Wave number selection in convection and related problems

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The wave number selection process induced by grain boundaries is studied beyond the framework of amplitude equations. It is shown that the process is an intrinsic property of the problem, being associated with its spatial symmetry. The process always results in discretization of possible values of the wave number. If the control parameter is small enough (so that pinning of the grain boundary to the small scale underlying structure may be neglected) the system possesses an extra restricting condition: the Lyapunov functional density for both coexisting structures must coincide. In this case the selected wave number provides a local minimum of the Lyapunov functional for the spatially uniform patterns. As an application of the theory we consider an extended Swift-Hohenberg equation for rolls with subcritical bifurcation.

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The range of experimentally observed wave numbers for spatially periodic patterns in extended dissipative systems with large aspect ratios usually is much narrower than that given by the corresponding standard stability theory (see, e.g., Ref. [1] and references therein). A possible explanation of this fact is the existence of a wave-number selection process induced by spatial inhomogeneities of the system such as side walls [2], spatial variation of the control parameter (ramp) [3], dislocations [4], etc. The wave number selection in each case is associated with the particular formulation of the problem, and/or with the approximation used.

On the other hand, in the case of bistable or multistable systems, we may expect the existence of domains (grains) occupied by different patterns. The domains are separated by grain boundaries (GB's) which can also induce wave number selection [5]. Up to now GB's have generally been considered to the lowest order in the amplitude equation approach [6]. It has been shown that for gradient systems a necessary condition for the existence of steady GB's is the coincidence of densities of the Lyapunov functional for both coexisting patterns [7]. The wave number selected is unique, and equals its critical value providing the minimum of the Lyapunov functional [5]. However, it is unclear whether these results are an intrinsic property of the problem or just a consequence of the approximation used. The goal of the present paper is to answer this question in the case of one-dimensional potential systems.

Let us consider a system with a real (generally speaking multicomponent) order parameter $u(x,t)$, whose time evolution is governed by the gradient equation

$$\frac{\partial u}{\partial t}=-\frac{\delta \mathcal{L}}{\delta u}, \tag{1}$$

where

$$\mathcal{L}=\int L(\varepsilon,u,u_x,u_{xx},\ldots)dx \tag{2}$$

is the Lyapunov functional and ε is a control parameter. Note that here L does not explicitly depend on x.

The system is assumed to be bistable or multistable, such that within the considered range of control parameter variations problem (1) has several qualitatively different types of *locally* stable steady solutions (see, e.g., Ref. [8]). We will study the steady GB's matching two of them. The problem is described by the stationary version of Eq. (1), i.e., with the Euler-Lagrange equation

$$\frac{\delta \mathcal{L}}{\delta u}=0 \tag{3}$$

together with the boundary conditions:

$$u \to u_-(x) \text{ at } x \to -\infty\ , \tag{4}$$

$$u \to u_+(x) \text{ at } x \to +\infty\ , \tag{5}$$

where the functions $u_\pm(x)$ describe spatially homogeneous coexisting patterns.

Note that Eq. (3) coincides with the equation of motion for a dynamical system if L is interpreted as the Lagrangian, u as spatial coordinates, and x as time. If L depends on u_{xx}, and/or higher derivatives, such a "dynamical system" is rather unusual because its dynamic equations contain fourth, or even higher, derivatives with respect to "time" x. Nevertheless, as already mentioned in Ref. [7], the independence of the Lagrangian L from x gives us an opportunity to apply Noether's theorem that provides the existence of the "energy" integral, i.e., a quantity $E(u,u_x,u_{xx},\ldots)$ which is invariant along the trajectory determined by problems (3)–(5).

In particular, when L depends only on u, u_x, and u_{xx}, the energy integral has the following form:

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$$E=L-u_x\frac{\partial L}{\partial u_x}-u_{xx}\frac{\partial L}{\partial u_{xx}}+u_x\frac{d}{dx}\frac{\partial L}{\partial u_{xx}} . \quad (6)$$

Taking into account dynamic equation (3), it is straightforward to see that $dE/dx=0$.

The energy integral is the only *exact* conserved quantity of the system. If the spatially uniform patterns at $x\rightarrow\pm\infty$ belong to different continuous families of steady solutions of the problem, one extra condition $E=\text{const}$ is not enough to provide either selection of unique wave number for the coexisting patterns or the equality

$$\bar{L}(-\infty)=\bar{L}(+\infty) , \quad (7)$$

where the bar denotes averaging over the periods of spatial oscillations for the functions $u_\pm(x)$.

