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1991 J. Phys.: Condens. Matter 3 1649

(http://iopscience.iop.org/0953-8984/3/11/022)

J. Phys.: Condens. Matter 3 (1991) 1649–1663. Printed in the UK

Disclination unbinding transition from the hexatic N + 6 phase to the nematic phase in discotic liquid crystals

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Received 14 June 1990, in final form 17 December 1990

Abstract. We investigate the disclination unbinding transition from the theoretically predicted hexatic N + 6 phase to the nematic phase in discotic liquid crystals. The free energy due to an equilibrium continuous density of disclinations in the hexatic N + 6 phase is derived. Two kinds of disclinations are considered, longitudinal wedge and twist disclinations, which decorrelate the sixfold orientational order, but do not break the cylindrical nematic order around the director. Two possible mechanisms for the transition are found. The longitudinal wedge free energy drives a transition of Kosterlitz type, which is the three-dimensional equivalent of the disclination unbinding transition in two-dimensional melting theory of Halperin and Nelson. Twist disclinations provide a different mechanism for the transition, which is peculiar to the hexatic phase as a quasi-two-dimensional system. The twist disclination free energy is not positive definite for some ranges of values of the Frank elastic constants. As a consequence, for strong coupling between the director distortions and the torsions around the axis of sixfold symmetry, a disclination unbinding instability, essentially due to repulsion between disclinations of opposite signs, develops in the system. In order to decide which of these two mechanisms is effective, we should know the physical values of the Frank constants in the hexatic phase.

1. Introduction

Recently there has been considerable interest in bond orientationally ordered phases [1–3] as intermediates between a fully disordered phase and a phase that is both orientationally and translationally ordered. For most of these phases there is as yet no 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 and have been proposed in a wide class of systems, including various kinds of liquid crystals, which show similar symmetry features despite different physical structures [3]. Stability against fluctuations of long-range orientational order is crucial for the actual existence of such new phases. Fluctuation-induced instability might be the reason why experimental observation of these phases is very difficult.

As regards discotic liquid crystals, we proposed a model for the melting of the hexagonal discotic phase into the nematic phase [4, 5], where we assumed an intermediate *hexatic* N + 6 *phase* [2, 4], which is still experimentally undiscovered. The hexatic phase is translationally invariant and therefore has homogeneous density like the ordinary nematic phase, but shows long-range sixfold orientational order around the director like the hexagonal discotic phase. The elastic stability of the N + 6 phase against fluctuation-induced breaking of long-range orientational order has been tested in a recent work [6].

We assumed such an intermediate phase because of some analogies with the two-dimensional melting theory of Halperin and Nelson [7]. As discussed in [4], the hexagonal discotic phase is a quasi-two-dimensional system consisting of an array of liquid columns parallel to each other and the axes of which are regularly positioned on a two-dimensional hexagonal lattice. The liquid-like behaviour along the columns stabilizes the two-dimensional lattice against thermal fluctuations.

In the previous works [4, 5], we considered the melting of the hexagonal discotic phase into the hexatic N + 6 phase, presenting also a defect model [8, 9] of this transition. Therefore we only dealt with the breaking of translational order. At such a transition the two-dimensional lattice of the hexagonal discotic phase is completely melted so that the hexatic phase, like an ordinary liquid, does not show resistance to shear. The orientational order, on the contrary, is maintained: the hexatic phase presents the same sixfold orientational order around the director as the hexagonal discotic phase, while the ordinary nematic phase shows cylindrical symmetry.

In the Halperin–Nelson theory of two-dimensional melting [7], two kinds of defects are considered: dislocations as defects of translational order and disclinations as defects of orientational order. Two second-order phase transitions are found. A transition, mediated by dissociation of dislocation–antidislocation pairs, occurs from the solid phase to an intermediate hexatic phase, which is translationally disordered but orientationally ordered. Another transition, mediated by unbinding of disclination–antidisclination pairs, takes place from the hexatic phase to the isotropic liquid phase. Such defect-mediated transitions have been extensively treated in several systems [1, 7, 10–12].

The present paper is devoted to developing a defect theory of the transition between the hexatic N + 6 phase and the nematic phase in discotic liquid crystals. The loss of orientational order is due to disclination unbinding, as in the Halperin–Nelson theory [7]. We shall consider the hexatic phase permeated by an equilibrium continuous density of unbound disclination loops, which decorrelate the sixfold orientational order and let the cylindrical order, typical of the nematic phase, alone. The derivation of the disclination free energy is somehow similar to that employed, in the dislocation unbinding transition, for obtaining the dislocation free energy [1, 8, 9].

The main result of this analysis is a new mechanism for the disclination unbinding transition, peculiar to the hexatic phase as a quasi-two-dimensional system. Normal stability of long-range orientational order requires some conditions on the Frank elastic constants [6]. Such a stability analysis involves long-wavelength non-singular fluctuations with respect to the uniform configuration. Disclinations, on the contrary, are non-homogeneous equilibrium configurations of the ordered medium which are singular along a line. The analysis of disclination energy imposes stronger conditions on the Frank constants. Therefore, the stability conditions against disclination unbinding can be violated even if the system is stable as regards non-singular fluctuations of orientational order.

The disclinations in the hexatic N + 6 phase are the same as in the hexagonal discotic phase, since these two phases share the same orientational symmetry. Beyond disclinations typical of a two-dimensional solid, like the so-called longitudinal wedge disclinations [13], there are the transverse wedge and twist disclinations [13], in which the modes of distortion of the nematic director are coupled to the strains of the two-dimensional lattice.

The hexatic phase is melted as regards the two-dimensional lattice, but it maintains a vestige of the singled out crystallographic axes in the hexagonal anisotropy. Therefore the nematic director is no longer sufficient to fix orientational order. We are forced to introduce a bond-angle field Ω_z, which gives the orientation of the local two-dimensional lattice in the plane orthogonal to the unperturbed nematic director $\boldsymbol{m}_0$, which is conventionally taken along the $\hat{z}$ axis. Such Ω_z can be defined as the rotation angle around the nematic director $\boldsymbol{m}_0$ between a given reciprocal lattice vector and a fixed $\hat{x}$ axis. In the hexatic phase there are no reciprocal lattice vectors, but only the 'directions' of such vectors, i.e. the crystallographic axes.

The full orientational order of the hexatic phase is therefore determined by the local rotation field $\boldsymbol{\Omega}$, which is defined as [4]

$$\boldsymbol{\Omega} = \Omega_z \boldsymbol{m}_0 + (\boldsymbol{m}_0 \times \delta\boldsymbol{m}) \tag{1}$$

where Ω_z is the local rotation of the two-dimensional lattice around $\boldsymbol{m}_0$, while $\delta\boldsymbol{m}$ is a small distortion of the unperturbed nematic director $\boldsymbol{m}_0$. The field $\boldsymbol{\Omega}$ locally fixes the orientation of the hexatic phase with respect to the uniform configuration in which Ω_z and $\delta\boldsymbol{m}$ vanish.

