Twisted Line Liquids

Randall D. Kamien
School of Natural Sciences
Institute for Advanced Study
Princeton, NJ 08540

and

T. C. Lubensky
Department of Physics
University of Pennsylvania
Philadelphia, PA 19104

We propose a model of directed lines where the average direction has the nature of a cholesteric liquid crystal. This model, for instance, would describe the liquid of screw dislocations in the twist-grain-boundary (TGB) phase of liquid crystals. We show that the presence of lines does not alter the long wavelength elasticity of a cholesteric and, therefore, does not stabilize Landau-Peierls instability of the cholesteric phase. We discuss other possible mechanisms for stabilizing the twist-grain-boundary phase.
1. Introduction and Summary

Directed line liquids have received attention recently in a variety of interesting physical situations. Composed of lines which are compelled on average to have tangent vectors parallel to an imposed axis, they are central to the long-wavelength physics of high-temperature superconductors in an external magnetic field, both as entangled flux liquids [1] and vortex glass states [2]. They are also of interest in nematic polymers [3], electrorheological fluids and ferrofluids [4]. In this paper, we will investigate a model for chiral line liquids in which tangent vectors of the lines are constrained to rotate in a helical fashion along some fixed pitch axis.

The entangled flux liquid in a superconductor is produced when thermal fluctuations cause the regular Abrikosov vortex lattice to melt. The close analogy between the smectic-A phase in liquid crystals and the superconducting phase in metals and that between the nematic-to-smectic-A and normal-metal-to-superconductor transition was pointed out some years ago by de Gennes [5]. This analogy leads to the theoretical expectation that a liquid crystal analog of the Abrikosov vortex phase should exist with dislocation lines replacing vortex lines. Recent experiments [6] confirm that such a phase does exist and that its properties are identical to those of the theoretically predicted TGB (twist-grain-boundary) phase [7] consisting of periodically repeated twist-grain-boundaries, each composed of periodically spaced screw dislocations whose axes rotate in a helical fashion from one boundary to the next. The TGB phase can presumably melt to a chiral line liquid just as the Abrikosov phase melts to a directed line liquid. The chiral line liquid we study in this paper is intended to model the melted TGB phase.

The entangled flux liquid phase in a superconductor is in fact the normal-metal phase, but with enhanced viscosities. Polymer nematics, on the other hand differ from normal nematics in that their splay elastic constant $K_1$ is infinite if all polymers extend from one end of the sample to the other [8]. Non-linearities constrained by full rotational invariance lead [9] to a renormalized theory in which elastic constants take on a momentum dependence. In particular, the twist and bend Frank constants diverge at small momentum while the splay modulus vanishes. It is thus natural to ask whether there are differences between the chiral line liquid and a cholesteric liquid crystal. Our calculations show that the long-wavelength properties of the chiral line liquid are identical to those of a cholesteric liquid crystal. A cholesteric is a one-dimensional layered structure with a long-wavelength Landau-Peierls elasticity and associated destruction of long-range periodic order [10]. The
TGB phase is also a one dimensional-layered structure, and though its elasticity is more complex than that of a cholesteric [11], its long-range order is also fluctuation destroyed. A chiral line liquid has the same long-wavelength Landau-Peierls elasticity as a cholesteric but with elastic constant renormalized by the presence of dislocations. The splay elastic constant $K_1$, which does not contribute to the Landau-Peierls energy, however, diverges as the square of an inverse wavenumber as it does in a polymer nematic [12].

In this paper we add explicit degrees of freedom to describe the dislocation line configurations. Though the energy of a smectic-$A$ screw dislocation tilted a small angle $\alpha$ away from the director goes as $\alpha^2 \log(1/\alpha)$, we will assume that we are at sufficiently long scales that the tipping energy becomes analytic [13]. In section II we derive a Landau theory for a melted, twisted line liquid, generalizing work on directed line liquids. In section III we derive the effective long-wavelength theory and find expressions for the new, effective Frank constants of the cholesteric. Finally in section IV we comment on a possible way for the non-harmonicity of the tipping energy to stabilize the Landau-Peierls instability of the twist-grain-boundary phase.

