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Critical Exponents for the Landau-De Gennes Model of the Nematic-Isotropic Phase Transition

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Critical Exponents for the Landau-De Gennes Model of the Nematic-Isotropic Phase Transition

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In this paper we report the application of Wilson's recursion relations to the numerical calculation of critical indices for the $d = 3$ Landau-de Gennes model near the isolated critical point on the nematic-isotropic phase transition line. We find that the calculated critical exponents namely $\gamma = 1.277$ and $\nu = 0.638$ in fair agreement with the best epsilon expansion results.

Keywords: Nematic liquid crystals; critical exponents; renormalization group; phase transition

PACS number(s): 64.70.Md, 61.30.Ak, 64.60.Ak, 64.60.Kw

INTRODUCTION

Although the nematic-isotropic (N-I) phase transition is the simplest and the most studied phase transition in liquid crystals, it is still of considerable current interest [1–10]. Therefore, it is surprising that until now there are no clear answers to some key questions concerning the nature of this phenomenon. First of all it is not quite clear what makes this transition so weakly first order. The low value of $(T_c - T^*)/T_c \approx 0.1\%$, where T_c is N-I transition temperature and T^* is the absolute stability limit of the isotropic phase poses a long standing puzzle. In some of our recent works [2–4] we looked into this problem both from the Landau mean-field theory and the

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renormalization group (RG) theory. Again in another work [5], Mukherjee *et al.* investigated the possibility of the critical region at the first order transition line of the N-I transition in the context of epsilon expansion. Recently Rzoska *et al.* [9] discussed the critical behavior of dielectric permitivity in the isotropic phase of nematogens. Keyes [11–12] suggested that the critical exponents for quantities diverging toward temperature T^* before being cut off by a first order transition at T_c, should be the characteristic of a tricritical point. Again considering the specific heat, Anisimov *et al.* [13–14] made a strong plea for tricritical hypothesis, fitting very precise specific heat measurements of MBBA and other compounds. In short, many questions remains about the nature of the N-I transition.

The renormalization-group approach to the theory of critical phenomena has been used by Wilson [15] to calculate critical exponents for the d-dimensional Ising model and by Wilson, Fisher, Pfeuty and Wegner to obtain perturbation expansion [16–19] in $\varepsilon = 4 - d$ of the critical indices for the classical Heisenberg, $X - Y$, and Ising models. Critical phenomena in liquid crystals have specific features due to the variety of the symmetries of the different phases and coupling of the different order parameters. These features complicate theoretical considerations and restrict methods which are well proved in other cases (RG method).

The transition of the isotropic phase of a liquid crystal to the nematic phase was investigated in detail in the paper of Vigman, Larkin and Filev [20]. This transition is first order. Appreciable pretransition phenomena indicate that the transition is close to being second order. There exists an appreciable region in which fluctuations become important and the Landau theory is not applicable. In the nematic phase the director fluctuations are "critical". Nelson and Pelcovits [21] pointed out that strongly developed director fluctuations could alter the character of the N-I transition and make it very weakly first order. They applied the RG method to the description of the fluctuation behaviour near the isolated critical point on the N-I transition line. At this point the cubic invariant in the effective Hamiltonian is equal to zero. With quadratic (r) and cubic (t) variables (in the Laboratory one could adjust the temperature and pressure of which r and t are smooth functions) we would get a first order transition except at an isolated point $r = t = 0$, where the jump in the order parameter vanishes. Baskakov, Semenchenko and Byankin [22] by extrapolating the experimental dependences of the specific-volume discontinuity on the temperature and pressure, concluded that an isolated critical point exists. Several workers [20, 23] investigated the Landau point with fluctuation by means of epsilon (ε) expansion method. At this point one can calculate the critical indices of the

transition to the isotropic phase by the methods of RG theory of expanding in $\varepsilon = 4 - d$ [16] and in $1/n$ [24]. RG calculations have been carried out for the vicinity of the isolated critical point and it has been found that when fluctuations effects are important the critical exponents should be those appropriate to an $n = 5$, $d = 3$ system [25]. The values of the critical exponents for the five component of the order parameter ($n = 5$) at $d = 3$, $\varepsilon = 1$, are obtained as $\beta \approx 0.38$, $\nu \approx 0.64$, $\tau \approx 1.27$, $\eta = 0$, and $\alpha = 0.04$.

