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Blue Phases in the Presence of Fluctuations. A One-Star Analysis

Jochen Englert [a], Lech Longa [b] & Hans-Miner Trebin [a]

[a] Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57/VI, Stuttgart, Germany

[b] Jagiellonian University, Department of Statistical Physics, Reymonta 4, Kraków, Poland

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BLUE PHASES IN THE PRESENCE OF FLUCTUATIONS. A ONE–STAR ANALYSIS.

JOCHEN ENGLERT*, LECH LONGA†,
and HANS-RAINER TREBIN*
* Institut für Theoretische und Angewandte Physik,
Universität Stuttgart, Pfaffenwaldring 57/VI, Stuttgart, Germany
† Jagiellonian University, Department of Statistical Physics,
Reymonta 4, Kraków, Poland

Abstract Conventional mean-field theory renders the *structure* of the cubic blue phases correctly, but not their *position* on the phase diagram. Also it has not been possible to suppress the artificial body centered cubic structure O^5. Within the framework of the weak crystallization theory we extend the Landau-Ginzburg-de Gennes free energy by including order parameter fluctuations. Calculations that involve one star of wave vectors destabilize the formerly dominant O^5 structure.

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The structure and properties of the blue phases (BPs) of chiral liquid crystals have been investigated thoroughly for more than 20 years now. Already in 1975 BRAZOVSKII[1] presented analytical calculations concerned with phase transitions in cholesteric liquid crystals, and he was the first to note that there may exist further ordered phases between the cholesteric and the isotropic (Iso) phases. However, no detailed phase diagrams were found at that time.

Experimentally it is well established that BPI has a body-centred cubic structure of $O^8(I4_132)$ space group symmetry, and that BPII is simple cubic $O^2(P4_232)$ (see e.g. [2]). The structure of BPIII, in turn, is still a matter of intensive theoretical and experimental studies[3–5], but many features of this phase are well reproduced by an isotropic model[3,4]. Mean field phase diagrams describing some of the properties of BPs were given in the work of GREBEL[6] *et al.* Using a Landau–Ginzburg–de Gennes free energy they considered the stability of phases with different space group symmetries as a function of temperature and chirality. Calculations were carried out by taking into account up to four shells (stars) of symmetry allowed wave vectors. The resulting phase diagram is sketched in Figure 1 (a). Note that at low temperatures only the cholesteric phase is stable. Additionally, with increasing chirality three cubic phases become stabilized: a simple cubic structure of space group symmetry $O^2(P4_232)$ and the body-centred cubic structures $O^8(I4_132)$ and

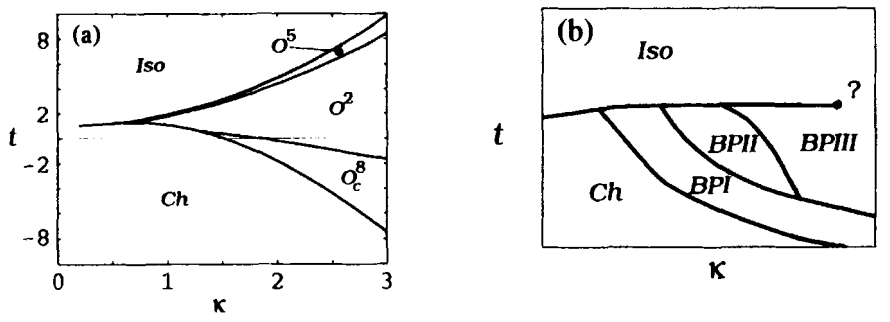

FIGURE 1: a) Theoretical phase diagram according to [2]. b) Sketch of the experimental phase diagram according to [7] and [5].

$O^5(P432)$. The O^5 structure is already stable at low chiralities ($\kappa \approx 0.5$), being the only phase except for the cholesteric one that shows a phase transition to Iso.