2. Derivation of Model

Our system is a collection of lines described by their locations $\mathbf{R}_i(s)$ and parameterized by arclength $s$ embedded in and interacting with a cholesteric liquid crystal with a unit director field $\mathbf{n}(r)$. We model the lines by a local density field $\rho$ and a local tangent-density vector $\mathbf{m}$. In terms of the paths of the lines $\mathbf{R}_i(s)$,

$$\rho(r) = \sum_i \int ds \delta^d(\mathbf{R}_i(s) - r), \quad (2.1)$$

and

$$\mathbf{m}(r) = \sum_i \int ds \frac{d\mathbf{R}_i(s)}{ds} \delta^d(\mathbf{R}_i(s) - r). \quad (2.2)$$

If our lines do not terminate, then $\mathbf{m}$ must be divergenceless:

$$\nabla \cdot \mathbf{m} = \sum_i \int ds \frac{d\mathbf{R}_i(s)}{ds} \cdot \nabla \delta^d(\mathbf{R}_i(s) - r) = -\sum_i \int ds \frac{d}{ds} \delta^d(\mathbf{R}_i(s) - r) = 0. \quad (2.3)$$

We will not consider the case of finite lines because dislocations cannot end within a sample.
In the TGB phase, screw dislocations align parallel on average along the local nematic director $\mathbf{n}$. We assume this remains true in the line liquid phase and propose the following free energy to describe the chiral line liquid:

$$F = \int d^3r \frac{A}{2}(\mathbf{m} - \rho_0 \mathbf{n})^2 + F_n[\mathbf{n}],$$

(2.4)

where

$$F_n[\mathbf{n}] = \frac{1}{2} \int d^3x \left[ K_1 (\nabla \cdot \mathbf{n})^2 + K_2 (\mathbf{n} \cdot [\nabla \times \mathbf{n}] - k_0)^2 + K_3 (\mathbf{n} \times [\nabla \times \mathbf{n}])^2 \right].$$

(2.5)

is the usual Frank free energy for a chiral liquid crystal and the constraint $\nabla \cdot \mathbf{m} = 0$ is understood. The free energy favors $\langle \mathbf{m} \rangle = \rho_0 \mathbf{n}$. We could have included an anisotropic tensor coupling of the form

$$F = \frac{1}{2} \int d^3x (m_\mu - \rho_0 n_\mu) I^{\mu\nu} (m_\nu - \rho_0 n_\nu).$$

(2.6)

By rotational invariance $I^{\mu\nu} = A \delta^{\mu\nu} + B n_\mu n_\nu$. If we keep only terms up to quadratic order in the fields, we are left only with the isotropic tensor $\delta^{\mu\nu}$. In principle, the self-coupling of the vector can be different along the pitch axis of the twist-grain-boundary phase than perpendicular to it, or in other words, if the pitch points along the $x$-axis, $I^{xx} \neq I^{yy} \equiv I^{zz}$. We might also include interactions of the defects with themselves involving $\mathbf{m}$ by itself. We believe, however, that in the long wavelength limit, this model captures the essential physics.

The ground state configuration of the liquid crystal has a spontaneously broken symmetry. We choose the pitch axis to lie along the $x$-axis and the equilibrium director,

$$\mathbf{n}_0(\mathbf{r}) = [0, \sin(k_0 x), \cos(k_0 x)],$$

(2.7)

to minimize the Frank Free energy. We introduce director fluctuations via $\mathbf{n} = \mathbf{n}_0 + \delta \mathbf{n}$. If we only work to quadratic order in fields, then because $\mathbf{n}$ is a unit vector, it is sufficient to consider only $\delta \mathbf{n}$ with $\delta \mathbf{n} \cdot \mathbf{n}_0 = 0$. Since $\langle \mathbf{m} \rangle$ is parallel to $\mathbf{n}_0$ in equilibrium, we set

$$\mathbf{m} = \rho \mathbf{n}_0 + \mathbf{t}.$$  

(2.8)

