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Dislocation melting for a discotic liquid crystal

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Abstract. A dislocation-loop mechanism for the melting of a discotic liquid crystal is presented. With respect to a previous similar work, the contribution of longitudinal edge dislocations is included. It is explicitly shown that a discotic liquid crystal permeated by an equilibrium density of unbound dislocation loops behaves like a nematic liquid crystal in the so-called $N+6$ phase. The interaction energy between parallel dislocations is calculated.

1. Introduction

Dislocations have long been proposed as a mechanism for the melting of three-dimensional crystalline solids into isotropic liquids [1]. More recently, a considerable interest rose about the effect of defects like dislocations and disclinations on melting of two-dimensional solids [2]. Helfrich first tried to develop a defect model for the melting of smectics into nematics [3]. Nelson and Toner explicitly showed that a finite density of dislocations makes a solid like a fluid, and applied the model to the melting of smectics [4].

In a previous paper [5] we presented a defect model for the melting of a discotic liquid crystal into a nematic liquid crystal in the so-called $N+6$ phase [6], which is still a theoretical prediction and, as yet, experimentally undiscovered. The main feature of the model, which closely follows the Nelson-Toner theory [4], is a finite density of unbound dislocation loops that decorrelate the two-dimensional hexagonal lattice of liquid rods. (For the structure of the hexagonal discotic phase, see [7].) Dislocations are effective for breaking translational order but they do not destroy sixfold orientational symmetry. In that way the melted phase is a fluid, i.e. a phase with homogeneous density and without resistance to shear, but maintains a residual stiffness to torsion not present in an isotropic liquid. A discotic liquid crystal shows some characteristics of a two-dimensional system and, in particular, the presence of a crystalline lattice in two dimensions, but each site of this lattice is occupied by a one-dimensional nematic structure. So we deal with the melting of a quasi-two-dimensional system. In particular, beyond dislocations typical of a two-dimensional solid, like the so-called longitudinal edge dislocations [8], there are transversal edge and screw dislocations [8], in which the modes of distortions of the nematic director play an important role. Some analogies with smectics follow. In some sense the bend mode in a discotic liquid crystal corresponds to the splay mode in a smectic liquid crystal: the former is an undulation of liquid rods, the latter is an undulation of liquid layers. The condensation of the two-dimensional lattice in discotics is similar to the condensation of one-dimensional

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positional order in smectics. We exploited the above-mentioned analogies in previous papers [9, 10], for developing a model of the phase transition between an hexagonal discotic phase and an intermediate nematic phase with sixfold orientational order ($N+6$ phase), and for computing the critical behaviour of Frank elastic constants. The Frank energy for a discotic liquid crystal shows, beyond the ordinary elastic modes of distortions of the director, some terms associated with strains of the field Ω_z, which describes local rotations of the lattice around the director (conventionally the $\hat{z}$ axis) [6, 10]. We refer to [9] for a more detailed discussion of the above-mentioned model and, in particular, for an explanation of the reasons for assuming such an intermediate nematic phase in the melting of a hexagonal discotic phase.

The proposed defect model [5] begins with the model free energy derived in [9, 10], which can be reduced to the case of a phase-only order parameter. The full elastic energy of the discotic liquid crystal so derived is analogous to the mixed elastic energy of smectics [11]. We therefore applied the general theory of Nelson and Toner [4] and derived the dislocation part of the free energy, which, in the hydrodynamic limit, becomes the free energy of the $N+6$ phase. From the dislocation free energy one can calculate the interaction energy between two transversal edge dislocations, which is analogous to the interaction energy between two edge dislocations in smectics. In the previous paper [5], as a first approximation, we neglected the contribution of longitudinal edge dislocations to the dislocation free energy, because their core energy is very large, by scaling arguments, and thus it is very hard to excite such defect lines.

The present paper is devoted to a more general treatment of the defect model, which includes the contribution of longitudinal edge dislocations. We will derive the full dislocation free energy and will show that, in the hydrodynamic limit, it becomes the full free energy of the $N+6$ phase, also including the terms associated with the torsion described by Ω_z. These terms are absent in the previous version, because of neglecting longitudinal edge dislocations, and they explicitly show the presence of sixfold rotational order in the plane orthogonal to the director.

We point out that, even if the defect unbinding transition described in this paper is assumed to be continuous, we cannot rule out the possibility of a first-order melting transition. In fact, Landau theory would imply that this transition is first order, rather than continuous. On the other hand, at present, we are not able to provide a renormalisation group calculation relative to our defect model. Therefore, we cannot state the existence of a stable fixed point, which would make the transition second order. Then we have to conclude that the transition may be first order.

The phase-only free energy for a discotic liquid crystal is briefly reviewed in § 2. In § 3 we develop the defect model, and show that a discotic liquid crystal permeated by an equilibrium density of unbound dislocation loops behaves like a nematic liquid crystal in the $N+6$ phase. In § 4 we calculate some interaction energies between dislocations.

