

Pattern formation: A Landau-type analysis of symmetry breaking

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Instabilities in nonequilibrium systems described by deterministic differential equations are investigated. Using group-theoretical arguments we find a rule similar to that valid for the equilibrium case: A spatial pattern appears necessarily through a first-order transition if a cubic invariant can be constructed from the amplitudes of the slow modes.

I. INTRODUCTION

A number of far-from-equilibrium systems exhibit instabilities leading to the formation of spatial patterns.¹⁻³ Familiar examples are the hydrodynamic instabilities,^{4,5} the pattern formation in chemical reactions,^{1,6} the morphogenesis,^{2,7} the Marangoni instability,⁸ some aspects of crystal growth,⁹ the buckling of spheres,¹⁰ etc. A basic feature of all the above nonequilibrium phase transitions is the spontaneous breakdown of symmetry: as some external control parameter is changed, the stable steady state of the system, which is invariant under a symmetry group G , loses its stability and a new steady state appears which is invariant only under a subgroup of G .

The simplest and best-understood examples of symmetry breaking are found in systems exhibiting equilibrium phase transitions. Since there is a great deal of similarity between the equilibrium and nonequilibrium phase transitions^{1,2,11} the theory of the latter is largely inspired by the concepts (order parameter, critical slowing down, universality and the relevance of the symmetry of the order parameter, etc.) and by the methods (mean-field approximation, scaling, renormalization group)^{1,2,6,11-13} worked out for equilibrium systems.

An interesting chapter in the theory of equilibrium phase transitions is the symmetry analysis by Landau¹⁴: with the use of the invariance properties of the thermodynamic potentials, it is possible to tell whether, in case of a given symmetry breaking, the order parameter could be continuous at the transition point or, in other words, whether the phase transition could be of second order. Although Landau's predictions are obtained within the framework of the mean-field theory, there are

only a few cases^{15,16} when the inclusion of fluctuations invalidates his results.

In case of nonequilibrium phase transitions, the mean-field theory seems to be an even better description (the critical region is expected to be extremely narrow¹¹) so it is natural to ask for the counterpart of Landau's symmetry analysis. The translation of Landau's results is not straightforward, however, since the nonequilibrium phase transitions are described by nonlinear differential equations and the symmetry breaking appears in the mathematics as the bifurcation of the stable stationary solution of those equations. The role of symmetry in analyzing the pattern formations and the corresponding bifurcations has already been recognized.^{10,17-20} Near the instability point there is a separation of characteristic time scales and, as a consequence, the essential features of the phenomenon can be described by a few relaxing modes, and the possible forms of the equations of motion for the amplitudes of the slow modes (order parameter) are severely restricted by the actual symmetry breaking. For example, special cases of breakdown of the translational¹⁹ and of the rotational²⁰ symmetries have been examined by Sattinger. He constructed the equation for the order parameter purely from symmetry arguments and determined whether the order parameter could change continuously at the transition point. He also pointed out²⁰ that the continuity properties of the transition could also be investigated for more complicated symmetries provided the equation of motion for the order parameter possessed a gradient structure, i.e., it was derivable from a potential.

Our aim with this paper is to carry out a Landau-type symmetry analysis for nonequilibrium phase transitions occurring in systems described by

deterministic differential equations. We derive the equations of motion for the slow modes making use of their symmetry properties (Sec. II). Then, without recourse to the possible gradient structure of those equations, the stability properties of the stationary solutions are examined (Sec. III) resulting in a necessary condition for the nonequilibrium phase transition to be of second order. This condition is similar to that known for the equilibrium case: the transition cannot be of second order if a cubic invariant can be constructed from the amplitudes of the slow (unstable and marginal) modes. Some applications of this result are discussed in Sec. IV.