Fluctuations of $\mathbf{m}$ along $\mathbf{n}_0$ are described by $\rho$ and fluctuations perpendicular to $\mathbf{n}_0$ described by $\mathbf{t}$. We, therefore, require $\mathbf{t} \cdot \mathbf{n}_0 = 0$. Fluctuations in the equilibrium average of $\mathbf{m}$ will point along $\mathbf{n}_0$. Thus $\langle \mathbf{t} \rangle = 0$, and $\langle \mathbf{m} \rangle = \langle \rho \rangle \mathbf{n}_0$. The constraint $\nabla \cdot \mathbf{m} = 0$ is now

$$\mathbf{n}_0 \cdot \nabla \rho + \nabla \cdot \mathbf{t} = 0.$$  

(2.9)
and our harmonic theory becomes

\[ F = \int d^3r \left\{ \frac{A}{2} (t - \rho_0 \delta n)^2 + \frac{A}{2} \delta \rho^2 \right\} + F_n[n], \]  

subject to \( n_0 \cdot \nabla \rho + \nabla \cdot t = 0. \) We have set \( \rho = \rho_0 + \delta \rho. \) and

\[ F_{\delta n}[\delta n] = F_n[n_0 + \delta n] \]

\[ = \frac{1}{2} \int d^3r \left[ K_1 (\nabla \cdot \delta n)^2 + K_2 (n_0 \cdot [\nabla \times \delta n])^2 + K_3 (k_0 \delta n \times n_0 + n_0 \times [\nabla \times \delta n])^2 \right]. \]  

We note that if \( k_0 = 0 \) then \( n_0 = \hat{z} \) and this theory reduces to the model derived for directed line liquids in [12].

In order to study the fluctuations in this system we, seek a parameterization of \( m \) and \( \rho \) satisfying the constraint (2.9) and the constraint \( n_0 \cdot t = 0. \) The first constraint is satisfied by setting

\[ \rho = \rho_0 - \rho_0 \nabla \cdot u \]  

\[ t = \rho_0 (n_0 \cdot \nabla) u - \rho_0 (u \cdot \nabla) n_0, \]  

where \( u \) is any vector. This equation is invariant under the transformation \( u \to u' = u + \nabla \times \lambda. \) This comes about because the constraint (2.9) only involves the longitudinal components of \( t. \) There is, therefore, a gauge-like symmetry of the transverse components. The constraint \( t \cdot n_0 = 0 \) implies

\[ n_0 \cdot \nabla (n_0 \cdot u) = 0. \]  

We can solve this constraint on \( u \) by choosing \( n_0 \cdot u = 0. \) This is tantamount to a choice of gauge in the sense that if we are given a \( u \) with \( n_0 \cdot u \neq 0 \) we can, without making \( u \) trivial, choose a \( \lambda \) such that \( n_0 \cdot (u + \nabla \times \lambda) = 0. \) Note that any vector \( u(r) \) that depends only on \( x, \) the component of \( r \) along the pitch axis, satisfies the constraint (2.13). Thus the free energy expressed in term of \( u \) will depend only on gradients of \( u \) in the \( yz \)-plane.

3. Rotational Symmetries and Long-wavelength Elasticity

The free energy for a chiral line liquid, like that for a cholesteric, is invariant with respect to uniform translations and rotations. It is precisely these invariances that lead to the Landau-Peierls elastic free energy and the destruction of long-range order in a one-dimensionally modulated structure. In order to obtain the effective long-wavelength free
energy, it is useful to understand how uniform translations and rotations are described by the variables $\mathbf{u}$ and $\delta \mathbf{n}$ describing deviations from the equilibrium ground state. Following the analysis in [14], we write our fields $\mathbf{u}$ and $\delta \mathbf{n}$ as

$$\mathbf{u} = [\phi, \theta \cos(k_0x), -\theta \sin(k_0x)], \quad (3.1a)$$

$$\delta \mathbf{n} = [f, g \cos(k_0x), -g \sin(k_0x)], \quad (3.1b)$$

thus enforcing both $\delta \mathbf{n} \cdot \mathbf{n}_0 = 0$ and $\mathbf{u} \cdot \mathbf{n}_0 = 0$. Because the ground state is not translationally invariant, it is convenient to decompose our fields into a sum over Brillouin zones. We write for any field $X$,

$$X(\mathbf{r}) = \sum_n X_n(\mathbf{r}) e^{i k_0 n \cdot \mathbf{x}}, \quad (3.2)$$

where $X_n(\mathbf{r})$ only has fourier modes with $x$-components $k_x \in (-\frac{k_0}{2}, \frac{k_0}{2}]$.