2. Phase-only free energy

The order parameter for the condensation of the two-dimensional hexagonal lattice [9] is a triple mass-density wave:

$$\delta\rho(\boldsymbol{r}) = \sum_{i=1}^{3} \eta_i(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{q}_i \cdot \boldsymbol{r}) + \mathrm{cc} \tag{1}$$

where the reciprocal lattice vectors $\boldsymbol{q}_i$ are defined in [9]. The full free energy of a discotic liquid crystal is [5, 9, 10]

$$F = F_1 + F_2 + F_3 \tag{2a}$$

with

$$F_1 = \int \mathrm{d}^3r\left[A\sum_{i=1}^{3}|\eta_i(\boldsymbol{r})|^2 + B\eta_1(\boldsymbol{r})\eta_2(\boldsymbol{r})\eta_3(\boldsymbol{r}) + C_1\left(\sum_{i=1}^{3}|\eta_i(\boldsymbol{r})|^2\right)^2 + C_2\sum_{i=1}^{3}|\eta_i(\boldsymbol{r})|^4\right] \tag{2b}$$

$$F_2 = \int \mathrm{d}^3r\left\{\frac{1}{2M_\parallel}\sum_{i=1}^{3}|[\nabla_z + \mathrm{i}\boldsymbol{q}_i\cdot\delta\boldsymbol{m}(\boldsymbol{r})]\eta_i(\boldsymbol{r})|^2 + \frac{1}{2M_\perp}\sum_{i=1}^{3}|[\boldsymbol{\nabla}_\perp - \mathrm{i}\Omega_z(\boldsymbol{r})\boldsymbol{m}_0\times\boldsymbol{q}_i]\eta_i(\boldsymbol{r})|^2\right\} \tag{2c}$$

$$F_3 = \frac{1}{2}\int \mathrm{d}^3r[K_1(\mathrm{div}\,\delta\boldsymbol{m})^2 + K_2(\boldsymbol{m}_0\cdot\mathrm{rot}\,\delta\boldsymbol{m})^2 + K_3(\boldsymbol{m}_0\times\mathrm{rot}\,\delta\boldsymbol{m})^2 + \gamma_1(\partial\Omega_z/\partial z)^2 + \gamma_2(\boldsymbol{\nabla}_\perp\Omega_z)^2 + \gamma_3(\boldsymbol{m}_0\cdot\mathrm{rot}\,\delta\boldsymbol{m})(\partial\Omega_z/\partial z)] \tag{2d}$$

where Ω_z describes the local orientation of the two-dimensional lattice, $\boldsymbol{m}_0$ is the director parallel to the liquid rods ($\hat{z}$ axis), and $\delta\boldsymbol{m}$ is a small fluctuation of $\boldsymbol{m}_0$.

The phase-only order parameter is suitable for the ordered phase in the presence of dislocations, because they decorrelate only the phase of the order parameter given in (1). It is given by [9]

$$\eta_i(\boldsymbol{r}) = \eta_0\exp[-\mathrm{i}\boldsymbol{q}_i\cdot\boldsymbol{u}(\boldsymbol{r})] \tag{3}$$

where η_0 is the constant amplitude, and $\boldsymbol{u}(\boldsymbol{r})$ is the fluctuation of the local displacement of the lattice in the XY plane. Substituting (3) in (2), we obtain the phase-only free energy. Equation (2*b*) becomes a constant, which can be neglected without loss of generality. The elastic energy F_2, (2*c*), by carrying out the sum over i [9], becomes

$$F_2 = \int \mathrm{d}^3r\left(\frac{3\eta_0^2}{4M_\parallel}q_0^2[\nabla_z\boldsymbol{u}(\boldsymbol{r}) - \delta\boldsymbol{m}(\boldsymbol{r})]^2 + \frac{3\eta_0^2}{4M_\perp}q_0^2\{u_{ik}(\boldsymbol{r})u_{ik}(\boldsymbol{r}) + 2[\Omega_z(\boldsymbol{r}) - \tfrac{1}{2}(\mathrm{rot}\,\boldsymbol{u}(\boldsymbol{r}))_z]^2\}\right) \tag{4}$$

where q_0 is defined in (7) of [9], and

$$u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right) \tag{5}$$

is the planar strain tensor of the lattice, with i, $k = x$, y.

