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Spiral and Antispiral Waves in Reaction-Diffusion Systems*

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Abstract *Spiral waves are ubiquitous phenomena in nonlinear chemical, physical, and biological systems. But antispiral waves are infrequent to date. The transition between spiral and antispiral waves has been rarely explored. We have analyzed the extended Brusselator model and the extended Oregonator model by linear stability analysis. We have demonstrated that it is possible and plausible to realize the transition between them by control of diffusion coefficient of inactivator from theoretical analysis and numerical simulations.*

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Key words: spiral waves, antispiral waves, extended Brusselator model, extended Oregonator model

1 Introduction

Spiral waves are ubiquitous phenomena since Zhabotinsky firstly observed them in the spatially extended Belousov–Zhabotinsky (BZ) reaction-diffusion system in 1968. Spirals are observed in nonlinear chemical,[1] optical,[2] and biological systems.[3] Spirals have been investigated in excitable systems,[2,3] oscillatory systems[4,5] and plane wave solution of the complex Ginsburg–Landau equation (CGLE).[6] Spiral core exists in single diffusion excitable medium.[7] A tip of spiral wave is considered as a wave source. A wave is sent out after the tip moves one circle along the core. The dynamical behavior of spiral waves in an excitable media is governed by the dispersion relation and the constitutive relation.[8,9] The former relates the speed to the period of the travelling waves, or rotating frequency and wavenumber, the latter relates the speed and rotating frequency. Spirals grow from the center, and move out from the center of their arc and disappear in the periphery. All spiral waves have a core, along which the tip of spiral wave meanders.[10]

However, antispiral waves are infrequent to date. Antispirals have been discovered in the spatially extended oscillatory BZ reaction dispersed in water droplets of a water-in-oil aerosol OT (BZ-AOT) microemulsion(BZ-AOT system),[11] the extended Oregonator model,[12] and (two-variable) typical reaction-diffusion systems.[13] The condition required for (two variables) reaction-diffusion systems close to Hopf bifurcation to form antispirals is determined: the frequency of the bulk oscillation must be larger than the asymptotic frequency of the antispiral waves.[13] The wave instability and negative group velocity suffice to generate inwardly propagating (IP) waves[12] in the extended Oregonator model with three variables, where the Hopf, Turing, and wave instability coexist, and the Turing and Hopf instabilities are not necessary conditions for IP waves to occur.[12] Antispirals grow from the periphery, move toward the center of their arc and annihilate in the center. To a precision of micrometers, the tip of an antispiral wave does not move.[11]

Spiral and antispiral waves have been investigated by control of concentration of species in experiments[1,4,9,10] and kinetic parameters in simulations.[1,12,13] Gong and Chrisini varied two real parameters and gave rich dynamical behaviors including spirals and antispirals.[13] In this paper, we will analyze the Brusselator model[12,14] and the extended Oregontor model[12] by linear stability analysis, and realize the transition between spirals and antispirals by control of diffusion coefficient of inactivator from numerical simulations.

2 Extended Brusselator Model

To study the transition between spirals and antispirals, we quote the Brusselator model.[12,14] Yang has extended the classic two-variable Brusselator model into a three-variable model, where a reversible inter-conversion between the activator X and unreactive fast diffusion species Z was considered. Three-variable partial differential equations take the following form

$$\frac{\partial x}{\partial t} = D_X \nabla^2 x + f(x,y) - cx + dz\,, \tag{1}$$

$$\frac{\partial y}{\partial t} = D_y \nabla^2 y + g(x,y)\,, \tag{2}$$

$$\frac{\partial z}{\partial t} = D_Z \nabla^2 z + cx - dz\,, \tag{3}$$

where x, y, and z are dimensionless concentrations of the activator X, the inhibitor Y, and the inactivator Z, whose corresponding diffusion coefficients are D_x, D_y, and

