10 January 2000

PHYSICS LETTERS A

ELSEVIER

Physics Letters A 264 (2000) 440–443

www.elsevier.nl/locate/physleta

Smectic–nematic phase transition as wrinkling transition in a stack of membranes

H. Kleinert *

Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Received 2 November 1999; accepted 26 November 1999
Communicated by P.R. Holland

Abstract

We point out that the smectic–nematic phase transition may considered as a transition of a stack of membranes in $2+\epsilon$ dimensions, in which the layers become so wrinkled that they interpenetrate each other are no longer distinguishable.

1. Introduction

It is often useful to study one and the same phase transition from various points of view. In the absence of an exact treatment, different approximate ways of describing a system may give valuable insights into complex phenomena such as phase transitions. A good example is the superfluid phase transition in three dimensions. It can be explained in terms of phase and size fluctuations of an order field in $4-\epsilon$ of in three dimensions, as a proliferation transition of vortex lines in a Villain model, which in turn can be reformulated as a complex disorder field theory coupled to a vector potential as in the Ginzburg–Landau theory of superconductivity, or as a transition in a system of pure massless phase fluctuations, as described by a so-called XY-model, which is a nonlinear σ-model on a lattice [1]. Each approach has given us important insights into the physics of the phase transition. Similarly, a Heisenberg model of ferromagnetism can be described by a vector field theory with quartic interactions in three and $4-\epsilon$ dimensions, by a vector model on a lattice, or by an O(3)-symmetric nonlinear σ-model in $2+\epsilon$ dimensions [2–5].

It is the purpose of this Letter to point out that there exists a new alternative way of looking at the smectic–nematic phase transition, which supplements the presently available descriptions by a model, comparable in spirit to the nonlinear σ-model approach to the Heisenberg model in $2+\epsilon$ dimensions. In the past, the transition has been studied in two ways. The first uses the Landau–De Gennes theory [6,7] which contains a complex field to describe the smectic order, and a vector field for the direction order of the molecules. The critical exponents of the phase transition are calculated in $4-\varepsilon$ dimensions. Initial difficulties [8] in explaining the continuous nature of the transition in a certain range of material parameters [9] have later been overcome

* E-mail: kleinert@physik.fu-berlin.de

[1] All these descriptions are discussed in detail in the textbook [1].

0375-9601/00/$ - see front matter
PII: S0375-9601(99)00834-8

[10,1]. An alternative description invokes the statistical mechanics of line-like defects [11,12] which, as in superfluid helium, can be formulated either as a Villain like model, or as a disorder field theory of the Ginzburg–Landau type [13].

2. Stack of membranes

In this Letter we propose a nonlinear theory for the smectic liquid crystal as a vertical stack of membranes, labeled by integer numbers $n = 0, \pm 1, \pm 2, \ldots$, whose positions are parametrized by functions $x^a(\xi, z)$, with $z = z_n = na$. The membranes are assumed to possesses only a curvature stiffness [14]. They are held at their average vertical distance a by quasi-harmonic forces [15–17]. In a continuum approximation of the stack, we shall write the energy as

$$E = \frac{1}{2\alpha}\int d(z/a)\int d^2\xi\rho(\xi,z) \times\left[\left(D^2x\right)^2 + \lambda^{ij}\left(\partial_i x\partial_j x - \delta_{ij}\rho\right) + b\left(N^a\partial_a x\right)^2\right] \tag{2.1}$$

The Lagrange multiplier field $\lambda^{ij}(\xi, z)$ ensures the intrinsic metric of the surfaces $x^a(\xi, z)$ to be in the conformal gauge $g_{ij}(\xi, z) = \partial_i x^a \partial_j x^a = \delta_{ij}\rho(\xi, z)$. The derivatives ∂_i apply to the conformal coordinates ξ^i of the individual membranes, and D^2 is the conformal Laplacian $\rho^{-1}\partial^2$. The vectors $N^a(\xi, z) = \frac{1}{2}\sqrt{g}\,\varepsilon^{ij}\varepsilon^{abc}\partial_i x^b \partial_j x^c$ describes the normal vectors of the membranes, and the elastic term proportional to b ensures an average spacing between the membranes in the normal direction. In a vertical stack, the normal vectors N^a point predominantly along the z-axis, and we may simplify the model by approximating $N^a \approx \hat{z}$, hopefully without an essential modification of the physical properties to be studied.