The local equilibrium values of $\delta\boldsymbol{m}$ and Ω_z, by minimising the free energy in (4), are

$$\delta\boldsymbol{m}(\boldsymbol{r}) = \nabla_z\boldsymbol{u}(\boldsymbol{r}) \tag{6}$$

$$\Omega_z(\boldsymbol{r}) = \tfrac{1}{2}(\mathrm{rot}\,\boldsymbol{u}(\boldsymbol{r}))_z. \tag{7}$$

Inserting (6) and (7) in (4), we obtain the local equilibrium elastic energy of the lattice:

$$F_2 = \int \mathrm{d}^3r\,\tfrac{1}{2}Cu_{ik}(\boldsymbol{r})u_{ik}(\boldsymbol{r}) \tag{8}$$

with

$$C = \frac{3}{2} \frac{\eta_0^2}{M_\perp} q_0^2. \tag{9}$$

Notice that, for this particular model, the shear and compression stiffnesses of the two-dimensional lattice are equal and given by (9). Substituting the local equilibrium values of $\delta \boldsymbol{m}$ and Ω_z, respectively, (6) and (7), in the Frank elastic energy, (2*d*), we have

$$F_3 = \int d^3r \, \tfrac{1}{2}\{K_1(\nabla_z \operatorname{div} \boldsymbol{u})^2 + K_0[\nabla_z(\operatorname{rot} \boldsymbol{u})_z]^2 + \tfrac{1}{4}\gamma_2[\boldsymbol{\nabla}_\perp(\operatorname{rot} \boldsymbol{u})_z]^2 + K_3[(\partial^2 u_x/\partial z^2)^2 + (\partial^2 u_y/\partial z^2)^2]\} \tag{10}$$

with

$$K_0 = K_2 + \tfrac{1}{4}\gamma_1 + \tfrac{1}{2}\gamma_3. \tag{11}$$

Equations (8) and (10) give $F_2 + F_3$ as the full elastic energy of the discotic liquid crystal, from which we will start, in the next section, by developing the defect model. It is analogous to the mixed elastic energy of smectics [11].

3. Melting of a discotic liquid crystal

The following can be considered as an application of the Nelson–Toner theory of dislocation-mediated melting [4] to our model of a discotic liquid crystal [9, 10].

Dislocation lines are topological singularities in the displacement field $\boldsymbol{u}$, characterised by a non-vanishing contour integral of $\boldsymbol{u}$ around such a line:

$$\oint d\boldsymbol{u} = -\boldsymbol{b} \tag{12}$$

which defines the Burger's vector $\boldsymbol{b}$, which in our case is a planar vector. The differential version of (12) is [4, 12]

$$\varepsilon_{ilm} \frac{\partial W_{mk}(\boldsymbol{r})}{\partial x_l} = -\tau_i b_k \delta^{(2)}(\boldsymbol{\xi}) \tag{13}$$

where $\delta^{(2)}(\boldsymbol{\xi})$ is a two-dimensional δ function of the radius vector $\boldsymbol{\xi}$ taken from the axis of the dislocation line in a plane orthogonal to the tangent vector $\boldsymbol{\tau}$, and

$$W_{mk}(\boldsymbol{r}) = \partial u_k(\boldsymbol{r})/\partial x_m \tag{14}$$

is the distortion tensor. At wavelengths long compared to the spacing between dislocation lines, we can ignore the discrete nature of dislocation lines. By averaging over a small volume containing many dislocations, (13) becomes

$$\varepsilon_{ilm} \frac{\partial W_{mk}(\boldsymbol{r})}{\partial x_l} = -\rho_{ik}(\boldsymbol{r}) \tag{15}$$

which defines $\rho_{ik}(\boldsymbol{r})$ as the density of Burger's vector carried by dislocation lines. Near the transition temperature the system should contain a large number of unbound dislocation loops of arbitrary size, and in this limit the density of dislocations $\rho_{ik}(\boldsymbol{r})$ can be considered a continuous tensor field. The density of dislocations is subject to the constraint

$$\partial \rho_{ik}(\boldsymbol{r})/\partial x_i = 0 \tag{16}$$

which follows directly from (15) and amounts to the conservation of Burger's vector. In our case, the second index of W_{ik} and ρ_{ik} can be only x, y, since the lattice is two dimensional.

Making a Fourier transform of (15), and solving for W_{ik}, we obtain

$$W_{ik}(\boldsymbol{q}) = \mathrm{i}q_i\psi_k(\boldsymbol{q}) - \mathrm{i}\varepsilon_{isj}(q_s/q^2)\rho_{jk}(\boldsymbol{q}) \tag{17}$$

with the definition

$$\mathrm{i}\psi_k(\boldsymbol{q}) = q_m W_{mk}(\boldsymbol{q})/q^2 \tag{18}$$

where $\boldsymbol{\psi}(\boldsymbol{q})$ is a planar vector to be determined. The constraint, (16), in Fourier-transformed variables is

$$q_i\rho_{ik}(\boldsymbol{q}) = 0. \tag{19}$$

In the following we only consider the singular part of the distortion tensor W_{ik}, given by (17), which is due to the presence of dislocations, and neglect the smooth background phonon field, since phonon field and dislocations are decoupled in the full free energy [4]. Our purpose is to determine the vector $\boldsymbol{\psi}(\boldsymbol{q})$, (18), as a function of the dislocation density ρ_{ik}. Afterwards, inserting W_{ik} as a function of ρ_{ik} in the free energy, we will obtain the dislocation free energy.