An experimental phase diagram[5,7] is sketched in Figure 1 (b). By comparing Figures 1 (a) and 1 (b) it is found that the structure of BPI and BPII could be associated with the space group symmetries O^8 and O^2, respectively. This observation is well supported by morphological studies[2]. But BPIII does not correspond to the theoretically found O^5 space group symmetry. Also, unlike the theoretical prediction, the first cubic phase appearing at low chiralities is BPI. At high chiralities BPIII dominates. Finally, in contrast with the theory, BPII vanishes at high chiralities.

It seems therefore, that at least two issues must be addressed to by an improved theory. The first one is a quantitive description of BPIII, that allows for systematic calculations of the free energy for all relevant structures. Another one is to reproduce phase transitions O^8–Iso and O^2–Iso, i.e. find a mechanism that destabilizes O^5. It can be shown that the mere introduction of an additional order parameter, such as a bond orientational one[8,9] or a pseudoscalar order parameter[3,4], does not solve the problem. Hence, in this paper we shall follow an alternative direction that allows for systematic studies of the effect of order parameter fluctuations on the phase diagrams of BPs. As the calculations are involved we restrict ourselves to the case when the cholesteric and the cubic structures are modelled by a single star of wave vectors. Generalization of the results to more than one star will be given elsewhere.

A first step towards taking into account the effect of fluctuations is to evaluate the two particle correlation function of the uniform phase

$$G^{(2)}(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{Z[0]} \frac{\delta^2 Z[\mathbf{J}]}{\delta \mathbf{J}(\mathbf{x}_1) \delta \mathbf{J}(\mathbf{x}_2)}\bigg|_{\mathbf{J}=\mathbf{0}}, \tag{1}$$

where

$$Z[\mathbf{J}] = \int \mathcal{D}\mathbf{Q} \exp\left(-\int \mathrm{d}\mathbf{x} \left(\mathcal{F}_0[\mathbf{Q}] + \lambda \mathcal{F}_I[\mathbf{Q}] + \mathbf{J}\mathbf{Q}\right)/k_B T\right) \tag{2}$$

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is the partition function, $\mathbf{J}$ is the external field conjugate to the alignment tensor $\mathbf{Q}(\mathbf{x})$, and $\mathcal{F}_0$ and $\lambda\mathcal{F}_I$ are the quadratic and higher orders of the Landau-Ginzburg-de Gennes functional[8], respectively.

Taylor expansion of the partition function (2) about $\lambda = 0$ leads to the well known analysis in terms of Feynman graphs. In particular, the effective free enthalpy $F = \ln Z$ for the disordered phase calculated up to the order of one loop is given by the two point vertex $\Gamma^{(2)}$[10], where

$$\Gamma^{(2)} = (G_0(\mathbf{k}))^{-1} - k_B T \Sigma(\mathbf{k}), \tag{3}$$

and where

$$G_0(\mathbf{k}) = \langle \mathbf{Q}(\mathbf{k})\mathbf{Q}(-\mathbf{k}) \rangle / k_B T = \frac{2}{t - \kappa^2 + \kappa^2(k - q_0)^2} \tag{4}$$

is the Fourier-transformed Gaussian propagator. $\Sigma(\mathbf{k})$ is the self energy function containing Feynman graphs without external legs. Neglecting higher order loop diagrams and off diagonal elements in $\mathbf{k}$ we arrive at the equation for the renormalized temperature in the isotropic phase given by (for comparison see [11])

$$\Delta_{iso} = \frac{\tau}{2} + \frac{\lambda k_B T}{2} \int^{q_0=1} dq\, G_0(q)(1 + 2\,|\mathrm{Tr}(\mathbf{M}_2(\mathbf{q})\mathbf{M}_2(-\mathbf{k})|^2)$$
$$\approx \tau/2 + (7\lambda k_B T)/(120\pi\kappa\sqrt{2\Delta_{iso}}), \tag{5}$$

where $\tau = t - \kappa^2$, $\mathbf{M}_2(\mathbf{k})$ are the spin $L = 2$ tensors with helicity $m = 2$ entering the plane waves expansion of the tensor field $\mathbf{Q}$ (see e.g. [9]). The last estimate in Eq. (5) is valid provided that Δ is small. Only the lowest lying branch ($m = 2$) of the excitation spectrum of $\mathcal{F}_0[\mathbf{Q}]$ is taken into account.