3. Nonperturbative approximation

Consider a planar background configuration of the stack $x^1 = \xi^1, x^2 = \xi^2, x^3 = z_n$, and allow only for vertical deviations $x^3(\xi, z) = z + u(\xi, z)$ at $z = z_n$. The vertical fluctuations $u(\xi, z)$ of the membranes are purely harmonic in the model, and can be integrated out, leaving only u- and λ fluctuations. These will be treated in mean-field approximation, an approximation which would be exact if the membrane were to fluctuate in a very large number of dimensions.

In this approximation, we may assume the metric g_{ij} and the multiplier field λ^{ij} to be constant and isotropic,

$$\lambda^{ij} = \lambda g^{ij} = \lambda\rho^{-1}\delta_{ij}, \text{with } \lambda = \text{const. and } \rho = \text{const.}$$

This simplifies the result of integrating out the u-fluctuations, yielding in the continuum the following reduced free energy density ($f = F/AT$ = free energy F per unit stack area A and temperature T)

$$f = \rho\left\{\frac{1}{2}\int\frac{d^2q}{(2\pi)^2}\int\frac{d\omega a}{2\pi}\ln\left(b\omega^2 + q^4 + \lambda q^2\right) - \frac{\lambda}{\alpha T} + \frac{\lambda}{\alpha\rho T}\right\} \tag{3.1}$$

where q_i and ω are the momenta in ξ^i- and z-directions, respectively. The temperature T is measured in natural units with $k_B = 1$.

In order to make the model renormalizable, we generalize the z-dimension to ε, and consider the model in $2+\varepsilon$ dimensions with small $\varepsilon > 0$. Then the ω-integral is finite in dimensional regularization.

Thus we apply the formula

$$\int\frac{d^\varepsilon(\omega a)}{(2\pi)^\varepsilon}\log\left(b\omega^2 + K^2\right) = \frac{1}{(4\pi)^{\varepsilon/2}}\frac{2}{\varepsilon}\Gamma(1-\varepsilon/2)\frac{a^\varepsilon}{b^{\varepsilon/2}}K^\varepsilon \equiv h_\varepsilon\frac{a^\varepsilon}{b^{\varepsilon/2}}K^\varepsilon, \tag{3.2}$$

to Eq. (3.1), leaving a q^i-integral over $f(\lambda) \equiv (q^4 + \lambda q^2)^{\varepsilon/2}$, which diverges like $(q^2)^{1+\varepsilon}$. The integral is conveniently regularized by a cutoff at $q^2 = \Lambda^2$, whose magnitude is determined by the inverse lateral size of the molecules in the membranes. By expanding near $\varepsilon = 0$ dimensions $(q^4 + \lambda q^2)^{\varepsilon/2} = (q^2)^\varepsilon + (\varepsilon/2)\lambda(q^2)^{\varepsilon-1} + \ldots$, we isolate the divergences. The remaining integral over the subtracted part of $f(\lambda)$, which may be written as $f_{\text{sub}}(\lambda) = f(\lambda) - f(0)$

$-\lambda f'(0)$, can be calculated with the help of the integral formula

$$\int_0^\infty dx x^{\mu-1}(1+x)^{-\nu} = \Gamma(\mu)\Gamma(\nu-\mu)\Gamma(\nu).$$

The resulting free energy density is

$$f = \rho\left\{ \frac{a^\epsilon h_\varepsilon}{b^{\varepsilon/2} 8\pi}\left(\frac{\Lambda^{2\varepsilon+2}}{1+\varepsilon} + \frac{\lambda}{2}\Lambda^{2\varepsilon}\right) - \frac{a^\varepsilon}{b^{\varepsilon/2}} \frac{h_\varepsilon c_\varepsilon \varepsilon}{8\pi(1+\varepsilon)} \lambda^{1+\varepsilon} a^\varepsilon - \frac{\lambda}{\alpha T} + \frac{\lambda}{\alpha\rho T}\right\}, \tag{3.3}$$

with

$$c_\varepsilon \equiv \frac{\Gamma(-\varepsilon)\Gamma(1+\varepsilon/2)}{\Gamma(-\varepsilon/2)} \approx \frac{1}{2} + \mathcal{O}(\varepsilon^2), \tag{3.4}$$

such that $h_\varepsilon c_\varepsilon \varepsilon \approx 1 + \mathcal{O}(\varepsilon)$. The leading divergence proportional to $\Lambda^{2\varepsilon+2}$ may be omitted since it can be removed by a counter term in the form of a surface tension, which is added to the initial energy functional (2.1) to obtain a finite theory.

