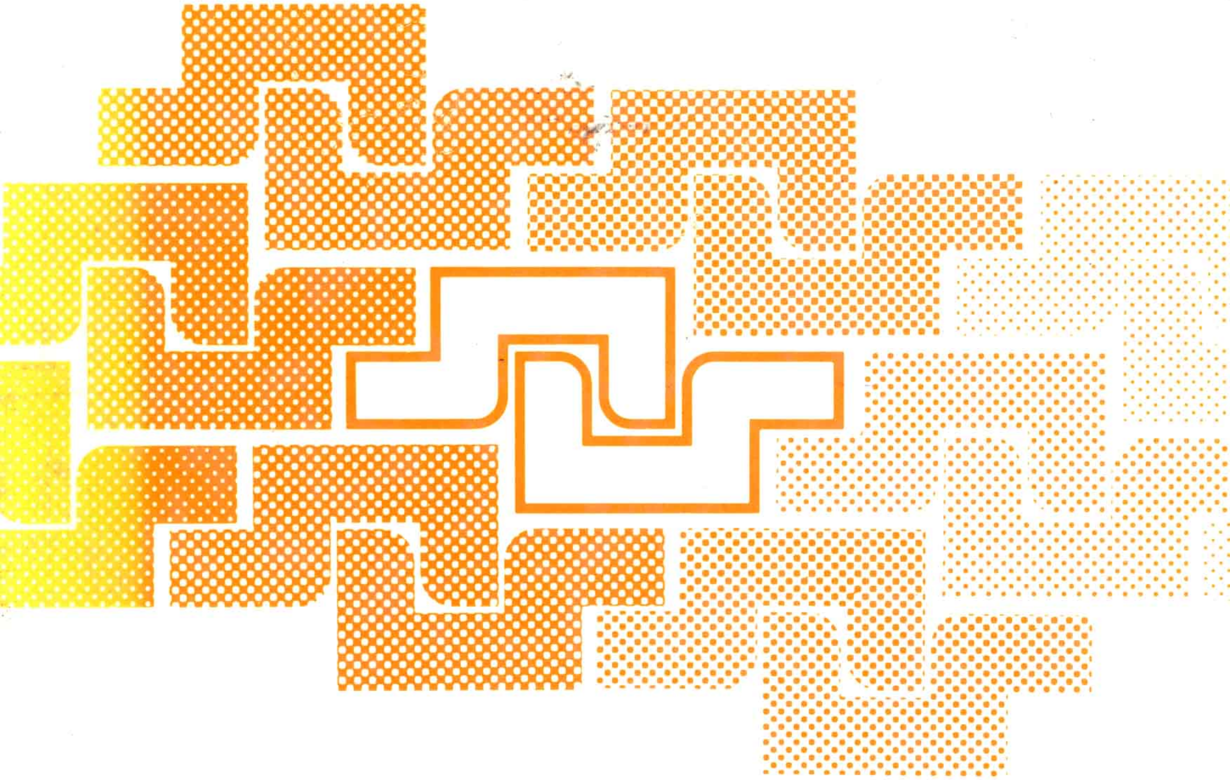

Patterns, Defects and Materials Instabilities

Edited by

D. Walgraef and N. M. Ghoniem

NATO ASI Series

Series E: Applied Sciences - Vol. 183

Patterns, Defects and Materials Instabilities

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Kluwer Academic Publishers

Dordrecht / Boston / London

Published in cooperation with NATO Scientific Affairs Division

Proceedings of the NATO Advanced Study Institute on
Patterns, Defects and Materials Instabilities
Cargèse, France
September 4–15, 1989

Library of Congress Cataloging in Publication Data

NATO Advanced Study Institute on Patterns, Defects, and Materials
Instabilities (1989 : Cargèse, France)
Pattern, defects and materials instabilities / edited by D.
Walgraef and N.M. Ghoniem.
p. cm. -- (NATO ASI series, Applied sciences ; 183)
"Proceedings of the NATO Advanced Study Institute on Patterns,
Defects, and Materials Instabilities, Cargese, France, September
4-15, 1989."
"Published in cooperation with NATO Scientific Affairs Division."
ISBN 0-7923-0753-4 (U.S. : alk. paper)
1. Chaotic behavior in systems--Congresses. 2. Space and time-
-Congresses. 3. Fluctuations (Physics)--Congresses. 4. Materials-
-Congresses. I. Walgraef, D. (David) II. Ghoniem, N. M. (Nars
Mostafa) III. North Atlantic Treaty Organization. Scientific
Affairs Division. IV. Title. V. Series: NATO ASI series. Series
E, Applied sciences ; no. 183.
Q172.5.C45N383 1989
530.4'1--dc20 90-34912

ISBN 0-7923-0753-4

Published by Kluwer Academic Publishers,
P.O. Box 17, 3300 AA Dordrecht, The Netherlands.

