

## Elastic stability for a discotic liquid crystal in the hexatic N+6 phase

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys.: Condens. Matter 2 3061

(<http://iopscience.iop.org/0953-8984/2/13/016>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.96

The article was downloaded on 10/05/2010 at 22:00

Please note that [terms and conditions apply](#).

## Elastic stability for a discotic liquid crystal in the hexatic $N + 6$ phase

C Giannessi

Dipartimento di Fisica dell'Università di Pisa, Istituto Nazionale di Fisica Nucleare,  
Sezione di Pisa, Piazza Torricelli 2, 56100 Pisa, Italy

Received 17 May 1989, in final form 20 September 1989

**Abstract.** The elastic stability of a discotic liquid crystal in the theoretically predicted hexatic  $N + 6$  phase against fluctuations of orientational order is tested. For this purpose, we derive the elastic stability conditions for Frank constants of a discotic liquid crystal, and find that the coupling constant  $\gamma_3$ , which couples the director distortions to local rotations of the hexagonal two-dimensional lattice, is forced to be weak with respect to the other Frank constants, in order to preserve the long-range sixfold orientational order. We then show that critical enhancements of Frank elastic constants, in the hexatic  $N + 6$  phase near the supposed continuous transition to the hexagonal discotic phase, fulfil the elastic stability conditions previously derived. Critical fluctuations of orientational order, therefore, are not able either to decorrelate the hexatic phase or to drive the transition to first order. Such a fluctuation-induced first-order transition, on the contrary, is known to play a role in smectic liquid crystals. We conclude that the  $N + 6$  phase remains orientationally correlated in the critical region, which proves the self-consistency of the model assuming such an intermediate phase, as yet experimentally undiscovered, between nematic and hexagonal discotic phases.

### 1. Introduction

In two previous papers [1, 2] we proposed a model for the hexagonal discotic–nematic phase transition. We considered, indeed, the phase transition between the hexagonal discotic phase and an intermediate hexatic phase ( $N + 6$  phase) [1, 3]. The hexatic phase is characterised by translational invariance in the plane orthogonal to the nematic director, so that it has homogeneous density like the ordinary nematic phase, but shows long-range sixfold orientational order around the director like the hexagonal discotic phase. Therefore, the symmetry group of the intermediate hexatic phase is  $D_{6h} \square R^3$ . We assumed such an intermediate phase, because of some analogies with the two-dimensional melting theory of Halperin and Nelson [4], as discussed in [1]. Anyway, it is only a theoretical prediction and as yet experimentally undiscovered.

There has been much recent theoretical interest in bond orientationally ordered phases [3, 5, 6] as intermediate phases between a more disordered phase and a phase that shows both orientational and translational order. Such new phases have been proposed in a wide class of systems, including Lifshitz point systems and various kinds of liquid crystals, which share some symmetry features despite different physical structures [6]. For most of these phases there is not yet experimental evidence, but they are, at least, possible on symmetry grounds and are of physical interest. They should be a

universal feature of ordered media, while the actual existence of a particular intermediate phase could depend on its stability against fluctuation-induced breaking of long-range orientational order. Stability against fluctuations, in its turn, is controlled by the effective values of some physical parameters. The aim of this paper is just to investigate the stability of the hexatic  $N + 6$  phase with respect to the fluctuations of local orientational order.

According to the aforementioned model [1], a triple mass-density wave in the plane orthogonal to the nematic director is the order parameter that describes the condensation of the hexagonal two-dimensional lattice. The requirement of local invariance under rotations [1, 5] yields the coupling between the order parameter and the local rotation field  $\mathbf{\Omega}$ , which is defined in equation (24) of [1] as

$$\mathbf{\Omega} = \Omega_z \mathbf{m}_0 + (\mathbf{m}_0 \times \delta \mathbf{m}) \quad (1)$$

where  $\Omega_z$  describes the local rotation of the two-dimensional lattice around  $\mathbf{m}_0$ , which is the unperturbed director (conventionally taken along the  $\hat{z}$  axis), while  $\delta \mathbf{m}$  is a small distortion of  $\mathbf{m}_0$ . The field  $\mathbf{\Omega}$  locally fixes the orientation of hexagonal phase with respect to the uniform configuration ( $\Omega_z = 0$ ,  $\delta \mathbf{m} = 0$ ).

Such a model [1] was developed in analogy with the nematic–smectic A transition, described as the onset of a plane density wave with wavevector along the nematic director [7]. In a smectic liquid crystal, the orientational order is fully characterised by the director  $\mathbf{m}$ . In a discotic liquid crystal, on the contrary, the director  $\mathbf{m}$  is not sufficient to describe the full orientational order of the phase. We must define also a bond-angle field  $\Omega_z$ , which gives the orientation of the two-dimensional lattice in the plane orthogonal to  $\mathbf{m}_0$ . Such  $\Omega_z$  can be defined as the rotation angle around  $\mathbf{m}_0$  between a given reciprocal lattice vector and a fixed  $\hat{x}$  axis.

As for smectics [7], free energy must be invariant under global rotations of the system, in this case under simultaneous rotations of the liquid columns and of the director. Anyway, for discotics, the director  $\mathbf{m}$  is not sufficient to fix orientational order, so that we are forced to introduce the full rotation field  $\mathbf{\Omega}$ , equation (1). Therefore, the requirement of global rotation invariance must be referred to  $\mathbf{\Omega}$ , as discussed in [1]. Also, the fluctuations of orientational order and elastic energy due to distortions of orientational order must be expressed in terms of the strains of the field  $\mathbf{\Omega}$  [2]. The full elastic energy of curvature for a discotic liquid crystal is therefore due to local variations of the three independent rotation fields  $\delta m_x$ ,  $\delta m_y$ ,  $\Omega_z$ , which are the components of  $\mathbf{\Omega}$ , equation (1). Such a Frank elastic energy controls the fluctuations of the three independent fields  $\mathbf{\Omega}$ .