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D_z, respectively. In order to introduce wave instability in the model, the inactivator must diffuse even faster than the inhibitor. The diffusion coefficients are that $D_x < D_y \ll D_z$. The Brusselator dynamic terms are given by the function $f(x, y)$ and $g(x, y)$ as follows:[12,14]

$$f(x, y) = a - (1 + b)x + x^2 y\,, \tag{4}$$

$$g(x, y) = bx - x^2 y\,, \tag{5}$$

where a, b, c, and d are re-scaled kinetic parameters. The steady state of the model is at

$$(x_{ss}, y_{ss}, z_{ss}) = \left(a, \frac{b}{a}, \frac{ac}{d}\right).$$

Although the system is a nonlinear system, because it has one steady state solution, linear stability analysis can be applied to the system when it lies in the onset of the bifurcation point. When parameters are selected at $(D_x, D_y, D_z) = (0.5, 1, 20)$, $c = d = 1$, typical spatial-temporal pattern transfers from outwardly propagating packet waves, $v_g = 0.957$, to inwardly propagating packet waves, $v_g = -0.24$, by control of dynamic parameters from $(a, b) = (1.0, 2.9)$ to $(a, b) = (3.0, 11.39)$.[14] Antispirals and antitargets are a special case of a more general phenomenon, where inwardly moving packet waves[15] consist of waves whose wavenumbers lie in a small range. We select parameters as $(a, b) = (3.0, 11.39)$, $c = d = 1$, $(D_x, D_y) = (0.5, 1)$. We take diffusion coefficient of inactivator D_z as variation, and then make linear stability analysis (Fig. 1), working out eignvalues λ from the characteristic equation. We may get either one real and one complex conjugate pair or three real solutions. However, we are interested in the complex pair. Wave instability occurs when $\mathrm{Re}(\lambda) = 0$, $\mathrm{Im}(\lambda) \neq 0$ at $k = k_c \neq 0$. k_c ($\mathrm{Re}(\lambda) = 0$) is critical wavenumber (we use *Mathematica*). We can calculate wave frequency $\omega = \mathrm{Im}\,(\lambda)$ and group velocity $v_g = \partial\omega/\partial k$ when $k = k_c$. We find that as the diffusion coefficient of inactivator D_z increases from 20 constantly, wavenumber will decrease from 0.376 slowly (Fig. 1 line B), and the group velocity of traveling wave will increase, varying from -0.24 to 0 and then to 0.162, and continue to increase (Fig. 1 line A). The travelling wave may vary from antispirals (Fig. 2(a)) to standing waves[14] to spiral waves (Fig. 2(b)). When the diffusion coefficient of inactivator D_z is less than 19, the maximum of Re (λ) will be less than -0.00449 (Fig. 1 line C), the system will be in steady state, and will not have travelling waves.

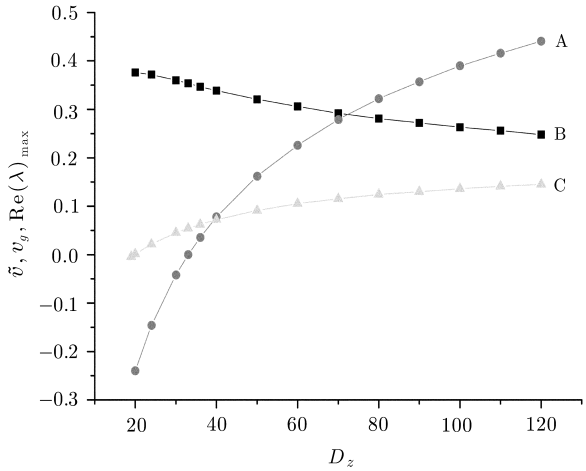

Fig. 1 Linear stable analysis for the extended Brusselator model, $(a, b) = (3.0, 11.39)$, $c = d = 1$, $(D_x, D_y) = (0.5, 1)$. Transverse axis D_z represents diffusion coefficient of inactivator. Curves A, B, and C, represent wavenumber, group velocity, and the maximum of $\mathrm{Re}(\lambda)$ each analysis, respectively.