Kluwer Academic Publishers incorporates the publishing programmes of
D. Reidel, Martinus Nijhoff, Dr W. Junk and MTP Press.

Sold and distributed in the U.S.A. and Canada
by Kluwer Academic Publishers,
101 Philip Drive, Norwell, MA 02061, U.S.A.

In all other countries, sold and distributed
by Kluwer Academic Publishers Group,
P.O. Box 322, 3300 AH Dordrecht, The Netherlands.

Printed on acid-free paper

Printed in the Netherlands

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NATO ASI Series

Advanced Science Institutes Series

A Series presenting the results of activities sponsored by the NATO Science Committee, which aims at the dissemination of advanced scientific and technological knowledge, with a view to strengthening links between scientific communities.

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Series E: Applied Sciences - Vol. 183

PREFACE

Understanding the origin of spatio-temporal order in open systems far from thermal equilibrium and the selection mechanisms of spatial structures and their symmetries is a major theme of present day research into the structures of continuous matter. The development of methods for producing spatially ordered microstructures in solids by non-equilibrium methods opens the door to many technological applications. It is also believed that the key to laminar/turbulence transitions in fluids lies in the achievement of spatio-temporal order.

Let us also emphasize the fact that the idea of self-organization in itself is at the origin of a reconceptualisation of science. Indeed, the appearance of order which usually has been associated with equilibrium phase transitions appears to be characteristic of systems far from thermal equilibrium. This phenomenon which was considered exceptional at first now appears to be the rule in driven systems. The chemical oscillations obtained in the Belousov-Zhabotinskii reaction were initially considered to be thermodynamically impossible and were rejected by a large number of chemists. Now these oscillations and related phenomena (waves, chaos, etc.) are the subject of intensive research and new classes of chemical oscillators have been recently discovered. Even living organisms have long been considered as the result of chance rather than necessity. Such points of view are now abandoned under the overwhelming influence of spatio-temporal organization phenomena in various domains ranging from physics to biology via chemistry, nonlinear optics, and materials science .

Today, materials science is undergoing a complete revolution. Indeed, by the use of new technologies (laser and particle irradiation, ion implantation, ultrafast quenches, etc.) it is possible to escape from the tyranny of the phase diagram and to process new materials with unusual properties. In order to describe and understand such materials, dynamical concepts related to nonequilibrium phenomena, irreversible thermodynamics, nonlinear dynamics, and bifurcation theory, are required.

The development of a theoretical framework to describe and interpret self-organization phenomena was made easier by the progress of thermodynamics of irreversible processes and by the introduction of the concept of dissipative structure. In this context it is clear that the nonlinearities of the dynamics and the distance from thermal equilibrium are at the origin of to spatio-temporal organization. Similar phenomena appear in very different systems : spiral waves in chemical systems (but also in the cortex or cardiac activity), the aggregation of micro-organisms, and convective rolls associated with hydrodynamical instabilities in normal fluids and liquid crystals. These varied appearances show that these phenomena are not induced by the microscopic properties of the systems but are triggered by collective effects including a large number of individuals (atoms, molecules, cells, etc.).

The role of fluctuations is also very important in such circumstances. Effectively, near instability points, the space and time scales are so large that the structures are particularly sensitive to even small fluctuations. When different states are simultaneously stable beyond an instability, such fluctuations or small external fields may affect the pattern selection mechanisms. Furthermore, in the case of spatial patterns, the position and orientation of the structure which are described by phase variables are usually fixed by the boundary conditions in small systems. This is of course not the case in large systems where phase fluctuations may trigger the nucleation of defects analogous to dislocations and disclinations. These effects show the importance of a stochastic description of self-organization phenomena far from equilibrium.