We now consider a rigid rotation described by the vector $\Omega$. Under this rotation $\mathbf{n}_0$ becomes:

$$\mathbf{n}_0' = \mathbf{n}_0 + [\Omega_y \cos(k_0x) - \Omega_z \sin(k_0x), -\Omega_x \cos(k_0x), \Omega_x \sin(k_0x)]$$

$$- (\Omega_y z - \Omega_z y) [0, k_0 \cos(k_0x), -k_0 \sin(k_0x)]. \quad (3.3)$$

We can now compare (3.1) and (3.3) to determine what fields $f$ and $g$ are generated by uniform rigid rotations. We find

$$f = \Omega_y \cos(k_0x) - \Omega_z \sin(k_0x) \quad (3.4a)$$

$$g = -\Omega_x - k_0 (\Omega_y z - \Omega_z y). \quad (3.4b)$$

If we write $t$ in terms of $\phi$ and $\theta$ and match the same rigid rotation, we find

$$\Omega_y = \partial_z \phi \quad (3.5a)$$

$$-\Omega_z = \partial_y \phi \quad (3.5b)$$

$$-\Omega_x - k_0 (\Omega_y z - \Omega_z y) = -k_0 \phi + \sin(k_0x) \partial_y \theta + \cos(k_0x) \partial_z \theta \quad (3.5c)$$

Then writing (3.4) and (3.5) in terms of the decomposition (3.2) gives (with $2X_+ = X_1 + X_{-1}$ and $2X_- = -i(X_1 - X_{-1})$)

$$f_+ = \Omega_y \quad (3.6a)$$

$$f_- = \Omega_z \quad (3.6b)$$

$$g_0 = -\Omega_x - k_0 (\Omega_y z - \Omega_z y) \quad (3.6c)$$

$$\partial_y \theta_- - \partial_z \theta_+ + k_0 \phi_0 = \Omega_x + k_0 (\Omega_y z - \Omega_z y) \quad (3.6d)$$

$$\partial_y \phi_0 = -\Omega_z \quad (3.6e)$$

$$\partial_z \phi_0 = \Omega_y \quad (3.6f)$$
The free energy cannot depend on the uniform rotation angle \( \Omega \). It will, however, depend on linear combinations of the fields \( \phi \), \( \theta \), \( f \), and \( g \) that do not depend on \( \Omega \). We can construct such combinations with the aid of (3.5). Note that \( \Omega \) only depends on \( \theta \) via the combination \( \partial_y \theta_+ - \partial_z \theta_- \). The combination \( \partial_y \theta_+ + \partial_z \theta_- \) does not generate a rotation, and the free energy can depend on it. Finally, we note that \( t \) will be nonzero if \( \partial_x \phi \) is nonzero. Thus, we expect on quite general grounds that \( F \) will have the form

\[
F = \frac{1}{2} \int d^3x \begin{cases}
  a \left[ (\partial_y g_0 - 2k_0 f_-)^2 + (\partial_z g_0 + 2k_0 f_+)^2 \right] \\
  + b \left[ (\partial_y \phi_0 + 2f_-)^2 + (\partial_z \phi_0 - 2f_+)^2 \right] \\
  + c(\partial_y \phi_0 + \partial_y \theta_+ - \partial_z \theta_+ + g_0)^2 \\
  + d(\partial_y \theta_+ + \partial_z \theta_- + \partial_x \phi_0)^2 \\
  + e \left[ (\partial_y \theta_+)^2 + (\partial_z \theta_+)^2 + (\partial_y \theta_-)^2 + (\partial_z \theta_-)^2 \right]
\end{cases}.
\] (3.7)

This form is dictated by the underlying rotational invariance. In terms of the original constants in (2.4) and (2.5), \( a = (K_1 + K_3)/2 \), and \( 2b = c = d = 2e = A\rho_0^2 \). The values of \( b, c, d \) and \( e \) are related by the underlying rotational invariance discussed in section II. There are other terms as well, in addition to higher powers and derivatives of the invariant combinations. We also note that because \( \rho = -\rho_0 \nabla \cdot \mathbf{u} \), \( \phi_n \) for \( n \neq 0 \) will be massive. Likewise, because of the energy of a splay configuration \( f_n \) will be massive for \( n \neq 0 \).