The longitudinal wedge disclinations [13] are characterized by $\delta\boldsymbol{m} = 0$ and only Ω_z is distorted (solid-like disclinations). In the transverse wedge and twist disclinations [13], on the contrary, the director distortions $\delta\boldsymbol{m}$ and the rotation strains of Ω_z are both involved. Longitudinal wedge disclination lines are straight lines along $\boldsymbol{m}_0$, while twist disclination lines lie along a direction orthogonal to $\boldsymbol{m}_0$. Both these kinds of disclinations are lines of singularities of the Ω_z component of $\boldsymbol{\Omega}$. Transverse wedge disclination lines, on the contrary, are orthogonal to $\boldsymbol{m}_0$ and are lines of singularities of a component of $\boldsymbol{\Omega}$ orthogonal to $\boldsymbol{m}_0$.

In the disclination unbinding transition from the hexatic N + 6 phase to the nematic phase only the longitudinal wedge and twist disclinations [13] play a role. In fact, the transverse wedge disclinations are characterized by large deformations of the nematic director [13], which undergoes a π rotation. In that way the transverse wedge disclinations would break the cylindrical nematic order too, making the system isotropic. Searching for the transition to the nematic phase, we therefore only consider the longitudinal wedge and twist disclinations. In those kinds of disclinations, the perturbations of the orientational order, $\delta\boldsymbol{m}$ and Ω_z, are small outside the disclination cores, so that they preserve $\boldsymbol{m}_0$ as the average nematic director and then the nematic order (figures 1 and 2). Thus equation (1), which assumes Ω_z and $\delta\boldsymbol{m}$ as small perturbations, makes sense in a perturbative approximation.

We shall derive the free energy due to an equilibrium density of disclinations in the hexatic N + 6 phase. The disclination density will be defined by considering the disclination lines as lines of topological singularities of the rotation field $\boldsymbol{\Omega}$. Since, as discussed above, we only deal with longitudinal wedge and twist disclinations, we will focus on Ω_z singularities. The curvature strains due to a finite density of disclinations, inserted in the Frank elastic energy of the hexatic phase previously obtained [5], give the disclination free energy. We then impose the equilibrium conditions to the elastic stresses yielded by disclinations, assuming an equilibrium continuous density of disclinations.

In fact, near the transition temperature, the system should contain a large number of unbound disclination loops of arbitrary size. Thus, the density of disclinations, in this limit, can be considered a continuous field. Finally, we get the free energy of the hexatic N + 6 phase permeated by an equilibrium continuous density of disclinations.

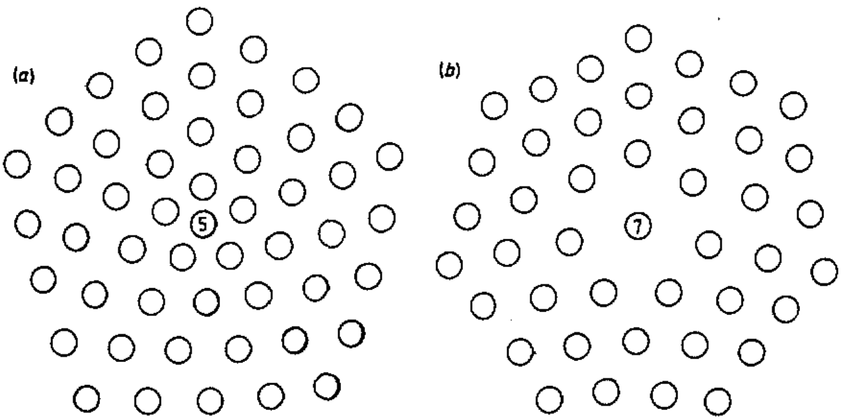

Figure 1. Longitudinal wedge disclinations of (*a*) $+\pi/3$ and (*b*) $-\pi/3$ of the planar hexagonal array of liquid columns. The tangent vector $\boldsymbol{\tau}$ of the singular core line is parallel to the director $\boldsymbol{m}_0$. Each circle represents the section of a liquid column in the plane orthogonal to $\boldsymbol{m}_0$, which remains undistorted (two-dimensional solid-like disclinations). Only the Ω_z angle of local orientation of the two-dimensional lattice undergoes distortions: the vector between two nearest neighbours rotates by (*a*) $+\pi/3$ and (*b*) $-\pi/3$ along any loop around the disclination core. As a consequence, the core sites of $+\pi/3$ and $-\pi/3$ disclinations are surrounded by five and seven nearest neighbours, respectively, while for every other site the number of nearest neighbours is six, as in a regular hexagonal lattice. The orientational configurations induced by disclinations in the hexatic phase are the same as in the hexagonal discotic phase to which the figures are referred, since the two phases share the same orientational symmetry.

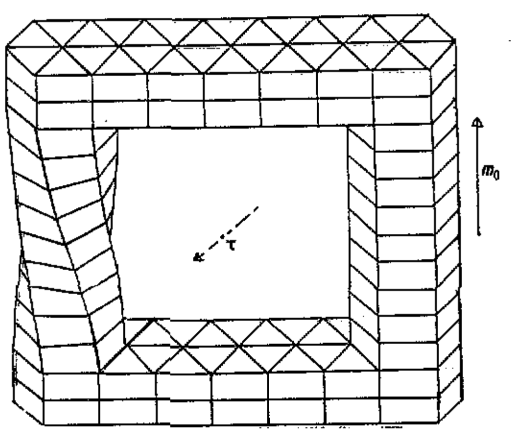

Figure 2. Twist disclination of $+\pi/3$. The tangent vector $\boldsymbol{\tau}$ of the disclination core line is orthogonal to the unperturbed director $\boldsymbol{m}_0$. For the sake of simplicity, the rotation is confined to a unique edge of the frame. Actually, if the elastic stresses are relaxed, the configuration of the rotation distortions spreads all over the plane orthogonal to the disclination line (see section 4). Each 'vertical' line represents a liquid column, while the 'horizontal' lines are the links of planar lattices. The twist disclination line is a line of singularities of the only Ω_i angle. However, it yields distortions of the director $\delta \boldsymbol{m}$, as well as Ω_z rotations of the local two-dimensional lattice, so that the liquid columns are just twisted. In this sense the twist disclination is typical of our quasi-two-dimensional system. Also this figure is referred to the hexagonal discotic phase, but the orientational configuration is the same as in the hexatic phase.