In this paper we present a numerical calculation of the critical exponents for the $d = 3$ Landau-de Gennes model near the isolated critical point on the (N-I) transition line from the recursion relation obtained by Wilson in the $\eta = 0$ approximation from RG theory. We find that our result fairly agrees with the best epsilon expansion results. The calculations are very similar to those which have already been reported for the Heisenberg model [26] and the $X-Y$ model [27].

MODEL AND THEORY

For purely geometrical reasons, the N-I transition is first order, as it was recognized by Landau [28]. The Landau-de Gennes model [29] containing a cubic term in the order parameter in the free energy expansion was proposed and used to describe the first order transition in liquid crystals.

The model we consider has the reduced Hamiltonian

$$\mathscr{H} = \int d^d x \left[\frac{1}{2}(r S_{ij} S_{ji} + \nabla_k S_{ij} \nabla_k S_{ij}) - t S_{ij} S_{jk} S_{ki} + u (S_{ij} S_{ji})^2 \right] \tag{1}$$

Here $d^d x$ indicates the integration in d dimension. The tensor S is 3×3, symmetric and traceless. The quadratic coefficient r is written as $r = r_0(T - T^*)$ and r_0, t and u are constants. If t becomes zero then T^* would be the mean field second order transition temperature. But since in our model $t > 0$, T^* would be the mean field absolute stability limit of the isotropic phase. In the isotropic phase $\langle S \rangle = 0$ and in the nematic phase $S_{11} = S$, $S_{22} = S_{33} = -(1/2)S$.

We start from Wilson's recursion formula [30]

$$Q_{p+1}(\mathbf{z}) = -2^d \ln[I_p(2^{1-d/2}\mathbf{z})/I_p(0)] \tag{2}$$

$$I_p(\mathbf{z}) = \int_{-\infty}^{+\infty} dy_1 \cdots dy_n \exp\left[-y^2 - \frac{1}{2} Q_p(y + \mathbf{z}) - \frac{1}{2} Q_p(-y + \mathbf{z}) \right] \tag{3}$$

The space of Q above is the parameter space on which RG transformation is applied.

For the Landau-de Gennes model of the N-I phase transition it may be written as

$$Q_{p+1}(S) = -8\ln\left\{\int_{-\infty}^{+\infty} dy_1 \cdots dy_n \exp\left[-y^2 - \frac{1}{2}(Q_p(2^{-1/2}S + y) + Q_p(2^{-1/2}S - y))\right]\right\} + 8\ln\left\{\int_{-\infty}^{+\infty} dy_1 \cdots dy_n \exp(-y^2 - Q_p(y))\right\} \quad (4)$$

To first order in epsilon (ε) the relevant fixed point controlling the Landau point (isolated critical point) is believed to be that for the isotropic n-vector model with $n = 5$, where n is the dimensionality of the order parameter. Wang and Keyes [8] calculated the fluctuations of all five components of the orientational order parameter of a nematic liquid crystals in a wide variety of circumstances involving several types of critical and multicritical points. Then the cubic term automatically becomes zero. So in the equation (4) we have taken $n = 5$. Then the integration (4) can be taken as $\int d^5 y \propto \int_0^{\infty} dy\ y^{5-1} \approx \int \exp(5 \ln y)\, dy$.

At the isolated critical point the length scale of correlation of the order parameter fluctuations becomes infinite and the series $\{Q_p\}$ is expected to approach a fixed point $Q^*(S)$ as $p \to \alpha$. The critical properties may be determined from the eigen functions and eigen values of (4) linearized about $Q^*(S)$.