The free energy $F_2 + F_3$ in (8) and (10) is a functional of derivatives of $\boldsymbol{u}$. Therefore, exploiting the definition of W_{ik}, (14), we obtain

$$\begin{aligned} F \equiv F_2 + F_3 = \int \mathrm{d}^3r [\![\tfrac{1}{8}C(W_{ik} + W_{ki})(W_{ik} + W_{ki}) \\ + \tfrac{1}{2}\{K_1(W_{xx,z} + W_{yy,z})^2 + K_0(W_{xy,z} - W_{yx,z})^2 + K_3(W_{zx,z}^2 + W_{zy,z}^2) \\ + \tfrac{1}{4}\gamma_2[(W_{xy,x} - W_{yx,x})^2 + (W_{xy,y} - W_{yx,y})^2]\}]\!] \end{aligned} \tag{20}$$

with $W_{ik,j} = \partial W_{ik}/\partial x_j$. For a given configuration of dislocation lines, $W_{ik}(\boldsymbol{r})$ must minimise the free energy (20). Exploiting the variational equation

$$\sum_{k,j} \frac{\mathrm{d}}{\mathrm{d}x_k}\left[\frac{\partial F}{\partial W_{ki}} - \frac{\mathrm{d}}{\mathrm{d}x_j}\frac{\partial F}{\partial W_{ki,J}}\right] = 0 \tag{21}$$

we obtain

$$\begin{aligned} C\left[\frac{\mathrm{d}}{\mathrm{d}x}W_{xx} + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}y}(W_{xy} + W_{yx})\right] \\ = K_1\frac{\mathrm{d}^2}{\mathrm{d}x\,\mathrm{d}z}(W_{xx,z} + W_{yy,z}) + K_0\frac{\mathrm{d}^2}{\mathrm{d}y\,\mathrm{d}z}(W_{yx,z} - W_{xy,z}) + K_3\frac{\mathrm{d}^2}{\mathrm{d}z^2}W_{zx,z} \\ + \tfrac{1}{4}\gamma_2\left[\frac{\mathrm{d}^2}{\mathrm{d}y\,\mathrm{d}x}(W_{yx,x} - W_{xy,x}) + \frac{\mathrm{d}^2}{\mathrm{d}y^2}(W_{yx,y} - W_{xy,y})\right] \end{aligned} \tag{22}$$

and an analogous equation by interchanging x with y. In Fourier space, the elastic free energy, (20), becomes

$$\begin{aligned} F = \frac{1}{2}\int \frac{\mathrm{d}^3q}{(2\pi)^3}[C(|W_{xx}|^2 + |W_{yy}|^2 + \tfrac{1}{2}|W_{xy} + W_{yx}|^2) + K_1q_z^2|W_{xx} + W_{yy}|^2 \\ + K_3q_z^2(|W_{zx}|^2 + |W_{zy}|^2) + (K_0q_z^2 + \tfrac{1}{4}\gamma_2q_\perp^2)|W_{xy} - W_{yx}|^2] \end{aligned} \tag{23}$$

where $\boldsymbol{q}_\perp$ is the projection of $\boldsymbol{q}$ in the XY plane, and the equilibrium equation (22) is

$$-C[q_x W_{xx} + \tfrac{1}{2}q_y(W_{xy} + W_{yx})] = K_1 q_x q_z^2(W_{xx} + W_{yy}) + q_y(K_0 q_z^2 + \tfrac{1}{4}\gamma_2 q_\perp^2)(W_{yx} - W_{xy}) + K_3 q_z^3 W_{zx} \qquad (24)$$

and an analogous equation is obtained by interchanging x with y.

In our model there are eight variables: ρ_{zx} and ρ_{zy} which are densities of longitudinal edge dislocations [8], ρ_{xy} and ρ_{yx} which are densities of transversal edge dislocations [8], ρ_{xx} and ρ_{yy} which are densities of screw dislocations [8], ψ_x and ψ_y defined in (18) as the part of W_{ik} longitudinal to the wavevector $\boldsymbol{q}$. These variables are constrained by four equations: the Burger's vector conservation (19) which amounts to two equations, and the two equilibrium equations, of which one is (24). Therefore we can express the free energy as a functional of four independent components of the tensor ρ_{ik}.