As a consequence of the coupling between the order parameter and  $\mathbf{\Omega}$ , the critical fluctuations of the order parameter drive the critical enhancements of the Frank elastic constants, which can be calculated by means of the response-function method [8]. In smectics, a similar coupling between the order parameter and the director yields critical enhancement of Frank elastic constants [8].

The above-mentioned mechanism for the melting of the hexagonal discotic phase into the nematic phase via an intermediate hexatic  $N + 6$  phase is a physically motivated conjecture [1]. Nevertheless, the actual existence and the range of stability of such an intermediate phase depend on the effects of thermal fluctuations. The local fluctuations of orientational order could yield an elastic instability in the  $N + 6$  phase near the second-order transition to the hexagonal discotic phase. In that case the fixed point describing the second-order transition would be unstable against fluctuations of orientational order and the system would undergo a cross-over to a first-order transition.

The question is whether a second-order transition is possible between a phase with  $D_{6h}$  symmetry and no translational order and a columnar phase with translational order in addition to  $D_{6h}$  symmetry, or whether fluctuations imply that such a transition is always first-order. As another possibility, the range of stability of the hexatic phase in the absence of effects due to fluctuations could be so narrow that instability driven by fluctuations would completely destroy long-range orientational order, so yielding a cross-over to a direct first-order transition between hexagonal discotic phase and nematic phase. All these possibilities, at last, could be realised in different ranges of values of physical parameters.

Fluctuations are known to have the above-mentioned effects, and the phenomenon of fluctuation-induced first-order phase transitions is well understood [9–14]. In particular, as regards the nematic–smectic A transition [12–14], the first-order transition is induced by the fluctuations of the director, which can be considered as a massless gauge field coupled to the smectic order parameter.

Since our model [1] is closely related to the De Gennes model [7] of the nematic–smectic A transition, we briefly review the theoretical insights into this transition. In mean-field theory, which neglects director fluctuations, this transition is continuous [7]. Director fluctuations can drive the transition to first order [12–14], but for some range of values of parameters the transition remains second order [15–17] even when all fluctuations are accounted for.

The elastic instability mechanism, which we take into account in this paper as a possible source either of a fluctuation-induced first-order transition or of a complete decorrelation of the hexatic phase, is somewhat different from that which makes the nematic–smectic A transition first-order. We consider that, as for smectics, the coupling between the order parameter and the ‘gauge’ field  $\Omega$  yields the critical enhancements of the Frank elastic constants as a consequence of the critical fluctuations of the order parameter near the second-order phase transition point. Such a critical behaviour of Frank constants might make the system unstable with respect to the fluctuations of  $\Omega$ , i.e. of orientational order. In renormalisation-group jargon, the fixed point controlling the transition would be unstable because some Frank constants could not reach stable values in parameter space.

The aim of this paper is to study the elastic stability of the hexatic phase, in particular near the supposed second-order transition to the hexagonal discotic phase, where the fluctuation effects are relevant. The main result of our analysis is that the instability described above does not develop, since critical enhancements of Frank constants still fulfil elastic stability conditions. Therefore, the hexatic phase is stable, at least in the theoretical framework of the model assumed.

We shall derive an inequality that the Frank elastic constants must fulfil, so that the elastic stability of discotic liquid crystals is preserved. Elastic stability is essential for the existence of discotic phases. The Frank elastic energy describes the stiffness of the system with respect to local distortions of orientational order. If the Frank energy does not fulfil the requirement of elastic stability, the system is not stable against breaking of the long-range orientational order by thermal fluctuations of  $\Omega$ . In that case the fluctuations of  $\Omega$  should make the system isotropic. No liquid-crystalline mesophase could be stable.

In particular, the coupling between  $\delta m$  and  $\Omega_z$  (see section 2) cannot be too strong, otherwise the system develops an unstable mode consisting of a mixing of twist and bend of the liquid tubes coupled to torsion of the two-dimensional lattice. As a consequence, the two-dimensional lattice is decorrelated over a macroscopic length scale. Therefore, preservation of sixfold symmetry requires weak coupling between the director distortion

$\delta\mathbf{m}$  and the local rotation angle  $\Omega_z$  of the two-dimensional lattice around the axis of liquid tubes.

Critical enhancements of the Frank elastic constants, calculated by means of the response-function method [8], fulfil the previously mentioned condition of elastic stability. So, critical behaviour in the hexatic  $N + 6$  phase, near the temperature of the phase transition to the hexagonal discotic phase, shows that the more disordered phase remains orientationally correlated in the critical region. Such a result can be considered as a self-consistency test of the model, in particular as regards the assumption of the intermediate  $N + 6$  phase. In spite of self-consistency, nevertheless, we cannot rule out different mechanisms for the hexagonal discotic to nematic phase transition, where the breaking of translational order is directly driven by the decorrelation of orientational order. Such a remark is valid in two-dimensional melting [4] as well.

The Frank elastic constant  $\gamma_3$ , which couples  $\delta\mathbf{m}$  to  $\Omega_z$ , shows critical enhancement. In this regard, the statement in [2] that  $\gamma_3$  is non-critical must be considered wrong. As a consequence, the director elastic modes  $\delta\mathbf{m}$  remain coupled to the 'rotation' elastic modes  $\Omega_z$ , near the transition temperature too. Incidentally, such a feature makes a renormalisation-group treatment of the transition harder, because the coupling between  $\delta\mathbf{m}$  and  $\Omega_z$  cannot be neglected. In fact the normal elastic modes are a mixing of  $\delta\mathbf{m}$  and  $\Omega_z$ , and the corresponding inverse propagators are not simply quadratic in the wavevector (see also [3]).

