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TURING INSTABILITY IN THE OREGONATOR MODEL

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Recently many studies have been carried in the formation process of the dissipative structure in non-equilibrium systems[1]. Ouyang and Swinney experimentally observed several interesting patterns, lamellar and triangular patterns by using the so-called gel reactor for CIMA (chlorite-iodide-malonic-acid) reaction[2]. On the other hand the Swift-Hohenberg equation known as the fundamental equation describing the formation dynamics of a roll pattern in the heat convection system[3] can not describe the formation of triangular pattern. This is due to the symmetry of the dynamics. In Ref.[4] the asymmetric Swift-Hohenberg equation (aSH) is derived for a general reaction diffusion equation by using the perturbation expansion near the Turing instability. Fujisaka, Ouchi and Egami studied the pattern dynamics in the aSH equation. The several patterns are observed for different parameter values contained in the aSH equation, roll and triangular patterns and the coexistence of rolls and triangular phase. They also discussed the formation process of a spot pattern and discovered that roll shrinks in time. The characteristic of the formation process to spot pattern is that lamella structure shrinks. The motivation of the present work is to study the formation process of the Turing pattern in a more realistic model.

We used the Oregonator model which is known as a model of the Belouzov-Zhabotinskii reaction. We have numerically solved the Oregonator model on a two-dimensional square lattice with a periodic boundary condition for the parameter region where the spatially uniform, steady reaction is unstable, and investigated the formation of Turing pattern by using spatial power spectra.

The dimensionless equations of motion for the Oregonator are given by

\[ \dot{x} = q(y - xy + px^2) + D_x \nabla^2 x, \quad \dot{y} = q^{-1}(-y - xy + fz) + D_y \nabla^2 y, \quad \dot{z} = r(x - y) + D_z \nabla^2 z \]

where \( x, y \) and \( z \) respectively stand for the dimensionless concentrations of \( \text{HBrO}_2, \text{Br}^- \) and \( 2\text{Ce}^{4+} \). The parameters representing reaction rates, \( q, p \) and \( r \) are set to be \( q = 77.27, p = 8.375 \times 10^{-6}, r = 0.161 k_5 \) and \( D_x, D_y \) and \( D_z \) are the diffusion coefficients. \( k_5 \) and \( f \) are chosen as the control parameters.

The spatially uniform solution is \( x_0^{(0)} = 0, x_0^{(\pm)} = (1 - p - f \pm \sqrt{(1 - p - f)^2 + 4p(1 + f)})/2p \)
\( y_0 = f x_0/(1 + x_0), x_0 = x_0 \). Since \( x_0^{(-)} < 0 \), it is physically meaningless. By changing either the parameters \( k_5 \) and \( f \) the system undergoes the Turing instability, and shows a spatially non-uniform structure. Control parameter values are chosen to be in the region where the uniform state is unstable, i.e. \( f = 1, k_5 = 570 \) and \( D_x = 0.6, D_y = 0.1, D_z = 1 \).

The numerical calculation was carried out on a square lattice with point \( 256 \times 256 \) with the mesh size 0.2 and the time step 0.001. As an initial condition a weak random noise is added around the unstable uniform steady state. Typical formation dynamics of \( x(r, t) \) is shown in Fig.1 for different times. The formation process of triangular pattern has three characteristic stages. The first is the formation of roll structure. The second is the pinching instability of the roll structure created in the first stage. The pattern is different from the spot pattern observed in Ref.[4]. The third stage is the formation of triangular pattern due to the adjustment of randomly distributed concentration. We studied a pattern dynamics for different values of \( f \).
and $k_s$, and found the same formation characteristic described above. In the present work we unfortunately did not succeed in finding the spot pattern observed in Ref.[4]. This may be reduced to the fact that since the parameter region of the existence of the spot pattern in aSH equation is narrow, the spot pattern may be found in a very narrow parameter region in the Oregonator model. Further studies will be needed to clarify the existence of the spot pattern in the Oregonator model.

To statistically characterize the formation dynamics we have calculated the two-dimensional spatial power spectrum $S(q,t) = \langle |\int x(r,t)e^{-iq\cdot r}dr|^{2} \rangle$, where $\langle \cdots \rangle$ is the angle average. The time evolution of formation process is investigated with the peak height $A(t)$ and the half width $W(t)$ of the power spectrum. The time evolution of $W(t)$ is shown in Fig. 2. It is found that $W(t)$ depends on time $t$ as $W(t) \propto t^{-\alpha}$ for the second and third stages. In the second stage (pinching process), the relaxation is very fast and the exponent $\alpha$ takes about 0.75. In the third stage (adjustment of distributed concentration), the relaxation is extremely slow, which lead to $\alpha \approx 0.15$. Also $A(t)$ satisfies the scale law $\propto t^\alpha$ in each stage. The fact that the exponent of $\alpha$ in the third stage is more smaller than that in the second implies the extremely slow relaxation in the third stage, which is due to the slow decrease of defects in the formation process of the triangular pattern.

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Fig. 1 The time evolution of $x(r,t)$. (a) $t = 2$, (b) 4, (c) 6, (d) 30. The white region corresponds to high values of $x$. The system size is $128 \times 128$. $f = 0.96$, $k_s = 440$, $D_x = 0.6$, $D_y = 0.1$ and $D_z = 1$.

Fig. 2 The time evolution of the half width of the power spectra

References
4. H.Fujisaka, K.Ouchi and K.Egami, 'Domain kinetics, earthworm structure and spotty pattern in the asymmetric Swift-Hohenberg model'