II. SYMMETRIES AND THE CONCEPT OF ORDER PARAMETER

Instabilities leading to the formation of spatial patterns are usually described by an equation of the following form:

$$\frac{\partial \rho}{\partial t} = F(\rho, \lambda), \quad (1)$$

where $\rho(x, t)$ is a space- and time-dependent field (e.g., the concentration of a chemical reactant, or a temperature field) and F stand for a nonlinear functional of both ρ and its spatial derivatives. The parameter λ is externally controlled; it characterizes the reservoirs surrounding the system. In most cases, ρ has several components but, for simplicity, we start with the one-component case and extend the results to many-component fields later.

Generally, Eq. (1) together with the given boundary conditions is covariant with respect to the symmetry operations of a group G' . It is supposed that, for λ smaller than a critical value λ_c , the steady state of the system, described by the stable stationary solution $\rho_0(x)$, is invariant under, generally speaking, a different group $G \subseteq G'$. At λ_c this state and the corresponding solution lose their stability against infinitesimal perturbations. For $\lambda > \lambda_c$, a new steady state is stable which is invariant under a subgroup of G and the problem is to determine whether the new symmetry could appear through a second-order transition.

Since the order of the transition is connected with the continuity of the order parameter, first the concept of how the order parameter arises as a consequence of the loss of stability of the symmetric solution, $\rho_0(x)$, should be discussed. The reasoning starts with steps analogous to those of Landau's symmetry analysis: consider a solution

$\rho(x, t)$ of Eq. (1). (Although the main interest is in the steady states of the system, i.e., in the stationary solutions, the time dependence of ρ will be needed to investigate the stability properties.) One expands $\rho(x, t)$ into a complete orthonormal set of functions. Under the transformations of G , these functions transform linearly among each other, i.e., they form a basis for a representation of G . After this representation is reduced, $\rho(x, t)$ can be written as

$$\rho(x, t) = \rho_0(x) + \sum_{n,i} C_i^{(n)}(t) \Phi_i^{(n)}(x), \quad (2)$$

where $\{\Phi_i^{(n)}(x), i = 1, \dots, m_n\}$ are the basis functions of the irreducible representation $\Gamma^{(n)}$ of G . Examples of $\Phi_i^{(n)}$ for two illustrative cases of symmetry breaking, discussed throughout the paper, are as follows.

Example A: Rotational symmetry is broken on the surface of a sphere; $\Phi_i^{(n)}$ are the spherical harmonics $Y_l^m(\theta, \varphi)$ with the correspondence $l \leftrightarrow n$ and $m \leftrightarrow i$.

Example B: Breakdown of translational and rotational symmetries; plane waves of fixed wavelength form the basis of an irreducible representation; $\Phi_i^{(n)}$ correspond to $e^{i \vec{k} \cdot \vec{x}}$ with $n \leftrightarrow |\vec{k}|$ and $i \leftrightarrow \vec{k} / |\vec{k}|$.

It should be noted that the physical quantity $\rho(x, t)$ is real so if $\Phi_i^{(n)}$ are complex, which is the general case, there are constraints among the complex coefficients $C_i^{(n)}$ in Eq. (2).

Having introduced the expansion of $\rho(x, t)$, the system is described by the variables $\{C_i^{(n)}\}$ and their equations of motion can be obtained by substituting Eq. (2) into Eq. (1) and re-expanding the right-hand side into $\{\Phi_i^{(n)}\}$. The result is an infinite set of ordinary differential equations:

$$\dot{C}_i^{(n)} = \omega^{(n)}(\lambda) C_i^{(n)} + f_i^{(n)}(\{C_j^{(m)}\}, \lambda), \quad (3)$$

where the term linear in $C_i^{(n)}$ is separated for convenience; thus, $f_i^{(n)}$ is a sum of forms quadratic, cubic, etc., in the variables $C_j^{(m)}$.

The transformation properties of $C_i^{(n)}$ follow from the fact that under the transformations of group G the functions $\{\Phi_i^{(n)}, i = 1, \dots, m_n\}$ transform among each other according to the irreducible representation $\Gamma^{(n)}$. As is obvious from Eq. (2), these transformations can be regarded as if not the functions $\Phi_i^{(n)}$ but the coefficients $C_i^{(n)}$ were transformed. Taking this view, one concludes that $\{C_i^{(n)}, i = 1, \dots, m_n\}$ transform according to $\Gamma^{(n)}$. Furthermore, the way Eq. (3) is constructed implies that the transformation properties of

$f_i^{(n)}$ and $C_i^{(n)}$ are the same.