In section 2 the elastic stability conditions are derived and, in particular, the inequality that involves the  $\delta\mathbf{m}$ - $\Omega_z$  coupling constant  $\gamma_3$ . In section 3 the critical enhancements of Frank elastic constants are calculated, and it is shown that they fulfil the elastic stability conditions. Finally, in the appendix, some calculational details are presented.

## 2. Elastic stability

The full elastic energy associated with the strains of the local rotation field  $\Omega$ , equation (1), for a discotic liquid crystal is [2]

$$F_D = \frac{1}{2} \int d^3r [K_1(\text{div } \delta\mathbf{m})^2 + K_2(\mathbf{m}_0 \cdot \text{rot } \delta\mathbf{m})^2 + K_3(\mathbf{m}_0 \times \text{rot } \delta\mathbf{m})^2 + \gamma_1(\nabla_{\parallel}\Omega_z)^2 + \gamma_2(\nabla_{\perp}\Omega_z)^2 + 2\gamma_3(\mathbf{m}_0 \cdot \text{rot } \delta\mathbf{m})(\nabla_{\parallel}\Omega_z)] \quad (2)$$

where a different (by a factor 2) definition of  $\gamma_3$ , with respect to [2], is adopted for convenience. The  $\gamma_4$  term present in equation (2) of [2] is omitted, since it is not invariant under reflections in planes passing through the  $\hat{z}$  axis. Therefore, by the chiral symmetry contained in the  $D_{6h}$  group, we have  $\gamma_4 = 0$ . Note that the hexagonal symmetry of the discotic phase entirely determines the elastic energy (2) and, in particular, implies cylindrical symmetry for elastic energy (see also [3]).

In Fourier space, elastic energy (2) is

$$F_D = \frac{1}{2} \int \frac{d^3q}{(2\pi)^3} \{ (K_1q_x^2 + K_2q_y^2 + K_3q_z^2) |\delta m_x(\mathbf{q})|^2 + (K_1q_y^2 + K_2q_x^2 + K_3q_z^2) |\delta m_y(\mathbf{q})|^2 + (K_1 - K_2)q_xq_y [\delta m_x(\mathbf{q})\delta m_y^*(\mathbf{q}) + \text{cc}] + (\gamma_1q_z^2 + \gamma_2q_{\perp}^2) |\Omega_z(\mathbf{q})|^2 + \gamma_3q_zq_x [\delta m_y(\mathbf{q})\Omega_z^*(\mathbf{q}) + \text{cc}] - \gamma_3q_zq_y [\delta m_x(\mathbf{q})\Omega_z^*(\mathbf{q}) + \text{cc}] \}. \quad (3)$$

Let us define the strain vector  $\mathbf{n}$ , the components of which are  $n_x \equiv \delta m_x$ ,  $n_y \equiv \delta m_y$ ,  $n_0 \equiv \Omega_z$ . The elastic energy (3), in terms of the strain  $\mathbf{n}$ , can be written as

$$F_D = \frac{1}{2} \int \frac{d^3q}{(2\pi)^3} Q_{\alpha\beta}(\mathbf{q}) n_\alpha(\mathbf{q}) n_\beta^*(\mathbf{q}) \quad (4)$$

with  $\alpha, \beta = x, y, 0$ . In equation (4),  $Q_{\alpha\beta}$  is the response function [8] relative to curvature distortions  $\mathbf{n}$ . The components of  $Q_{\alpha\beta}$ , by comparing (4) with (3), are

$$Q_{xx} = K_1 q_x^2 + K_2 q_y^2 + K_3 q_z^2 \quad (5a)$$

$$Q_{yy} = K_1 q_y^2 + K_2 q_x^2 + K_3 q_z^2 \quad (5b)$$

$$Q_{xy} = Q_{yx} = (K_1 - K_2) q_x q_y \quad (5c)$$

$$Q_{00} = \gamma_1 q_z^2 + \gamma_2 q_\perp^2 \quad (5d)$$

$$Q_{0x} = Q_{x0} = -\gamma_3 q_z q_x \quad (5e)$$

$$Q_{0y} = Q_{y0} = \gamma_3 q_z q_y \quad (5f)$$

Elastic stability requires that the quadratic form  $Q_{\alpha\beta} n_\alpha n_\beta^*$  in (4) is positive definite. In that case any distortion  $\mathbf{n}$  yields an energy increase, so that the uniform configuration  $\mathbf{n} = 0$  is stable. Therefore, the coefficients  $Q_{\alpha\beta}$  of the quadratic form in (4) must fulfil the well known inequalities

$$Q_{xx} > 0 \quad Q_{yy} > 0 \quad Q_{00} > 0 \quad (6a)$$

$$Q_{xx} Q_{yy} - Q_{xy}^2 > 0 \quad (6b)$$

$$\det Q = Q_{xx}(Q_{yy} Q_{00} - Q_{y0}^2) + Q_{xy}(Q_{y0} Q_{x0} - Q_{00} Q_{xy}) \\ + Q_{x0}(Q_{xy} Q_{y0} - Q_{0x} Q_{yy}) > 0 \quad (6c)$$

which make  $Q_{\alpha\beta} n_\alpha n_\beta^*$  positive definite.