The contribution of longitudinal wedge disclinations to the above-mentioned free energy is completely similar to the free energy that drives the disclination unbinding transition in two-dimensional melting [7], since the longitudinal wedge disclinations are solid-like disclinations. Therefore, as regards longitudinal wedge disclinations, the transition should be of Kosterlitz type [10, 11].

However, we have to consider also the contribution due to twist disclinations, which are not solid-like. The twist disclination free energy is not positive definite for some ranges of values of the Frank elastic constants, which still fulfil the elastic stability conditions [6]. As a consequence, the interaction between disclinations of opposite signs can become repulsive, so yielding a twist disclination unbinding transition as a new type of phase transition.

At present, without direct knowledge of the ranges of values of physical parameters in the hexatic N + 6 phase, we are not able to state which of the two mechanisms described above is effective. We only conclude that there is the possibility of a disclination unbinding transition peculiar to the hexatic N + 6 phase as a quasi-two-dimensional system.

In section 2 we define the disclination density field. In section 3 we derive the disclination free energy, which drives the disclination unbinding transition from the hexatic N + 6 phase into the nematic phase. In section 4 we calculate the pair-interaction energy between disclinations and the deformations due to an isolated disclination. Finally, in the appendix, we explicitly calculate the interaction energy of twist disclinations.

2. Disclination density in the hexatic N + 6 phase

Disclination lines in the hexatic phase are topological singularities of the rotation field $\mathbf{\Omega}$ (equation (1)) characterized by a non-vanishing contour integral of $\mathbf{\Omega}$ around such a line. We only consider Ω_z singularities, and then longitudinal wedge and twist disclinations, since only this kind of singularity is effective in the disclination-mediated hexatic N + 6 phase to nematic phase transition. Thus our disclination lines are characterized by

$$\oint \mathrm{d}\Omega_z = 2\pi(n/6) \tag{2}$$

where the contour integral is made along any loop around such a line, and $n = \pm 1, \pm 2, \pm 3$ is an integer measure of the disclinicity of the line [7, 13]. In equation (2), n can take only the integer values $\pm 1, \pm 2, \pm 3$ in order to preserve locally the hexagonal symmetry.

Disclinations can be viewed as linear defects of orientational order, i.e. non-homogeneous equilibrium configurations of the ordered medium that are singular along a line. In section 4 we will compute the configuration of $\mathbf{\Omega}$ around such a singular line. A non-homogeneous configuration is characterized by a non-vanishing curvature strain tensor

$$A_{ij} = \partial A_j/\partial x_i \tag{3}$$

where the vector $\mathbf{A}$ is defined as

$$A_z = \Omega_z \qquad A_x = \delta m_x = \Omega_y \qquad A_y = \delta m_y = -\Omega_x. \tag{4}$$

Equation (2) can be written in terms of the curvature strain tensor as

$$\oint A_{kz}\, \mathrm{d}x_k = 2\pi(n/6). \tag{5}$$

The following is in full analogy with dislocation theory [1, 14]. The application of Stokes' theorem to equation (5) gives the differential version of (2),

$$\varepsilon_{ijk}\, \partial A_{kz}/\partial x_j = 2\pi(n/6)\tau_i \delta^{(2)}(\boldsymbol{\xi}) \tag{6}$$

where $\delta^{(2)}(\boldsymbol{\xi})$ is a two-dimensional δ function of the radius vector $\boldsymbol{\xi}$ taken from the axis of the disclination line in a plane orthogonal to the tangent vector $\boldsymbol{\tau}$. For longitudinal wedge disclinations $\boldsymbol{\tau}$ is along the unperturbed nematic director $\boldsymbol{m}_0$ ($\hat{z}$ axis), while for twist disclinations $\boldsymbol{\tau}$ is orthogonal to $\boldsymbol{m}_0$ [13].

For an arbitrary number of disclinations, one can define the disclination density

$$\boldsymbol{\alpha} = 2\pi \sum_a (n_a/6)\delta^{(2)}(\boldsymbol{\xi} - \boldsymbol{\xi}_a)\boldsymbol{\tau}_a \tag{7}$$

and then, by equation (6),

$$\alpha_i = \varepsilon_{ijk}\, \partial A_{kz}/\partial x_j. \tag{8}$$

The disclination density is subject to the constraint

$$\nabla \cdot \boldsymbol{\alpha} = 0 \tag{9}$$

which follows from (8) and amounts to the conservation of the disclinicity carried by disclination lines. As a consequence of equation (9), *the disclination lines must either close or terminate at external boundaries of the system.*

At a length scale long compared to the spacing between disclination lines, we can ignore the discrete nature of disclination lines and consider $\boldsymbol{\alpha}$ to be a continuous field. This is meaningful near the transition temperature, since the system contains a large number of disclination loops of arbitrary size.

Making a Fourier transform of (8) and solving for A_{iz}, we obtain

$$A_{iz}(\boldsymbol{q}) = q_i\psi(\boldsymbol{q}) + \mathrm{i}\varepsilon_{ijk}(q_j/q^2)\alpha_k(\boldsymbol{q}) \tag{10}$$

with

$$\psi(\boldsymbol{q}) = (q_i/q^2)A_{iz}(\boldsymbol{q}). \tag{11}$$

Equation (9) in Fourier space is

$$\boldsymbol{q} \cdot \boldsymbol{\alpha}(\boldsymbol{q}) = 0 \tag{12}$$

which means that $\boldsymbol{\alpha}(\boldsymbol{q})$ is transverse to $\boldsymbol{q}$. Let us note that α_z is the density of longitudinal wedge disclinations, while α_x and α_y are the densities of twist disclinations. By equation (9) or (12), $\boldsymbol{\alpha}$ has only two independent components.

3. Hexatic N + 6 phase with continuous density of disclinations

The full elastic energy associated with the rotation strains for a discotic liquid crystal in the hexatic N + 6 phase is [5]

$$F = \frac{1}{2}\int \mathrm{d}^3r\,[K_1(\mathrm{div}\,\delta\boldsymbol{m})^2 + K_2(\boldsymbol{m}_0 \cdot \mathrm{rot}\,\delta\boldsymbol{m})^2 + K_3(\boldsymbol{m}_0 \times \mathrm{rot}\,\delta\boldsymbol{m})^2 + \gamma_1(\nabla_z\Omega_z)^2 + \gamma_2(\nabla_\perp\Omega_z)^2 + 2\gamma_3(\boldsymbol{m}_0 \cdot \mathrm{rot}\,\delta\boldsymbol{m})(\nabla_z\Omega_z)] \tag{13}$$

where $\boldsymbol{\Omega}$ is the local rotation field defined in equation (1).

