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LETTER TO THE EDITOR

Renormalisation group study of liquid crystalline order in two dimensions

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Abstract. We apply the Migdal-Kadanoff real space renormalisation group method to study the Lebwohl-Lasher lattice model of liquid crystal behaviour in two dimensions. The model supports a phase transition similar to the Kosterlitz-Thouless transition in the two-dimensional XY model of magnetism. However, the liquid crystalline order at low temperatures is unstable to any symmetry breaking crystalline field. This suggests that thin nematic films may be experimentally unrealisable.

Two-dimensional liquid crystals are particularly promising for theoretical as well as experimental studies of phase transitions (see, for example, [1]). This is because the theory of phase transitions in two dimensions is simpler than its counterpart in three dimensions and has a rich structure [2]. On the experimental side, liquid crystal films almost as thin as a monolayer can be fabricated and studied in order to test this theory. In this connection it is noteworthy that the liquid crystal films fabricated so far are smectic films and it appears impossible to produce thin nematic films stable against rupture. In this letter, we study the theory of two-dimensional nematic order and the effect of symmetry breaking crystalline fields on the ordered state. We find that the two-dimensional nematic order is strongly unstable to any symmetry breaking crystalline field. We feel that this may be the explanation for the failure to produce thin nematic films in the laboratory.

We take up the Lebwohl-Lasher lattice model of a nematic liquid crystal [3]. This is given by the Hamiltonian

$$H = -J \sum_{i,j} (\cos^2 \theta_{ij} - 1) \qquad \theta_{ij} = \theta_i - \theta_j \tag{1}$$

where the sum is over pairs of nearest-neighbour sites on a square lattice, J is a parameter characterising the strength of the interaction and θ_i is the angle that the axis of symmetry of the molecule at the site i makes with some reference axis. We apply the Migdal-Kadanoff real space renormalisation group method to study the phase transition supported by the above Hamiltonian [4]. The first step of the renormalisation transformation consists of a bond moving operation whereby the square lattice of a spacing a is converted into a more sparse square lattice of spacing $2a$ by moving alternate vertical columns of bonds to the right and alternate horizontal rows of bonds down as indicated in figure 1(a). Figure 1(b) shows a unit cell of the new lattice obtained as a result of the above bond moving operation. The site at the centre of the square is completely isolated and contributes an unimportant constant of integration to the partition function of the system. The next step in the transformation

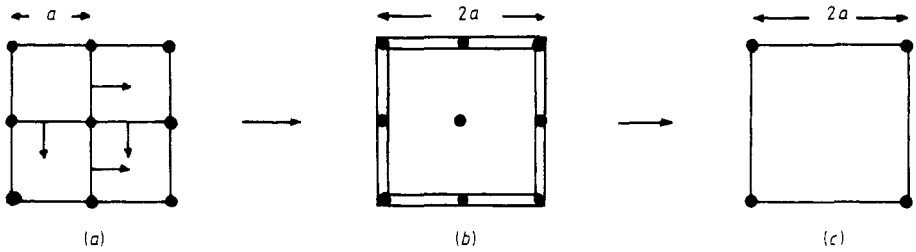

Figure 1. (*a*) Original lattice, (*b*) lattice after bond moving, (*c*) lattice after bond moving and decimation.

is to integrate over the sites situated at mid-points of the sides of the square cell in figure 1(*b*). This is a one-dimensional problem and can be done exactly. The resulting new unit cell is shown in figure 1(*c*). The results of bond moving and decimation on the interaction is most conveniently expressed in terms of the Fourier-Bessel components of the reduced pair interaction $V(K, \theta_{12})$. The initial pair interaction in the Lebwohl-Lasher model is $V(K, \theta_{12}) = K(\cos^2 \theta_{12} - 1)$, with $K = J/k_B T$. However, successive steps of the renormalisation group transformation change the form of the interaction and therefore it is necessary to write the renormalisation group equations for an arbitrary pair interaction. Let us write

$$\exp[V(K, \theta_{12})] = \sum_{m=-\infty}^{+\infty} f_m(K) \exp(\mathrm{i}m\theta_{12}). \tag{2}$$

