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Layered structures in twodimensional nonequilibrium systems

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Résumé. — Le rôle des défauts dans les structures bidimensionnelles en rouleaux est analysé. On montre que la fusion de ces structures à grandes amplitudes peut être interprétée en termes de solitons.

Abstract. — The role of the defects in twodimensional layered structures is analysed. It is shown that the melting of these structures at large amplitudes can be understood within a soliton picture.

Many instabilities lead to twodimensional layered *dissipative structures* [1] such as for instance the Rayleigh-Bénard instability [2] and the convective instabilities in nematic liquid crystals [3]. It has been suggested that when one decreases the bifurcation parameter a Kosterlitz-Thouless type melting may occur. However, these structures also vanish when one increases the constraint (contrary to the equilibrium situation where perfect rigidity is reached for $T = 0$). We here want to study these two possible transitions leading to the destruction of the layered pattern. It is well known that these structures can be described in terms of a Landau type generalized potential for the order parameter $\sigma(\mathbf{r})$ [4, 5, 6] :

$$\sigma(\mathbf{r}) = R \cos(qz + \varphi(\mathbf{r})). \quad (1)$$

In the convecting region, we may ignore the amplitude fluctuations and take $R = R_0 \simeq [(\lambda - \lambda_c)/\lambda_c]^{1/2}$. Here λ is the bifurcation parameter, λ_c the mean-field critical point and $2\pi/q_c$ the critical wavelength. The potential for the phase fluctuations which dominate at long wavelengths may then be written

$$V = \frac{1}{T} \int dx \int dz \left\{ \left[\frac{D_{\parallel}}{2} \left(\frac{\partial \varphi}{\partial z} \right)^2 + \frac{D_{\perp}}{2} \left(\frac{\partial \varphi}{\partial x} \right)^2 + C \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial z^2} \right)^2 \right] + u R_0^4 \cos[2(qz + \varphi)] \right\} \quad (2)$$

where

$$\begin{aligned} D_{\parallel} &= 2[4 D q^2 R_0^2 + 2 D R_0^2 (q^2 - q_c^2)] \\ D_{\perp} &= 4 D R_0^2 (q^2 - q_c^2) + E \\ C &= D R_0^2 \end{aligned} \quad (3)$$

with

$$D \propto q_c^{-2}$$

and u depends on the specific parameters of the problem.

The field E tends to orient the layers perpendicularly to the z axis. It mimics the anisotropies which raise the orientational degeneracy of the structure in many convective instabilities. Moreover an experimental study of the diffusive phase behaviour in the case of Rayleigh-Bénard shows that $D_{\parallel} \gg D_{\perp}$ [7]. The first part of the functional (2) favours layered structures with small phase variations, while the second which models the contribution of the harmonics generated by the nonlinearities [8] only becomes important for high amplitudes ($\lambda \gg \lambda_c$) and favours homogeneous states.

A. We first consider small values of the bifurcation parameter when the first part of (2) dominates. The corresponding phase fluctuations destroy the translational order. The absence of true long range order shows up in the behaviour of the correlation function $C(\mathbf{r})$ for the order parameter $\Psi(\mathbf{r}) = R_0 \exp i\varphi(\mathbf{r})$. Indeed, in the ordered region we have at large distances [10] :

$$C(\mathbf{r}) = \langle \Psi(\mathbf{r}) \Psi^*(\mathbf{r}) \rangle \simeq \left(\frac{D_{\parallel}}{D_{\perp}} x^2 + z^2 \right)^{-\eta} \quad (4)$$

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where

$$\eta = \frac{\Gamma}{4\pi\sqrt{D_{\perp}D_{\parallel}}} \quad (5)$$

This algebraic decay is characteristic of quasi long range order [9], when $D_{\perp} = 0$, one recovers the exponential decay of the short range order [10, 4]. Following Kosterlitz and Thouless [11], one suspects that defects play an important role in the behaviour of large systems. The energy of an isolated dislocation embedded in a layered structure is given by

$$E_D \simeq \frac{m^2}{\Gamma q^2} \sqrt{D_{\parallel}D_{\perp}} \ln\left(\frac{L}{a}\right) \quad (6)$$