In pioneering fields, such as hydrodynamics or nonlinear chemistry, the comparison between theoretical predictions and experimental observations has long been qualitative but has reached the quantitative level recently. This is because of new experimental methods using laser and computer technology and of theoretical progress based on the theory of dynamical systems, on bifurcation calculus, and on the development of supercomputers which make numerical simulations feasible.

While quantitative and systematic experimental analysis followed theoretical analysis in the case of nonlinear chemistry, the evolution has been quite different in the field of hydrodynamics. Despite the fact that convective instabilities and turbulence have been studied for more than a century , definite progress in understanding pattern formation, selection and stability, and the origin of chaotic behavior were achieved only recently It is worth noting that these problems present severe difficulties. From the experimental point of view, the absence of any operational definition of turbulence, the lack of sensitivity of traditional measurement techniques to the temporal behavior of hydrodynamical flows, and a poor resolution of boundary effects limited the progress until the last decade. From the theoretical viewpoint, a major difficulty has been finding analytic solutions because of the complexity of the Navier-Stokes equations.

Significant progress have been achieved in the experimental analysis of instabilities and hydrodynamical flows because of new techniques (laser velocimetry, cryogenic techniques, image processing, etc.) , the systematic use of computer science in data processing and experiment control, and the linkage with new theoretical approaches based on instability and bifurcation theory. On the other hand, the study of the succession of instabilities obtained by increasing the bifurcation parameter requires nonlinear analysis which extends far beyond the classical studies in the field. Hence a few relatively simple systems (Rayleigh-Benard, Taylor-Couette, Benard-

Marangoni, etc.) became very popular as prototypes of complex behavior where nonlinear theories of pattern formation may easily be tested.

Although the Rayleigh-Benard type of instabilities have been discussed at length in the literature and are still providing new challenges for theorists and experimentalists, some of their basic aspects bear reviewing. When a thin horizontal layer of fluid is heated from below or cooled from above, a temperature gradient is generated across the sample. For small gradients, the fluid remains in a conductive state but, on increasing the temperature difference between the horizontal fluid boundaries, the gradient may reach a threshold where this conductive state becomes unstable. Beyond this threshold (instability or bifurcation point), convection sets as cellular structures associated with periodic spatial variations of the hydrodynamic fluid velocity field and of the temperature field. Several types of structures may be obtained according to the working conditions: rolls, hexagons, squares, traveling or standing waves. On increasing further the bifurcation parameter, these patterns may in turn become unstable causing successive bifurcations to occur driving the system to chaos.

From the theoretical point of view, while the first bifurcation may easily be determined from the Navier-Stokes equation, it is a formidable task to determine the behavior of the system beyond the hydrodynamic instabilities with these equations. Fortunately, the derivation of amplitude equations for the patterns led to definite progress in the study of their formation, selection and stability properties. These equations which are usually of the Ginzburg-Landau type, correspond to reduced versions of the complete dynamics which contain all the symmetries of the problem. They may be solved more easily and describe correctly the dynamics of the system on long space-time scales close to the bifurcation point.

Because of the permanent interactions between theory, experiment and numerical analysis, significant progress have been made during the past 20 years on the mathematical methods of nonlinear dynamics and in the understanding of simple fluids instabilities. It has become quite clear that such instabilities manifest themselves in the form of various patterns which vary from the simple to the complex. More recently, the growth in the body of knowledge of liquid-crystal hydrodynamics furnished an exciting ground for further experimental observations on the nature of transitions from one pattern structure to another. Nonlinear interactions at the micro level can explain, to a large degree, the onset and propagation of instabilities at the macro level. Instabilities are saturated through the formation of what is now commonly known as "dissipative" structures. The geometry and properties of these structures can be well explained by a competition between local and nonlocal transport reactions. This framework appears to be quite general, at least conceptually, and can be seen in many physical phenomena (e.g. laser-material interactions, energetic particle-material interactions, magnetic fluids, plastic instabilities, plasma and electric systems). General observations of these vastly diverse physical systems show striking similarities in the nature and occurrence of patterns as manifestations of instabilities.