If we only consider the cholesteric, then \( \rho_0 = 0 \). In this case we are only left with the term proportional to \( a \) in (3.7). By integrating out \( f_\pm \) we see that \( \partial_x g \) and \( \partial_y g \) cannot appear quadratically. Thus they will first appear quartically, and we find the classic Landau-Peierls instability. Including the lines, we see that \( \theta \) appears without \( x \)-derivatives and always in combination with other fields. Upon integrating out \( \theta \) both the terms proportional to \( c \) and \( d \) disappear.

The preceding analysis showed that we must keep all the modes in the first Brillouin zone as well as \( f_+ \) and \( f_- \). Returning to our proposed model (2.10), we integrate out the modes in the second zone, as well as \( \phi_0 \). We find, to leading order in all derivatives, an effective free energy for \( g_0 \):

\[
F_g = \int d^3x \left\{ \left( \frac{A\rho_0^2}{3k_0^2} + K_2 \right)(\partial_x g_0)^2 + \frac{K_2 + 3K_3}{8k_0^2} \left[ (\partial_y^2 + \partial_z^2)g_0 \right]^2 \right\}.
\] (3.8)

Thus the fluctuation \( g_0 \) suffers from the Landau-Peierls instability. The penetration depth of the smectic, \( \lambda \), is

\[
\lambda^2 = \frac{3(K_2 + 3K_3)}{8k_0^2(3K_2 + A\rho_0^2)},
\] (3.9)
and thus the effect of the defects is to decrease the penetration depth. Though there is no long range order, $\lambda$ sets the scale over which it is possible to see the dephasing of the ground state. Consider two defects in the same plane of constant phase. Their mutual repulsion forces them apart, and as they move they drag the plane with them. Thus the effect of the repulsion should be to make the system “less” ordered.

Additionally, the free energy for the remaining director mode $f_0$ is

$$\frac{1}{2} \int d^3x \left[ K_1(\partial_x f_0)^2 + \frac{K_2 + K_3}{2} [ (\partial_y f_0)^2 + (\partial_z f_0)^2 ] + (A\rho_0^2 + K_3 k_0^2) f_0^2 \right], \quad (3.10)$$

and so the $f_0$ fluctuations become massive. In analogy with results on polymer nematics [12] we could interpret part of this as a defect density dependent divergent shift in $K_1$, namely

$$K_1'(q) = K_1 + \frac{A\rho_0^2}{q_x^2}. \quad (3.11)$$

4. Stabilization of the Twist-Grain-Boundary Phase

Because the Landau-Peierls instability in the twist-grain-boundary phase is due to the underlying rotational invariance, it is hard to imagine how any long-wavelength description of the phase could have long range order. As mentioned above, the energy of a defect tilted at an angle $\alpha$ with respect to the layer normal is proportional to $\alpha^2 \log(1/\alpha)$. While it is true that upon integrating out short-distance modes, the effective energy will become analytic in $\alpha$, the coarse-graining procedure will be cutoff by length scales inherent to the system. In particular, as we coarse-grain, the distance between the screw dislocations decreases. When the distance between them becomes on the order of the penetration depth, we must stop. If the screw dislocations are close enough (i.e. $k_0$ is sufficiently large), then the defect energy will remain non-analytic. The argument in the previous section would break down, because now we could have a term such as $-\log(q_t(q) \cdot t(-q))$ in the free energy in addition to those in (2.4). Though again, we would expect that $t$ would always appear in combination with $\delta n$, it is hard to see how non-analytic momentum dependence would change things. Since the energy cost of a bend in the direction of the cholesteric pitch will pick up this logarithmic energy in the twist-grain-boundary phase, we might consider, as a toy model, a slightly more rigid cholesteric described by a phase field $u$ with free energy