Substituting (5) in (6), one can see immediately that equations (6a) are valid for

$$K_1 > 0 \quad K_2 > 0 \quad K_3 > 0 \quad \gamma_1 > 0 \quad \gamma_2 > 0 \quad (7)$$

i.e. the Frank elastic constants  $K_1$ ,  $K_2$  and  $K_3$ , relative to  $\delta \mathbf{m}$  distortions, and the rotational stiffnesses  $\gamma_1$  and  $\gamma_2$ , relative to  $\Omega_z$  distortions, must be positive. Inequality (6b) can be put in the form

$$(K_3 q_z^2 + K_1 q_\perp^2)(K_3 q_z^2 + K_2 q_\perp^2) > 0$$

(with  $q_\perp^2 = q_x^2 + q_y^2$ ), which is always fulfilled by (7).

Finally, the inequality (6c) is equivalent to

$$(K_3 q_z^2 + K_1 q_\perp^2)[(\gamma_1 q_z^2 + \gamma_2 q_\perp^2)(K_3 q_z^2 + K_2 q_\perp^2) - \gamma_3^2 q_z^2 q_\perp^2] > 0$$

or, by (7), to

$$\gamma_1 K_3 q_z^4 + \gamma_2 K_2 q_\perp^4 + (\gamma_1 K_2 + \gamma_2 K_3 - \gamma_3^2) q_z^2 q_\perp^2 > 0. \quad (8)$$

Such an inequality involves a quadratic form in  $q_z^2$  and  $q_\perp^2$  variables, which has to be positive definite. Generally, equation (8) holds good for  $\gamma_1 K_3 > 0$ ,  $\gamma_2 K_2 > 0$ , which are fulfilled by (7), and for

$$4\gamma_1 K_2 \gamma_2 K_3 - (\gamma_1 K_2 + \gamma_2 K_3 - \gamma_3^2)^2 > 0$$

or

$$\gamma_3^4 - 2\gamma_3^2(\gamma_1 K_2 + \gamma_2 K_3) + (\gamma_1 K_2 - \gamma_2 K_3)^2 < 0. \quad (9)$$

But (9) is too restrictive, because in its derivation  $q_z^2$  and  $q_\perp^2$  variables of quadratic form (8) are assumed to take either positive or negative values, while they can be only positive. For positive values of  $q_z^2$  and  $q_\perp^2$  variables and by (7), the quadratic form (8) is positive whenever

$$\gamma_1 K_2 + \gamma_2 K_3 > \gamma_3^2 \quad (10)$$

independently of (9). By solving (9) with respect to  $\gamma_3$  we get the inequality

$$[(\gamma_1 K_2)^{1/2} - (\gamma_2 K_3)^{1/2}]^2 < \gamma_3^2 < [(\gamma_1 K_2)^{1/2} + (\gamma_2 K_3)^{1/2}]^2. \quad (11)$$

Therefore, (8) is fulfilled if  $\gamma_3$  is in accordance with inequality (10) or, inclusively, with inequality (11). Putting together these two inequalities, one gets

$$\gamma_3^2 < [(\gamma_1 K_2)^{1/2} + (\gamma_2 K_3)^{1/2}]^2$$

or

$$|\gamma_3| < (\gamma_1 K_2)^{1/2} + (\gamma_2 K_3)^{1/2}. \quad (12)$$

Inequalities (7) and (12) are the conditions of elastic stability. In particular, (12) means that the modulus of the coupling constant  $\gamma_3$ , i.e. the strength of the coupling between  $\delta\mathbf{m}$  and  $\Omega_z$ , cannot be too large with respect to the other Frank elastic constants. The sign of  $\gamma_3$  can be either positive or negative. The unstable mode, which develops if  $\gamma_3$  does not fulfil inequality (12), is a mixing of the twist and bend modes of the director with the torsion mode of the two-dimensional lattice, since  $\gamma_3$  couples  $\mathbf{m}_0 \cdot \text{rot } \delta\mathbf{m}$  to  $\nabla_{\parallel}\Omega_z$ , as shown in equation (2). In fact  $\mathbf{m}_0 \cdot \text{rot } \delta\mathbf{m} \neq 0$  implies that  $\delta\mathbf{m}$  and then liquid tubes are twisted, while  $\nabla_{\parallel}\Omega_z \neq 0$  represents a rotation angle  $\Omega_z$  that is non-uniform along the  $\hat{z}$  axis and then a torsion of the two-dimensional lattice. Indeed, the normal elastic modes, which can be obtained from the quadratic form (3), contain a bend component too, in addition to twist and torsion modes.

### 3. Critical enhancements of Frank elastic constants

In this section we closely follow [1, 2], and thus we only outline the general lines of the derivation. We exploit the response-function method [8] in order to calculate enhancements of Frank constants, in the hexatic  $N + 6$  phase, just above the phase transition temperature to the hexagonal discotic phase. Such a method was first applied by Jahnig and Brochard to evaluate critical enhancements of Frank constants in smectics [8], described by the De Gennes model [7]. Our model [1] is analogous with the De Gennes model and the only differences are the following: the order parameter is a triple density wave while the smectic order parameter is a plane density wave; the 'gauge' field is  $\Omega$ , equation (1), while for smectics  $\delta\mathbf{m}$  is sufficient to express the global rotational invariance of the system. Some consequences follow on the form of gauge coupling between order parameter and gauge field [1], and therefore on the critical behaviour of Frank constants [1, 2].