Physicists and mathematicians have already observed that beyond the onset of instability, patterns which form to "dissipate" the instability are rarely perfect. Imperfections, or defects, can be shown to develop in all pattern-forming instabilities. In some simplified models, one can mathematically find conditions for defect creation in otherwise regular structures. On the other hand, it is already known to materials scientists that defects play an important role in determining material properties. Point defects play a major role in all macroscopic material properties which are related to atomic diffusion mechanisms, and to electronic properties in semiconductors. Line defects, or dislocations, are unquestionably recognized as the basic elements which lead to metal plasticity and fracture. As a consequence, the study of the individual properties of solid state defects is at an advanced level. However, studies of the collective behavior of line defects are still elementary. At the present time, it is important to note that the collective behavior of point defects is well described within the rate theory framework, in analogy to the concepts developed earlier for chemical kinetics. Theoretical description of point-defect interactions can be described as reaction-diffusion equations. On the other hand, major theoretical challenges are encountered in the development of statistically based models of the collective behavior of line defects. Nonetheless, significant progress has been made in the field of dislocation dynamics and plastic instabilities over the past several years.

Physical systems which comprise many interacting entities (e.g. fluids, solids, plasmas, etc.) have been described at different levels. (1) The most fundamental and detailed level is a description based on the equations of motion (EOMs) for the individual entities. Hence, the framework of Newtonian or quantum mechanics is appropriate. (2) A higher level in the hierarchy is statistical mechanics, where the concern is with distribution functions in phase space, rather than the individual EOMs. Thus we are able at this level of description to discuss collective properties such as diffusion, conduction, viscosity, permeability, etc.. (3) The description of continuum mechanics is more appropriate for studying macroscopic length and time scale resolutions. Navier-Stokes, continuity and compatibility equations provide the primary vehicles for a macroscopic description of the continuum. At this level, constitutive relations are needed to complete the framework. It is hoped that such constitutive relations are derivable at the statistical mechanics level. However, this is not usually the case. More often, a phenomenological model is used to obtain the needed constitutive relations. (4) Continuous media deform generally homogeneously if the externally perturbing field induces small deviations from equilibrium. Critical levels of non-equilibrium perturbing field lead to dynamical instabilities in the continuous distribution of matter and to the eventual emergence of patterns or dissipative structures. In past few decades astonishingly rapid progress has been made in our understanding of the nature of pattern-forming instabilities. The appropriate framework at this level of analysis is nonlinear dynamics, where the dynamical equations which describe the bifurcations and instabilities are obtained from appropriate con-