We explicitly write the constraint, (19), as

$$\rho_{zx} = -\frac{q_x}{q_z}\rho_{xx} - \frac{q_y}{q_z}\rho_{yx} \qquad (25a)$$

$$\rho_{zy} = -\frac{q_x}{q_z}\rho_{xy} - \frac{q_y}{q_z}\rho_{yy}. \qquad (25b)$$

The components of (17) are

$$W_{xx} = \mathrm{i}q_x\psi_x + \mathrm{i}\frac{q_z}{q^2}\rho_{yx} - \mathrm{i}\frac{q_y}{q^2}\rho_{zx} \qquad (26a)$$

$$W_{yy} = \mathrm{i}q_y\psi_y - \mathrm{i}\frac{q_z}{q^2}\rho_{xy} + \mathrm{i}\frac{q_x}{q^2}\rho_{zy} \qquad (26b)$$

$$W_{xy} = \mathrm{i}q_x\psi_y + \mathrm{i}\frac{q_z}{q^2}\rho_{yy} - \mathrm{i}\frac{q_y}{q^2}\rho_{zy} \qquad (26c)$$

$$W_{yx} = \mathrm{i}q_y\psi_x - \mathrm{i}\frac{q_z}{q^2}\rho_{xx} + \mathrm{i}\frac{q_x}{q^2}\rho_{zx} \qquad (26d)$$

$$W_{zx} = \mathrm{i}q_z\psi_x - \mathrm{i}\frac{q_x}{q^2}\rho_{yx} + \mathrm{i}\frac{q_y}{q^2}\rho_{xx} \qquad (26e)$$

$$W_{zy} = \mathrm{i}q_z\psi_y + \mathrm{i}\frac{q_y}{q^2}\rho_{xy} - \mathrm{i}\frac{q_x}{q^2}\rho_{yy} \qquad (26f)$$

and the definition of $\boldsymbol{\psi}$, (18), is

$$\mathrm{i}\psi_x = \frac{1}{q^2}(q_x W_{xx} + q_y W_{yx} + q_x W_{zx}) \qquad (27a)$$

$$\mathrm{i}\psi_y = \frac{1}{q^2}(q_y W_{yy} + q_x W_{xy} + q_z W_{zy}). \qquad (27b)$$

Now it is a matter of algebra, tedious and very long to be carried out but straightforward. We have to solve the equilibrium equations (24) and its analogues for W_{zx} and W_{zy}, and insert them in (27). Then we substitute (26a–d) in (27), and also exploiting (25), we obtain ψ_x and ψ_y as functions of ρ_{xx}, ρ_{yy}, ρ_{xy} and ρ_{yx}, which are taken as the four independent dislocation densities. Such expressions of ψ_x and ψ_y, and the following expressions of W_{ik}, are very cumbersome and not interesting enough to report here. We directly write the quadratic invariant combinations of W_{ik} in terms of which the free energy, (23), is given:

$$|W_{xy}-W_{yx}|^2=\frac{|K_3q_z^4\,\mathrm{Tr}\,\rho+Cq_\perp^2\,\mathrm{Tr}\,P\rho|^2}{q_z^2(K_3q_z^4+K_0q_z^2q_\perp^2+\frac{1}{4}\gamma_2q_\perp^4+\frac{1}{2}Cq_\perp^2)^2} \tag{28}$$

$$|W_{xx}+W_{yy}|^2=\frac{|K_3q_z^4\,\mathrm{Tr}\,\varepsilon\rho+Cq_\perp^2\,\mathrm{Tr}\,\varepsilon P\rho|^2}{q_z^2(K_3q_z^4+K_1q_z^2q_\perp^2+Cq_\perp^2)^2} \tag{29}$$

$$|W_{zx}|^2+|W_{zy}|^2=\frac{|(K_0q_z^2q_\perp^2+\frac{1}{4}\gamma_2q_\perp^4+\frac{1}{2}Cq_\perp^2)\,\mathrm{Tr}\,\rho-Cq_\perp^2\,\mathrm{Tr}\,P\rho|^2}{q_\perp^2(K_3q_z^4+K_0q_z^2q_\perp^2+\frac{1}{4}\gamma_2q_\perp^4+\frac{1}{2}Cq_\perp^2)^2}+\frac{|(K_1q_z^2q_\perp^2+Cq_\perp^2)\,\mathrm{Tr}\,\varepsilon\rho-Cq_\perp^2\,\mathrm{Tr}\,\varepsilon P\rho|^2}{q_\perp^2(K_3q_z^4+K_1q_z^2q_\perp^2+Cq_\perp^2)^2} \tag{30}$$

$$|W_{xx}|^2+|W_{yy}|^2+\tfrac{1}{2}|W_{xy}+W_{yx}|^2=\frac{1}{2}\frac{|K_3q_z^4\,\mathrm{Tr}\,\rho-2(K_3q_z^4+K_0q_z^2q_\perp^2+\frac{1}{4}\gamma_2q_\perp^4)\,\mathrm{Tr}\,P\rho|^2}{q_z^2(K_3q_z^4+K_0q_z^2q_\perp^2+\frac{1}{4}\gamma_2q_\perp^4+\frac{1}{2}Cq_\perp^2)^2}+\frac{|K_3q_z^4\,\mathrm{Tr}\,\varepsilon\rho-(K_3q_z^4+K_1q_z^2q_\perp^2)\,\mathrm{Tr}\,\varepsilon P\rho|^2+(K_3q_z^4+K_1q_z^2q_\perp^2+Cq_\perp^2)^2|\mathrm{Tr}\,\varepsilon P\rho|^2}{q_z^2(K_3q_z^4+K_1q_z^2q_\perp^2+Cq_\perp^2)^2} \tag{31}$$