The gradient terms of the order parameter in the free energy, locally invariant under  $\Omega$  rotations, are given by

$$F_2 = \int d^3r \left( \frac{1}{2M_{\parallel}} \sum_{i=1}^3 |[\nabla_z + i\mathbf{q}_i \cdot \delta\mathbf{m}(\mathbf{r})] \eta_i(\mathbf{r})|^2 + \frac{1}{2M_{\perp}} \sum_{i=1}^3 |[\nabla_{\perp} - i\Omega_z(\mathbf{r})\mathbf{m}_0 \times \mathbf{q}_i] \eta_i(\mathbf{r})|^2 \right) \quad (13)$$

as in equation (28) of [1]. The order parameter is represented by the three complex amplitudes  $\eta_i$  (with  $i = 1, 2, 3$ ) of the triple mass-density wave

$$\delta\rho(\mathbf{r}) = \text{Re}[\eta_1(\mathbf{r}) \exp(i\mathbf{q}_1 \cdot \mathbf{r}) + \eta_2(\mathbf{r}) \exp(i\mathbf{q}_2 \cdot \mathbf{r}) + \eta_3(\mathbf{r}) \exp(i\mathbf{q}_3 \cdot \mathbf{r})]$$

where  $\{\mathbf{q}_i\}$  is a set of shortest reciprocal lattice vectors (defined in equations (3)–(6) of [1]) characteristic of the planar hexagonal lattice orthogonal to the nematic director. Such an order parameter describes the condensation of the planar hexagonal lattice from the homogeneous hexatic phase, as the De Gennes order parameter [7] (only one complex amplitude) describes the condensation of smectic layers from the nematic phase.

The increment of free energy due to a small external distortion  $\mathbf{n}$  can be written as

$$\delta F = - \int d^3r \mathbf{h}(\mathbf{r}) \cdot \mathbf{n}(\mathbf{r}) \quad (14)$$

where  $\mathbf{h}(\mathbf{r})$  is the response of the system to the external perturbation  $\mathbf{n}(\mathbf{r})$ . The response function [8]  $Q_{\alpha\beta}$  is defined by

$$h_{\alpha} = Q_{\alpha\beta} n_{\beta}. \quad (15)$$

The hydrodynamic contribution to  $Q_{\alpha\beta}$  comes from the variation of elastic energy, equation (4), and is given by equations (5), in Fourier space. The fluctuating contribution to equation (15) comes from the variation of  $F_2$ , equation (13), and can be calculated by statistical averaging over thermal fluctuations of the order parameter.

In Fourier-transformed variables, the fluctuating response function is given by the thermal average

$$\tilde{Q}_{\alpha\beta}(\mathbf{q}) = - \frac{1}{k_B T} [\langle \tilde{h}_{\alpha}(\mathbf{q}) \tilde{h}_{\beta}^*(\mathbf{q}) \rangle - \langle \tilde{h}_{\alpha}(0) \tilde{h}_{\beta}^*(0) \rangle] \quad (16)$$

where the components of  $\tilde{\mathbf{h}}(\mathbf{q})$  are

$$\tilde{h}_0(\mathbf{q}) = \frac{i}{M_{\perp}} \sum_{i=1}^3 (\mathbf{m}_0 \times \mathbf{q}_i) \cdot \int \frac{d^3p}{(2\pi)^3} \mathbf{p}_{\perp} \eta_i^*(\mathbf{p} - \mathbf{q}/2) \eta_i(\mathbf{p} + \mathbf{q}/2) \quad (17a)$$

$$\tilde{h}_j(\mathbf{q}) = - \frac{i}{M_{\parallel}} \sum_{i=1}^3 (q_i)_j \int \frac{d^3p}{(2\pi)^3} p_z \eta_i^*(\mathbf{p} - \mathbf{q}/2) \eta_i(\mathbf{p} + \mathbf{q}/2) \quad (17b)$$

with  $j = x, y$ .

In Gaussian approximation [1, 8], the response function  $\tilde{Q}_{\alpha\beta}$  is

$$\tilde{Q}_{00}(\mathbf{q}) = - \frac{1}{k_B T M_{\perp}^2} \sum_{i=1}^3 \int \frac{d^3p}{(2\pi)^3} [(\mathbf{m}_0 \times \mathbf{q}_i) \cdot \mathbf{p}_{\perp}]^2 \times [G(\mathbf{p} - \mathbf{q}/2)G(\mathbf{p} + \mathbf{q}/2) - G^2(\mathbf{p})] \quad (18a)$$



$$\bar{Q}_{jk}(\mathbf{q}) = -\frac{1}{k_B T M_{\parallel}^2} \sum_{i=1}^3 (q_i)_j (q_i)_k \int \frac{d^3 p}{(2\pi)^3} p_z^2 [G(\mathbf{p} - \mathbf{q}/2)G(\mathbf{p} + \mathbf{q}/2) - G^2(\mathbf{p})] \quad (18b)$$

$$\begin{aligned} \bar{Q}_{0j}(\mathbf{q}) = \bar{Q}_{j0}(\mathbf{q}) &= \frac{1}{k_B T M_{\parallel} M_{\perp}} \sum_{i=1}^3 (q_i)_j \int \frac{d^3 p}{(2\pi)^3} [(m_0 \times \mathbf{q}_i) \cdot \mathbf{p}_{\perp}] p_z \\ &\times [G(\mathbf{p} - \mathbf{q}/2)G(\mathbf{p} + \mathbf{q}/2) - G^2(\mathbf{p})] \end{aligned} \quad (18c)$$

with

$$\langle \eta_i^*(\mathbf{q}) \eta_j(\mathbf{q}') \rangle = G(\mathbf{q}) (2\pi)^3 \delta_{ij} \delta(\mathbf{q} - \mathbf{q}') \quad (19)$$