Since Eq. (1) and consequently Eq. (3) are covariant with respect to the transformations of group $G \subseteq G'$, the coefficient of the linear term, $\omega^{(n)}(\lambda)$, in Eq. (3) is independent of i (Schur's lemma). This means that in the particular case of spherical symmetry (example A) ω is independent of the "magnetic index" m , while in example B ω depends only on $|\vec{k}|$.

Additional information about $\omega^{(n)}(\lambda)$ follows from the stability properties of $\rho_0(x)$. For $\lambda < \lambda_c$, $\rho_0(x)$ is stable against infinitesimal perturbations, i.e., a perturbation $\delta\rho(x,t) = \sum C_i^{(n)}\Phi_i^{(n)}$ will die out provided the $C_i^{(n)}$'s are sufficiently small, implying $\text{Re}\omega^{(n)}(\lambda < \lambda_c) < 0$ for all n . The loss of stability of $\rho_0(x)$ means that $\text{Re}\omega^{(n)}$ changes sign at λ_c for some $n=s$ and so $\text{Re}\omega^{(s)}(\lambda \gtrsim \lambda_c) > 0$. The corresponding $C_i^{(s)}$'s transforming according to $\Gamma^{(s)}$ grow in a general perturbation, $\delta\rho$, and a new stationary state with nonzero $C_i^{(s)}$ appears. Of course, to have a *symmetry breaking instability*, $\Gamma^{(s)}$ should not be the identity representation.

Expanding $\omega^{(s)}(\lambda)$ near λ_c , we have

$$\omega^{(s)}(\lambda) = a^{(s)}(\lambda - \lambda_c), \quad (4)$$

where $\text{Re}a^{(s)} > 0$ and the vanishing of $\text{Im}\omega^{(s)}(\lambda_c)$ is the consequence of considering the formation of time-independent patterns only (soft-mode instabilities).

In special cases, it might happen that $\text{Re}\omega^{(s)}(\lambda \gtrsim \lambda_c) > 0$ for several $s = n_1, \dots, n_q$. If none of $\Gamma^{(s)}$ is the identity representation, all of our forthcoming conclusions apply to those cases as well.

The modes described by $C_i^{(s)}$ exhibit critical slowing down. This leads to an enormous reduction in the effective degrees of freedom since the slow modes govern the time evolution of the rapidly relaxing variables $C_i^{(r)}$, $r \neq s$, thus making possible the adiabatic elimination of the fast modes near the instability point.² The amplitudes of the slow modes obey an equation similar to Eq. (3) but with new nonlinear terms containing only the slow variables:

$$\dot{\vec{u}} = \omega(\lambda)\vec{u} + \vec{g}(\vec{u}), \quad (5)$$

where the notation $\vec{u} = \{C_1^{(s)}, C_2^{(s)}, \dots, C_{m_s}^{(s)}\}$, $\omega(\lambda) = \omega^{(s)}(\lambda)$ has been introduced. The nonlinear terms, $\vec{g}(\vec{u})$, are generally smooth functions of λ , therefore their λ dependence has been neglected.

Since Eq. (5) completely specifies the behavior of the system near λ_c , including the symmetry prop-

erties of the stationary states, the amplitudes of the slow modes $\{C_i^{(s)}\} = \vec{u}$ are together called the order parameter of the system. The number of components of the order parameter is given by the dimension m_s of $\Gamma^{(s)}$ provided $\Gamma^{(s)}$ is real. If it is complex then, due to the constraint of $\rho(x,t)$ being real, the dimension of the physically irreducible representation is $2m_s$ and so the order parameter is specified by $2m_s$ real parameters. For example, if the spherical symmetry is broken (example A) and the unstable mode is associated with the irreducible representation $\Gamma^{(l)}$, the order parameter has $2l + 1$ real components. The breakdown of rotational and translational symmetries (example B) is exotic in the sense that the number of components of the order parameter is infinite although the unstable modes are associated with one irreducible representation.^{6,21}

Having reduced the original problem [Eq. (1)] to the equation of motion for the order parameter [Eq. (5)], it is now possible to connect the symmetry and stability properties of the stationary solutions.