L is the size of the systems, a the core diameter and the charge m is defined by [4]

$$\oint \nabla\varphi \cdot d\mathbf{l} = m\left(\frac{2\pi}{q}\right). \quad (7)$$

The generalized potential for a neutral array of dislocations breaks into two parts $V = V_0 + V_D$ where V_0 is the regular part of (2) and

$$V_D = \frac{\pi}{2\Gamma q^2} \sum_{i,j} m_i m_j \sqrt{D_{\parallel}D_{\perp}} \ln \left[\frac{D_{\parallel}}{D_{\perp}} (x_i - x_j)^2 + (z_i - z_j)^2 \right] \quad (8)$$

for

$$|\mathbf{r}_i - \mathbf{r}_j| > b$$

where b is an estimation of the size of the region below which the effects of the second order curvature elasticity coefficient C become important.

As in the isotropic case ($D_{\parallel} = D_{\perp}$) the lowering of the bifurcation parameter could induce a phase transition due to the dislocation unbinding when [11] :

$$2 = K_d = \frac{\pi}{2\Gamma q^2} \sqrt{D_{\parallel}D_{\perp}} \simeq \sqrt{\frac{2\pi^2 DE}{\Gamma^2 q^2}} R_0.$$

For $K_d < 2$ the quasi long range translational order is destroyed and if $E < \Gamma q^2/\pi$, the remaining quasi long range orientational order (« biatic phase ») persists until $\pi C = \pi D R_0^2 = 2\Gamma$ where the disclinations unbind. When $E > \Gamma q^2/\pi$, one has the simultaneous unbinding of dislocations and disclination pairs at $K_d = 2$. The transitions to the homogeneous steady state then happen in a single step without biatic phase.

However for sufficiently small values of R_0 ($\lambda \rightarrow \lambda_c$) the amplitude correlation length $\xi = \sqrt{D/R_0}$ grows and eventually becomes of the order of the size of the region below which the phase fluctuations are unessential, this occurs when

$$\xi = L_m = q^{-1} \exp \sqrt{D_{\perp}D_{\parallel}}/2\Gamma.$$

In this case the separation between phase and amplitude is no more justified. If the dislocation mediated transition has not occurred when $\xi = L_m$, then the transition to the homogeneous state is driven by the amplitude fluctuations which obey a Landau-Hopf equation [12].

Whatever the mechanism of the transition, dislocations do appear in the layered structures. The coupling between these dislocations given by (8) implies that they should be nucleated by pairs of opposite Burger's vectors and the distance between these dislocations should increase essentially perpendicularly to the axis of the rolls leading to an increase of the characteristic wavelength in agreement with experiments on the convective structures in nematics [13].

B. When the bifurcation parameter increases, the amplitude of the pattern grows and the nonlinearities coming from the quartic term in (2) become important. By first neglecting the transverse phase fluctuations ($D_{\perp} \ll D_{\parallel}$), one obtains a potential similar to that describing the commensurate-incommensurate transition in solids [14, 15] :

$$F = \frac{K}{\Gamma} \int dx \int dz' \left[\frac{1}{2} \left(\frac{\partial \phi}{\partial z'} - h \right)^2 + \cos \phi \right] \quad (9)$$

where

$$h = \left(\frac{Dq^4}{4R_0^2} \right)^{1/2}, \quad K = \left(\frac{Dq^2 u R_0^6}{2} \right)^{1/2} \quad (10)$$

and

$$z' = 2qz/h \\ \phi = 2(qz + \varphi).$$

As discussed in various works [15] the minimum of this potential is given by the solution of the sine-Gordon equation which is the amplitude of the elliptic function of the first kind

