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R. G. Priest [a]

[a] Naval Research Laboratory Washington, D.C., 20375

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RENORMALIZATION GROUP CALCULATION APPLIED TO THE NEMATIC-ISOTROPIC PHASE TRANSITION

R. G. PRIEST
Naval Research Laboratory
Washington, D. C. 20375

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ABSTRACT: The renormalization group technique is used to calculate the difference between T_c, the nematic-isotropic transition temperature and T* the temperature at which the reciprocal of the light scattering intensity extrapolates to zero. The model free energy is the Landau de Gennes form. This calculation gives results which are in better agreement with experiment than the mean field approximation results.

The Landau de Gennes second rank tensor phenomenology[1] qualitatively predicts the principle experimental results for nematic liquid crystal systems. On close examination however, one quantitative discrepancy between the theory and experiment is found to be much larger than reasonably expected. It is customary to define T_c as the nematic-isotropic phase transition temperature. The phenomenological theory contains another temperature commonly called T*, which is the absolute limit of stability of the isotropic phase. The theory predicts that $T_c > T^*$ and that the intensity of light scattering in the isotropic phase is proportional to $1/(T - T^*)$. The experimental result[2] for $T_c - T^*$, as determined by light scattering, is approximately 1°C for p-azoxyanisole (PAA). However, pointed out by Shih et al.[3], any reasonable choice of parameters in the phenomenological free energy leads to values more than 10 times as large. The Maier-Saupe model[4] also predicts far too large a result for $T_c - T^*$.

It was suggested in reference 3 that the source of the large discrepancy may be that the mean field approximation is used to analyze the theoretical models. These authors put forward a renormalization group analysis supporting an earlier hypothesis that the coherence length (and hence the light scattering intensity) diverges at a temperature higher than T*.

In view of this development it seems worthwhile to consider a renormalization group analysis of the de Gennes model that does not involve any special hypotheses. In an earlier publication[5] a renormalization group analysis of the de Gennes model in the form:

$$\begin{aligned} F = \int d^d x \, [\tfrac{1}{4} (r \, Q_{ij}Q_{ij} + \nabla_k Q_{ij} \nabla_k Q_{ij}) \\ - b \, Q_{ij} Q_{jk} Q_{ki} + u \, (Q_{ij}Q_{ij})^2 \\ - H_{ij} Q_{ij}] \end{aligned} \qquad (1)$$

was reported. Here $d^d x$ indicates a functional integral in d dimensions over the tensor field Q = Q(x). The tensor Q is 3 x 3, symmetric and traceless. The quadratic coefficient r is linear in the temperature T and the coefficients b, u and H are temperature independent. In the isotropic state $< Q > = 0$. If H_{ij} is uniaxial, $< Q >$ is diagonal in the nematic state with $< Q_{11} > = S$, $< Q_{22} > = < Q_{33} > = -\frac{1}{2}S$. The quantity S is the usual order parameter.

The analysis in reference 5 employed the ε expansion technique.[6] This method relies on the fact that the mean field approximation is exact for $d > 4$. It is a perturbation expansion about the solution for $d = 4$. The small parameter is $\varepsilon = 4-d$. The fixed point of the renormalization group corresponds to a second order phase transition with $b = 0$. The cubic coupling was found to be a "relevant" term so b was treated as a perturbation. One of the results obtained was an expression for the equation of state in scaling form:

$$\frac{H}{S^{\delta}} + \frac{t}{S^{w}} = 1 + X + \frac{\varepsilon}{26}\,[3(3+X)\ \ln\ (3+X) \qquad (2)$$

$$+4(1+X)\ \ln\ (1+X) + 6X\ \ln\ (2) - 9(1+X)\ \ln\ 3]$$

Here $X = t/S^{1/\beta}$, $\delta = 3+\varepsilon$, $w = 1+7\varepsilon/13$ and $\beta = .5(1-3\varepsilon/13)$. The quantity t is the reduced temperature $t = (T-T^*)/T^*$. The temperature T* is the temperature at which the second order phase transition would take place if b were zero. Therefore T* retains its significance as the temperature at which the light scattering intensity would diverge if there were no cubic coupling and hence no first order phase transition. In deriving Eq. (2) the external field H_{ij} was set to the uniaxial form $H_{11} = H$, $H_{22} = H_{33} = -\frac{1}{2} H$.

From general thermodynamic arguments we know that $H = -\partial F/\partial S$. The free energy may therefore be found by integrating the equation of state with respect to S. The conditions that the free energies of the isotropic and nematic states be equal and that the free energy be a local minimum with respect to S can be expressed as:

$$\int_0^S H(S')\,dS' = 0 \qquad (3a)$$

$$H(S) = 0 \qquad (3b)$$

For fixed b these equations are to be solved for $S = S_c$ and $t = t_c$. The resulting value of t_c is then interpreted as $t_c = (T_c - T^*)/T^*$. Since the equation of state, Eq. (2), exhibits Van der Waals loops, Eq. (3) may be viewed as a Maxwell construction.

Of course the coefficient b is unknown. However it is well known[4] that $S_c \cong .4$. A reasonable approach is to choose b such that S_c is equal to this experimental value. This requires a numerical solution of Eq. (3) as a function of b. It is also desirable to do this calculation in the mean field approximation. It can be easily verified that this is equivalent to setting $\varepsilon = 0$ in Eq. (2) and using Eq. (3). The results are given in Table 1.

TABLE 1

	$\varepsilon = 1$	$\varepsilon = 0$ (mean field)
S_c	.4	.4
t_c	.04283	.08
b	.3819	.6
$\frac{dS}{dt}$	-6.08	-5.0
$T_c - T^*$	12.8°	24°

The values for $\frac{dS}{dt}$ are included to show that reasonable values for the variation of order parameter with temperature are obtained. A value of -5. for this quantity corresponds to a few per cent per degree. The values for $T_c = T^*$ are for the case $T^* = 300°K$. As can be seen from the table, the renormalization group result is approximately one half as large as the mean field result while still being too large in comparison with experiment. The improvement over the mean field result is however, encouraging.

In hopes of obtaining still better results there are three aspects of this calculation that could be explored in more detail. First, the cubic coupling b is treated as a perturbation in the calculation of the equation of state. Perhaps this is not adequate for $b \sim 1/3$. Second the ε expansion was used to calculate the equation of state. For $d < 10/3$ the quintic (Q^5) coupling becomes relevant. Since the ε expansion is based at $d = 4$ it does not reflect the quintic coupling. Third, the validity of the Maxwell construction has never been examined in the context of the renormalization group. Unfortunately these are all difficult points which may have to await further progress in the theory of phase transitions for clarification.

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