III. SYMMETRIES AND THE STABILITY OF STEADY STATES

At the instability point, the symmetric solution ($\vec{u} = 0$) bifurcates into stationary solutions of lower symmetry ($\vec{u} \neq 0$). For the corresponding transition to be of second order, the order parameter must be continuous in the stationary state realized by the system. Then, sufficiently close to λ_c , the order parameter can be made arbitrarily small and it is enough to consider Eq. (5) and keep the lowest-order nonlinear term. Doing so, one finds stationary solutions with continuously varying order parameter but the conclusion about the order of the transition does not follow yet. The stability properties are to be investigated: if all the stationary solutions are found to be unstable then the transition cannot be of second order since the fluctuations, always present in reality, drive the system out of the unstable state into a stable state and a jump in the order parameter occurs (i.e., the transition is of first order).

One would expect that the actual physical situation (coupling constants) play an important role in determining the stability of the stationary solutions. There is an exception, however, when general conclusions can be drawn about the stability properties without recourse to the physical parameters. This case is the simplest in the sense that the

lowest-order nonvanishing nonlinear term is quadratic, i.e., the equation of motion to leading order is given by

$$\dot{\vec{u}} = \omega(\lambda)\vec{u} + \vec{B}(\vec{u}, \vec{u}), \quad (6)$$

where $\vec{B}(\vec{u}, \vec{u})$ is a set of forms quadratic in the components of the order parameter. Of course, \vec{B} transforms according to the same representation as \vec{u} . We shall find a first-order transition in this case, i.e., we conclude that a transition can be of second order only if the symmetry of the order parameter excludes the existence of a quadratic term in the equation of motion, Eq. (5).

In order to prove that Eq. (6) leads to a first-order transition, consider an arbitrary stationary solution \vec{w} :

$$0 = \omega(\lambda)\vec{w} + \vec{B}(\vec{w}, \vec{w}). \quad (7)$$

To investigate the stability of this solution, one must linearize Eq. (6) around \vec{w} and calculate the eigenfrequencies of the system. If at least one of them has a positive real part, the solution is unstable.

The eigenfrequencies are determined as the eigenvalues of the Jacobian matrix \hat{J} formed from the partial derivatives of the right-hand side of Eq. (6) taken at \vec{w} . The action of \hat{J} on an arbitrary vector $\vec{v} = \{v_1, v_2, \dots, v_{m_s}\}$, having the same transformation properties as \vec{u} , is easily shown to be

$$\hat{J}\vec{v} = \omega(\lambda)\vec{v} + 2\vec{B}(\vec{w}, \vec{v}). \quad (8)$$

The instability of \vec{w} for $\lambda > \lambda_c$ follows immediately from Eq. (8). Since the trace of \hat{J} is invariant under the transformations of group G , it can be written as

$$\text{Tr}\hat{J} = m_s \omega(\lambda). \quad (9)$$

The contribution of \vec{B} into $\text{Tr}\hat{J}$ vanishes because the possible terms would be linear in \vec{w} and it is well known that no linear invariant can be formed from quantities which transform according to an irreducible representation of a group.

Since $\text{Re}\omega(\lambda) > 0$ for $\lambda > \lambda_c$, the eigenvalues, q_i , of \hat{J} satisfy the following inequality

$$\text{Re}\text{Tr}\hat{J} = \sum_i \text{Re}q_i > 0. \quad (10)$$

Thus at least one of the eigenvalues of \hat{J} has a positive real part, i.e., we have shown that all stationary solutions \vec{w} are unstable for $\lambda > \lambda_c$.