with

$$P_{ik}=\frac{q_iq_k}{q_\perp^2}\qquad i,k=x,y \tag{32}$$

$$\mathrm{Tr}\,\rho=\rho_{xx}+\rho_{yy} \tag{33}$$

$$\mathrm{Tr}\,P\rho=\frac{1}{q_\perp^2}[q_x^2\rho_{xx}+q_y^2\rho_{yy}+q_xq_y(\rho_{xy}+\rho_{yx})] \tag{34}$$

$$\mathrm{Tr}\,\varepsilon P\rho=\frac{1}{q_\perp^2}[q_y^2\rho_{yx}-q_x^2\rho_{xy}+q_xq_y(\rho_{xx}-\rho_{yy})] \tag{35}$$

$$\mathrm{Tr}\,\varepsilon\rho=\rho_{yx}-\rho_{xy} \tag{36}$$

ε being the antisymmetric unit tensor in two dimensions with $\varepsilon_{xy}=-\varepsilon_{yx}=1$, $\varepsilon_{xx}=\varepsilon_{yy}=0$. We observe that (33)-(36) are the only independent invariants linear in ρ_{ik} that can be built with ρ_{ik} and $\mathbf{q}_\perp$.

Substituting (28)-(31) in (23), the free energy becomes

$$F_D=F_{D1}+F_{D2} \tag{37a}$$

with

$$F_{D1}=\frac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}[q_z^2q_\perp^2(K_3q_z^4+K_1q_z^2q_\perp^2+Cq_\perp^2)]^{-1}[K_3q_z^4(K_1q_z^2q_\perp^2+Cq_\perp^2)|\mathrm{Tr}\,\varepsilon\rho|^2+Cq_\perp^2[2(K_3q_z^4+K_1q_z^2q_\perp^2)+Cq_\perp^2]|\,\mathrm{Tr}\,\varepsilon P\rho|^2-K_3q_z^4Cq_\perp^2(\mathrm{Tr}\,\varepsilon P\rho\,\mathrm{Tr}\,\varepsilon\rho^*+\mathrm{cc})] \tag{37b}$$

which is the K_1-controlled term, and

$$F_{D2}=\frac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}[q_z^2q_\perp^2(K_3q_z^4+K_0q_z^2q_\perp^2+\tfrac{1}{4}\gamma_2q_\perp^4+\tfrac{1}{2}Cq_\perp^2)]^{-1}$$
$$\times[K_3q_z^4(K_0q_z^2q_\perp^2+\tfrac{1}{4}\gamma_2q_\perp^4+\tfrac{1}{2}Cq_\perp^2)|\operatorname{Tr}\rho|^2$$
$$+2Cq_\perp^2(K_3q_z^4+K_0q_z^2q_\perp^2+\tfrac{1}{4}\gamma_2q_\perp^4)|\operatorname{Tr}P\rho|^2$$
$$-K_3q_z^4Cq_\perp^2(\operatorname{Tr}P\rho\operatorname{Tr}\rho^*+\mathrm{cc})] \tag{37c}$$

which is the (K_0, γ_2)-controlled term. Equations (37) give the dislocation part of the free energy for a discotic liquid crystal. Now we have to add the phenomenological core energy [4] E_s of screw dislocations, E_e of transversal edge dislocations and E_0 of longitudinal edge dislocations. As usual, we have

$$F_{\mathrm{core}}=\frac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}[2E_s(|\rho_{xx}|^2+|\rho_{yy}|^2)+2E_e(|\rho_{xy}|^2+|\rho_{yx}|^2)+2E_0(|\rho_{zx}|^2+|\rho_{zy}|^2)]. \tag{38}$$

By scaling arguments, similar to that employed by Nelson and Toner [4], we have (see also [5])

$$E_s\sim E_e\sim\xi_\parallel \tag{39a}$$
$$E_0\sim\xi_\parallel^{-1}\xi_\perp^2 \tag{39b}$$

where $\xi_\parallel$ and $\xi_\perp$ are the correlation lengths, respectively, parallel and orthogonal to the director. Therefore we can put $E_s=E_e\equiv E_c$, in the renormalised sense, and (38) becomes

$$F_{\mathrm{core}}=\frac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}[2E_c(|\rho_{xx}|^2+|\rho_{yy}|^2+|\rho_{xy}|^2+|\rho_{yx}|^2)+2E_0(|\rho_{zx}|^2+|\rho_{zy}|^2)] \tag{40}$$

which is given in terms of quadratic invariant combinations of ρ_{ik}. Expressing ρ_{zx} and ρ_{zy} with (25), and using the same quadratic invariants in terms of which F_D, (37), is given, the core free energy of dislocations can be written as

$$F_{\mathrm{core}}=\frac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\bigg(2E_0\frac{q_\perp^2}{q_z^2}(|\operatorname{Tr}P\rho|^2+|\operatorname{Tr}\varepsilon P\rho|^2)$$
$$+2E_c[|\operatorname{Tr}\rho|^2+2|\operatorname{Tr}P\rho|^2-(\operatorname{Tr}P\rho\operatorname{Tr}\rho^*+\mathrm{cc})+|\operatorname{Tr}\varepsilon\rho|^2+2|\operatorname{Tr}\varepsilon P\rho|^2$$
$$-(\operatorname{Tr}\varepsilon P\rho\operatorname{Tr}\varepsilon\rho^*+\mathrm{cc})]\bigg). \tag{41}$$