However, law (7) can be obtained as an *approximate* law if the characteristic spatial scale of GB's (macroscale) is large in comparison with the scale of underlying spatially periodic patterns (microscale). In this case use of Whitham's method [9], i.e., averaging the Lagrangian L over rapid spatial oscillations, yields a new quantity $\bar{L}(\varepsilon, A, A_X, A_{XX}, \ldots)$, where A stands for the envelope of $u(x)$, and X is a new slow-varying coordinate. The averaging does not break the symmetry of the problem. Therefore the evolution equation for the envelope also must have an energy integral similar to that given by Eq. (6), where L should be replaced by $\bar{L}$, u by A, and x by X. However, now the boundary conditions for the envelope demand that

$$A_X\rightarrow 0 \text{ at } X\rightarrow\pm\infty . \quad (8)$$

which ensures condition (7); see Eq. (6).

The physics of this result is clear: Two patterns with different values of $\bar{L}$ may coexist matched by a steady GB, only if the GB is trapped by pinning effects [5,7,8]. If at a certain approximation the equation for the envelope can be derived in a closed form, being independent of local characteristics of the small scale underlying structure, this means that pinning effects are neglected, which immediately excludes any possibility of equilibrium if $\bar{L}(-\infty)\neq\bar{L}(+\infty)$.

Let us illustrate these general speculations considering as a particular example the extended Swift-Hohenberg equation with subcritical bifurcation proposed in Ref. [8]:

$$\frac{\partial u}{\partial t}=\left[\varepsilon-\left[1+\frac{\partial^2}{\partial x^2}\right]^2\right]u+\mu u^3-u^5 , \quad (9)$$

where ε and μ are two control parameters: $\varepsilon<0$ and $|\varepsilon|\sim\mu^2\ll 1$. The Lagrangian for Eq. (9) is

$$L=-u_x^2+\tfrac{1}{2}u_{xx}^2-\frac{\varepsilon-1}{2}u^2-\frac{\mu}{4}u^4+\frac{u^6}{6} . \quad (10)$$

Then the energy integral may be written as

$$E=u_x^2-\tfrac{1}{2}u_{xx}^2+u_xu_{xxx}-\frac{\varepsilon-1}{2}u^2-\frac{\mu}{4}u^4+\frac{u^6}{6} . \quad (11)$$

Equation (9) has *locally* stable steady solutions of two different types—the trivial state $u\equiv 0$ and the family of spatially periodic states [8]:

$$u(x)=\sqrt{\mu}[u_0\cos kx+\mu^2u_1\cos 3kx+\cdots] , \quad (12)$$

where

$$u_0^2\simeq\frac{3}{5}\left\{1+\left[1+\nu\left[1-\frac{(1-k^2)^2}{\varepsilon}\right]\right]^{1/2}\right\} \quad (13)$$

and $\nu\equiv 40\varepsilon/9\mu^2$ $(-1\leq\nu<0)$.

In the case under consideration $(-1\leq\nu<0)$ in four-dimensional phase space for the steady $(\partial u/\partial t=0)$ version of Eq. (9), the GB corresponds to a heteroclinic orbit matching the fixed point $u\equiv 0$ (a focus with two stable and two unstable manifolds) with the periodic solution belonging to the family (12). The existence of the energy integral (11) means that the phase space is stratified by a family of three-dimensional hyperplanes $E=\text{const}$ and any phase trajectory, including the heteroclinic orbit, lays completely on the corresponding three-dimensional hyperplane.

In what follows μ is considered a fixed small parameter. In this case the family (12) is parametrized by two independent quantities ν (or ε) and k, i.e., at a fixed ν we still have a band of wave numbers k $(|1-k|\sim\mu)$. The heteroclinic orbit belongs to the isoenergetic surface $E=0$. This condition selects from the band a discrete number of k $[k=k_j(\nu)]$. Note that ν is still a *free parameter* of the problem. The pinning effect allows freedom for its variation within the exponentially narrow domain [8]:

$$|\nu-\nu_c|\leq\tfrac{3}{8}\alpha^{3/2}e^{-\alpha} \quad (14)$$

(here $\alpha\equiv 2\pi|\varepsilon|^{-1/2}$, $\nu_c=-\frac{3}{4}$ *with a corresponding variation of the selected wave numbers.*