The elastic energy (13) in terms of the strain tensor A_{ij}, equation (3), is

$$F = \frac{1}{2}\int \mathrm{d}^3r\,[K_1(A_{xx} + A_{yy})^2 + K_2(A_{xy} - A_{yx})^2 + K_3(A_{zx}^2 + A_{zy}^2) + \gamma_1 A_{zz}^2 + \gamma_2(A_{xz}^2 + A_{yz}^2) + 2\gamma_3 A_{zz}(A_{xy} - A_{yx})]. \tag{14}$$

In the presence of disclinations, it is more suitable to express the elastic free energy as a functional of the strain tensor A_{ij}. In that way each component of A_{ij}, rather than each component of $\mathbf{\Omega}$ as in equation (13), can be treated as an independent fluctuating field variable. In fact, the singular components A_{iz} of the strain tensor, equation (10), cannot be represented by equation (3) everywhere. In the disclination cores $\boldsymbol{\alpha}$ does not vanish, while the representation (3) of A_{ij} in terms of $\mathbf{\Omega}$ components, by equation (8), would make $\boldsymbol{\alpha}$ vanishing everywhere. Therefore we have to consider A_{iz} as independent fields, which are not equivalent to a varying Ω_z, since disclination cores are lines of physical singularities of Ω_z. At the end of this section we will comment about such a choice of independent variables.

For a given configuration of disclination lines, $A_{ij}(\boldsymbol{r})$ must minimize the free energy (14). Exploiting the variational equation

$$\frac{\mathrm{d}}{\mathrm{d}x_i}\frac{\partial F}{\partial A_{ij}}=0 \tag{15}$$

we obtain the equilibrium equations

$$K_1\nabla_{\perp a}(A_{xx}+A_{yy})-\varepsilon_{ab}\nabla_{\perp b}[\gamma_3A_{zz}+K_2(A_{xy}-A_{yx})]+K_3\nabla_zA_{za}=0 \tag{16a}$$

$$\gamma_2\nabla_{\perp a}A_{az}+\gamma_1\nabla_zA_{zz}+\gamma_3\nabla_z(A_{xy}-A_{yx})=0 \tag{16b}$$

where ε_{ab} is the antisymmetric unit tensor in two dimensions and a, $b=x, y$ (sum over repeated indices a, b is implied). If one takes, respectively, the curl and the divergence in two dimensions (xy plane) of equation (16a), one gets

$$(K_2\nabla_\perp^2+K_3\nabla_z^2)\varepsilon_{ab}A_{ab}+\gamma_3\nabla_\perp^2A_{zz}=0 \tag{17}$$

$$(K_1\nabla_\perp^2+K_3\nabla_z^2)A_{aa}=0 \tag{18}$$

where we have exploited the relation $\nabla_iA_{ka}=\nabla_kA_{ia}$ with $a=x, y$, which follows from equation (3) for the non-singular components A_{ia} ($a\neq z$) of the strain tensor. Note that, here and in the following, the indices $i, j, k, \ldots$ are three-dimensional indices, while a, $b, c, \ldots$ are two-dimensional indices (in the xy plane).

In Fourier space, the elastic free energy (14) is

$$F=\frac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}[K_1|A_{aa}|^2+K_2|\varepsilon_{ab}A_{ab}|^2+K_3|A_{za}|^2+\gamma_1|A_{zz}|^2+\gamma_2|A_{az}|^2$$
$$+\gamma_3(A_{zz}^*\varepsilon_{ab}A_{ab}+\mathrm{cc})] \tag{19}$$

and the equilibrium equations (16b), (17) and (18) are, respectively,

$$\gamma_2q_{\perp a}A_{az}(\boldsymbol{q})+\gamma_1q_zA_{zz}(\boldsymbol{q})+\gamma_3q_z\varepsilon_{ab}A_{ab}(\boldsymbol{q})=0 \tag{20a}$$

$$(K_2q_\perp^2+K_3q_z^2)\varepsilon_{ab}A_{ab}(\boldsymbol{q})+\gamma_3q_\perp^2A_{zz}(\boldsymbol{q})=0 \tag{20b}$$

$$(K_1q_\perp^2+K_3q_z^2)A_{aa}(\boldsymbol{q})=0 \tag{20c}$$

with $\boldsymbol{q}_\perp=(q_x, q_y, 0)$. From equation (20$c$) we have

$$A_{aa}(\boldsymbol{q})=0 \tag{21}$$

which stands for div $\delta\boldsymbol{m}=0$. Therefore, in the presence of only twist and longitudinal wedge disclinations, at equilibrium, the splay mode of the director vanishes.

By solving (20*a*) and (20*b*) with respect to the singular components A_{az} of the strain tensor, we get

$$A_{zz} = \frac{-\gamma_2(K_2 q_\perp^2 + K_3 q_z^2)}{q_z[(K_2\gamma_1 - \gamma_3^2)q_\perp^2 + K_3\gamma_1 q_z^2]} q_{\perp a} A_{az} \tag{22}$$

$$\varepsilon_{ab} A_{ab} = \frac{\gamma_2\gamma_3 q_\perp^2}{q_z[(K_2\gamma_1 - \gamma_3^2)q_\perp^2 + K_3\gamma_1 q_z^2]} q_{\perp a} A_{az}. \tag{23}$$

Equation (23) gives the twist mode of the director at equilibrium as a function of the singular components of the strain tensor. In order to obtain A_{za}, which is the bend mode, at equilibrium, we exploit the relation $q_i A_{za} = q_z A_{ia}$, valid for non-singular components, which gives

$$A_{za} = -\varepsilon_{ab}(q_{\perp b} q_z / q_\perp^2)(\varepsilon_{cd} A_{cd}) \tag{24}$$

and then, by equation (23),

$$A_{za} = -\varepsilon_{ab} q_{\perp b} \frac{\gamma_2\gamma_3}{(K_2\gamma_1 - \gamma_3^2)q_\perp^2 + K_3\gamma_1 q_z^2} q_{\perp c} A_{cz}. \tag{25}$$

Substituting equations (21), (22), (23) and (25) in equation (19) we get the free energy at elastic equilibrium as a functional of the two independent components A_{az} of the strain tensor,

$$F = \tfrac{1}{2}\gamma_2 \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \left(\frac{\gamma_2(K_2 q_\perp^2 + K_3 q_z^2)}{[(K_2\gamma_1 - \gamma_3^2)q_\perp^2 + K_3\gamma_1 q_z^2] q_z^2} q_{\perp a} q_{\perp b} + \delta_{ab} \right) A_{az} A_{bz}^*. \tag{26}$$

