Symmetry-breaking instabilities under nonclassical bifurcation conditions

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We analyze the bifurcation of spatial-temporal dissipative structures beyond a hard-mode instability in open reacting systems operating far from equilibrium when a symmetry group (isomorphic to Z_2) acts on the diffusion space. The transversality condition which we study is not the classical Hopf bifurcation situation: Let us denote $\theta_1(\nu)\pm i\theta_2(\nu)$ the eigenvalues of the linearized reaction-diffusion problem that cross the imaginary axis for certain $\nu=\nu_c$ (ν is the bifurcation parameter) and for certain critical spatial wave number. Then our transversality condition reads $\theta_1(\nu_c)=0$, $d^j\theta_1(\nu=\nu_c)/d\nu^j=0$, and $d^l\theta_1(\nu=\nu c)/d\nu^l\neq 0$, $2\leq j<l$, while in the Hopf picture we had $\theta_1(\nu_c)=0$, and $d\theta_1/d\nu(\nu=\nu_c)\neq 0$. The system is assumed to have reflection symmetry. If the wave number is odd, the bifurcation diagram presents an additional nonthermodynamic branch which is not present in the Hopf case. The three possible bifurcation diagrams are investigated. Several laws of motion are derived from the restriction that the bifurcation equations should be covariant with respect to the action of the symmetry group.

I. INTRODUCTION

The classical picture of Hopf for the onset of symmetry-breaking instabilities was investigated in connection with reaction-diffusion systems and the occurrence of dissipative spatial-temporal organizations by a number of people.[1–4] Sattinger,[4,5] applying group representation methods, studied the existence of Turing instabilities when a symmetry group (the reflection group on an interval consisting of two elements, isomorphic to $\mathbb{Z}_2$) acts on the diffusion space and established the covariant nature of the bifurcation equations with respect to this symmetry group. (See also Ruelle.[6])

Our reaction-diffusion system is assumed to be subject to no flux boundary conditions and the diffusion space endowed with reflexion symmetry. To fix some notation, $\theta_1(\nu)\pm i\theta_2(\nu)$ are the conjugated eigenvalues of the linearized diffusion-reaction problem that cross the imaginary axis for a critical value $\nu=\nu_c$ of the bifurcation parameter and for a certain spatial wave number n_c. The rest of the eigenvalues live in the left half plane for all ν in a neighborhood of ν_c. The Hopf bifurcation condition is

$$\theta_1(\nu_c)=0,\quad \frac{d\theta_1(\nu=\nu_c)}{d\nu}\neq 0\ . \tag{1}$$

The aim of the paper is to prove that under the transversality condition

$$\theta_1(\nu_c)=0, \frac{d\theta_1(\nu=\nu_c)}{d\nu}=0, \ldots, \frac{d^l\theta_1(\nu=\nu_c)}{d\nu^l}=0\ ,$$
$$\frac{d^k\theta_1(\nu=\nu_c)}{d\nu^k}\neq 0,\quad 1<l<k\ . \tag{2}$$

The degeneracy of the thermodynamic branch for n_c odd is bigger than in the case of a Hopf bifurcation from a hard mode instability. This degeneracy is lifted by symmetry-breaking perturbations. Our derivation has only one restriction; we assume that the bifurcation parameter ν is an analytic function of the amplitude α and also that θ_1 is analytic in ν. This is a mild restriction which is given as thesis in the classical Hopf picture[4,5] and it is assumed in the mean-field Ginzburg-Landau theory of chemical kinetics under critical regimes where the bifurcation equation has the form

$$-(\nu-\nu_c)\alpha+\gamma\alpha^3=0$$

(α is the amplitude).

The covariant nature of the bifurcation equations impose certain laws of motion that are not present in the standard Hopf picture.

II. COVARIANT BIFURCATION EQUATIONS

Consider the general formulation of the reaction diffusion problem:

$$\dot{\vec{X}}=\vec{F}(\vec{X})+\underline{D}\frac{\partial^2}{\partial y^2}\vec{X},\quad y\in[0,\ \beta] \tag{3}$$

(β is the length of the reactor, $\underline{D}$ is the diffusion matrix, and $\vec{F}$ is the kinetic map smoothly dependent on the bifurcation parameter ν),

$$\vec{X}\in L^2[0,\ \beta]\times L^2[0,\ \beta]$$

with no flux boundary conditions:

$$\left.\frac{\partial\vec{X}}{\partial y}\right|_{y=0}=\left.\frac{\partial\vec{X}}{\partial y}\right|_{y=\beta}=0,\quad t\geq 0 \tag{4}$$

and an homogeneous steady state $\vec{X}=\vec{X}_0$.