Adding F_{core}, (41), to F_D, (37), we obtain the full dislocation free energy for a discotic liquid crystal. Such a free energy can be reduced to the free energy of the $N+6$ phase [6, 10], at long enough wavelengths [4]. In fact we take the hydrodynamic limit $q\to 0$, or $\lambda q\ll 1$, of the full dislocation free energy, where λ is defined as

$$\lambda=\left(\frac{K}{C}\right)^{1/2} \tag{42}$$

with K any one of the Frank constants K_1, K_0, K_3, γ_2.

It is tedious but straightforward to evaluate correlation functions of δm_x, δm_y and Ω_z in the presence of continuous density of dislocations, making use of (28), (30), (37), (41), and exploiting also (6) and (7), and the definition of W_{ik}, (14), which imply $W_{zx}=\delta m_x$, $W_{zy}=\delta m_y$, and $|W_{xy}-W_{yx}|=2\Omega_z$. In the hydrodynamic limit, and in the approximation $E_0 \gg E_c \gg K_3$ which follows from scaling arguments [5], one finds that the fluctuations are described by

$$F_{N+6} = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}\{(K_3q_z^2 + 2E_cq_\perp^2)(|\delta m_x|^2 + |\delta m_y|^2) + (4K_0'q_z^2 + \gamma_2'q_\perp^2)|\Omega_z|^2 - 2E_cq_z[(q_x\delta m_y^* - q_y\delta m_x^*)\Omega_z + \text{cc}]\} \tag{43}$$

with

$$\gamma_2' = \gamma_2 + 2E_0 \tag{44}$$

$$K_0' = K_0 + \tfrac{1}{2}E_c. \tag{45}$$

Equation (43) is the free energy of the $N+6$ phase, with $K_1 = K_2 = 2E_c$ and $\gamma_3 = -2E_c$. The dislocation melted phase is actually a $N+6$ phase, as the Ω_z terms in (43) explicitly shows, and having lost any stiffness to shear is a liquid. In particular, note that (43) is just like (2*d*), and therefore has the symmetry of the free energy of the $N+6$ phase [6, 10], whose elastic terms represent the residual sitffness to torsion. If one does not take the $E_0 \gg E_c \gg K_3$ limit, one gets more complex expressions of the various elastic constants in terms of the dislocation parameters, which are not very interesting to be reported here. Anyway, the free energy has still the form of (2*d*), as is even clear on symmetry grounds. So we have shown that a discotic liquid crystal with a finite density of unbound dislocation loops does indeed behave like a mematic liquid crystal in the $N+6$ phase.

We observe that $K_1 = K_2 = 2E_c$ and (39*a*) give

$$K_1 \sim K_2 \sim \xi_\parallel \tag{46}$$

while (44) and (39*b*) give the critical enhancement of γ_2:

$$\gamma_2 \sim \xi_\parallel^{-1}\xi_\perp^2. \tag{47}$$

Equations (46) and (47) are in accordance with the critical behaviour of Frank constants, derived in [9, 10] on the basis of mean-field theory.

At last, we have to comment on the character of the defect unbinding transition, which has been assumed second order. Actually, according to Landau theory, the transition is predicted to be first order, because of the cubic term in (2*b*). Renormalisation group calculation applied to our defect model is not, at present, available, so that we cannot conclude in favour of the existence of a stable fixed point. Therefore, we point out that the transition may be first order.

4. Interaction energies between dislocations

The dislocation free energy F_D, (37), can be considered as the interaction energy between dislocations, which are described by the continuous density ρ_{ik}. Let F_D be written as

$$F_D = \frac{1}{2}\int \frac{d^3q}{(2\pi)^3} U_{ij,kl}(\boldsymbol{q})\rho_{ij}(\boldsymbol{q})\rho_{kl}^*(\boldsymbol{q}) \tag{48}$$

where $U_{ij,kl}$ is a pair interaction energy [13]. As a particular case, we can consider only two dislocations in the bulk, in order to calculate their coupling energy. The interaction energy for unit length between two transversal edge dislocations parallel, e.g., to the $\hat{y}$ axis is therefore (see also [13])