Calculations similar to [1] give the corresponding equation for Δ in the ordered state ($\mu \equiv \mu_2$ is the mean field value). It reads

$$\Delta(\mathbf{k}) = \tau/2 + \mu^2 s(\mathbf{k})/N + (7k_B T)/(120\pi\kappa\sqrt{2\Delta}), \tag{6}$$

where

$$s(\mathbf{k}) = \frac{1}{6}\left(N + 2\sum_{\mathbf{k}_l \in {}^*\mathbf{k}} |\mathrm{Tr}(\mathbf{M}_2(\mathbf{k}_l)\mathbf{M}_2(-\mathbf{k})|^2\right) \tag{7}$$

and where N is the number of prongs of the star. Restricting to $m = 2$ modes (also for the cholesteric phase) we arrive at the following values for the function $s(\mathbf{k})$: 2/3 (cholesteric), 17/12 (O^2), 269/96 (O^5, O^8). Note that by rescaling the original Hamiltonian the parameter λ could be set to one[6]. Finally, the $m = 2$ Fourier component of the external field is given by

$$J(\mathbf{k}_m) \equiv J = \frac{\partial F}{\partial \mu} = \Delta\mu - \frac{1}{2}\mu^2 \sum_{\mathbf{k}_j} (\mathrm{Tr}(\mathbf{M}_2(-\mathbf{k}_j - \mathbf{k}_m)\mathbf{M}_2(\mathbf{k}_j)\mathbf{M}_2(\mathbf{k}_m))$$
$$+ 2\mathrm{Tr}(\mathbf{M}_2(-\mathbf{k}_j - \mathbf{k}_m)\mathbf{M}_2(\mathbf{k}_m)\mathbf{M}_2(\mathbf{k}_j))) - s(\mathbf{k})\mu^3 +$$
$$\frac{1}{12}\mu^3 \sum_{jk} (\mathrm{Tr}(\mathbf{M}_2(-\mathbf{k}_j - \mathbf{k}_k - \mathbf{k}_m)\mathbf{M}_2(\mathbf{k}_j))\mathrm{Tr}(\mathbf{M}_2(\mathbf{k}_k)\mathbf{M}_2(\mathbf{k}_m))$$
$$+ \mathrm{Tr}(\mathbf{M}_2(-\mathbf{k}_j - \mathbf{k}_k - \mathbf{k}_m)\mathbf{M}_2(\mathbf{k}_m))\mathrm{Tr}(\mathbf{M}_2(\mathbf{k}_k)\mathbf{M}_2(\mathbf{k}_m))). \tag{8}$$

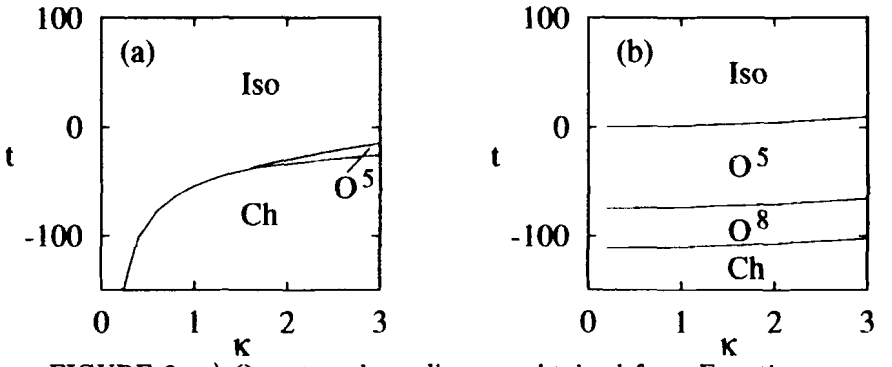

FIGURE 2: a) One star phase diagram obtained from Equations (10) and (11) with renormalized energies. b) The corresponding one star mean field phase diagram.