For completeness we also prove that all the non-

trivial ($\vec{w} \neq 0$) stationary solutions of Eq. (6) are unstable below λ_c as well. Setting $\vec{v} = \vec{w}$ in Eq. (8) and using Eq. (7), one can see that \vec{w} is an eigenvector of \hat{J} ,

$$\hat{J}\vec{w} = -\omega(\lambda)\vec{w}, \quad (11)$$

with the eigenvalue $q_1 = -\omega(\lambda)$. For $\lambda < \lambda_c$, we have $\text{Re}q_1 = -\text{Re}\omega(\lambda) > 0$ hence the above statement follows.

As it has been discussed, the order parameter might be more complicated; several modes belonging to different representations might become unstable at λ_c [$\text{Re}\omega^{(s)}(\lambda \geq \lambda_c) > 0$ for $s = n_1, \dots, n_q$]. If none of the modes transform according to the identity representation, the trace of the corresponding Jacobian matrix can again be calculated easily since the terms linear in the components of the order parameter vanish:

$$\text{Tr}\hat{J} = \sum_{s=n_1}^{n_q} m_s \omega^{(s)}(\lambda). \quad (12)$$

Then the inequality $\text{Re}\text{Tr}\hat{J} > 0$ follows for $\lambda > \lambda_c$ thus implying that all stationary states are unstable above λ_c . This conclusion does not change if one of the slow modes is marginal [$\omega^{(m)}(\lambda) \equiv 0$] since its contribution to $\text{Tr}\hat{J}$ is zero and the positivity of $\text{Re}\text{Tr}\hat{J}$ is ensured by the unstable modes.

Thus the above Landau-type symmetry analysis is summarized in the following rule. A transition with unstable and marginal modes transforming according to a representation Γ of G can be of second order only if there is no quadratic form constructed from the amplitudes of the slow modes, which would transform according to the same representation Γ .

The group-theoretical formulation of this condition is that the symmetric square of Γ should not contain Γ itself.

Yet another way of describing this condition follows from realizing that, if $\vec{B}(\vec{u}, \vec{u})$ and \vec{u} transform according to Γ , then their scalar product $\langle \vec{u}, \vec{B}(\vec{u}, \vec{u}) \rangle$ is an invariant under the transformations of group G and, reversely, a quadratic form transforming like \vec{u} can always be derived from a cubic invariant. Thus the transition is necessarily a first-order one if a cubic invariant can be constructed from the components of the slow modes.

The existence of the invariant $\langle \vec{u}, \vec{B}(\vec{u}, \vec{u}) \rangle$ does not mean that the equation of motion [Eq. (6)] possesses a gradient structure. If, however, the tri-

linear form $\langle \vec{u}, \vec{B}(\vec{u}', \vec{u}'') \rangle$ is completely symmetric in \vec{u}, \vec{u}' , and \vec{u}'' , then Eq. (6) is derivable from a potential and the above rule is entirely analogous with that of Landau worked out for the equilibrium phase transitions. The complete symmetry of the trilinear form is ensured if the order parameter transforms according to an *irreducible* representation of a *simple reducible* group.²² This case has been investigated in detail by Sattinger.²⁰ His results concerning the order of the transitions are in agreement with the predictions following from our rule.

There are, of course, limits to the validity of the above results. First, even if the symmetry of the slow modes would permit its presence, the quadratic form in Eq. (6) might vanish due to special physical circumstances (an example is the convective instability in a Boussinesq fluid²¹). Secondly, the starting point of our symmetry analysis, Eq. (5), was obtained by neglecting all the fluctuations of the unstable modes. Fluctuations might, in principle, change a transition first order by symmetry, into a second-order one. We believe, however, that this happens rarely as in the case of equilibrium phase transitions.^{15,16}

Finally, two remarks are in order.

First, we have tacitly assumed that every irreducible representation appears only once in the expansion of $\rho(x, t)$ [Eq. (2)]. If this was not the case, the linear parts of the equations for $C_i^{(n)}$ and $\tilde{C}_i^{(n)}$, both transforming according to $\Gamma^{(n)}$, would couple to each other and then an equation similar to Eq. (3) could be obtained only after a diagonalization procedure. From that point on, however, the argumentation and the final result is unchanged.

