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Gauge field theory of dislocations in smectic A liquid crystals

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Résumé. — De l'énergie de courbure des cristaux liquides smectiques A : $\frac{B}{2}(\partial_z\varphi)^2 + \frac{K}{2}(\partial_\perp^2\varphi)^2$, nous déduisons une théorie de champ de jauge du type Ginzburg-Landau. Celle-ci comprend un champ complexe qui décrit les fluctuations des lignes de dislocations dans un ensemble grand-canonique et un champ de jauge rendant compte des interactions élastiques entre les lignes.

Abstract. — Starting from the bending energy $\frac{B}{2}(\partial_z\varphi)^2 + \frac{K}{2}(\partial_\perp^2\varphi)^2$ of smectic A liquid crystals, we derive a gauge field theory of dislocation lines which is of the Ginzburg-Landau type with a complex field describing the grand canonical ensemble of dislocation lines and the gauge field accounting for the long-range « elastic » interactions among these.

Recently, the phase transition smectic A to nematic liquid crystal has been studied as a three dimensional example for the destruction of order by line-like defects [1-3]. We would like to point out that in analogy with other physical systems [4] containing line-like defects there is a simple way to *derive* a Ginzburg-Landau type of gauge field theory which is the perfect tool for studying this transition. In it, there appear two fields, one complex disorder field which describes the vortex lines, and a gauge field which generates the long-range « elastic » forces between these.

The starting point is a Landau expression for some real order parameter $\rho(\mathbf{x})$ of the smectic liquid crystal

$$F = \int d^3x \,\{\, [(\partial^2 + q_0^2)\,\rho(\mathbf{x})]^2 + V(\rho(\mathbf{x}))\,\} \tag{1}$$

which is minimized by some layered solution along, say, the z direction

$$\rho(\mathbf{x}) = \rho_0 + A\cos(q_0 z + \gamma(\mathbf{x}))\,. \tag{2}$$

The phase $\gamma(\mathbf{x})$ has long-range fluctuations whose bending energies can be extracted from (1) as [5]

$$F = \int d^3x \frac{B}{2}\,[(\partial_z\gamma)^2 + \lambda^2(\partial_\perp^2\gamma)^2]\,. \tag{3}$$

Typically (in octyloxy-cyanobiphenyl)

$$q_0 \sim 0.197\,\text{Å}^{-1}\,, \qquad \lambda q_0 \sim 1.55\,t^{-0.13} \tag{4}$$

(from light scattering [6]), where $t \equiv 1 - \frac{T}{T_c}$. The quantities

$$\eta \equiv kT/8\,\pi B\lambda\,, \qquad K \equiv B(\lambda q_0)^2$$

have the values (0.17, 8.4×10^{-7} dyn), (0.23, 7.1×10^{-7} dyn), (0.38, 7.7×10^{-7} dyn) at $t = 9 \times 10^{-4}$, 5.9×10^{-4}, 4×10^{-6}, respectively.

A line-like defect in the phase field $\gamma(\mathbf{x})$ is characterized by the circuit integral $\oint \mathrm{d}\gamma(\mathbf{x}) = 2\pi n$ around the line. It may be considered as the boundary line of a surface S across which the phase $\gamma(\mathbf{x})$ has a discontinuity by $2\pi n$.

The partition function which describes small $\delta\gamma(\mathbf{x})$ fluctuations as well as these defect lines can most easily be written down on a simple cubic lattice in the following form (1) :

$$Z = \prod_{\mathbf{x}} \int_{-\pi}^{+\pi} \frac{\mathrm{d}\gamma(\mathbf{x})}{2\pi} \sum_{\{n_i(\mathbf{x})\}} \exp\left\{ -\frac{Ba}{2T} \sum_{\mathbf{x}} \left[(\nabla_3 \gamma(\mathbf{x}) - 2\pi n_3(\mathbf{x}))^2 + \left(\frac{\lambda}{a}\right)^2 (\boldsymbol{\nabla}_\perp(\nabla_1 \gamma - 2\pi n_1))^2 + \right.\right.$$
$$\left.\left. + \left(\frac{\lambda}{a}\right)^2 (\boldsymbol{\nabla}_\perp(\nabla_2 \gamma - 2\pi n_2))^2 \right] \right\}. \tag{5}$$