The reflection symmetry group acting on $L^2[0,\ \beta]\times L^2[0,\ \beta]$ operates as follows.

The nontrivial operation g is

$$gy=\beta-y\ . \tag{5}$$

Then we can define the representation T_g on $L^2[0, \beta]\times L^2[0, \beta]$ simply by

$$T_g f(y)=f(gy)=f(\beta-y) . \tag{6}$$

Clearly the operator $\vec{F}+\underline{D}\partial^2/\partial y^2$ is covariant with respect to

$$T_g:\ T_g\left[\vec{F}+\underline{D}\frac{\partial^2}{\partial y^2}\right]=\left[\vec{F}+\underline{D}\frac{\partial^2}{\partial y^2}\right]T_g . \tag{7}$$

It is also true, therefore, that T_g commutes with the linearized operator

$$J(\vec{F})\Big|_{\vec{X}_0}+\underline{D}\frac{\partial^2}{\partial y^2}=\mathscr{L} \tag{8}$$

$J(\vec{F})\,|_{\vec{X}_0}$ is the Jacobian matrix of $\vec{F}$ at $\vec{X}_0$. Therefore, it is possible to define an action on each eigenspace E_n of $\mathscr{L}$ given by

$$E_n=\left\{\vec{v}_1\cos\left[\frac{n\pi}{\beta}y\right],\ \vec{v}_2\cos\left[\frac{n\pi}{\beta}y\right]\right\} , \tag{9}$$

where $\vec{v}_1$ and $\vec{v}_2$ are eigenvectors of

$$J(\vec{F})\,|_{\vec{X}_0}-\frac{n^2\pi^2}{\beta^2}\underline{D}=\mathscr{L}_n . \tag{10}$$

This action is

$$\begin{aligned} T_g\vec{v}\cos\frac{n\pi}{\beta}y&=\vec{v}\cos\frac{n\pi}{\beta}(\beta-y)\\ &=\begin{cases}\vec{v}\cos\dfrac{n\pi}{\beta}y & \text{for } n \text{ even}\\ -\vec{v}\cos\dfrac{n\pi}{\beta}y & \text{for } n \text{ odd} .\end{cases}\end{aligned} \tag{11}$$

Suppose that at $\nu=\nu_c$ the conjugated eigenvalues $\theta_1(0)\pm i\theta_2(0)$ of $\mathscr{L}$ cross the imaginary axis for $n=n_c$, then the spatial-temporal locally attractive solutions (traveling waves) tangent at $\vec{X}_0$ to E_{n_c} will have the form[7,8]

$$\vec{X}(y,t)=\vec{X}_0+\alpha\,\mathrm{Re}\left[e^{it/\tau}\vec{v}\cos\left[\frac{n\pi}{\beta}y\right]\right] , \tag{12}$$

α is the amplitude of the nonthermodynamic branch, τ is the period of the wave [to a first approximation $\tau=2\pi/\theta_2(\nu_c)$]. The representation T_g on E_{n_c} induces one on the α space given by

$$\widetilde{T}_g\alpha=\begin{cases}\alpha & \text{if } T_g \text{is the identity on } E_{n_c}\\ -\alpha & \text{otherwise}\end{cases} \tag{13}$$

or

$$\widetilde{T}_g\alpha=\begin{cases}\alpha & \text{if } n_c \text{ is even}\\ -\alpha & \text{if } n_c \text{ is odd} .\end{cases}$$

Assume α is given in terms of $\nu-\nu_c=\overline{\nu}$ by the equation $B(\alpha,\overline{\nu})=0$, then since $\vec{F}+\underline{D}\partial^2/\partial y^2$ is T_g covariant, the following covariant relation holds:[4,7]

$$B(\widetilde{T}_g\alpha,\overline{\nu})=\widetilde{T}_g B(\alpha,\overline{\nu}) . \tag{14}$$

Relation (14) is trivial for n_c even but for n_c odd it imposes restrictions on B:

$$B(-\alpha,\overline{\nu})=-B(\alpha,\overline{\nu}) . \tag{14$'$}$$

Consider problem (3) restricted to the space tangent to E_{n_c}. After we perform the translation $\vec{X}-\vec{X}_0=\vec{Y}$, there exists a linear transformation to convert this problem into Poincaré normal form.[8] The change of variables is

$$\begin{aligned}&\vec{Y}_n=\underline{Q}\vec{Z} ,\\ &\underline{Q}=[\mathrm{Re}\vec{v}_1,\ \mathrm{Im}\vec{v}_1] .\end{aligned} \tag{15}$$

After these two linear transformations, the problem (3) reads (in complex variables)

$$\dot{z}=[\theta_1(\nu)+i\theta_2(\nu)]z+\sum_{2\le i+j\le M} g_{ij}(\nu)\frac{z^i\overline{z}^j}{i!j!} . \tag{16}$$