$$G(\mathbf{q}) = \frac{k_B T}{A(1 + \xi_{\parallel}^2 q_z^2 + \xi_{\perp}^2 q_{\perp}^2)} \quad (20)$$

where  $A = A'(T - T^*)$ ,  $T^*$  being a second-order phase transition temperature, and  $\xi_{\parallel} = (2AM_{\parallel})^{-1/2}$ ,  $\xi_{\perp} = (2AM_{\perp})^{-1/2}$  are the correlation lengths parallel and orthogonal, respectively, to the director  $\mathbf{m}_0$ . Carrying out the sum over  $i$  in equations (18), one gets

$$\bar{Q}_{00}(\mathbf{q}) = -\frac{3}{2} \frac{q_0^2}{k_B T M_{\perp}^2} \int \frac{d^3 p}{(2\pi)^3} p_{\perp}^2 [G(\mathbf{p} - \mathbf{q}/2)G(\mathbf{p} + \mathbf{q}/2) - G^2(\mathbf{p})] \quad (21a)$$

$$\bar{Q}_{jk}(\mathbf{q}) = -\frac{3}{2} \frac{q_0^2}{k_B T M_{\parallel}^2} \delta_{jk} \int \frac{d^3 p}{(2\pi)^3} p_z^2 [G(\mathbf{p} - \mathbf{q}/2)G(\mathbf{p} + \mathbf{q}/2) - G^2(\mathbf{p})] \quad (21b)$$

$$\begin{aligned} \bar{Q}_{0j}(\mathbf{q}) = \bar{Q}_{j0}(\mathbf{q}) &= \frac{3}{2} \frac{q_0^2}{k_B T M_{\parallel} M_{\perp}} \varepsilon_{jk} \\ &\times \int \frac{d^3 p}{(2\pi)^3} p_z p_{\perp k} [G(\mathbf{p} - \mathbf{q}/2)G(\mathbf{p} + \mathbf{q}/2) - G^2(\mathbf{p})] \end{aligned} \quad (21c)$$

where  $q_0$  is the modulus of the vectors  $\mathbf{q}_i$  and  $\varepsilon_{jk}$  is the antisymmetric unit tensor in two dimensions.

In the hydrodynamic limit [1, 8]  $\xi q \ll 1$ , the integrations in equations (21) give

$$\bar{Q}_{00} = \frac{q_0^2 k_B T}{16\pi} (2\xi_{\parallel}^2 q_z^2 + \xi_{\perp}^2 \xi_{\parallel}^{-1} q_{\perp}^2) \quad (22a)$$

$$\bar{Q}_{ij} = \frac{q_0^2 k_B T}{16\pi} \xi_{\parallel} (q_x^2 + q_y^2) \delta_{ij} \quad (22b)$$

$$\bar{Q}_{0i} = \bar{Q}_{i0} = \frac{q_0^2 k_B T}{16\pi} \xi_{\parallel} q_z \varepsilon_{ij} q_j \quad (22c)$$

Comparing equations (22) with equations (5), we obtain the critical contributions to the Frank constants

$$\delta K_1 = \delta K_2 = \frac{q_0^2 k_B T}{16\pi} \xi_{\parallel} \quad (23a)$$

$$\delta K_3 = 0 \quad (23b)$$

$$\delta \gamma_1 = \frac{q_0^2 k_B T}{8\pi} \xi_{\parallel} = 2\delta K_2 \quad (23c)$$

$$\delta\gamma_2 = \frac{q_0^2 k_B T}{16\pi} \xi_{\parallel}^{-1} \xi_{\perp}^2 \quad (23d)$$

$$\delta\gamma_3 = -\frac{q_0^2 k_B T}{16\pi} \xi_{\parallel} = -\delta K_2. \quad (23e)$$

For  $T \rightarrow T^*$ ,  $\xi_{\parallel}$  and  $\xi_{\perp}$  diverge, so that the critical contributions (23) to Frank constants become larger than the background values. Therefore, the elastic stability condition (12) for  $T \rightarrow T^*$  becomes

$$|\delta\gamma_3|^2 < \delta\gamma_1 \delta K_2. \quad (24)$$

The critical enhancements (23) fulfil inequality (24), since

$$(\delta\gamma_3)^2 = (\delta K_2)^2 < 2(\delta K_2)^2 = \delta\gamma_1 \delta K_2.$$

Note that the critical contribution to the response function  $Q_{\alpha\beta}$ , equations (21), fulfils elastic stability conditions (6), even if one does not perform the hydrodynamic limit of equations (21). Let us define, for convenience, the rescaled wavevector

$$\hat{q}_{\parallel} \equiv \xi_{\parallel} q_z \quad \hat{q}_{\perp} \equiv \xi_{\perp} q_{\perp} \quad (25)$$

and the rescaled components of response function

$$C^{-1} \xi_{\perp}^{-2} \tilde{Q}_{00} \equiv \tilde{\mathcal{Q}}_{00} = - \int \frac{d^3 p}{(2\pi)^3} p_{\perp}^2 [G(\mathbf{p} - \hat{\mathbf{q}}/2)G(\mathbf{p} + \hat{\mathbf{q}}/2) - G^2(\mathbf{p})] \quad (26a)$$

$$C^{-1} \xi_{\parallel}^{-2} \tilde{Q}_{ij} \equiv \tilde{\mathcal{Q}}_{ij} = -\delta_{ij} \int \frac{d^3 p}{(2\pi)^3} p_z^2 [G(\mathbf{p} - \hat{\mathbf{q}}/2)G(\mathbf{p} + \hat{\mathbf{q}}/2) - G^2(\mathbf{p})] \quad (26b)$$