$$F = \frac{1}{2} \int \frac{d^3q}{(2\pi)^3} u(-q) \left[ B \log |1/aq_x| q_x^2 u + K(q_y^2 + q_z^2)^2 \right] u(q). \quad (4.1)$$
In this model, there is still a Landau-Peierls instability, in that

\[ \langle u^2(x) \rangle = \int \frac{d^3q}{(2\pi)^3} \frac{1}{-B \log |aq_x|q_x^2 + K(q_y^2 + q_z^2)^2} = \int \frac{dq_x dq_{\perp}}{(2\pi)^2} \frac{1}{-B \log |aq_x|q_x^2 + K q_{\perp}^4} = \frac{1}{32\pi \sqrt{KB}} \int_{1/L}^{1/a} dq_x \frac{dq_x}{q_x \sqrt{-\log aq_x}} = \frac{\sqrt{\log(L/a)}}{16\pi \sqrt{KB}} \]

and so there will still be a divergence with system size, but it will scale as the square-root of the logarithm instead of the logarithm itself.

Unless there are sufficiently long-ranged interactions it appears that the underlying rotational invariance will always destabilize the twist-grain-boundary phase.

5. Acknowledgements

It is a pleasure to acknowledge stimulating discussions with J. Toner. RDK was supported in part by the National Science Foundation, through Grant No. PHY92-45317, and through the Ambrose Monell Foundation. TCL was supported in part by the National Science Foundation through grants No. DMR91-20668 and No. DMR91-22645.
References

[1] D.R. Nelson, Phys. Rev. Lett. 60, 1973 (1988); D.R. Nelson and H.S. Seung, Phys. Rev. B 39, 9153 (1989).
[2] M.P.A. Fisher, Phys. Rev. Lett. 62, 1415 (1989).
[3] J.V. Selinger and R.F. Brunisma, Phys. Rev. A 43, 2910, 2922 (1991).
[4] R.D. Kamien and D.R. Nelson, J. Stat. Phys. 71, 23 (1993).
[5] P.G. de Gennes, Solid State Commun. 14, 997 (1973).
[6] J. Goodby, M.A. Waugh, S.M. Stein, R. Pindak, and J.S. Patel, Nature 337, 449 (1988); J. Am. Chem. Soc. 111, 8119 (1989); G. Strajer, R. Pindak, M.A. Waugh, J.W. Goodby, and J.S. Patel, Phys. Rev. Lett. 64, 13 (1990); K.J. Ihn, J.A.N. Zasadzinski, R. Pindak, A.J. Slaney, and J. Goodby, Science 258, 275 (1992).
[7] S.R. Renn and T.C. Lubensky, Phys. Rev. A 38, 2132 (1988); 41, 4392 (1990).
[8] P.G. de Gennes, in Polymer Liquid Crystals, edited by A. Ciferri, W.R. Kringbaum, and R.B. Meyer (Academic, New York, 1982), Chap. 5; R.B. Meyer, Chap. 6. See also [12]and [3].
[9] J. Toner, Phys. Rev. Lett. 68, 1331 (1992).
[10] L.D. Landau and E.M. Lifshitz, Statistical Physics, 3rd Ed., Part I, Chap. XIII (Pergamon Press, Oxford, 1980); A. Caille, C.R. Acad. Sci., Ser. B 274, 891 (1972); T.C. Lubensky, Phys. Rev. Lett. 29, 206 (1972).
[11] J. Toner, Phys. Rev. B 43, 8289 (1991); 46, 5715 (1992).
[12] R.D. Kamien, P. Le Doussal, and D.R. Nelson, Phys. Rev. A 45, 8727 (1992).
[13] This follows, for instance, from Toner’s theorem, J. Toner, private communication.
[14] T.C. Lubensky, T. Tokihiro, and S.R. Renn, Phys. Rev. A 43, 5449 (1991)