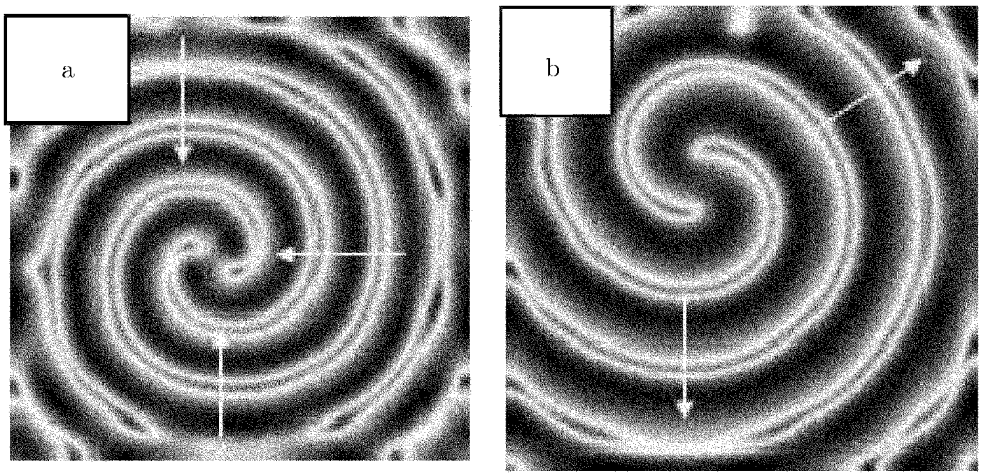

Fig. 2 Pattern formation in simulations of the extended Brusselator model with zero-flux boundary and random initial condition. The time step is set as 0.001. Snapshots are taken as 20 000 time units. (a) Snapshot of antispiral ($D_z = 20$); (b) Snapshot of spiral ($D_z = 39$). Arrows indicate the direction of wave propagation. The frame size is 128 × 128 space units.

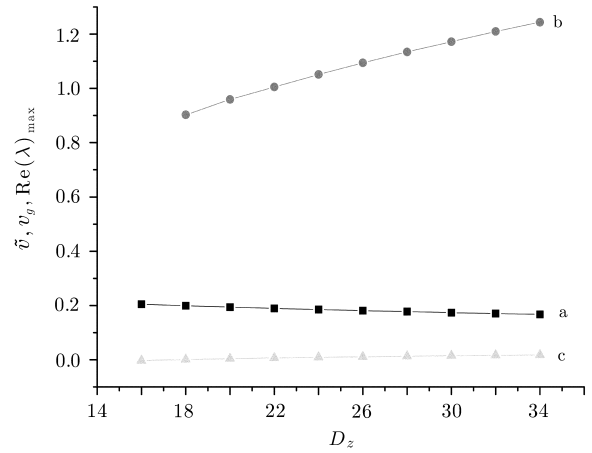

Fig. 3 Linear stable analysis for the extended Brusselator model, $c = d = 1$, $(a, b) = (1.0, 2.9)$, $(D_x, D_y) = (0.5, 1)$. Transverse axis D_z represents diffusion coefficient of inactivator. Curves a, b, and c represent wavenumber, group velocity, and the maximum of $\mathrm{Re}(\lambda)$ each analysis, respectively.

Can spiral waves become antispiral waves at any case in the extended reaction-diffusion systems? The outwardly propagating packet waves, $k_c = 0.194$, $v_g = 0.957$, were found in the extended Brusselator model, where parameters were selected at $(D_x, D_y, D_z) = (0.5, 1, 20)$, $c = d = 1$, $(a, b) = (1.0, 2.9)$.[14] We take diffusion coefficient of inactivator D_z as control parameter. From theoretical analysis, we find that the wavenumber will decrease from 0.1989 (Fig. 3 line a), group velocity will gradually increase from 0.903 (Fig. 3 line b) and no negative velocity is gained as diffusion coefficient of inactivator increases from 18. Nevertheless, when diffusion coefficient of inactivator gets 16 and the maximum of $\mathrm{Re}(\lambda)$ is -0.032, the system lies in steady state. In such systems, outwardly propagating packet waves will not transform into inwardly propagating waves. Then the system cannot come into antispiral waves. $D_x < D_y \ll D_z$ is a radical premise of wave instability that make systems form either spiral or antispiral waves.