NUMERICAL PROCEDURE AND RESULTS

The integrations were performed numerically by the two-point Gaussian integration formula, varying S for 0 to 4 with mesh spacing $\Delta = 0.1$. All calculations were performed in double-precision. Linear interpolation was used to compute $Q_p(S)$ for points in between the mesh point. The integral over y was calculated by neglecting the region $|y| > 3.2$ and dividing the region $-3.2 < y < 3.2$ into equally spaced intervals. In order to find $Q^*(S)$ for the $d = 3$ Ladau-de Gennes model of the N-I transition we consider an initial interaction with $Q_0(S) = r_0 S^2 + 0.5S^4$. In the initial interaction we put the cubic coefficient $t = 0$. If we put $t = 0$ in (1) and (4) then the free

energy depends only on one invariant $\mathrm{Tr}(S^2)$. The value of $\mathrm{Tr}(S^2)$ can be represented as the square of the modulus of a five-dimensional vector whose components are the independent components of the tensor S_{ij}. Thus at $t=0$ the thermodynamic free energy has the symmetry group O_5 of rotations in five dimensional space. In this case the number of Goldstone fluctuations is four. Hence the relevant fixed point merges to an isolated critical point. But for $t \neq 0$ only two Goldstone fluctuations connected with the transverse directions of the director are possible and the isolated critical point is impossible. Hence the integration in Eq. (4) was performed in five dimensional space. Eq. (4) was used to compute the series $\{Q_p(r,s)\}$ integrating numerically by the two-point Gaussian formula over $S/2^{1/2}+y$ and $S/2^{1/2}-y$. For $S>4.0$, a S^6 extrapolation was assumed. The coefficient r_0 is a parameter which one varies in order to locate the critical temperature r_c. It is not difficult to locate the critical value of r_c for r_0. For $r_0 > r_c$ the values of $Q_p(S)$, for fixed S, went rapidly to $+\alpha$ as $p \to \alpha$; for $r_0 < r_c$ the values of $Q_p(S)$ were erratic. In practice, r_c was found by finding the sequence of values r_{cp} for which the pth function $Q_p(S)$ satisfies $Q_p(r_p, 1.5)=0$. This sequence appeared to be converging rapidly with increasing p. The $\{r_p\}$ converges to r_c the critical value, as $p \to \alpha$. To do this one generates on the computer a sequence

$$Q_1(S) \to Q_2(S) \to \cdots \to Q_p(S) \to \tag{5}$$

for a given r_0. This sequence is examined for a fixed value of S, say $S=1.5$. What one wants is a sequence tending to a limit for $p \to \alpha$ as depicted in Figure 1. This never happens in practice. This happens only for a certain values of p. If r_0 is chosen too large, the sequence (5) goes off to infinity because one is above the critical point and the Gaussian term $r_p S^2$ dominates for large p. To compensate, one lowers r_0 and generates a new sequence Q_p. If r_0 were chosen too low, the sequence will tend to oscillate badly for large p. In practice one compromises between these two extremes by choosing an r_0 such that Q_p falls within a preassigned range after a preassigned number p' of iteration. This procedure is then repeated for larger values of p'. Once one has a sequence with $Q_p(S)$ stabilized over many iterations p' ($p' \geqslant 12$ in practice), one has a good approximation to the fixed point function Q^*. The value for r_c was found to be $r_c = -3.2144645$. This determined the isolated critical point as $Q_c(r_c, S)$ and an estimate of $Q^*(S)$ was obtained from the Q_p versus p in Figure 1 for the value of $r_p = -3.2144645$. When $r_0 \simeq r_c$, it was found that the function $Q_p(S)$, as p increased, first approached a critical function $Q_c(S)$, then for very large p