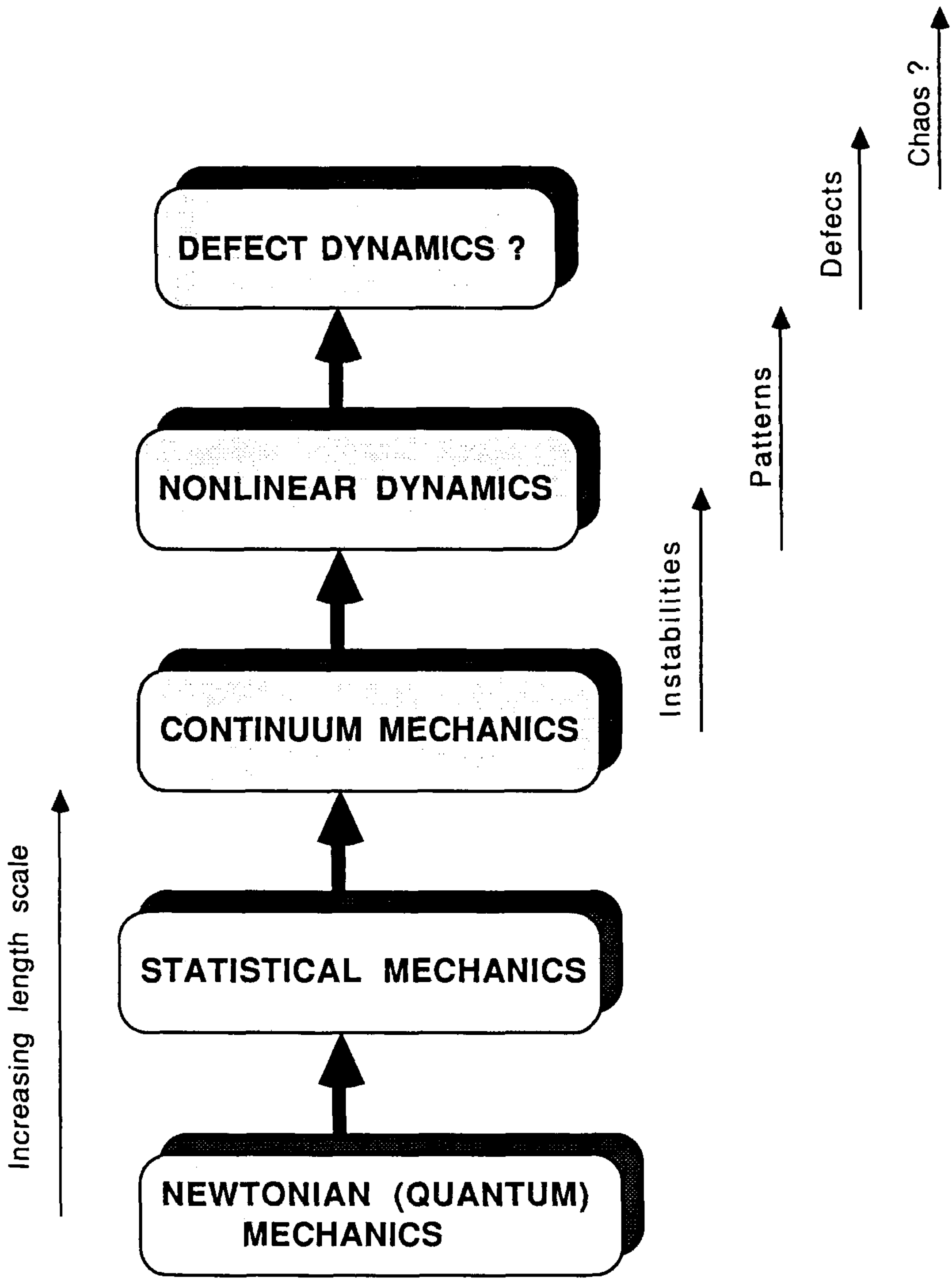

Fig. 1: Schematic representation of a hierarchical framework for describing material instabilities, patterns, and defects.

tinuum equations. Thus from Navier-Stokes or reaction-diffusion equations, for instance, one is able to develop dynamical equations of the Ginzburg-Landau type, which are capable of describing the instabilities in a manner reminiscent of phase transitions in thermodynamic systems. (5) Solutions of these dynamical equations lead to conditions where "defects" are obtained in otherwise periodically perfect structures. This has, in fact, already been observed in several systems, most notably in liquid crystals. At this level of description, the system characteristics are manifest in the dynamics of interaction between such defects, and one may be able to develop the framework of "defect dynamics". This ascension of levels is shown schematically in Fig.1.

Physicists, chemists, material scientists, and mathematicians have the goal of developing a unified framework for explaining pattern-forming instabilities and defects. To this end, the proceedings of this meeting represent a combination of lectures and contributed presentations on patterns, defects, and material instabilities and we hope that this ASI has advanced this goal within the community. We are grateful to the NATO Scientific Affairs Division, to the Directorate General for Science, Research and Development of the Commission of the European Communities, to the CNRS (France) and to the International Solvay Institutes for their generous financial support. Special thanks are also due to the secretarial staff in Brussels and Cargèse, in particular Ms M.F.Hanseler and N.Sardo, for its efficiency.

N. M. Ghoniem D. Walgraef

January 1990

CONTENTS

ONE-DIMENSIONAL CELLULAR PATTERNS

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ABSTRACT. A classification of the generic instabilities that one-dimensional cellular patterns can suffer is presented.

1. Introduction

Stationary cellular patterns are frequently observed in nature. Recently a classification of the various bifurcations of one-dimensional periodic patterns has been proposed [1]. In this paper we summarize these bifurcations on the basis of symmetry considerations.

Our initial hypothesis is the existence of a one-dimensional stationary cellular pattern which can be described by a solution $U_0(x)$ of an evolution equation

$$\partial_t U = f(U) \tag{1}$$

where $U = (U_1, ..., U_N)$ are, for the sake of simplicity chosen to be scalar quantities. This evolution equation is assumed to describes one-dimensional physical systems which are invariant under the following symmetries

$$\mathcal{T}_\theta \quad : \quad t \to t + \theta \tag{2}$$

$$T_\sigma \quad : \quad x \to x + \sigma \tag{3}$$

$$P \quad : \quad x \to -x \tag{4}$$

Since U is a scalar $PU(x) \equiv U(-x)$. The solution U_0 which describes the periodic cellular pattern is such that

$$\mathcal{T}_\theta U_0 = U_0 \tag{5}$$

$$T_a U_0 = U_0 \tag{6}$$

$$PU_0 = U_0 \tag{7}$$

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In words, U_0 is stationary, periodic in space with a period a, and can be chosen even by an appropriate coordinate change.