Here the sum over all integers $n_i(\mathbf{x})$ accounts for all possible discontinuities by $2\pi n_i(\mathbf{x})$ across surface elements in the direction of **i**. The symbols ∇_i denote lattice derivatives, $\nabla_i \gamma(\mathbf{x}) = \gamma(\mathbf{x} + \mathbf{i}) - \gamma(\mathbf{x})$ along the oriented basis vectors, i.e. $\mathbf{i} \equiv a(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$ for $i = 1, 2, 3$. Let also $\nabla_i^* \gamma(\mathbf{x}) \equiv \gamma(\mathbf{x}) - \gamma(\mathbf{x} - \mathbf{i})$ be the lattice derivative arising in « partial integrations » on a lattice, i.e. $\sum_{\mathbf{x}} \gamma'(\mathbf{x}) \nabla_i \gamma(\mathbf{x}) = -\sum_{\mathbf{x}} \nabla_i^* \gamma'(\mathbf{x}) \gamma(\mathbf{x})$.

Introducing an auxiliary field $b_i(\mathbf{x})$, (5) can be rewritten as

$$Z = \prod_{\mathbf{x}} \left[\int_{-\pi}^{+\pi} \frac{\mathrm{d}\gamma(\mathbf{x})}{2\pi} \prod_i \int_{-\infty}^{+\infty} \frac{\mathrm{d}b_i(\mathbf{x})}{\sqrt{2\pi Ba/T}} \right] \sum_{\{n_i(\mathbf{x})\}} \exp\left\{ -\frac{T}{2Ba} \sum_{\mathbf{x}} \left[b_3^2 - \left(\frac{a}{\lambda}\right)^2 \mathbf{b}_\perp \cdot ((\boldsymbol{\nabla}_\perp^* \cdot \boldsymbol{\nabla}_\perp)^{-2} \mathbf{b}_\perp) \right] + \right.$$
$$\left. + i \sum_{\mathbf{x}} b_i (\nabla_i \gamma - 2\pi n_i) \right\}. \tag{6}$$

Performing the sum over $n_i(\mathbf{x})$ forces the integrals over the fields $b_i(\mathbf{x})$ to become a sum over integers $b_i(\mathbf{x})$ due to Poisson's relation $\sum_{n=-\infty}^{\infty} \exp(2\pi i b n) = \sum_{k=-\infty}^{\infty} \delta(b - k)$. After partial integration, the γ-integrals lead to a vanishing lattice divergence of the b_i's : $\nabla_i^* b_i = 0$. Thus the smectic liquid crystal has the following simple representation (N = number of lattice points)

$$Z = (2\pi Ba/T)^{-N/2} \sum_{\{b_i(\mathbf{x})\}} \delta_{\nabla_i^* b_i(\mathbf{x}),0} \exp\left\{ -\frac{T}{2Ba} \left[\sum_{\mathbf{x}} b_3^2 - \left(\frac{a}{\lambda}\right)^2 \sum_{\mathbf{x},\mathbf{x}'} \mathbf{b}_\perp(\mathbf{x}) (\boldsymbol{\nabla}_\perp^* \cdot \boldsymbol{\nabla}_\perp)^{-2} (\mathbf{x}, \mathbf{x}') \, \mathbf{b}_\perp(\mathbf{x}') \right] \right\} \tag{7}$$

a representation which appears in similar form in many other lattice theories [9, 10].