Note that for ϵ close to unity, the theory is nonrenormalizable since the fluctuations generate a divergence of the form λ^2/ε. To absorb this infinity, we would have to add a term $\propto \lambda^2$ to the initial energy (2.1), a term describing in-plane elasticity.

Minimizing f in ρ, and maximizing it in λ, gives the saddle point equations

$$\lambda = 0 \quad \text{or} \quad \frac{1}{\alpha}\left(\frac{1}{T} - \frac{1}{T_c}\right) = -\frac{h_\varepsilon c_\varepsilon}{8\pi b^{\varepsilon/2}} \frac{\lambda^\varepsilon a^\varepsilon}{1+\varepsilon} \tag{3.5}$$

and

$$\frac{1}{\rho} = 1 - \frac{T}{T_c} + \alpha T \frac{h_\varepsilon c_\varepsilon}{8\pi b^{\varepsilon/2}} \lambda^\varepsilon a^\varepsilon \tag{3.6}$$

where we have introduced the critical temperature

$$T_c = \left(\alpha \frac{a^\varepsilon h_\varepsilon}{b^{\varepsilon/2}} \frac{\Lambda^{2\varepsilon}}{8\pi}\right)^{-1}. \tag{3.7}$$

The energy density at the extremum is

$$f = \frac{\lambda}{\alpha}. \tag{3.8}$$

The $\lambda \neq 0$-solution is found in the high-temperature phase, $T > T_c$, where the order parameter λ is given by

$$\lambda = a^{-1}\left[\frac{8\pi b^{\varepsilon/2}(1+\varepsilon)}{\alpha h_\varepsilon c_\varepsilon \varepsilon}\left(\frac{1}{T} - \frac{1}{T_c}\right)\right]^{1/\epsilon} \tag{3.9}$$

and (3.6) is solved by

$$\rho^{-1} = \varepsilon\left(\frac{T}{T_c} - 1\right). \tag{3.10}$$

At $T = T_c$, the system undergoes a phase transition to the low temperature phase with $\lambda = 0$ and

$$\rho^{-1} = 1 - \frac{T}{T_c}. \tag{3.11}$$

Since ρ characterizes the ratio between intrinsic area and base area, we see that the surface becomes infinitely wrinkly at the transition. This destroys the layered structure.

4. Physical properties

The free energy density $f = \lambda/\alpha$ is $\propto (T - T_c)^{1/\varepsilon}$ above and $\equiv$ below T_c, which is characteristic for a second order phase transition. The critical exponent α governing the divergence of the specific heat near T_c like $|T - T_c|^{-\alpha}$ is $\alpha = 2 - 1/\epsilon$. Experimentally, this exponent is the same as in superfluid helium [9], i.e., close to zero. This does not agree too well with $\alpha = 2 - 1/\epsilon$ for $\varepsilon = 1$. Such a disagreement, however, is typical for this type of expansion: The nonlinear σ-model yields $\alpha = 2 - 3/\epsilon$ for all O(n) symmetries [2], which is negative at $\epsilon = 1$, and thus much worse than our result.

The properties of the transition are better understood by looking at the effective energy of long-wave-length fluctuations. In the low temperature phase with $\lambda = 0$ it reads

$$E_{\text{eff}} = \frac{1}{2\alpha}\int d(z/a)\int d^2\xi \left[(\partial^2 u)^2 + b(\partial_z u)^2\right] \tag{4.1}$$

This is an approximate energy for the smectic phase used a long time ago by De Gennes [18]. It can be

derived from a gradient energy of a particle density $n(\xi,z)$.

$$E=\int d(z/a)\int d^2\xi\left[\left(\partial^2+k_0^2\right)n(\xi,z)\right]^2, \qquad (4.2)$$

by inserting a periodic layer ansatz for the ground state density.

$$n(\xi,z)\sim\cos\left[k_0 z+u(\xi,z)\right].$$

The wave fronts are smoothly displaced in the vertical direction by $u(\xi,z)$. Expanding (4.2) in powers of u and its gradients, and averaging over many layers one finds (4.1) with $b\equiv 4k_0{}^2$.

