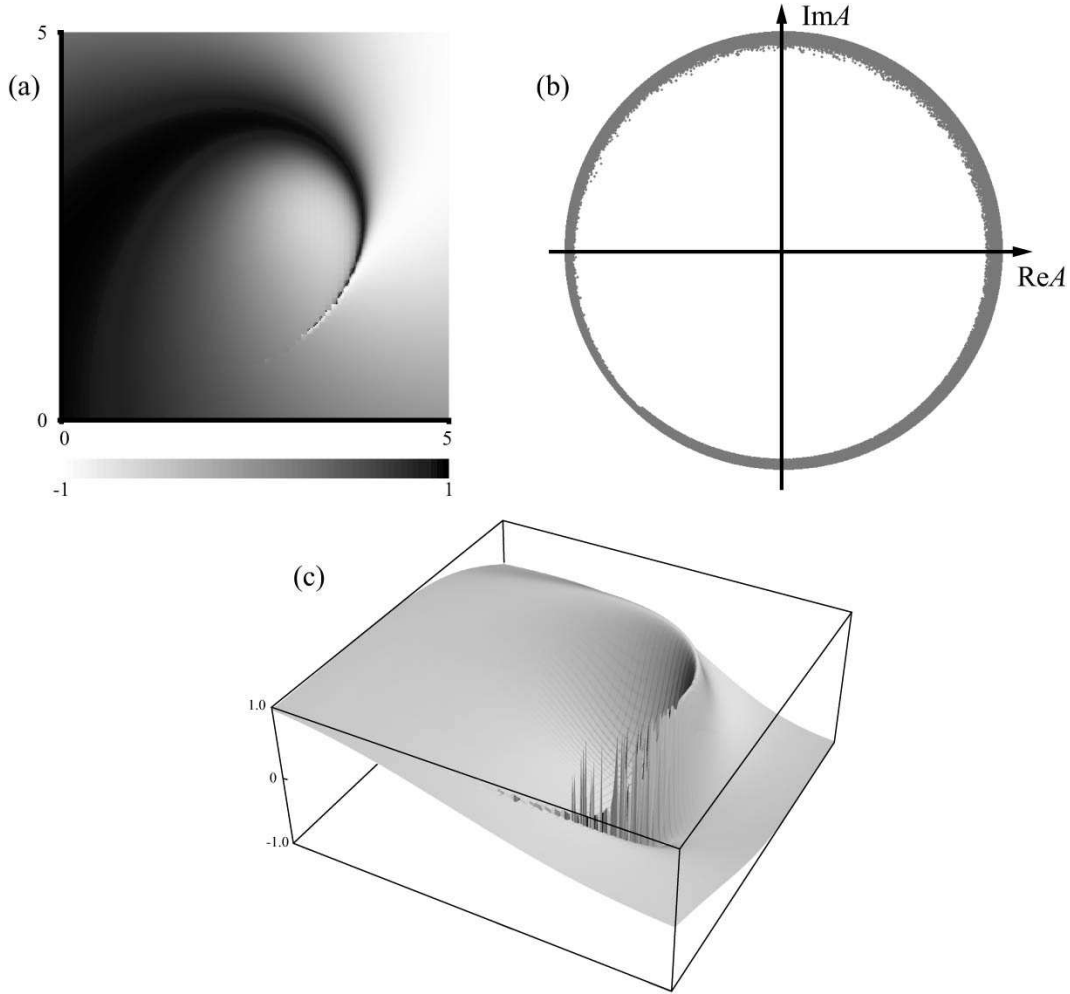


Fig. 5. (a) and (b) are similar to Fig. 3 (a) and (b), respectively, but for much smaller value of K , i.e., $K = 0.1$. (c) shows a 3D pattern of $\text{Re} A$.

scenario starting from a normal behavior changing to increasingly complex behavior are not available yet. Still the following rough scenario seems to be correct at least. Rigid rotation of the pattern first becomes unstable at some K (say, $K = K_1$, which should definitely be less than 1), and successive bifurcations will occur up to another K (say, $K = K_2$) above which the core becomes turbulent. In the turbulent regime, the pattern is spatially continuous at first, but there is a third critical value of K (say, $K = K_3$) at which such continuity is lost and the a group of oscillators inside the core lose mutual synchrony.

We are particularly interested in the situation near the transition when the synchrony is first lost and independent motion of the oscillators sets in. From a theoretical point of view, there are good reasons to believe that over some finite range of K preceding this transition, the pattern loses spatial smoothness in a mathematical

sense. The reason may most roughly be stated as follows. As we pointed out in §2, something anomalous is expected to occur when the coupling becomes so weak that the characteristic wavelength of the pattern which was denoted by l_p becomes comparable or even smaller than the effective coupling radius. The quantity l_p may be chosen as the core radius in our case. This means that inside the core our system has no intrinsic length scale down to the zero value as long as a continuum limit of oscillator distribution is assumed. Thus, the inside region of the core is so to speak a *scale-free world*. Once turbulent fluctuations occurred in this scale-free world, they should also be scale-free. In other words, fluctuations should exist over all scales below the coupling radius down to infinitesimal scales in a self-similar manner, which implies loss of spatial smoothness.