If the equilibrium state is characterized by a continuous density of disclinations, the singular components A_{az} and A_{zz} of the strain tensor are given in terms of $\boldsymbol{\alpha}$ by equation (10). Taking account of the constraint (12), which allows only two independent components of $\boldsymbol{\alpha}$, and exploiting (22), which comes from the equilibrium equations, we can solve (10) with respect to the equilibrium disclination density:

$$q_{\perp a} A_{az} = \frac{-\mathrm{i} q_z q_\perp [(K_2\gamma_1 - \gamma_3^2)q_\perp^2 + K_3\gamma_1 q_z^2]}{K_3\gamma_1 q_z^4 + K_2\gamma_2 q_\perp^4 + (K_3\gamma_2 + K_2\gamma_1 - \gamma_3^2) q_\perp^2 q_z^2} \alpha_t \tag{27a}$$

$$A_{az}^* A_{az} = \frac{1}{q_\perp^2} |\alpha_z|^2 + q_z^2 \frac{(K_2\gamma_1 - \gamma_3^2)q_\perp^2 + K_3\gamma_1 q_z^2}{K_3\gamma_1 q_z^4 + K_2\gamma_2 q_\perp^4 + (K_3\gamma_2 + K_2\gamma_1 - \gamma_3^2) q_\perp^2 q_z^2} |\alpha_t|^2. \tag{27b}$$

We have chosen α_z and α_t as independent components of disclination density: α_z is the density of longitudinal wedge disclinations while α_t, defined as

$$\alpha_t = (1/q_\perp)(q_x \alpha_y - q_y \alpha_x) \tag{28}$$

is the density of twist disclinations transverse to $\boldsymbol{q}_\perp$.

Substituting equations (27) in (26) we get the disclination free energy at equilibrium,

$$F_{\mathrm{D}}=\frac{1}{2}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\left(\frac{\gamma_2}{q_\perp^2}|\alpha_z|^2 + \gamma_2\frac{(K_2\gamma_1-\gamma_3^2)q_\perp^2+K_3\gamma_1q_z^2}{K_3\gamma_1q_z^4+K_2\gamma_2q_\perp^4+(K_3\gamma_2+K_2\gamma_1-\gamma_3^2)q_\perp^2q_z^2}|\alpha_t|^2\right). \tag{29}$$

Then we have to add the phenomenological core energy

$$F_{\mathrm{core}}=\int\frac{\mathrm{d}^3q}{(2\pi)^3}[E_{\mathrm{W}}|\alpha_z|^2+E_{\mathrm{T}}(|\alpha_x|^2+|\alpha_y|^2)] \tag{30}$$

where E_{W} and E_{T} are the core energies of, respectively, a longitudinal wedge disclination and a twist disclination. At last we obtain the full free energy of the hexatic N + 6 phase permeated by an equilibrium continuous density of disclinations,

$$F_{\mathrm{tot}}=F_{\mathrm{D}}+F_{\mathrm{core}}. \tag{31}$$

The disclination free energy (29) can be written as

$$F_{\mathrm{D}}=\frac{1}{2}\iint\mathrm{d}^3r_1\,\mathrm{d}^3r_2\,\alpha_i(\boldsymbol{r}_1)U_{ij}(\boldsymbol{r}_1-\boldsymbol{r}_2)\alpha_j(\boldsymbol{r}_2) \tag{32}$$

with

$$U_{ij}(\boldsymbol{r})=\int\frac{\mathrm{d}^3q}{(2\pi)^3}U_{ij}(\boldsymbol{q})\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \tag{33}$$

and

$$U_{ij}(\boldsymbol{q})=U_{zz}(\boldsymbol{q})\delta_{zi}\delta_{zj}+U_{\mathrm{tt}}(\boldsymbol{q})(\delta_{\perp ij}-\hat{q}_{\perp i}\hat{q}_{\perp j}) \tag{34}$$

where $\hat{\boldsymbol{q}}_\perp=\boldsymbol{q}_\perp/q_\perp$, $\delta_{\perp ij}$ is the two-dimensional (in the xy plane) Kronecker δ, and

$$U_{zz}(\boldsymbol{q})=\gamma_2/q_\perp^2 \tag{35a}$$

$$U_{\mathrm{tt}}(\boldsymbol{q})=\frac{\gamma_2[(K_2\gamma_1-\gamma_3^2)q_\perp^2+K_3\gamma_1q_z^2]}{K_3\gamma_1q_z^4+K_2\gamma_2q_\perp^4+(K_3\gamma_2+K_2\gamma_1-\gamma_3^2)q_\perp^2q_z^2}. \tag{35b}$$

From equations (32)–(35) one can see that F_{D} is the interaction energy between disclinations and has two separate contributions: one comes from interaction between longitudinal wedge disclinations and the other one comes from interaction between twist disclinations. Longitudinal wedge and twist disclinations are decoupled.

The full free energy of disclinations therefore has two decoupled contributions,

$$F_{\mathrm{tot}}=F_{\mathrm{W}}+F_{\mathrm{T}} \tag{36}$$

where

$$F_{\mathrm{W}}=\frac{1}{2}\iint\mathrm{d}^3r_1\,\mathrm{d}^3r_2\,\alpha_z(\boldsymbol{r}_1)U_{zz}(\boldsymbol{r}_1-\boldsymbol{r}_2)\alpha_z(\boldsymbol{r}_2)+\int\mathrm{d}^3r\,E_{\mathrm{W}}[\alpha_z(\boldsymbol{r})]^2 \tag{37}$$

is the contribution of longitudinal wedge disclinations, and

$$F_{\mathrm{T}}=\frac{1}{2}\iint\mathrm{d}^3r_1\,\mathrm{d}^3r_2\,\alpha_a(\boldsymbol{r}_1)U_{ab}(\boldsymbol{r}_1-\boldsymbol{r}_2)\alpha_b(\boldsymbol{r}_2)+\int\mathrm{d}^3r\,E_{\mathrm{T}}\,\alpha_a(\boldsymbol{r})\alpha_a(\boldsymbol{r}) \tag{38}$$

is the contribution of twist disclinations.

As regards the contribution of longitudinal wedge disclinations, by carrying out the three-dimensional Fourier transform of $U_{zz}(\boldsymbol{q})$, equation (35*a*), we get

$$F_{\mathrm{W}} = -\frac{\gamma_2}{4\pi}\iint \mathrm{d}^2r_{\perp 1}\,\mathrm{d}^2r_{\perp 2}\int \mathrm{d}z\;\alpha_z(\boldsymbol{r}_{\perp 1}, z)\log\left(\frac{|\boldsymbol{r}_{\perp 1}-\boldsymbol{r}_{\perp 2}|}{r_0}\right)\alpha_z(\boldsymbol{r}_{\perp 2}, z)$$
$$+\int \mathrm{d}^3r\,E_{\mathrm{W}}[\alpha_z(\boldsymbol{r})]^2 \qquad (39)$$

where r_0 is a disclination core radius. By equation (39), one can see that the longitudinal wedge disclination free energy is a three-dimensional transcription of the free energy of disclinations in two-dimensional melting [7]. Therefore, longitudinal wedge disclinations should drive a disclination unbinding transition [7] of Kosterlitz type [10, 11]. Such a result is trustworthy, and somehow expected, since the longitudinal wedge disclinations are solid-like disclinations.