2. Normal modes of a perturbation

The stability analysis of U_0 proceeds as follows. Let

$$U(x,t) = U_0(x) + u(x,t) \tag{8}$$

where $u(x,t)$ is a small perturbation. At the first order in $u(x,t)$ the equation for the perturbation reads

$$\Lambda u = 0 \tag{9}$$

where $\Lambda = \partial_t - \mathcal{L}(x)$ and $\mathcal{L}(x) = \partial f(U)/\partial U|_{U=U_0(x)}$ is the Jacobian operator. Λ has the following properties:

$$[\Lambda, \mathcal{T}_\theta] = 0 \tag{10.a}$$

$$[\Lambda, T_a] = 0 \tag{10.b}$$

$$[\Lambda, P] = 0 \tag{10.c}$$

where $[A, B] = AB - BA$. These properties are now used to solve Eq. (9). Since Λ commutes with $\mathcal{T}_\theta$, T_a and P, they have a common spectral decomposition,

$$u = \sum_j u_j e_j(x,t) \tag{11}$$

where, in the space of bounded functions, a typical element of this basis

$$e_j(x,t) = B_j(x) exp(s_j t) \tag{12}$$

is such that

$$\mathcal{T}_\theta e_j(x,t) = \lambda_\theta e_j(x,t) \tag{13.a}$$

with $\lambda_\theta = exp(s_j \theta)$ and

$$T_a e_j(x,t) = \lambda_a e_j(x,t) \tag{13.b}$$

with $|\lambda_a| = 1$. The eigenfunction of the discrete translation T_a are Bloch functions. They have the general form $B(x) = \eta(x)\exp(ikx)$, with $T_a \eta(x) = \eta(x)$. The condition of boundness ($|\lambda_a| = 1$) is satisfied by three different type of eigenvalues (spatial analogs of Floquet multipliers)

(a) $\lambda_a = 1$
(b) $\lambda_a = \exp(i\phi), \exp(-i\phi)$
(c) $\lambda_a = -1$

In case (b), in general, $\phi/2\pi \neq n/m$. The corresponding Bloch functions are

(a) $B(x) = \eta(x)$ $(k = 0)$
(b) $B(x) = \eta(x)\exp(ik_0 x), \bar{\eta}(x)\exp(-ik_0 x)$ $(k = k_0)$
(c) $B(x) = \eta(x)\exp(i\pi x/a) \equiv \hat{\eta}(x)$ $(k = \pi/a)$

In case (a), the eigenvector has the same period as the basic pattern U_0 and the corresponding eigenvalue is generically simple. In case (b) it is bi-periodic (modulation with a period $2\pi/k_0$ generally irrationaly related to a). The corresponding eigenvalue is generically double. In case (c), the eigenvalue is generically simple and the eigenvector has twice the period of the basic pattern. The spectral decomposition can be pushed further when one takes into account the parity. In case (a) the eigenspace naturally splits into two components which correspond to the two eigenspaces of P, namely the even functions of x ($P\eta_E(x) = \eta_E(x)$) and the odd function of x ($P\eta_O(x) = -\eta_O(x)$). The same property is true for case (c), where $\hat{\eta}(x)$ splits into even and odd parts ($\hat{\eta}_E(x)$ and $\hat{\eta}_O(x)$ respectively). In case (b), the eigenspace has already a dimension two, no further splitting occurs since even and odd functions of x can be generated in this space. The spectral decomposition is summarized in Table I (Case I and Case II respectively correspond to real and complex s).