The matrix $g_{ij}(\nu)$ can be made diagonal via the Ruppelt-Schneider transformation (the reader can consult Ref. 9 for details)

$$z=\xi+\sum_{Z\le i+j\le M} X_{ij}(\nu)\frac{\xi^i\overline{\xi}^j}{i!j!} , \tag{17}$$

$X_{ij}\equiv 0$ for $i=j+1$. The restriction to (3) to the attractive mode ξ reads now

$$\dot{\xi}=[\theta_1(\nu)+i\theta_2(\nu)]\xi+\sum_{j=1}^{[M/2]}\rho_j(\nu)\xi\,|\,\xi\,|^{2j} . \tag{18}$$

The amplitude α of the bifurcating solution (18) is derived from

$$\frac{d\,|\,\alpha\,|^2}{dt}=\frac{d(\xi\overline{\xi})}{dt}=\dot{\xi}\overline{\xi}+\xi\dot{\overline{\xi}}=0 \tag{19}$$

or

$$\frac{d\alpha^2}{dt}=2\xi\overline{\xi}\left[\theta_1(\nu)+\sum_{j=1}^{M}[\mathrm{Re}\rho_j(\nu)](\xi\overline{\xi})^j\right]=0 . \tag{20}$$

Therefore, we get

$$\theta_1(\nu(\alpha))+\sum_{j=1}^{M}\{[\mathrm{Re}\rho_j(\nu(\alpha))]\alpha^{2j}\}=0 . \tag{21}$$

In order to derive the bifurcation equations we shall impose the additional mild restriction that $\overline{\nu}$ is analytic in α and θ_1 in ν (cf. Refs. 8 and 10). That means

$$\nu=\nu_c+\sum_{j=1}^{\infty}\nu_j\alpha^j , \tag{22}$$

$$\begin{aligned}\theta_1&=\sum_{i=1}^{\infty}[\theta_1^{(i)}(\nu_c)(\nu-\nu_c)^i]\\ &=\sum_{i=1}^{\infty}\left[\theta_1^{(i)}(\nu_c)\left[\sum_{j=1}^{\infty}\nu_j\alpha^j\right]^i\right] .\end{aligned} \tag{23}$$

Equation (22) multiplied by α can be regarded as the bifurcation equation once the coefficients ν_j are evaluated. The equation should be multiplied by α to allow for the solution $\alpha\equiv 0$ corresponding to the thermodynamic branch.

Equation (21) allows us to derive the coefficients ν_j. By substituting (22) and (23) in (21), we get

$$\theta_1'(\nu_c)\sum_{j=1}^{\infty}\nu_j\alpha^j+\frac{\theta''(\nu_c)}{2}\left[\sum_{j=1}^{\infty}\nu_j\alpha^j\right]^2+\cdots+[\mathrm{Re}\rho_1(\nu_c)]\alpha^2+[\mathrm{Re}\rho'(\nu_c)]\left[\sum_{j=1}^{\infty}\nu_j\alpha^j\right]\alpha^2$$
$$+\cdots+[\mathrm{Re}\rho_2(\nu_c)]\alpha^4+\cdots=0\ . \qquad (24)$$

When n_c is odd, the relation (14′) holds, therefore, the bifurcation equation is

$$-\bar{\nu}\alpha+\sum_{j=1}^{\infty}\nu_{2j}\alpha^{2j+1}=0\ . \qquad (25)$$

That is, $\nu_i=0$ for i odd.

Observation: From Eq. (24) the condition (2) cannot hold for $k>2$ except in the special case $\mathrm{Re}\rho_1(\nu_c)=0$ (since we get this last relation at order α^2). We shall examine therefore, the case $k=2$ in condition (2).

At $O(\alpha^2)$ in (24) we get the relation

$$\frac{\theta_1''(\nu_c)}{2}\nu_1^2+\mathrm{Re}\rho_1(\nu_c)=0\ . \qquad (26)$$

Hence

$$\mathrm{Re}\rho_1(\nu_c)=0 \ \text{ for } n_c \text{ odd}\ . \qquad (27)$$

At $O(\alpha^4)$ in (24) we obtain

$$\nu_2^2\frac{\theta''(\nu_c)}{2}+[\mathrm{Re}\rho_1'(\nu_c)]\nu_2+\mathrm{Re}\rho_2(\nu_c)=0\ . \qquad (28)$$