The above reasoning regarding the loss of spatial smoothness could be made a little more mathematical as follows. One may ask first what physical quantities carry information on the smoothness and continuity of the pattern. The most convenient quantities to work with seem to be various moments of amplitude increment between two spatial points with infinitesimal mutual distance. Let such amplitude increment over the distance x be denoted by y , and its q th moments by $\langle y^q \rangle$. Detailed definition of "amplitude" is irrelevant. Real or imaginary part of A as well as $|A|$ may be chosen as y if we are working with complex CGL, while X or Y (but not B) would be appropriate for y for the reaction-diffusion system given by Eqs. (2.1)~(2.3). In what follows, we use terms appropriate for the non-local CGL.

The amplitude vs. x curve which is fluctuating may be regarded as continuous and differentiable to an arbitrary degree if

$$\langle y^q \rangle \sim x^q \quad (5.1)$$

in the limit $x \rightarrow 0$. It was argued in previous works^{5),6),12)} that non-locally coupled oscillator systems of the type we are now working with give moments $\langle y^q \rangle$ different from Eq. (5.1). Remember that, as stated toward the end of §3, our system may be regarded as an assembly of independent oscillators driven by a common forcing. The forcing field $Z(\mathbf{x}, t)$ is temporally nonperiodic in general and its spatial variation should be smooth with typical wavelength comparable with the coupling radius or core radius. Since the feedback from the motion of a given oscillator to the forcing field acting on it is totally negligible, one may introduce a local Lyapunov exponent $\lambda(t)$ and its mean $\bar{\lambda}$ defined for the individual oscillator. Well inside the core, $\lambda(t)$ and $\bar{\lambda}$ are expected to be space-independent. Thus, regarding possible statistics of $\langle y^q \rangle$, one may apply a previous theory on multi-affine spatio-temporal chaos in non-locally coupled oscillatory fields. The theory tells that the behavior of $\langle y^q \rangle$ depends crucially on the sign of $\bar{\lambda}$. If $\bar{\lambda} < 0$, it is given by

$$\langle y^q \rangle \sim x^{\zeta(q)} \quad (5.2)$$

with some nonlinear function of q , while if $\bar{\lambda} > 0$, we have

$$\langle y^q \rangle \sim \delta + x^{\zeta(q)}, \quad (5.3)$$

where δ is a positive constant signifying spatial discontinuity. If $\bar{\lambda}$ is negative for a given oscillator, its motion should be synchronized with the forcing field, so that

a small group of oscillators composed of its neighbors will also be mutually synchronized, thus leading to spatial continuity. If $\bar{\lambda}$ becomes positive, such mutual synchrony is lost and individual motion of the oscillators sets in. This type of transition is expected to occur at a certain critical value of K .

It can further be shown that the exponent $\zeta(q)$ is identical with q up to some value $q = \beta$, while it completely saturates to a constant, i.e., $\zeta(q) = \beta$ for $q > \beta$. Thus, prior to the onset of discontinuity, the pattern loses complete smoothness in the sense that the moments of y higher than the order β behaves anomalously. β is shown to tend to zero as the onset of discontinuity is approached, by which all moments become anomalous. It should also be remarked that the pattern becomes fractal if $\beta < 1$.

In a previous work,¹³⁾ these theoretical results were confirmed by numerical simulation for systems with statistical homogeneity in space. For the present type spiral-core anomaly, in contrast, the turbulent regime is strongly localized, so that such comparison between the theory and numerical experiment would not be easy.

§6. Concluding remarks

We have shown that in non-locally coupled systems spiral core is the weakest part of rotating spiral waves in the sense that localized turbulence without spatial smoothness and even spatial continuity is initiated there. We have also shown that such behavior is not restricted to systems of genuine non-local coupling but may also arise in an important class of reaction-diffusion systems where some of the chemical components are diffusion-free. The non-local CGL obtained near the codimension-two point proved to be extremely useful for the study of the dynamics peculiar to non-locally coupled self-oscillatory fields.

Complete absence of local coupling on which the whole argument of the present paper relies would not be very realistic in real reaction-diffusion systems. How the spiral dynamics changes when weak diffusive coupling has been introduced could be an interesting future problem.

References

- 1) D. Barkeley, in *Chemical Waves and Patterns*, ed. R. Kapral and K. Showalter, Dordrecht, Kluwer, Ch. 5 p. 163 (1995).
- 2) E. Mihaliuk et al., *Faraday Discuss.*, **120**, 383 (2001).
- 3) J. P. Keener, *Physica D* **31**, 269 (1988).
- 4) A preliminary results of this work were reported in: Y. Kuramoto, in *Nonlinear Dynamics and Chaos: Where do we go from here?*, ed. S. J. Hogan et al., IoP, p. 209 (2003).
- 5) Y. Kuramoto, *Prog. Thor. Phys.* **94**, 321 (1995).
- 6) Y. Kuramoto, D. Battogtokh and H. Nakao, *Phys. Rev. Lett.* **81**, 3543 (1998).
- 7) Y. Kuramoto, H. Nakao and D. Battogtokh, *Physica A* **288**, 244 (2000).
- 8) V. K. Vanag and I. R. Epstein, *Phys. Rev. Lett.* **88**, 088303 (2002).
- 9) Y. Kuramoto, *Chemical Oscillations, Waves, and Turbulence*, Springer-Verlag,(1984).
- 10) D. Tanaka and Y. Kuramoto, in preparation.
- 11) A. T. Winfree, *The Geometry of Biological Time* (2nd Ed.), Springer, (2000).
- 12) Y. Kuramoto and H. Nakao, *Phys. Rev. Lett.* **76**, 4352 (1996).
- 13) H. Nakao and Y. Kuramoto, *Eur. Phys. J. B* **11**, 345 (1999).