$$\phi = 2am(z'/k + \xi) \quad (11)$$

where k is such that $hk = 4E(k)/\pi$; $E(k)$ is the complete elliptic function of the second kind and ξ an arbitrary constant. This solution only exists for

$$h > h_M = 4/\pi. \quad (12)$$

For $h \gg h_M$, the phase varies quasi linearly with z and the structure is layered with a well defined wavelength. When h decreases, regions appear where $\phi(z)$ is almost constant; between these regions the phase grows nearly like $\pi q/2 E(k)$ (see Fig. 1). The corresponding structure consists of layered domains separated by quasi homogeneous regions. These domains are regularly separated by a distance $l = 4E(k)K(k)/\pi q$ (where $K(k)$ is the first kind complete elliptic function). When h further decreases, the homogeneous regions become larger as l grows

Fig. 1. — Spatial variation of the phase perpendicular to the axis of the layers in the mean-field approximation (schematic).

and for $h \rightarrow h_M$ the phase becomes the one soliton solution of the sine-Gordon equation [13, 14]. There l behaves as $\ln(h - h_M)^{-1}$. When $h = h_M$ a continuous transition occurs to the homogeneous state $\phi = \pi/2$. It corresponds to the destruction of the layered structure at large values of the bifurcation parameter via the increase of the size of the homogeneous domains.

In this context the fluctuations also play an essential role and may deeply alter the preceding mean-field analysis. Writing $\phi(z)$ as $\phi(z - \theta(x, z))$ one obtains an additional term in the Ginzburg-Landau functional corresponding to the elastic deformation energy of the homogeneous regions lattice (soliton lattice)

$$V = F + \frac{D_{\parallel}}{2q^2\Gamma} \int dz \int dx \left(\frac{\partial \phi}{\partial z} \right)^2 \times \left[\left(\frac{\partial \theta}{\partial z} \right)^2 + \frac{D_{\perp}}{D_{\parallel}} \left(\frac{\partial \theta}{\partial x} \right)^2 \right]. \quad (13)$$

As usual θ may be decomposed into a regular part (« phasons ») the effect of which is to increase the value of h_M [16] and a singular part describing the topological defects.

For $h \gg h_M$, $(\partial \phi / \partial z)^2 \sim q^2$ which corresponds to

the situation described in the first part of this note as (13) directly leads to (8). When h decreases, larger and larger regions appear where $(\partial \phi / \partial z)^2$ also decreases and for $h \rightarrow h_M$ the one soliton form of ϕ induces

$$\frac{\partial \phi}{\partial z} \simeq \frac{\pi q}{2} \operatorname{sech} \pi q z. \quad (14)$$

As a consequence, in this regime, isolated dislocations may appear destroying the quasi long range order of the soliton lattice as the one dislocation contribution to V , given by

$$\frac{D_{\parallel} D_{\perp}}{2\Gamma} \cdot \frac{m^2}{q^4} \int dz \int dx \left(\frac{\partial \phi}{\partial z} \right)^2 \frac{1}{D_{\perp} z^2 + D_{\parallel} x^2} \quad (15)$$

remains finite even in infinitely extended systems. So before the mean-field transition point ($h = h_M$) is reached a dislocation mediated melting occurs ($h = h_T > h_M$).

Therefore in the present model the structure which is created at the critical value λ_c of the bifurcation parameter is periodic in one direction but with topological defects such as dislocation pairs. When the bifurcation parameter increases, a lattice of nearly homogeneous domains may form. Its wavelength (l) increases with λ and defects are also present up to a threshold where isolated dislocations may appear leading to the melting of the structure.

In most experiments a transition to a twodimensional pattern takes place before the melting of the rolls [3b, 17].

However, in view of the results of reference [3b], we expect a similar scenario to be of some relevance in the explanation of the melting of these 2D structures. Indeed, there also the size of the square like domains decreases progressively in favour of a homogeneous phase.

In this situation one should however take into account the intersection energy of the homogeneous walls. Work in this direction is in progress.

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