Let us now find the selected wave numbers in the explicit form. We start from the amplitude equation. In the lowest approximation, we take

$$u\simeq\frac{1}{2}\left[\frac{3\mu\zeta}{5}\right]^{1/2}(Ae^{ix}+\text{c.c.}) , \quad (15)$$

where $\zeta\equiv\nu+\sqrt{1+\nu}$. The slow-varying amplitude A depends on slow variables $X\equiv(\varepsilon/\nu)^{1/2}x/2$, $T\equiv\varepsilon t/\nu$. Setting expression (15) into Eq. (9) and neglecting higher-order terms in the leading approximation, we obtain the generalized Ginzburg-Landau equation

$$A_T=A_{XX}+(1-|A|^2)(\nu+\zeta^2|A|^2)A , \quad (16)$$

that may be written in the equivalent form of two coupled equations:

$$R_T=R_{XX}-R\varphi_X^2+(1-R^2)(\nu+\zeta^2R^2)R , \quad (17)$$

$$\varphi_T=\frac{1}{R^2}(R^2\varphi_X)_X , \quad (18)$$

with

$$A=\text{R}e^{i\varphi} . \quad (19)$$

Equation (16), or equivalently, Eqs. (17) and (18), have the trivial solution $A\equiv 0$ and a family of *exact* spatially periodic solutions of the following form:

$$\varphi_X = K = \text{const} , \quad (20)$$

$$R^2 = \frac{1 \pm \sqrt{1+\nu-K^2}}{\zeta} , \quad (21)$$

which are reduced to Eqs. (12) and (13) by the transformation

$$K^2 = \frac{4\nu(k-1)^2}{\varepsilon} , \quad R^2 = \frac{5u_0^2}{3\zeta} . \quad (22)$$

It is straightforward to see from Eq. (16) that the trivial solution $A \equiv 0$ is locally stable. As for the family (20)–(21), the linear stability analysis shows that the stable solutions correspond to the upper sign in Eq. (21), cf. Eq. (13), and K must be smaller than a certain limit:

$$K^2 \le K_E^2 \equiv \frac{1}{2}\left[\frac{3}{4} + \nu + \left[\frac{9}{16} + \frac{\nu}{2}\right]^{1/2}\right] < 1 + \nu , \quad (23)$$

with $-1 < \nu < 0$.

Note that contrary to Eq. (9), Eqs. (17) and (18) now have *two* first integrals: In addition to the "energy" conservation, we also have another invariant quantity, the angular momentum

$$M = R^2 \varphi_X , \quad (24)$$

as it occurs with the conventional Ginzburg-Landau equation; see, e.g., Ref. [10].

Taking into account that, for the trivial state ($A \equiv 0$), M vanishes, we immediately obtain the wave number selection law: The only spatially periodic state that may coexist with the trivial one matched by the steady GB is the state with $K = 0$, i.e., with $k = 1$; see Eq. (22). On the other hand, at $K = 0$ condition $E(A, A^*) = 0$, together with Eqs. (13), (19), (21), and (22), selects the unique value of the control parameter $\nu = \nu_c = -\frac{3}{4}$; cf. Eq. (14).

Thus, within the framework of Eq. (16), the wave-number selection law is a consequence of the angular momentum conservation. In its turn this conservation law follows from the symmetry of Eq. (16) and the corresponding Lagrangian with respect to an arbitrary rotation in complex plane (the transformation $A \to Ae^{i\varphi}$, $\varphi = \text{const}$). But this symmetry is a *specific* symmetry of the approximation used. The initial problem does not possess this symmetry and has only one first integral; see Eqs. (9) and (11). For this reason the possibility of the wave number selection law obtained beyond the framework of the Ginzburg-Landau equation (16) is worth exploring.

To do so let us consider the quantity $\bar{L}$, where L is given by Eq. (10). As mentioned earlier, neglecting pinning effects, i.e., within the exponential accuracy of $|\varepsilon|^{-1/2}$ [see Eq. (14)], we have that $\bar{L}$ of a spatially periodic state ($\bar{L}_{\text{sp}}$) must be equal to $\bar{L}$ of the trivial state, i.e., to zero. Together with the condition $E = 0$, this yields

$$\nu = \nu_c , \quad (25a)$$

$$\overline{u_x^2} = \overline{u_{xx}^2} . \quad (25b)$$

Setting Eq. (12) into Eqs. (25), and taking into account that $k + 1 \simeq 2$, we obtain the wave number selection law

$$k_s = 1 - \frac{36u_1^2}{u_0^2}\mu^4 + O(\mu^8) . \quad (26)$$

Being an amplitude of a slaved mode, the quantity u_1 may be expressed using u_0:

$$u_1 \simeq -\tfrac{1}{256}(\tfrac{5}{4}u_0^2 - 1)u_0^3 . \quad (27)$$

Finally, the value of u_0 is fixed by the condition $\nu = \nu_c \equiv -\frac{3}{4}$, see Eq. (13). Then we obtain

$$k_s - 1 \simeq -\frac{1}{2^{16}5^2}(\tfrac{3}{2})^6\mu^4 \simeq -6.9 \times 10^{-6}\,\mu^4 . \quad (28)$$

Note that the departure of the selected wave number from the value $k = 1$ is extremely small—a fourth power of the small parameter μ together with a rather small numerical coefficient.