3 Extended Oregonator Model

We further adapt an extended Oregonator model given by Yang[12] while reversible transition between the activator and the inactivator was considered. The additional reaction is responsible for the emergence of the wave instability. Three-variable reaction-diffusion equations are obtained,

$$\frac{\partial x}{\partial t} = D_x \nabla^2 x + \frac{1}{\varepsilon}\left(x - x^2 - fz\frac{x-q}{x+q} - (cx - dr)\right), \quad (6)$$

$$\frac{\partial z}{\partial t} = D_z \nabla^2 z + x - z\,, \quad (7)$$

$$\frac{\partial r}{\partial t} = Dr\nabla^2 r + \frac{1}{\epsilon_1}(cx - dr)\,, \quad (8)$$

where variables x, z, and r, are dimensionless concentrations of the activator X, the oxidized form of catalyst Z, and the inactivator R, respectively. Parameters ϵ, ε_1, q, c, and d are rescaled kinetic parameters. The steady state solution is at $x_{ss} = z_{ss} = (1 - q - f + \sqrt{1 - 2f + 2q + f^2 + 6fq + q^2})/2$ and $r_{ss} = x_{ss}c/d$. One four-arm, one one-arm antispiral and one antitarget wave have been obtained by computer simulation with parameters $c = 0.2$, $q = 0.009$, $d = 1$, $\epsilon_1 = 2$, $(\epsilon, f) = (0.325, 0.910)$, $(D_x, D_z, D_r) = (0.025, 0.12, 0.8)$.[12]

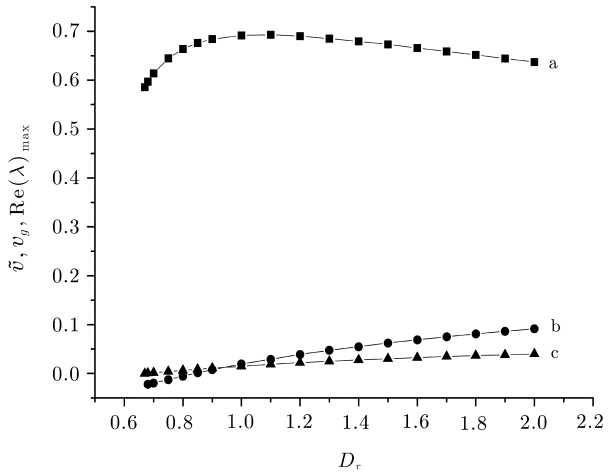

Fig. 4 Linear stable analysis for the extended Oregonator model, where $c = 0.2$, $q = 0.009$, $d = 1$, $\epsilon_1 = 2$, $(\epsilon, f) = (0.325, 0.910)$, $(D_x, D_z) = (0.025, 0.12)$. Transverse axis D_r represents diffusion coefficient of inactivator. Curves a, b, and c represent wavenumber, group velocity, and the maximum of $\mathrm{Re}(\lambda)$ each analysis, respectively.