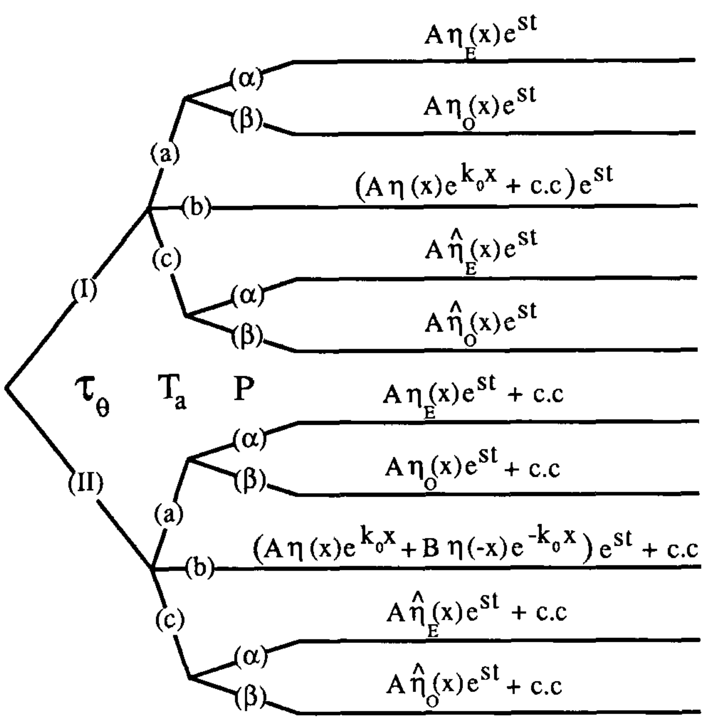

Table I

3. Instabilities

A bifurcation occurs whenever $\mathcal{R}e(s) = 0$. Replacing s by 0 or $\pm i\omega_0$, the previous table turns into the classification of the ten generic instabilities that one-dimensional periodic patterns can suffer [1]. Case (I) corresponds to stationary bifurcations. The associated marginal eigenvector does not break time translations. Case (II) corresponds to oscillatory or Hopf bifurcations. The marginal eigenfunctions do break time translations. In case (a) the discrete translational symmetry T_a is not broken. Case (b) and case (c) do break it. Case (b) is associated with a spatial modulation of the pattern and case (c) corresponds to a spatial period doubling bifurcation. In case (α) the parity is not broken, while it is in case (β). In case (b) the parity is also generically broken.

4. Normal forms

As usual, the next step in the bifurcation analysis consists in establishing the equations for the amplitudes of the weakly off marginal modes. We first remark that $u = \partial_x U_0(x)$ is a solution of Eq. (9) with $s = 0$. It is a straightforward consequence of the translational symmetry (T_σ) which has been broken by the cellular pattern $U_0(x)$

$$\partial_x f(U_0(x)) = \mathcal{L}(x)\partial_x U_0(x) = 0 \tag{14}$$

A simple way to account explicitely for this degree of freedom (phase order parameter) consists in replacing Eq.(8) by

$$U(x,t) = U_0(x+\phi) + u(x+\phi,t) \tag{15}$$

together with an orthogonality condition

$$\langle u, \partial_x U_0 \rangle = 0$$

where $\langle V, W\rangle = \int_{-\infty}^{+\infty} \sum_j V_j(x)\bar{W}_j(x)dx$. In order to get the equations for the phase and amplitude perturbations, we now insert (14) into Eq. (1) and keep only first order terms in ϕ and u

$$\partial_t \phi = \langle \mathcal{L}u, \partial_x U_0\rangle / |\partial_x U_0|^2 \tag{16.a}$$

$$\partial_t u = L(x)u \tag{16.b}$$

where $L(x)u = \mathcal{L}(x)u - \partial_x U_0 \langle \mathcal{L}u, \partial_x U_0\rangle/|\partial_x U_0|^2$. These equations describe, in the linear theory, the coupling between the phase order parameter ϕ and the amplitude modes. Near an instability, in the linear approximation, u becomes one of the eigenmodes given in Table I, where $s = 0$ or $s = \pm i\omega_0$. The amplitudes of these marginal modes turn into order parameters associated with the instability. Center manifold theorem allows to express, near the bifurcation threshold, the amplitudes of all other modes in terms of the order parameters. The equations for ϕ and for these order parameters are the normal forms associated with the bifurcation. Simple symmetry arguments can be used in order to establish the form of these equations.

5. An example of bifurcation: the parity breaking instability.

Let us now illustrate this method for finding the amplitude equations. Case (I.a.β) corresponds to a stationary instability characterized by a mode which has the same period than the basic cellular pattern, but with a different parity. From Table I one