Let us prove now that k_s selected by the conditions $E = 0$ and $\bar{L}_{\text{sp}} = 0$ provides a local minimum of $\bar{L}_{\text{sp}}$ at arbitrary μ. To do this, we write a formal solution of Eq. (9) in the form

$$u = \sum_{-\infty}^{\infty} U_n \exp(inkx) , \quad (29)$$

$$U_n^* = U_{-n} , \quad n = \pm 1, \pm 3, \ldots . \quad (30)$$

That gives the following expression for $\bar{L}_{\text{sp}}$:

$$\bar{L}_{\text{sp}} = -\tfrac{1}{2}\sum[\varepsilon - (1 - n^2k^2)^2]|U_n|^2 + F(U_{\pm 1}, U_{\pm 3}, \ldots, U_{\pm n}, \ldots) , \quad (31)$$

where the quantity F does not depend explicitly on k. For the uniform spatially periodic solution, the Euler-Lagrange equation (3) now transforms into the set of equations

$$\frac{\partial \bar{L}_{\text{sp}}}{\partial U_n} = 0 . \quad (32)$$

In this case

$$\frac{d\bar{L}_{\text{sp}}}{dk} = \frac{\partial \bar{L}_{\text{sp}}}{\partial k} + \sum \frac{\partial \bar{L}_{\text{sp}}}{\partial U_n}\frac{dU_n}{dk} = \frac{\partial \bar{L}_{\text{sp}}}{\partial k} = -2k\sum n^2(1 - n^2k^2)|U_n|^2 . \quad (33)$$

On the other hand, for any uniform, spatially periodic solution the quantity $E \equiv \bar{E}$ may be expressed by $\bar{L}_{\text{sp}}$ according to the relation [see Eqs. (10) and (11)]:

$$E = \bar{L}_{\text{sp}} + 2(\overline{u_x^2} - \overline{u_{xx}^2}) . \quad (34)$$

which, using Eqs. (29), (30), and (33), becomes

$$E = \bar{L}_{\text{sp}} - k\frac{d\bar{L}_{\text{sp}}}{dk} , \quad (35)$$

Thus conditions $E = \bar{L}_{\text{sp}} = 0$ result in the vanishing of $d\bar{L}_{\text{sp}}/dk$ at any $k_s \neq 0$. At $k_s = 0$ the same conclusion follows from the continuity of the dependence of this quantity on the parameters of the problem.

Finally, taking into account that $E = \bar{L}_{\text{sp}} =$

$d\bar{L}_{sp}/dk=0$ at $k=k_s$, and differentiating Eq. (33) with respect to k, we obtain

$$\frac{d^2\bar{L}_{sp}}{dk^2}=\frac{\partial^2\bar{L}_{sp}}{\partial k^2}$$

$$=-2\sum n^2(1-n^2k^2)|U_n|^2+4k^2\sum n^4|U_n|^2$$

$$=4k^2\sum n^4|U_n|^2>0 \quad (36)$$

at $k=k_s$, as expected.

Let us summarize the main results obtained for the model considered:

(1) Steady GB existence gives rise to a strict wave number selection law: at small μ a unique value of k corresponds to each value of ε.

(2) The wave number selection law is an intrinsic property of the problem, and a consequence of its symmetry associated with existence of a Noether invariant.

(3) Neglect of pinning effects results in the additional condition $\bar{L}_{sp}=0$, which fixes the unique value of the control parameter $\varepsilon=\varepsilon_c$. In this case the selected wave number provides a local minimum of $\bar{L}_{sp}$.

(4) Pinning brings about a finite domain of possible values of the control parameter related to a steady GB. Inside this domain ε and k_s are in one-to-one correspondence. Any variation of ε must induce wave-number alteration starting from the creation or annihilation of rolls at GB's with further relaxation of the perturbation by the phase-diffusion mechanism in accordance with the scenario proposed by Pomeau [7]. However, the wave number selected by this process does not minimize $\bar{L}_{sp}$ for any $\varepsilon\neq\varepsilon_c$.

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