Second, $\rho(x, t)$ might have several components, $\rho_\alpha(x, t)$, some of them being scalars while others transforming like the components of a vector or a tensor. Then the expansion Eq. (2) must be viewed as an expansion for every component. The coefficients $C_i^{(n)}$ acquire a suffix α and the $C_{i\alpha}^{(n)}$'s transform according to $\Gamma^{(n)}$ in the suffix i , while they transform according to some other representation $\tilde{\Gamma}$ of G in the suffix α . The reduction of the direct-product representation $\Gamma^{(n)} \times \tilde{\Gamma}$ is extra work but otherwise the reasoning is not changed and our results apply to the case of many component $\rho(x, t)$ as well.

IV. DISCUSSION

As an application of the rule developed above, we discuss now the two examples of Sec. II.

A. Broken rotational symmetry on the surface of a sphere

Cubic invariants can only be constructed from quantities transforming according to the irreducible representation $\Gamma^{(l)}$ with l even.²⁰ Thus non-equilibrium phase transitions occurring on spherical surfaces (morphogenesis, Marangoni effect, buckling of a sphere, chemical reactions, etc.) are always of first order if there are modes among the unstable and marginal ones which transform according to $\Gamma^{(l)}$ with $l=2k$.

This is a generalization of Sattinger's result²⁰ since we allow instabilities with slow modes transforming according to a reducible representation. The growth of a spherical crystal provides a typical example⁹: the first instability is connected with the $l=2$ mode but the marginal $l=1$ mode should be also included in the analysis. As a consequence, the existence of a potential is not *a priori* ensured. Actually, an explicit nonlinear analysis shows²³ that, treating the $l=1$ and $l=2$ modes on equal footing, the equation of motion for the slow modes does not possess a gradient structure. Nevertheless, our rule can be applied and the prediction is that the new shape growing out of a spherical crystal appears through a first-order transition.

B. Translational and rotational symmetry is broken (Ref. 24)

In all known cases, the instabilities are associated with *one* critical wave number q_c and, consequently, with one irreducible representation $\Gamma^{(q_c)}$. The components of the order parameter $C_{\vec{q}}, |\vec{q}| = q_c$ transform among each other like plane waves of fixed wavelength. Third-order invariants are easily constructed from such quantities: the only condition is that the wave vectors $\vec{q}_1, \vec{q}_2, \vec{q}_3$ ($|\vec{q}_i| = q_c$) should form an equilateral triangle. Thus the formation of spatial patterns in a homogeneous and isotropic system is expected, in general, to be a first-order transition.

Even the pattern of the new steady state can be predicted if the transition is only weakly first order (there is only a small jump in the order parameter). As it can be easily shown, the equation of motion for C_q [Eq. (6)] can be derived from a potential. Then, one repeats the argument by Alexander and McTague²⁵ about the minimalization of the third-order term in the potential to arrive at the result that the transition is into a body-centered cubic

structure in three dimensions, while hexagonal pattern is selected in the two-dimensional case. These results are in agreement with finding obtained for special systems.^{2,6} It should be added that potential exists also in example A, provided the order parameter is associated with one irreducible representation $\Gamma^{(l)}$ with l even.²⁰ This case has been investigated in detail by Busse²⁶ who found that an axisymmetric and a cubic pattern is selected for $l=2$ and $l=4$, respectively, while for $l=6$ the symmetry of the preferred state is that of an icosa-

hedron.

As a summary, we can say that although the nonequilibrium phase transitions are much more complicated than the equilibrium ones, a Landau-type analysis is equally useful in both cases.

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- ²²A group is simple reducible if (a) every element is equivalent to its inverse (i.e., for every p there is an h such that $p=hp^{-1}h$) and (b) the tensor product of any two irreducible representations contains no irreducible representation more than once. Examples of the simple reducible groups are the three-dimensional rotation group, most of the crystal point groups, etc. See, e.g., M. Hamermesh, *Group Theory and Its Application to Physical Problems* (Addison-Wesley, Reading, Mass., 1962).
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