However, we have to take into account also the contribution of twist disclinations. In the appendix we explicitly calculate $U_{ab}(\boldsymbol{r}_1 - \boldsymbol{r}_2)$, i.e. the interaction between twist disclinations, which is peculiar to our quasi-two-dimensional system. The elastic stability conditions [6] make the denominator of $U_{\mathrm{tt}}(\boldsymbol{q})$, equation (35*b*), positive definite, so that $U_{ab}(\boldsymbol{r})$ is given by a Fourier integral which does not suffer divergences. On the other hand the numerator of $U_{\mathrm{tt}}(\boldsymbol{q})$ is not positive definite for $\gamma_3^2 > K_2\gamma_1$, which is still consistent with the above-mentioned elastic stability conditions. As a consequence, for $\gamma_3^2 > K_2\gamma_1$, twist disclinations of opposite signs can be coupled by repulsive interaction, while twist disclinations of the same sign can feel attractive interaction. The mechanism described above yields twist disclination unbinding, driven by an increasing density of disclinations which decorrelate the long-range sixfold orientational order, but preserve the nematic order. Such a twist disclination unbinding transition is peculiar to the hexatic N + 6 phase as a quasi-two-dimensional system.

The twist disclination unbinding transition from the hexatic N + 6 phase to the nematic phase should take place for

$$\gamma_3^2 = K_2\gamma_1. \qquad (40)$$

In fact, the twist disclination-mediated instability of the N + 6 phase occurs for $\gamma_3^2 > K_2\gamma_1$, while for $\gamma_3^2 < K_2\gamma_1$ the N + 6 phase is stable. On the other hand, in [6] we found that, near the transition between the N + 6 phase and the hexagonal discotic phase, the Frank constants fulfil $\gamma_3^2 < K_2\gamma_1$, i.e. a more restrictive version of elastic stability conditions, which prevents disclination unbinding besides fluctuation instability. Therefore, in this consistent scheme, the N + 6 phase takes a range of stability between the condensation of the hexagonal discotic phase and the disclination-mediated melting into the nematic phase.

The elastic stability conditions against fluctuation-induced breaking of sixfold order [6] were derived assuming the components of $\boldsymbol{\Omega}$ to be independent fluctuating variables. In the presence of disclinations, nevertheless, Ω_z is not defined in the disclination cores so that it cannot be taken as an independent field. Thus we are forced to assume A_{ij} as independent fields, since the singular components A_{iz} of the strain tensor are not equivalent to a varying Ω_z in the disclination cores. The elastic free energy (14), written in terms of A_{ij} as independent fields, is just positive definite for $\gamma_3^2 < K_2\gamma_1$ besides K_1, K_2, K_3, γ_1 and $\gamma_2 > 0$. This inequality is more restrictive than the previously derived [6] $|\gamma_3| < (K_2\gamma_1)^{1/2} + (K_3\gamma_2)^{1/2}$, which refers to non-singular deformations of $\boldsymbol{\Omega}$. Therefore, the stability condition against disclination unbinding can be violated when the system is still stable as regards non-singular fluctuations of orientational order.

The elastic equilibrium equations, e.g. equation (15), implicitly contain boundary conditions on the independent fields, which have to vanish at external boundaries of the system. For non-singular deformations, $\mathbf{\Omega}$ can be taken vanishing at boundaries. In the presence of an isolated disclination, on the contrary, the Ω_z increase along any loop around the singular core is $2\pi(n/6)$, as in equation (2), so that Ω_z cannot be taken vanishing at boundaries even if the configuration is asymptotically homogeneous. Therefore, at external boundaries, the medium is locally, but not globally, uniform, which is just due to the singularity in the disclination core. On the other hand A_{iz}, given by $\nabla_i\Omega_z$ outside the disclination core, vanish at boundaries and can therefore be taken as independent fields in the equilibrium equations when unbound disclinations are present.

In conclusion, we have described two possible mechanisms for the disclination unbinding transition of the hexatic N + 6 phase into the nematic phase. The longitudinal wedge disclination part of the free energy should drive a Kosterlitz transition [10, 11], as in two-dimensional systems [7]. The twist disclination free energy shows the possibility of a different kind of disclination unbinding transition, peculiar to the hexatic N + 6 phase as a quasi-two-dimensional system, due to repulsion between disclinations of opposite signs.

4. Pair-interaction energy and deformations of isolated disclinations

In this section we will compute the deformations of $\mathbf{\Omega}$ yielded by an isolated disclination, and then the pair-interaction energy between two isolated disclinations.

The curvature strain tensor due to the presence of disclinations is a function of disclination density. Exploiting equations (22), (23), (25) and (27) we get

$$A_{za}(q) = \mathrm{i}\varepsilon_{ab}q_{\perp b}[\gamma_2\gamma_3 q_z q_\perp/\Delta(q)]\alpha_t(q) \tag{41a}$$

$$\varepsilon_{ab}A_{ab}(q) = -\mathrm{i}[\gamma_2\gamma_3 q_\perp^3/\Delta(q)]\alpha_t(q) \tag{41b}$$

$$A_{zz}(q) = \mathrm{i}\gamma_2[(K_2q_\perp^2 + K_3q_z^2)/\Delta(q)]q_\perp\alpha_t(q) \tag{41c}$$

$$A_{az}(q) = -\mathrm{i}\,\frac{q_z q_{\perp a}}{q_\perp}\frac{(K_2\gamma_1 - \gamma_3^2)q_\perp^2 + K_3\gamma_1 q_z^2}{\Delta(q)}\,\alpha_t(q) + \mathrm{i}\,\frac{\varepsilon_{ab}q_{\perp b}}{q_\perp^2}\,\alpha_z(q) \tag{41d}$$

with

$$\Delta(q) = K_3\gamma_1 q_z^4 + K_2\gamma_2 q_\perp^4 + (K_3\gamma_2 + K_2\gamma_1 - \gamma_3^2)q_\perp^2 q_z^2. \tag{42}$$

Equations (41*a*) and (41*b*) give, respectively, the bend mode and the twist mode of the director, while (41*c*) and (41*d*) are the singular components of the strain tensor, i.e. the Ω_z torsion modes. The splay mode of the director, by equation (21), vanishes in the presence of only twist and longitudinal wedge disclinations.

