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Statistical scaling laws for chemical oscillators

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HIGHLIGHTS

- Definition of universality classes for the nonlinear, oscillatory Belousov–Zhabotinsky (BZ) reaction.
- Convergence to equilibrium described by phenomenological and analytical approaches.
- Analysis supported by numerical data via computer simulation and confirmed with analytical solution.
- Dependence on initial conditions, and variation of control parameters mark the convergence to the equilibrium.
- General, and universal formalism for the study of systems exhibiting Hopf bifurcations.

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ABSTRACT

Universality classes are defined for the nonlinear, oscillatory Belousov–Zhabotinsky (BZ) reaction. We examine the decay to asymptotic steady state for supercritical Hopf bifurcation by considering a phenomenological approach supported by numerical simulations and confirmed by a analytical description. The formalism is general and it is expected to be universal for systems exhibiting Hopf bifurcations.

1. Introduction

In statistical mechanics, scaling laws are generally associated with changes in the spatial structure of dynamical systems due to variations of control parameters [1–4]. A bifurcation is the scientific terminology given to these particular qualitative change in the dynamics [5]. In the local bifurcation theory, when an equilibrium point changes stability from stable to unstable and a stable limit cycle shows up, we say the system has undergone into a Hopf bifurcation [6,7]. In general, the study of the Hopf bifurcation is of great practical concern as well as of fundamental scientific interest, once it is present in a variety of systems including electrical circuits [8–10], dynamical population [11,12] , lasers [12,13] and many others. Although, some of the basic questions that remain to be explored about Hopf bifurcation are the regimes for which certain scaling laws exist and whether the exponents obtained for system obeying kinds of dynamics are valid for others.

In this paper, we examine the nonlinear, oscillatory Belousov–Zhabotinsky (BZ) reaction. In general, nonlinear chemical oscillators are found in a variety of biological systems including neural network, circadian clocks and vascular systems [14–17]. The BZ reaction is a particularly interesting nonlinear phenomenon, in contrast to the most chemical reactions where a state of homogeneity and equilibrium is quickly reached, this remarkable chemical reaction maintains a prolonged state of non-equilibrium leading to temporal oscillations and spatial pattern formation (see Fig. 1).

Our main goal in this paper is to apply the scaling formalism to explore the evolution towards equilibrium of the BZ reaction near the Hopf bifurcation. Here, two different procedures are adopted. The first one is mostly phenomenological

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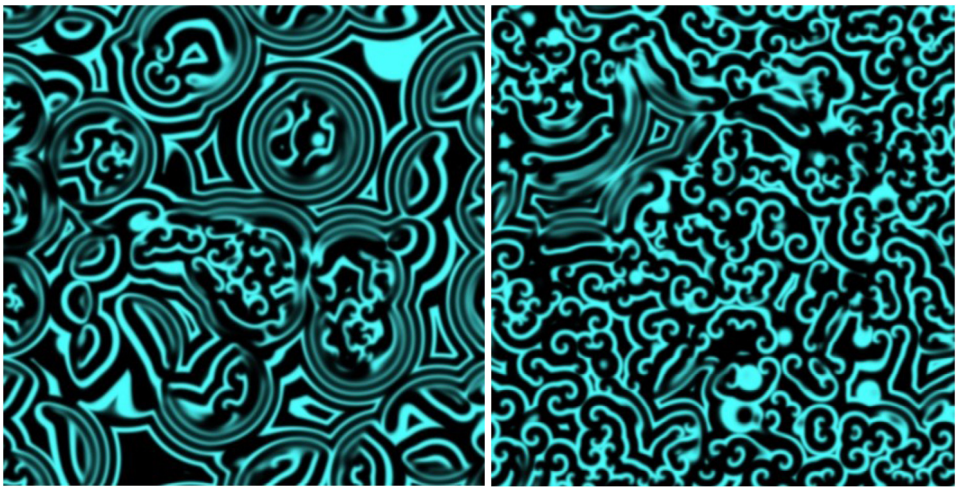

(a) (b)

Fig. 1. Spiral waves of chemical activity of the Belousov–Zhabotinsky (BZ) reaction. (BZ) reaction is an example of a temporally oscillating chemical reaction. (a) Processing simulation of the spatial oscillations of an idealized BZ reaction after 100 frames; (b) state after approximately 400 frames.

with scaling hypotheses ending up with scaling laws of seven critical exponents. The second one considers an analytical description confirming the results obtained by numerical simulation. The scaling analysis presented in this paper suggests that the same critical exponents as well the scaling properties studied should also be valid for other multidimensional systems that exhibit Hopf bifurcation [18].

This paper is organized as follows. In Section 2, a theoretical model of the BZ reaction is presented and its normal-form derived. Section 3 is devoted to describe the phenomenological approach based on scaling hypotheses leading to critical exponents, and hence to scaling laws. In Section 4 an analytical description is made and scaling exponents derived through the direct solution of the differential equations. Moving on, conclusions are made in Section 5.

2. The dynamics and normal-form computation

2.1. The mathematical model and dynamics

The first theoretical attempt to explain oscillating reactions was accomplished by G. Nicolis and Ilya Prigogine and it is called Brusselator [19]. A *Brusselator* is a scientific terminology given to auto-catalytic chemical reactions at which one of the reactants in the reaction mechanism is also a product and vice-versa. The dimensionless form [19,20] of the rate equations for an idealized auto-catalytic BZ reaction is fundamentally nonlinear and given by

$$\begin{cases} \dot{x}_1 = & a - (1+b)x_1 + x_2x_1^2, \\ \dot{x}_2 = & bx_1 - x_2x_1^2. \end{cases} \tag{1}$$

where x_1, x_2, a and $b \in \mathbb{R}$. For further developments, a is assumed constant and b treated as a control parameter. BZ reaction's model expressed in Eq. (1) has one fixed point at $P_0 = (a, \frac{b}{a})$. Near the fixed point P_0 we have the Jacobian matrix

$$J_{P_0} = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix}. \tag{2}$$

The eigenvalues of the matrix (2) considering the fixed point P_0 are

$$\lambda_{1,2} = \alpha(b) \pm i\beta(b), \tag{3}$$

where $\alpha(b) = \frac{(b-a^2-1)}{2}$ and $\beta(b) = \frac{\sqrt{4a^2-(b-a^2-1)^2}}{2}$.

According to the linear stability theory when $\alpha < 0$, the fixed point turns a stable spiral whose sense of rotation depends on β. For $\alpha = 0$, an stable spiral dictates the dynamics however the speed of convergence is different from $\alpha < 0$. Finally, for $\alpha > 0$, there is an unstable spiral at the origin and, a stable and periodic limit cycle bifurcates from the fixed point.