Therefore, disregarding in (25) infinitesimals of order higher than α^3 we obtain two bifurcation equations instead of one as in the classical Hopf picture, one for each root of Eq. (28):

$$B_1(\alpha,\bar{\nu})=-\bar{\nu}\alpha+\nu_{2,1}\alpha^3=0$$
$$=-\bar{\nu}\alpha+\left[-\frac{\mathrm{Re}\rho_1'(\nu_c)}{\theta_1''(\nu_c)}+\frac{\{[\mathrm{Re}\rho_1'(\nu_c)]^2-2\theta_1''(\nu_c)\mathrm{Re}\rho_2(\nu_c)\}^{1/2}}{\theta_1''(\nu_c)}\right]\alpha^3=0\ , \qquad (29)$$

$$B_2(\alpha,\bar{\nu})=-\bar{\nu}\alpha+\nu_{2,2}\alpha^3=0$$
$$=-\bar{\nu}\alpha+\left[-\frac{\mathrm{Re}\rho_1'(\nu_c)}{\theta_1''(\nu_c)}-\frac{\{[\mathrm{Re}\rho_1'(\nu_c)]^2-2\theta_1''(\nu_v)\mathrm{Re}\rho_2(\nu_c)\}^{1/2}}{\theta_1''(\nu_c)}\right]\alpha^3=0\ . \qquad (30)$$

The bifurcation diagram presents two nonthermodynamic branches except in the case (degenerate) $\mathrm{Re}\rho_1'(\nu_c)^2=2\theta_1''(\nu_c)\mathrm{Re}\rho_2(\nu_c)$ or in the case $\mathrm{Re}\rho_2(\nu_c)=0$. If

$$0<2\theta_1''(\nu_c)\mathrm{Re}\rho_2(\nu_c)<[\mathrm{Re}\rho_1'(\nu_c)]^2$$

both branches appear for $\nu>\nu_c$.

When $\mathrm{sgn}\,\mathrm{Re}\rho_2(\nu_2)\neq\mathrm{sgn}\theta_1''(\nu_c)$ one branch bifurcates for $\nu>\nu_c$ and the other one appears for $\nu<\nu_c$.

III. FLUCTUATIONS

Consider again the case in which the degeneracy of the thermodynamic branch is doubled, that is

$$o<2\theta_1''(\nu_c)\mathrm{Re}\rho_2(\nu_c)<[\mathrm{Re}\rho_1'(\nu_c)]^2$$

for n_c odd. A symmetry breaking perturbation lifts the degeneracy and two nonthermodynamic branches bifurcate from the homogeneous steady state. The system will preferentially evolve to the nonthermodynamic branch corresponding to the smallest amplitude $\sqrt{\bar{\nu}/\nu_{2,1}}$.

In order to rigorously define the meaning of the term "preferentially" in the preceding paragraph, one should consider each component x_i of the reaction mixture in a fixed volume V of the open system. An estimation of the preference can thus be given by taking the quotient between the difference in population of the two branches $(\Delta N)_D$ and the thermal fluctuations $(\Delta N)_{\mathrm{th}}$,

$$(\Delta N)_{D,i}=[\sqrt{\bar{\nu}/\nu_{2,2}}-\sqrt{\bar{\nu}/\nu_{2,1}}]N_a v_i V\ , \qquad (31)$$

N_a is Avogadro's number, v_i is the ith component of vector $\vec{v}$ [cf. Eq. (12)],

$$(\Delta N)_{\mathrm{th},i}=\sqrt{N_a X_{0,i} V}\ , \qquad (32)$$

$X_{0,i}$ is the ith component of the steady-state vector. Then the preference $\mathscr{P}$ increases as the bifurcation parameter departs from the critical value ν_c according to

$$\mathscr{P}_i=\frac{(\Delta N)_{D,i}}{(\Delta N)_{\mathrm{th,i}}}=\left[\left[\frac{\bar{\nu}}{\nu_{2,2}}\right]^{1/2}-\left[\frac{\bar{\nu}}{\nu_{2,1}}\right]^{1/2}\right]\left[\frac{N_a v_i^2 V}{X_{0,i}}\right]^{1/2}\ . \qquad (33)$$

IV. CONCLUSION

We have demonstrated that the control parameter for the onset of hard mode instabilities in open reactive systems operating far from equilibrium is an analytic function of the amplitude of the bifurcating solution only in two cases:

(a) the classical Hopf picture,
(b) under the transversality condition

$$\theta_1'(\nu_c)=0, \quad \theta_1''(\nu_c)\neq 0 \ .$$

We have studied in detail case (b) to derive that the degeneracy of the thermodynamic branch of the system is higher than in case (a) except if an unstable solution (whose amplitude is proportional to $\sqrt{|\bar{\nu}|}$) exists when the homogeneous steady state is asymptotically stable. In this last case only one nonthermodynamic branch appears beyond the symmetry-breaking instability.

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