$$U_{ll}(x, z) = a^2 \int\int_{-\infty}^{+\infty} [U_{yx,yx}(\boldsymbol{q})]_{q_y=0} \exp[\mathrm{i}(xq_x + zq_z)] \frac{\mathrm{d}q_x}{2\pi}\frac{\mathrm{d}q_z}{2\pi} \qquad (49)$$

where a is the spacing of the lattice. From the examination of (37) and taking account of the expressions of the invariants in (33)-(36), one can get $U_{yx,yx}(\boldsymbol{q})$. The result is

$$U_{ll}(x, z) = a^2 \int\int_{-\infty}^{+\infty} \frac{K_3 q_z^2(C + K_1 q_z^2)}{K_3 q_z^4 + q_x^2(C + K_1 q_z^2)} \exp[\mathrm{i}(xq_x + zq_z)] \frac{\mathrm{d}q_x}{2\pi}\frac{\mathrm{d}q_z}{2\pi} \qquad (50)$$

which is the same as (44) of [5]. For large z compared to $\lambda_1 = (K_1/C)^{1/2}$ ($\lambda_1 q_z \ll 1$), we have [5]

$$U_{ll}(x, z) \simeq a^2 C \int\int_{-\infty}^{+\infty} \frac{K_3 q_z^2}{K_3 q_z^4 + C q_x^2} \exp[\mathrm{i}(xq_x + zq_z)] \frac{\mathrm{d}q_x}{2\pi}\frac{\mathrm{d}q_z}{2\pi} \qquad (51)$$

which is analogous to the interaction energy between edge dislocations in smectics, by interchanging x with z. Therefore, following the arguments of Nelson and Toner about anisotropic scaling [4], one should argue that $\xi_\perp \sim \xi_\parallel^2$, which would give $\nu_\perp = 2\nu_\parallel$, as in [5]. Nevertheless, those arguments themselves are known to be untrustworthy [14], while other more reliable theoretical approaches give isotropic scaling for smectics [14]. As regards our model of discotics, in the absence of an understanding of the renormalisation group fixed point, we cannot make any definite statement about the ratio $\nu_\parallel/\nu_\perp$.

In a similar way we can calculate the interaction energy for unit length between two screw dislocations parallel, e.g., to the $\hat{x}$ axis, which is

$$U_{ss}(y, z) = a^2 \int\int_{-\infty}^{+\infty} [U_{xx,xx}(\boldsymbol{q})]_{q_x=0} \exp[\mathrm{i}(yq_y + zq_z)] \frac{\mathrm{d}q_y}{2\pi}\frac{\mathrm{d}q_z}{2\pi} \qquad (52)$$

and then

$$U_{ss}(y, z) = a^2 \int\int_{-\infty}^{+\infty} \frac{K_3 q_z^2(\frac{1}{2}C + K_0 q_z^2 + \frac{1}{4}\gamma_2 q_y^2)}{K_3 q_z^4 + q_y^2(\frac{1}{2}C + K_0 q_z^2 + \frac{1}{4}\gamma_2 q_y^2)} \exp[\mathrm{i}(yq_y + zq_z)] \frac{\mathrm{d}q_y}{2\pi}\frac{\mathrm{d}q_z}{2\pi}. \qquad (53)$$

The interaction energy between a screw and a transversal edge dislocation, mutually parallel, vanishes, since, e.g.,

$$[U_{yx,yy}]_{q_y=0} = 0. \qquad (54)$$

Analogously, in a three-dimensional solid, a screw and an edge dislocation, mutually parallel, are not coupled.

Finally, it is interesting to calculate the coupling between two longitudinal edge dislocations, which are solid-like dislocations. For this purpose we have to take ρ_{zx}, ρ_{zy}, ρ_{yx}, ρ_{xy}, as independent densities, by solving (25) with respect to ρ_{xx} and ρ_{yy}, and substituting them in (37). We obtain, for the interaction energy for unit length between two longitudinal edge dislocations, with both Burger's vectors along the $\hat{x}$ axis,

$$U_{00}(x, y) = a^2 \int\int_{-\infty}^{+\infty} (Cq_y^2/q_\perp^4 + \gamma_2 q_x^2/q_\perp^2) \exp[i(xq_x + yq_y)] \frac{dq_x}{2\pi}\frac{dq_y}{2\pi} \qquad (55)$$

which, by performing the integral, becomes

$$U_{00}(x, y) = \frac{Ca^2}{4\pi}(-\ln r + x^2/r^2) + \frac{\gamma_2 a^2}{2\pi}\frac{y^2 - x^2}{r^4} \qquad (56)$$

with $r = (x^2 + y^2)^{1/2}$.

Note that the first term in (56) is the ordinary interaction between two dislocations in a two-dimensional solid, due to first-order elastic constants. The second term in (56), on the other hand, corresponds to the contribution of second-order elastic constants, just like the torsion constant γ_2, and should be present in a solid as well, if higher-order elastic constants were included in elastic theory of dislocations.

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