$$C^{-1} \xi_{\parallel}^{-1} \xi_{\perp}^{-1} \tilde{Q}_{0i} \equiv \tilde{\mathcal{Q}}_{0i} = \varepsilon_{ij} \int \frac{d^3 p}{(2\pi)^3} p_z p_j [G(\mathbf{p} - \hat{\mathbf{q}}/2)G(\mathbf{p} + \hat{\mathbf{q}}/2) - G^2(\mathbf{p})] \quad (26c)$$

with

$$C \equiv 6q_0^2 k_B T (\xi_{\parallel} \xi_{\perp}^2)^{-1}. \quad (27)$$

It can be shown (see the appendix) that

$$- \int \frac{d^3 p}{(2\pi)^3} p_{\alpha} p_{\beta} [G(\mathbf{p} - \hat{\mathbf{q}}/2)G(\mathbf{p} + \hat{\mathbf{q}}/2) - G^2(\mathbf{p})] = f(\hat{q}) (\delta_{\alpha\beta} - \hat{q}_{\alpha} \hat{q}_{\beta} / \hat{q}^2) \quad (28)$$

with  $\alpha, \beta = x, y, z$ , which corresponds to the transverse response function of a smectic liquid crystal [8]. Therefore, equations (26) take the form

$$\tilde{\mathcal{Q}}_{00} = [f(\hat{q})/\hat{q}^2] (2\hat{q}_z^2 + \hat{q}_{\perp}^2) \quad (29a)$$

$$\tilde{\mathcal{Q}}_{ij} = [f(\hat{q})/\hat{q}^2] \hat{q}_{\perp}^2 \delta_{ij} \quad (29b)$$

$$\tilde{\mathcal{Q}}_{0i} = [f(\hat{q})/\hat{q}^2] \varepsilon_{ij} \hat{q}_z \hat{q}_j. \quad (29c)$$

In the hydrodynamic limit  $f(\hat{q})/\hat{q}^2 \approx \text{const}$ , and we get equations (22). As shown in the appendix, the function  $f(\hat{q})$  is positive. It is straightforward to show that the response function in equations (29) fulfils the elastic stability conditions (6), since  $f(\hat{q}) > 0$ .

In conclusion, we have tested the stability of the hexatic  $N + 6$  phase, a theoretically predicted intermediate phase between the hexagonal discotic and nematic phases [1], against fluctuations of orientational order, which could decorrelate the phase. We have

taken account of a possible development of Frank elastic instability due to critical behaviour of Frank constants in the  $N + 6$  phase near the supposed continuous transition to the hexagonal discotic phase. As possible consequences of such an instability, the transition could be driven to first order or the range of stability of the hexatic phase could vanish.

Such fluctuation effects are well known in various systems [9–14]. In particular, as regards the De Gennes model [7] of smectics, with which our model shows several analogies, director fluctuations can drive the nematic–smectic A transition to first order [12–14].

As the main result of our calculations, critical behaviour of Frank constants shows that, even though the coupling constant  $\gamma_3$  undergoes critical enhancement, elastic stability conditions are still fulfilled for the  $N + 6$  phase in the critical region. Therefore, the sixfold orientational order is actually preserved at the continuous transition between hexatic and hexagonal discotic phases. We can conclude that, in the theoretical framework of our model, the hexatic phase is stable against fluctuations of orientational order. As in two-dimensional melting [4], nevertheless, we cannot rule out other mechanisms, e.g. driven by disclination unbinding [4], for a direct first-order transition between hexagonal discotic and nematic phases. We only state that our model [1, 2] is stable and self-consistent.

### Acknowledgment

This research is supported by funds from the Ministero della Pubblica Istruzione (Italy).

### Appendix

In this appendix, we derive equation (28) and show that  $f(\hat{q}) > 0$ . Generally, such a quantity as that on the left-hand side of equation (28) can depend only on the tensors  $\delta_{\alpha\beta}$  and  $\hat{q}_\alpha\hat{q}_\beta/\hat{q}^2$ . Therefore, we put

$$-\int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta [G(\mathbf{p} - \hat{q}/2)G(\mathbf{p} + \hat{q}/2) - G^2(\mathbf{p})] \\ = f(\hat{q})(\delta_{\alpha\beta} - \hat{q}_\alpha\hat{q}_\beta/\hat{q}^2) + g(\hat{q})\hat{q}_\alpha\hat{q}_\beta/\hat{q}^2 \quad (\text{A1})$$

where  $f(\hat{q})$  and  $g(\hat{q})$  are the transverse and longitudinal parts, respectively. In order to get  $g(\hat{q})$ , we contract equation (A1) with  $\hat{q}_\beta$ :

$$\hat{q}_\beta \int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta [G^2(\mathbf{p}) - G(\mathbf{p} - \hat{q}/2)G(\mathbf{p} + \hat{q}/2)] = \hat{q}_\alpha g(\hat{q}). \quad (\text{A2})$$

Let us calculate

$$\int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta G^2(\mathbf{p}) = \delta_{\alpha\beta} \int p_\gamma^2 G^2(\mathbf{p}) \frac{d^3p}{(2\pi)^3}$$

since  $G(\mathbf{p})$ , equation (20), is isotropic in rescaled wavevector (25). By a partial integration on  $p_\gamma$ , one has

$$\int \frac{d^3p}{(2\pi)^3} G(\mathbf{p}) = 2 \int \frac{d^3p}{(2\pi)^3} p_\gamma^2 G^2(\mathbf{p})$$

and then

$$\int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta G^2(\mathbf{p}) = \frac{1}{2} \delta_{\alpha\beta} \int \frac{d^3p}{(2\pi)^3} G(\mathbf{p}). \tag{A3}$$