The divergencelessness of $b_i(\mathbf{x})$ can be used to decompose

$$b_i(\mathbf{x}) = (\boldsymbol{\nabla} \times \mathbf{a})_i \equiv \varepsilon_{ijk} \nabla_j^* a_k(\mathbf{x} - \mathbf{k}) \tag{8}$$

which is invariant under gauge transformations

$$a_k(\mathbf{x}) \rightarrow a_k(\mathbf{x}) + \nabla_k \Lambda(\mathbf{x}). \tag{9}$$

In this way we arrive in the gauge $\boldsymbol{\nabla}_\perp \mathbf{a}_\perp = 0$ at

$$Z = \prod_{\mathbf{x},i} \int_{-\infty}^{+\infty} \frac{\mathrm{d}A_i(\mathbf{x})}{\sqrt{2\pi Ba/T}} \delta(\boldsymbol{\nabla}_\perp . \mathbf{A}_\perp) \times$$
$$\times \exp\left\{ -\frac{T}{2Ba} \sum_{\mathbf{x}} \left[(a/\lambda)^2 A_3^2 - \mathbf{A}_\perp \left(\boldsymbol{\nabla}_\perp^* . \boldsymbol{\nabla}_\perp + \frac{a^2}{\lambda^2} \frac{\nabla_3^* \nabla_3}{\boldsymbol{\nabla}_\perp^* . \boldsymbol{\nabla}_\perp} \right) \mathbf{A}_\perp \right] \sum_{\{l_i(\mathbf{x})\}} \delta_{\nabla_i^* l_i,0} \exp\left(2\pi i \sum_{\mathbf{x}} l_i A_i \right). \right. \tag{10}$$

Here the sums over integer fields $a_i(\mathbf{x})$ has been replaced by integrals over continuous $A_i(\mathbf{x})$ fields with an extra sum over integer $l_i(\mathbf{x})$'s ensuring that nothing has been changed, due to Poisson's formula. The condition $\nabla_i^* l_i = 0$ is required by gauge invariance. The sum over $l_i(\mathbf{x})$ with $\nabla_i^* l_i = 0$ may be interpreted as a sum over all closed defect lines. The coupling to the gauge fields $A_i(\mathbf{x})$ gives rise to their long-range interactions.

(1) This form is inspired by Villain's [8] treatment of the planar spin model.

As a matter of fact, if we integrate out the A_i fields we obtain

$$Z = \sum_{\{l_i(\mathbf{x})\}} \delta_{\nabla_i^* l_i, 0} \exp\left[-\frac{1}{2} \frac{(2\pi)^2}{T} Ba \sum_{\mathbf{x}} l_3^2(\mathbf{x}) \right] \times \exp\left\{ -\frac{1}{2} \frac{(2\pi)^2}{T} Ba \sum_{\mathbf{x},\mathbf{x}'} l_\perp(\mathbf{x})_\alpha \, v_{\alpha\beta}(\mathbf{x}-\mathbf{x}') \, l_\perp(\mathbf{x}')_\beta \right\} \quad (11)$$

with

$$v_{\alpha\beta}(\mathbf{x}-\mathbf{x}') = \sum_{\mathbf{k}} e^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')} \frac{|\mathbf{K}_\perp|^2}{|\mathbf{K}_\perp|^4 + \frac{a^2}{\lambda^2}|\mathbf{K}_3|^2} (\delta_{\alpha\beta} - K_\alpha^* K_\beta / |\mathbf{K}|^2) \quad (12)$$

being the long-range potential between the lines.