With the help of Eqs. (5)–(8) the calculations of the equilibrium free energy of various phases could proceed in a similar way as in [1]. In particular, the difference of the free energy between the ordered and the isotropic phase is given by

$$\delta E = \int_0^{\mu_{\rm ord}} NJ \mathrm{d}\mu \tag{9}$$

Explicit calculations of the integral (9) for the cholesteric and the cubic structures yield the free energy differences relative to the isotropic phase. They read

$$E_{Ch/O^2} = -c_1\Delta^2 - c_2\Delta_{iso}^2 + \frac{Nc}{2s\kappa}(\sqrt{\Delta} - \sqrt{\Delta_{iso}}) \tag{10}$$

$$E_{O^5/O^8} = c_3(\Delta^2 - \Delta_{iso}^2) + \frac{Nc}{2s\kappa}(\sqrt{\Delta} - \sqrt{\Delta_{iso}}) - c_4\mu^3 - c_5\mu^4, \tag{11}$$

where $c_1 = c_2 = 3/4$ for the cholesteric phase, $c_1 = 117/34, c_2 = 18/17$ for O^2, $c_3 = 288/269, c_4 = 23/32\sqrt{12}, c_5 = 13/3072$ for O^5 and $c_3 = 288/269, c_4 = -5/16\sqrt{6}, c_5 = 89/9216$ for O^8, $\mu = d_1(1-\sqrt{1+d_2\Delta})$ with $d_1 = -828/13\sqrt{12}, d_2 = 832/4761$ for O^5 and $d_1 = 1080/89\sqrt{6}, d_2 = 712/675$ for O^8. Finally, c is a free parameter proportional to $k_{\rm B}T$.

A representative phase diagram is given in Figure 2 (a). For comparison the mean field diagram in one star approximation is additionally presented in Figure 2 (b). In order to understand the effect of fluctuations on various cubic structures we also calculated the phase diagrams with cholesteric and O^8 phases being suppressed. They are given in Figures 3 (a) and 3 (b). Generally we find that the body-centred cubic phases are strongly destabilized for $\kappa \lesssim 2$. The effect is attributed to correlations between the Fourier components of the **Q** tensor, induced by the quartic term of the Landau-Ginzburg-de Gennes functional. At high chiralities the quartic term becomes negligible with the self energy corrections being proportional to κ^{-1}. In this regime the free energy of the system is dominated by the quadratic part of the free energy ($\sim \kappa^2\mu^2$) and by the Gaussian part ($\sim \ln\kappa$), which is nearly

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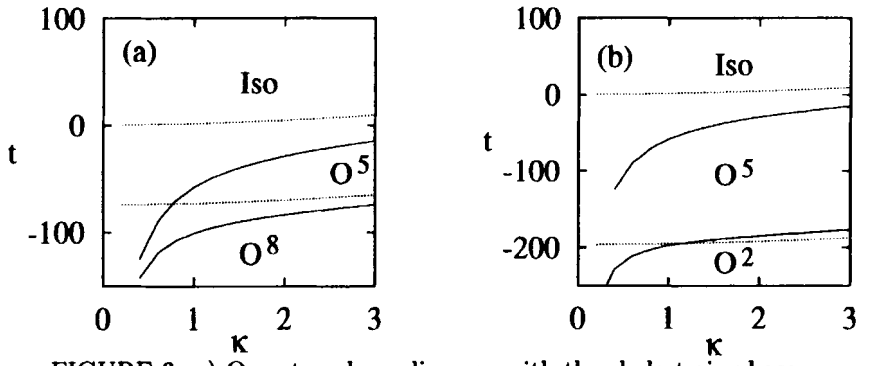

FIGURE 3: a) One star phase diagram with the cholesteric phase being suppressed. b) O^8 is also suppressed. The dashed lines represent the corresponding mean field diagrams.

the same for all structures. This implies that, effectively, phase diagrams approach mean field high chirality limit. In conclusion we could show that the stability of O^5 is lowered by the influence of fluctuations. In order to get proper phase sequences, however, it might be necessary to modify the Landau coefficient λ of the quartic order. This will be published elsewhere.

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