The disclination density for an isolated longitudinal wedge disclination is

$$\alpha_z = 2\pi(n/6)\delta^{(2)}(r_\perp) \qquad \alpha_x = \alpha_y = 0 \tag{43}$$

with $r_\perp = (x, y, 0)$. Substituting the Fourier transform of equations (43) in equations

(41), and carrying out the Fourier transforms of (41), the only non-vanishing components are

$$A_{xz}(\boldsymbol{r}) = -(n/6)(y/r_\perp^2) \qquad A_{yz}(\boldsymbol{r}) = (n/6)(x/r_\perp^2). \tag{44}$$

The bend and twist modes of the director, which depend only on α_t, in addition to the splay mode, vanish for a longitudinal wedge disclination, so that $\delta\boldsymbol{m} = 0$. The torsion mode A_{zz} vanishes as well, and then Ω_z depends only on x and y. Outside the disclination core, i.e. for $r_\perp \neq 0$, $A_{az} = \nabla_a \Omega_z$. Therefore, the integration of equation (44) gives the deformation of $\boldsymbol{\Omega}$ around the singular core of a longitudinal wedge disclination

$$\Omega_z = (n/6)\arctan(y/x) \tag{45a}$$

$$\delta\boldsymbol{m} = 0 \tag{45b}$$

which is just valid for $r_\perp \neq 0$. The deformation (45) is essentially two-dimensional. Incidentally, equation (44) shows that A_{az} vanish for $r_\perp \to \infty$, while Ω_z, equation (45a), does not become constant for $r_\perp \to \infty$, as observed at the end of the previous section.

An isolated twist disclination along the $\hat{x}$ axis, for example, is characterized by the disclination density

$$\alpha_x = 2\pi(n/6)\delta^{(2)}(y,z) \qquad \alpha_y = \alpha_z = 0 \tag{46}$$

which in Fourier space is

$$\alpha_t(\boldsymbol{q}) = -(2\pi)^2(n/6)\delta(q_x) \qquad \alpha_z(\boldsymbol{q}) = 0. \tag{47}$$

Substituting (47) in (41) we get the Fourier transformed strain tensor. As a result, $A_{zy}(\boldsymbol{r}) = \nabla_z \delta m_y$ vanishes. Moreover, any deformation yielded by the isolated disclination does not depend on x, because of $\delta(q_x)$ in equation (47). As a consequence, equation (21) gives $A_{yy}(\boldsymbol{r}) = \nabla_y \delta m_y = 0$. Therefore, δm_y is constant, and then can be taken vanishing. Furthermore the strains of δm_x are

$$\begin{aligned} A_{zx}(\boldsymbol{q}) &= \mathrm{i}q_z\delta m_x(\boldsymbol{q}) = -\mathrm{i}(2\pi)^2(n/6)\gamma_2\gamma_3[q_z q_y^2/\Delta(\boldsymbol{q})]\delta(q_x) \\ \varepsilon_{ab}A_{ab}(\boldsymbol{q}) &= -\mathrm{i}q_y\delta m_x(\boldsymbol{q}) = \mathrm{i}(2\pi)^2(n/6)\gamma_2\gamma_3[q_y^3/\Delta(\boldsymbol{q})]\delta(q_x) \end{aligned} \tag{48}$$

and then

$$\delta m_x(\boldsymbol{q}) = -(2\pi)^2(n/6)\gamma_2\gamma_3[q_y^2/\Delta(\boldsymbol{q})]\delta(q_x) \tag{49}$$

while the strains of Ω_z are

$$\begin{aligned} A_{yz}(\boldsymbol{q}) &= \mathrm{i}(2\pi)^2\frac{n}{6}q_z\frac{(K_2\gamma_1 - \gamma_3^2)q_y^2 + K_3\gamma_1 q_z^2}{\Delta(\boldsymbol{q})}\delta(q_x) \\ A_{zz}(\boldsymbol{q}) &= -\mathrm{i}(2\pi)^2\frac{n}{6}q_y\frac{\gamma_2(K_2q_y^2 + K_3q_z^2)}{\Delta(\boldsymbol{q})}\delta(q_x) \\ A_{xz}(\boldsymbol{q}) &= 0. \end{aligned} \tag{50}$$

The Fourier transforms of (49) and (50) can be calculated by factorizing the denominator $\Delta(\boldsymbol{q})$, equation (42), as in equation (A6) of the appendix, and reducing the integrand expressions into the sum of fractions whose denominators are quadratic in q_z and q_y. As a result, outside the core, i.e. for $y^2 + z^2 > r_0^2$, we get

$$\delta m_x = \frac{n}{24} \frac{\gamma_2 \gamma_3}{k_3 \gamma_1} \frac{1}{B} \left[(A-B)^{-1/2} \log \left(\frac{(A-B)z^2 + y^2}{r_0^2} \right) - (A+B)^{-1/2} \log \left(\frac{(A+B)z^2 + y^2}{r_0^2} \right) \right] \tag{51}$$

and

$$A_{yz} = \frac{\partial \Omega_z}{\partial y} = -\frac{n}{24B} \frac{\partial}{\partial z} \left[(A+B)^{-1/2}(A+B-C) \log \left(\frac{(A+B)z^2 + y^2}{r_0^2} \right) + (A-B)^{-1/2}(B+C-A) \log \left(\frac{(A-B)z^2 + y^2}{r_0^2} \right) \right] \tag{52a}$$

$$A_{zz} = \frac{\partial \Omega_z}{\partial z} = \frac{n}{24B} \frac{\partial}{\partial y} \left[(A+B)^{1/2}(A+B-C) \log \left(\frac{(A+B)z^2 + y^2}{r_0^2} \right) + (A-B)^{1/2}(B+C-A) \log \left(\frac{(A-B)z^2 + y^2}{r_0^2} \right) \right] \tag{52b}$$

where r_0 is a core radius, while A, B and C are defined in equations (A7) and (A9) of the appendix. The integration of equation (52) gives the torsion

$$\Omega_z = \frac{n}{12B} \left[(B+A-C) \arctan \left(\frac{(A+B)^{1/2} z}{y} \right) + (B-A+C) \times \arctan \left(\frac{(A-B)^{1/2} z}{y} \right) \right]. \tag{53}$$

Equations (51) and (53) together with $\delta m_y = 0$ represent the $\mathbf{\Omega}$ deformations around a twist disclination parallel to the $\hat{x}$ axis. From equation (51) δm_x is proportional to the coupling constant γ_3, which just couples the director distortions to the Ω_z torsions. The Ω_z twist singularity drives, by γ_3 coupling in equation (13) or (14), $\delta \boldsymbol{m}$ distortions. As $\delta \boldsymbol{m}$, in equation (1), was assumed to be small, the result (51) is only valid for weak γ_3 coupling, otherwise the logarithmic increase breaks down the perturbative approximation. The twist disclination unbinding transition, described in the previous section, takes place for strong γ_3 coupling, so that (51) fails near such a transition.