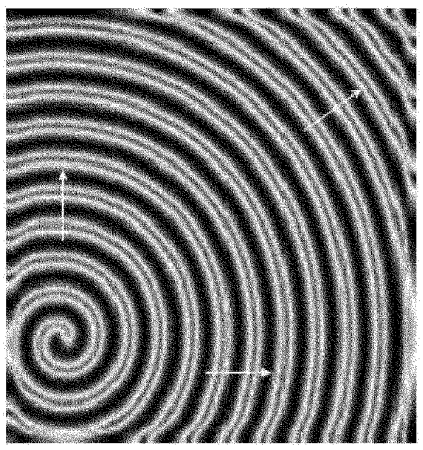

Fig. 5 Spiral waves in simulation of the extended Oregoantor model with zero-flux boundary and random initial condition ($D_z = 1.7$). The time step is set as 0.002. A snapshot is taken as 10000 time units. Arrows indicate the direction of wave propagation. The frame size is 128×128 space units.

This system is also a nonlinear system with one steady state solution, and so we may apply linear stability analysis to the system when it lies in the onset of bifurcation point. We take D_r as variable and other parameters as constant, then make linear stability analysis (Fig. 4). We obtain that the group velocity of travelling wave varies from -0.022 to 0.0915, and continues to increase (Fig. 4 line b). Waves may be transformed from antispirals[14] to spiral waves (Fig. 5), and the wavenumber increases from 0.597 to 0.693 at first and then decreases slowly as parameter D_r increases from 0.68 (Fig. 4 line a). The last case is very different from the extended Brusselator model. When parameter D_r is lower than 0.67, and the maximum of $\mathrm{Re}(\lambda)$ is less than -0.000495 (Fig. 4 line c), this system will be in a steady state for any perturbation and will not produce travelling waves.

4 Conclusion

The Brusselator model has a cubic autocatalytic term, but the Oregonator model does not. From the above we have mentioned, although two models have different dynamical terms, we may gain similar results. While spiral and antispiral waves have contrary notions and different behavior, it is plausible and possible to realize the transition between them by control of diffusion coefficient of inactivator from theoretical analysis and numerical simulations. To our knowledge, the transition between them has rarely been explored until now. We further provide a hint to find antispirals (spirals) in reaction-diffusion systems in which spirals (antispirals) have been observed.

References

[1] W. Jahnke, W.E. Skaggs, and A.T. Winfree, J. Phys. Chem. **93** (1989) 740.

[2] Wang Peng-Ye, Lu Wei-Ping, Yu De-Jin, and G. Robert, Harrison Optics Commun. **189** (2001) 127.

[3] M. Jorge, Davidenko, Arcady V. Pertov, Remy Salomonsz, Willam Baxter, and José Jalife, Nature **355** (1992) 349.

[4] Zhou Lu-Qun and Ou-Yang Qi, Phys. Rev. Lett. **85** (2000) 1650.

[5] Yang Ling-Fa and Irving R. Epstein, Phys. Rev. Lett. **90** (2003) 178303.

[6] Mads Ipsen, Lorenz Kramer, and Preben Graae Sørensen, Phys. Rep. **337** (2000) 193.

[7] David A. Kesseler, Herbert Levine, and William N. Reynolds, Phys. Rev. Lett. **68** (1992) 401.

[8] Ou-Yang Qi, *Pattern Formation in Reaction Diffusion Systems*, Shanghai Scientific and Technological Education Publishing House, Shanghai (2000) (in Chinese).

[9] Zhou Lu-Qun and Ou-Yang Qi, J. Phys. Chem. (2001) **A105** (2001) 112.

[10] Ou-Yang Qi, Harry L. Swinney, and Li Ge, Phys. Rev. Lett. **84** (2000) 1047.

[11] Vladimir K. Vanag, and Irving R. Epstein, Science **249** (2001) 835.

[12] Yang Ling-Fa, Milos Dolinik, Antol M. Zhabotinsky, and Irving R. Epstein, J. Chem. Phys. **117** (2002) 7259.

[13] Gong Yun and David J. Christini, Phys. Rev. Lett. **90** (2003) 088302.

[14] Yang Ling-Fa and Irving R. Epstein, J. Phys. Chem. **A106** (2002) 11676.

[15] Vladiniv K. Vanag and Irving R. Epstein, Phys. Rev. Lett. **88** (2002) 088303.