Here $K_i \equiv \frac{1}{i}(e^{ik_i a} - 1)$, $K_i^* = \frac{1}{i}(1 - e^{-ik_i a})$, and α, β run from 1 to 2. Using the condition $\nabla_i^* l_i = 0$ the second exponent becomes

$$\sum l_3(\mathbf{x})\, v_3(\mathbf{x}-\mathbf{x}')\, l_3(\mathbf{x}') + \mathbf{l}_\perp(\mathbf{x})\, v_\perp(\mathbf{x}-\mathbf{x}')\, \mathbf{l}_\perp(\mathbf{x}') \quad (13)$$

with

$$\begin{aligned} v_3(\mathbf{x}) &\equiv \sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{x}} \frac{|\mathbf{K}_\perp|^2}{|\mathbf{K}_\perp|^4 + \frac{a^2}{\lambda^2}|K_3|^2}, \\ v_\perp(\mathbf{x}) &\equiv \sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{x}} \frac{|K_3|^2}{|\mathbf{K}_\perp|^4 + \frac{a^2}{\lambda^2}|K_3|^2}. \end{aligned} \quad (14)$$

It is useful to separate out the large contributions $v_3(0)$, $v_\perp(0)$ and define $v'(\mathbf{x}) \equiv v(\mathbf{x}) - \delta_{\mathbf{x},0}\, v(0)$. Then (11) becomes

$$Z = \sum_{\{l_i(\mathbf{x})\}} \delta_{\nabla_i^* l_i, 0} \exp\left\{ -\frac{1}{2} \frac{(2\pi)^2}{T} Ba \left[(1 + v_3(0)) \sum_{\mathbf{x}} l_3(\mathbf{x})^2 + v_\perp(0) \sum_{\mathbf{x}} l_\perp^2(\mathbf{x}) \right] \right\} \times$$
$$\times \exp\left\{ -\frac{1}{2} \frac{(2\pi)^2}{T} Ba \sum_{\mathbf{x},\mathbf{x}'} [l_3(\mathbf{x})\, v_3'(\mathbf{x}-\mathbf{x}')\, l_3(\mathbf{x}') + (3 \to \perp)] \right\}. \quad (15)$$

The second factor can be transformed back to the form (10), and (12) becomes

$$Z = \prod_{\mathbf{x}} \int \frac{dA(\mathbf{x})}{\sqrt{2\pi Ba/T}} \exp\left\{ -\frac{T}{2\,Ba} \sum_{\mathbf{x}\mathbf{x}'} [A_3(\mathbf{x})\, v_3'^{-1}(\mathbf{x},\mathbf{x}')\, A_3(\mathbf{x}') + (3 \to \perp)] \right\} Z^A_{\text{loops}}$$

where

$$Z^A_{\text{loops}} \equiv \sum_{\{l_i(\mathbf{x})\}} \delta_{\nabla_i^* l_i(\mathbf{x}), 0} \exp\left\{ -\frac{1}{2} \frac{(2\pi)^2}{T} Ba \left[(1 + v_3(0)) \sum_{\mathbf{x}} l_3^2 + v_\perp(0) \sum_{\mathbf{x}} l_\perp^2 \right] \right\} \exp\left(2\pi i \sum_i l_i A_i \right) \quad (16)$$

is the partition function of closed defect loops coupled to the field A_i. We can now follow Peskin [10] and observe that this sum can be rewritten in the form

$$Z^A_{\text{loops}} = \prod_{\mathbf{x}} \int_{-\pi}^{+\pi} \frac{d\theta(\mathbf{x})}{2\pi} \sum_{\{n_i(\mathbf{x})\}} \exp\left\{ -\frac{T}{2(2\pi)^2 Ba} \sum_{\mathbf{x}} \left[\frac{1}{1 + v_3(0)} (\nabla_3 \theta - 2\pi A_3 - 2\pi n_3)^2 + \right.\right.$$
$$\left.\left. + \frac{1}{v_\perp(0)} (\nabla_\perp \theta - 2\pi \mathbf{A}_\perp - 2\pi \mathbf{n}_\perp)^2 \right] \right\}. \quad (17)$$