Moreover, by equations (20) and (25), we have the equality

$$\hat{q} \cdot \mathbf{p} = \frac{1}{2} [G^{-1}(\mathbf{p} + \hat{q}/2) - G^{-1}(\mathbf{p} - \hat{q}/2)]$$

and then

$$\hat{q}_\beta \int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta G(\mathbf{p} - \hat{q}/2) G(\mathbf{p} + \hat{q}/2) = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} p_\alpha [G(\mathbf{p} - \hat{q}/2) - G(\mathbf{p} + \hat{q}/2)]. \tag{A4}$$

As

$$\int \frac{d^3p}{(2\pi)^3} p_\alpha G(\mathbf{p} - \hat{q}/2) = \int \frac{d^3p}{(2\pi)^3} (p_\alpha + \hat{q}_\alpha/2) G(\mathbf{p}) = \frac{1}{2} \hat{q}_\alpha \int \frac{d^3p}{(2\pi)^3} G(\mathbf{p})$$

and analogously for the other part of the integral in equation (A4), we find

$$\hat{q}_\beta \int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta G(\mathbf{p} - \hat{q}/2) G(\mathbf{p} + \hat{q}/2) = \frac{1}{2} \hat{q}_\alpha \int \frac{d^3p}{(2\pi)^3} G(\mathbf{p}). \tag{A5}$$

Finally, equations (A3) and (A5) yield

$$\hat{q}_\beta \int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta [G^2(\mathbf{p}) - G(\mathbf{p} - \hat{q}/2) G(\mathbf{p} + \hat{q}/2)] = 0$$

and then, by equation (A2),

$$\hat{q}_\alpha g(\hat{q}) = 0 \tag{A6}$$

i.e. the longitudinal part in equation (A1) vanishes. Therefore, equation (A1) becomes

$$- \int \frac{d^3p}{(2\pi)^3} p_\alpha p_\beta [G(\mathbf{p} - \hat{q}/2) G(\mathbf{p} + \hat{q}/2) - G^2(\mathbf{p})] = f(\hat{q}) (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta / \hat{q}^2) \tag{A7}$$

which is the same as equation (28).

At last, we will show that  $f(\hat{q}) > 0$ . Taking the trace of equation (A7), we have

$$f(\hat{q}) = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} p^2 [G^2(\mathbf{p}) - G(\mathbf{p} - \hat{q}/2) G(\mathbf{p} + \hat{q}/2)] \tag{A8}$$

while the trace of equation (A3) yields

$$\int \frac{d^3p}{(2\pi)^3} p^2 G^2(\mathbf{p}) = \frac{3}{2} \int \frac{d^3p}{(2\pi)^3} G(\mathbf{p}). \tag{A9}$$

Moreover, we use the following relation

$$\begin{aligned} \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{[1 + (\mathbf{p} + \hat{q}/2)^2][1 + (\mathbf{p} - \hat{q}/2)^2]} &= \int \frac{d^3p}{(2\pi)^3} \frac{1}{1 + p^2} - \left(1 + \frac{\hat{q}^2}{4}\right) \\ &\times \int \frac{d^3p}{(2\pi)^3} \frac{1}{[1 + (\mathbf{p} + \hat{q}/2)^2][1 + (\mathbf{p} - \hat{q}/2)^2]} \end{aligned} \tag{A10}$$

which can easily be verified. Substituting equations (A9) and (A10) in equation (A8), we get

$$f(\hat{q}) = \frac{1}{4} \int \frac{d^3 p}{(2\pi)^3} G(\mathbf{p}) + \frac{1}{2}(1 + \hat{q}^2/4) \int \frac{d^3 p}{(2\pi)^3} G(\mathbf{p} - \hat{q}/2)G(\mathbf{p} + \hat{q}/2) \quad (\text{A11})$$

which is always positive, since the expressions in the integrals are positive.

## References

- [1] Giannesi C 1983 *Phys. Rev. A* **28** 350
- [2] Giannesi C 1986 *Phys. Rev. A* **34** 705
- [3] Toner J 1983 *Phys. Rev. A* **27** 1157
- [4] Nelson D R and Halperin B I 1979 *Phys. Rev. B* **19** 2457
- [5] Nelson D R and Toner J 1981 *Phys. Rev. B* **24** 363
- [6] Grinstein G, Lubensky T C and Toner J 1986 *Phys. Rev. B* **33** 3306
- [7] De Gennes P G 1972 *Solid State Commun.* **10** 753
- [8] Jahnig F and Brochard F 1974 *J. Physique* **35** 301
- [9] Mukamel D and Krinsky S 1976 *Phys. Rev. B* **13** 5065
- [10] Bak P, Krinsky S and Mukamel D 1976 *Phys. Rev. Lett.* **36** 52
- [11] Bak P, Knak Jensen S J and Mouritsen O G 1977 *Phys. Rev. Lett.* **39** 629
- [12] Halperin B I and Lubensky T C 1974 *Solid State Commun.* **14** 997
- [13] Halperin B I, Lubensky T C and Shang-Keng Ma 1974 *Phys. Rev. Lett.* **32** 292
- [14] Lubensky T C and Jing-Huei Chen 1978 *Phys. Rev. B* **17** 366
- [15] Toner J 1982 *Phys. Rev. B* **26** 462
- [16] Lubensky T C 1983 *J. Chim. Phys.* **80** 31
- [17] Dasgupta C and Halperin B I 1981 *Phys. Rev. Lett.* **47** 1556