In the high-temperature phase, the effective energy becomes

$$E\approx\frac{1}{2\alpha}\int d(z/a)\times\int d^2\xi\left[(\partial^2 u)^2+\lambda(\partial_i u)^2+b(\partial_z u)^2\right], \qquad (4.3)$$

which describes, at long wavelengths where the curvature term is much smaller than the others, the elastic energy of an ordinary *continuum* in all directions, without preference of the z-direction.

During the phase transition, the undulations of a layer change from a long-range algebraic correlation in the transverse direction ($r\equiv|\xi|$)

$$\langle u(\xi)u(0)\rangle\approx T\int\frac{d^2q}{(2\pi)^2}\frac{d\omega}{2\pi}\frac{\alpha a\,e^{iq\xi}}{q^4+b\omega^2}=T\pi\frac{\alpha a}{\sqrt{b}}\frac{1}{2\pi}\ln r$$

to a short-range correlation

$$\langle u(\xi)u(0)\rangle\approx T\int\frac{d^2q}{(2\pi)^2}\frac{d\omega}{2\pi}\frac{\alpha a\,e^{iq\xi}}{\lambda q^2+b\omega^2}=T\pi\frac{\alpha a}{\sqrt{b\lambda}}\frac{1}{2\pi r}.$$

In the first case, the surface is smooth, in the second case, it is so wrinkled that the layers interpenetrate each other and become indistinguishable.

These are signals that the stack of layers has entered a homogeneous phase which is anisotropic in the third direction.

At this point we establish contact of this transition with the nematic–smectic transition in liquid crystals. For this we imagine vertical rod-like molecules to be attached to the surfaces of the model. Then the two phases of the stack of membranes can be considered as the layered smectic, and the direction-ordered nematic phase of a liquid crystal.

5. Outlook

For a more complete description of the system it will be necessary to include the transverse elastic properties of the membranes and study the behavior of the shear resistance near the transition. In addition, a vector field will be necessary to account for the directional properties of the molecules on the layers before and after transition.

Acknowledgements

The author thanks M.E. Borelli for useful discussions.

References

[1] H. Kleinert, Gauge Fields in Condensed Matter, Vol. I Superflow and Vortex Lines, World Scientific, Singapore 1989, pp. 1–744. (See www.physik.fu-berlin.de/~kleinert/re0.html#b1.)
[2] E. Brézin, S. Hikami, cond-mat/9612016.
[3] S. Hikami, E. Brézin, J. Phys. A 11 (1978) 1141.
[4] W. Bernreuther, F.J. Wegner, Phys. Rev. Lett. 57 (1986) 1383.
[5] H. Kleinert, Variational Resummation of ϵ-Expansions of Critical Exponents in Nonlinear $O(N)$-Symmetric σ-Model in $2+\epsilon$ Dimensions, FU-Berlin preprint 1998, hep-th/9808145.
[6] P.G. De Gennes, Solid State Commun. 10 (1972) 753.
[7] P.G. De Gennes, Mol. Cryst. Liq. Cryst. 21 (1973) 498.
[8] B.I. Halperin, T.C. Lubenski, S.-K. Ma, Phys. Lett. 32 (1974) 292.
[9] J. Thoen, M. Maynissen, W. Van Dael, Phys. Rev. Lett. 52 (1984) 204.
[10] H. Kleinert, Lett. Nuovo Cimento 35 (1982) 405.
[11] J. Toner, D.R. Nelson, Phys. Rev. B 23 (1981) 316.
[12] A.R. Day, T.C. Lubensky, A.J. McKane, Phys. Rev. A 27 (1983) 146.
[13] H. Kleinert, J. Phys. (Paris) 44 (1983) 353.
[14] W. Helfrich, Z. Naturforsch. C 29 (1974) 510.
[15] W. Helfrich, Z. Naturforsch. A 33 (1987) 305.
[16] W. Helfrich, R.M. Servuss, Nuovo Cimento D 3 (1984).
[17] W. Janke, H. Kleinert, Phys. Rev. Lett. 58 (1987) 144.
[18] P.D. De Gennes, J. Phys. (Paris) 30 (1969) C4.