This follows in the same way as (6) did from (5). It may be considered as the Villain approximation to the partition function of an asymmetric XY model (up to a trivial factor)

$$Z^A_{XY} = \prod_{\mathbf{x}} \int_{-\pi}^{+\pi} \frac{d\theta(\mathbf{x})}{2\pi} \times$$
$$\times \exp\left\{ \frac{T}{(2\pi)^2 Ba} \sum_{\mathbf{x}} \left[(1 + v_3(0))^{-1} \cos(\nabla_3 \theta - 2\pi A_3) + v_\perp^{-1}(0) \sum_{\alpha=1,2} \cos(\nabla_\alpha \theta - 2\pi A_\alpha) \right] \right\}. \quad (18)$$

For $A_i = 0$, this can be rewritten as a classical planar Heisenberg model involving the « spins » $S(\mathbf{x}) = (\cos\theta, \sin\theta)(\mathbf{x})$:

$$Z_{XY}^A = \prod_{\mathbf{x}} \int_{-\pi}^{+\pi} \frac{d\theta(\mathbf{x})}{2\pi} \times \\ \times \exp\left\{\frac{T}{(2\pi)^2 Ba} \sum_{\mathbf{x}} \left[(1 + v_3(0))^{-1} S_a(\nabla_3 + 1) S_a + v_\perp^{-1}(0) \sum_{\alpha=1,2} S_a(\nabla_\alpha + 1) S_a\right]\right\}. \tag{19}$$

Moreover, using parity invariance we can replace $\nabla_i + 1$ by $\frac{1}{2}(\nabla_i^* \nabla_i + 2)$.

Now we are ready to introduce the field theory of defects as a two component auxiliary field φ_a such that

$$Z_{XY}^A = \prod_{\mathbf{x}} \int_{-\pi}^{+\pi} \frac{d\theta(\mathbf{x})}{2\pi} \iint_{-\infty}^{+\infty} \frac{d\varphi_1\, d\varphi_2(\mathbf{x})}{[T/\pi Ba]} \exp\left\{-\frac{(2\pi)^2 Ba}{4T} \sum_{\mathbf{x}} \varphi_a^2 + \sum_{\mathbf{x}} \psi_a S_a\right\} \tag{20}$$

where

$$\psi_a \equiv [(1 + v_3(0))^{-1} (\tfrac{1}{2} \nabla_3^* \nabla_3 + 1) + v_\perp^{-1}(0) (\tfrac{1}{2} \nabla_\perp^* \nabla_\perp + 2)]^{1/2} \varphi_a .$$

Here the integrations over $d\theta(\mathbf{x})$ produce Bessel functions and we arrive at

$$Z_{XY}^A = \prod_{\mathbf{x}} \iint_{-\infty}^{+\infty} \frac{d\varphi_1\, d\varphi_2(\mathbf{x})}{[T/\pi Ba]} e^{S[\varphi,\varphi^+]} \tag{21}$$

with a defect entropy

$$S[\varphi, \varphi^+] = -\frac{(2\pi)^2 Ba}{4T} \sum_{\mathbf{x}} \varphi_a^2 + \sum_{\mathbf{x}} \log I_0(\psi_a^2) . \tag{22}$$

Close to the critical temperature we can use a Landau expansion (see the last of refs. [4])

$$S[\varphi, \varphi^+] \sim -\sum_{\mathbf{x}} \left\{\left[\frac{(2\pi)^2 Ba}{4T} - \frac{1}{4}\left(\frac{1}{1 + v_3(0)} + \frac{2}{v_\perp(0)}\right)\right] \varphi_a^2 \right. \\ \left. + \frac{1}{8}\left(\frac{1}{1 + v_3(0)} (\nabla_3 \varphi_a)^2 + \frac{1}{v_\perp(0)} (\nabla_\perp \varphi_a)^2\right) + \frac{1}{16.4}\left(\frac{1}{1 + v_3(0)} + \frac{2}{v_\perp(0)}\right)^2 (\varphi_a^2)^2\right\} \tag{23}$$

which shows that the disordered phase sets in at

$$T = T_c \equiv (2\pi)^2 Ba\left(\frac{1}{1 + v_3(0)} + \frac{2}{v_\perp(0)}\right) \tag{24}$$