Finally, we calculate the pair-interaction energy between two parallel disclinations. For two isolated longitudinal wedge disclinations, the disclination density is

$$\begin{aligned} \alpha_z(\boldsymbol{r}) &= 2\pi(n_1/6)\delta^{(2)}(\boldsymbol{r}_\perp - \boldsymbol{r}_{\perp 1}) + 2\pi(n_2/6)\delta^{(2)}(\boldsymbol{r}_\perp - \boldsymbol{r}_{\perp 2}) \\ \alpha_x &= \alpha_y = 0 \end{aligned} \tag{54}$$

where n_1, n_2 and $\boldsymbol{r}_{\perp 1}$, $\boldsymbol{r}_{\perp 2}$ are, respectively, the disclinicities and the positions of the two disclination lines. Inserting (54) in the disclination free energy (32) we obtain, besides the self-interaction energies, the pair-interaction energy between the two lines. The interaction energy for unit length between two longitudinal wedge disclinations is then

$$U_{\mathrm{WW}}(r_\perp) = -2\pi(n_1 n_2/36)\gamma_2 \log(r_\perp/r_0) \tag{55}$$

where $\boldsymbol{r}_\perp$ is the distance between the two lines.

In a similar way, the interaction energy for unit length between two twist disclinations parallel, for example, to the $\hat{x}$ axis is

$$U_{TT}(y,z) = -\frac{\pi n_1 n_2}{36}\frac{\gamma_2}{2B}\left[\frac{A+B-C}{(A+B)^{1/2}}\log\left(\frac{(A+B)z^2+y^2}{r_0^2}\right) + \frac{B-A+C}{(A-B)^{1/2}}\log\left(\frac{(A-B)z^2+y^2}{r_0^2}\right)\right]. \tag{56}$$

The coupling between a twist and a longitudinal wedge disclination, just discussed in the previous section, as well as the coupling between two orthogonal twist disclinations, vanishes.

Acknowledgment

This research is supported by funds of Ministero dell'Università e della Ricerca Scientifica e Tecnologica (Italy).

Appendix

The interaction between twist disclinations is given, in equation (38), in terms of $U_{ab}(r)$, which is the three-dimensional Fourier transform of

$$U_{ab}(q) = U_{tt}(q)(\delta_{ab} - \hat{q}_{\perp a}\hat{q}_{\perp b}) \tag{A1}$$

where $U_{tt}(q)$ is given in equation (35*b*). Therefore

$$U_{ab}(r) = \int \frac{d^3q}{(2\pi)^3}(\delta_{ab} - \hat{q}_{\perp a}\hat{q}_{\perp b})U_{tt}(q)\,e^{iq\cdot r} \tag{A2}$$

is a symmetric tensor of rank 2, built up with the components of $r_\perp = (x, y, 0)$, so that we have

$$U_{ab}(r) = \tfrac{1}{2}\delta_{ab}U(r) + (\hat{r}_{\perp a}\hat{r}_{\perp b} - \tfrac{1}{2}\delta_{ab})\tilde{U}(r) \tag{A3}$$

with $\hat{r}_\perp = r_\perp/r_\perp$.

Taking the trace of (A3) we have $U_{aa}(r) = U(r)$ and then, from (A2),

$$U(r) = \int \frac{d^3q}{(2\pi)^3} U_{tt}(q)\,e^{iq\cdot r}. \tag{A4}$$

Contraction of $U_{ab}(r)$, equation (A3), with the traceless tensor $\hat{r}_{\perp a}\hat{r}_{\perp b} - \frac{1}{2}\delta_{ab}$ gives

$$\tilde{U}(r) = 2(\hat{r}_{\perp a}\hat{r}_{\perp b} - \tfrac{1}{2}\delta_{ab})U_{ab}(r)$$

and then, by (A2),

$$\tilde{U}(r) = \int \frac{d^3q}{(2\pi)^3}[1 - 2(\hat{q}_\perp\cdot\hat{r}_\perp)^2]U_{tt}(q)\,e^{iq\cdot r}. \tag{A5}$$

In order to perform the Fourier transforms in (A4) and (A5), it is convenient to factorize the denominator of $U_{tt}(q)$ as

$$K_3\gamma_1 q_z^4 + K_2\gamma_2 q_\perp^4 + (K_3\gamma_2 + K_2\gamma_1 - \gamma_3^2)q_\perp^2 q_z^2 = K_3\gamma_1[q_z^2 + (A+B)q_\perp^2][q_z^2 + (A-B)q_\perp^2] \tag{A6}$$

where

$$A = \frac{K_3\gamma_2 + K_2\gamma_1 - \gamma_3^2}{2K_3\gamma_1} \qquad B = \left(A^2 - \frac{K_2\gamma_2}{K_3\gamma_1}\right)^{1/2} \tag{A7}$$

so that $U_{tt}(\boldsymbol{q})$ can be written as

$$U_{tt}(\boldsymbol{q}) = \frac{\gamma_2}{2B}\left(\frac{A+B-C}{q_z^2 + (A+B)q_\perp^2} - \frac{A-B-C}{q_z^2 + (A-B)q_\perp^2}\right) \tag{A8}$$

with

$$C = (K_2\gamma_1 - \gamma_3^2)/K_3\gamma_1. \tag{A9}$$

Substituting (A8) in (A4) and (A5), the Fourier transforms give, respectively,

$$U(\boldsymbol{r}) = \frac{\gamma_2}{8\pi B}\left(\frac{A+B-C}{(A+B)^{1/2}}[(A+B)z^2 + r_\perp^2]^{-1/2} + \frac{B-A+C}{(A-B)^{1/2}}[(A-B)z^2 + r_\perp^2]^{-1/2}\right) \tag{A10}$$

and

$$\tilde{U}(\boldsymbol{r}) = \frac{\gamma_2}{8\pi B}\left(\frac{A+B-C}{(A+B)^{1/2}}\,\frac{\{[1+(A+B)z^2/r_\perp^2]^{1/2} - (A+B)^{1/2}|z|/r_\perp\}^2}{[(A+B)z^2 + r_\perp^2]^{1/2}} + \frac{B-A+C}{(A-B)^{1/2}}\,\frac{\{[1+(A-B)z^2/r_\perp^2]^{1/2} - (A-B)^{1/2}|z|/r_\perp\}^2}{[(A-B)z^2 + r_\perp^2]^{1/2}}\right). \tag{A11}$$

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