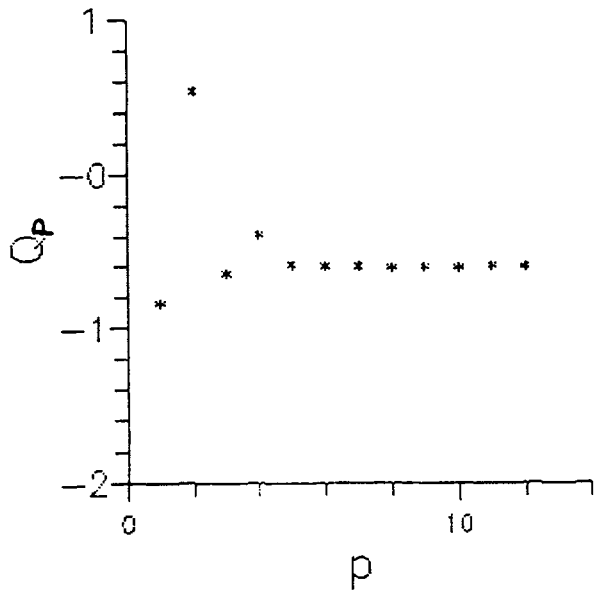

FIGURE 1 An ideal plot of the approach of $Q_p(1.5)$ to a fixed point.

moved away from $Q_c(S)$, just as predicted earlier. The critical function $Q_c(S)$ is plotted in Figure 2. This is nothing but the fixed point function $Q^*(S)$.

Now for the other values of S, one can also obtain the same fixed point function Q^*. But in that case fixed point function Q^* remains same upto $p \to 6$. On the other hand when fix the value of $S = 1.5$, we obtain the fixed point function upto $p \to 12$.

Once one has found the critical function $Q^*(S)$, further numerical studies of the recursion formula yield the critical exponent ν. For this purpose, one begins the iteration scheme with $r_0 \simeq r_c$, but not equal to r_c. One then observes how $Q_p(S)$ departs from Q^*. For reasonably large p, one expects that Q_p has the form

$$Q_p \simeq Q^* + (r_0 - r_c)\lambda^p R^*(S) \tag{6}$$

with

$$\lambda = 2^{Y_1} = 2^{1/\nu} \tag{7}$$

where $R^*(S)$ is function independent of p and r_0. An estimate of Y_1, the eigenvalue for temperature like perturbations, was obtained from

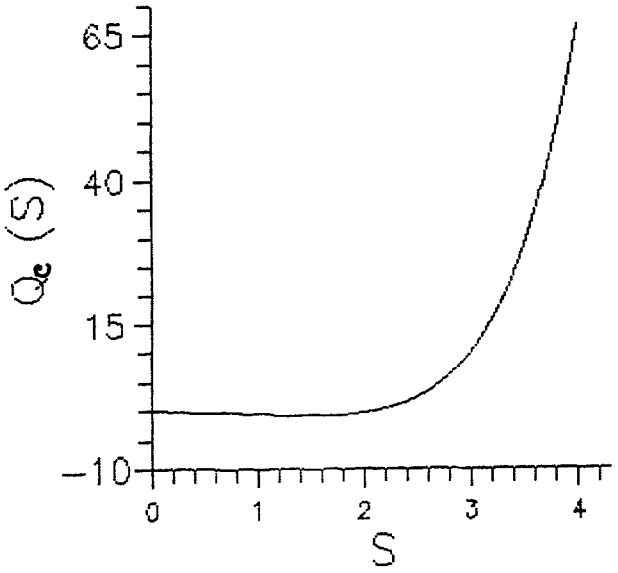

FIGURE 2 Fixed point function $Q^*(S)$ as determined numerically from the approximate recursion formula.

TABLE I Critical exponents for the N-I transition

Exponents	*This work*	*ε-expansion*
v	0.638	0.64
γ	1.277	1.277

$$2^{Y_1} = (Q_2(S) - Q_1(S))/(Q_1(S) - Q_0(S)) \tag{8}$$

It was yielded the estimate $Y_1 = 1.5651$, $v = 0.638$, $\gamma = 2v = 2/Y_1 = 1.277$ in good agreement with the best ε-expansion series [2,4]. The results are summarized in Table I.

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[30] Equations (3.41) and (3.43) of paper II of reference (1); Equations (3) and (4) of reference (2).