above which φ_a^2 acquires a non-zero expectation value. This is an XY model transition with the reversed temperature axis, due to the disorder nature of the field φ_a. The coupling to A can now be introduced simply by the gauge invariant replacement $\nabla_i \to D_i$ which in the complex notation $\varphi \equiv \varphi_1 + i\varphi_2$ reads

$$\nabla_i \varphi(\mathbf{x}) \to D_i \varphi(\mathbf{x}) = \varphi(\mathbf{x} + \mathbf{i})\, e^{-2\pi i A_i(\mathbf{x})} - \varphi(\mathbf{x}) \\ \nabla_i^* \varphi(\mathbf{x}) \to D_i^* \varphi(\mathbf{x}) = \varphi(\mathbf{x}) - \varphi(\mathbf{x} - \mathbf{i})\, e^{2\pi i A_i(\mathbf{x} - \mathbf{i})} . \tag{25}$$

In this way we arrive at the following reformulation of the smectic liquid crystal partition function (5) as a gauge field theory of defect lines

$$Z = \prod_{\mathbf{x}} \left[\prod_i \int \frac{dA_i(\mathbf{x})}{\sqrt{2\pi Ba/T}} \int \frac{d\varphi\, d\varphi^+}{T/\pi Ba}\right] \exp\left(-\frac{1}{T} F[\varphi, \varphi^+, A]\right) \tag{26}$$

where the energy F has the Landau expansion in φ :

$$\frac{1}{T} F \approx \sum_{\mathbf{x}} \left\{\frac{1}{4}\left[\frac{(2\pi)^2}{T} Ba - (1 + v_3(0))^{-1} - 2 v_\perp^{-1}(0)\right] |\varphi|^2 + \right. \\ \left. + \frac{1}{16.4}((1 + v_3(0))^{-1} + 2 v_\perp^{-1}(0)) |\varphi|^4 + \frac{1}{8}[(1 + v_3(0))^{-1} |D_3 \varphi|^2 + v_\perp^{-1}(0) |D_\perp \varphi|^2]\right\} \\ + \frac{1}{2} \frac{T}{Ba} \sum_{\mathbf{x},\mathbf{x}'} [A_3(\mathbf{x}) v_3'^{-1}(\mathbf{x}, \mathbf{x}') A_3(\mathbf{x}') + \mathbf{A}_\perp(\mathbf{x}) v_\perp'^{-1}(\mathbf{x}, \mathbf{x}') \mathbf{A}_\perp(\mathbf{x}')] \tag{27}$$

with $\mathbf{D} \simeq \partial - i\, 2\pi \mathbf{A}$.

This energy should be useful for a quantitative study of the critical phenomena near the smectic A-nematic phase transition. Notice that contrary to other approaches [3], there are no free parameters in our energy, all being completely determined in terms of the two smectic parameters.

The potentials $v_3(0)$, $v_\perp(0)$ required for the calculation of T_c can be calculated approximately from the formulae ($\lambda' = \lambda/a$)

$$v_3(0) \sim (\lambda'^2 + \lambda'^5)/(1 + 2\,\lambda' + 2\,\pi\lambda'^4)$$

$$v_\perp(0) \sim \tfrac{1}{2}\,\lambda'(1 + \lambda'(\log \lambda' + \pi)/2\,\pi)/(1 + \lambda'^2)$$

which provide a smooth interpolation between the $\lambda' \to 0, \infty$ limiting behaviours

$$v_3(0) \to \lambda'^2, \frac{\lambda'}{2\,\pi}$$

$$v_\perp(0) \to \frac{\lambda'}{2}, (\log \lambda')/4\,\pi$$

with the maximal mistake around $\lambda' \sim 0.4$. The curve $T_c/(2\,\pi)^2\,Ba$ has roughly the shape $\dfrac{4}{\lambda'} + 8\,\pi/\log(4\,\pi^2\,\lambda')$.

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