Under bond moving operation f_m goes into f_m^{b} where

$$f_m^{\mathrm{b}} = \sum_{n=-\infty}^{+\infty} f_n f_{m-n}. \tag{3}$$

Under decimation f_m goes into f_m^{d} where

$$f_m^{\mathrm{d}} = f_m^2 \left(\sum_{m=-\infty}^{+\infty} f_m^2 \right)^{-1}. \tag{4}$$

For the initial Lebwohl-Lasher pair interaction the Fourier-Bessel coefficients are

$$\begin{aligned} f_{2m}(K) &= \exp(-\tfrac{1}{2}K) I_m(\tfrac{1}{2}K) \\ f_{2m+1}(K) &= 0 \qquad m = 0, 1, 2, \ldots \end{aligned} \tag{5}$$

where I_m is the modified Bessel function of integer order m.

The renormalisation group method consists in starting with the set of coefficients given by equation (5) and computing the new coefficients with the help of equations (3) and (4). This procedure is repeated with the newly obtained coefficients as the input coefficients for the next iteration. The even character of the coefficients, as embodied in equation (5), is preserved by the renormalisation group transformation. The result of repeated application of the transformation on the Hamiltonian (1) falls into two categories, one corresponding to low temperature behaviour and the other corresponding to high temperature behaviour. At high temperatures the initial set of coefficients rapidly converge to a high temperature fixed point. At low temperatures

the initial coefficients quickly approach the form

$$f_{2m}(T) = (T/\pi)^{1/2} \exp(-4m^2 T)$$
$$f_{2m+1}(T) = 0 \qquad m = 0, 1, 2, \ldots . \tag{6}$$

Here, and in the following discussion, we have set the Boltzmann constant k_B equal to unity for convenience. The above form of the coefficients remains almost unaltered under further iterations. It may be noted that equation (6) is the leading term in the asymptotic expansion of equation (5) for large K which corresponds to low T. The difference between the input coefficient f_{2m} given by equation (6) and the corresponding renormalised coefficient as obtained by the application of equations (3) and (4) is exponentially small of the order of $\exp(-\pi^2/4T)$ as T goes to zero. Thus over an entire range of low temperatures, a few iterations of the renormalisation group transformation reduce the initial interaction (5) to the form (6) which remains almost fixed under further renormalisations.

In order to determine the dividing line between the low T and high T behaviour, it is instructive to characterise the system by a single parameter which measures the effective temperature of the system. We define

$$T' = \frac{f_0(1/T) - f_4(1/T)}{2f_2(1/T)}. \tag{7}$$

For the initial coefficients the effective temperature defined by equation (7) is in fact equal to the real temperature of the system. This can be easily verified by using the recursion relations satisfied by the modified Bessel functions. As the form of the interaction is altered by the renormalisation group transformation, T' begins to deviate from T but it still serves as a useful parameter to characterise the effective temperature of the system. After the first step of the renormalisation group transformation the effective temperature of the system becomes

$$T' = T\left(\frac{I_0(1/T)}{I_1(1/T)} - T\right). \tag{8}$$

Thus the change in the effective temperature under a scale change of 2 is given by

$$\Delta = (T' - T)/\ln 2. \tag{9}$$

In figure 2 we have plotted Δ against T. The graph shows a fixed point at $T^* = 0.647$ separating the low T behaviour from the high T behaviour. If the temperature of the system is greater than T^*, the renormalisation group transformation increases the effective temperature of the system so that successive iterations of the transformation would take the system to the infinite temperature fixed point. On the other hand, if the initial temperature of the system is less than T^*, the renormalisation group transformation decreases the effective temperature of the system and the system flows to the zero temperature fixed point under successive applications of the renormalisation group transformation. We identify T^* with the Kosterlitz-Thouless transition temperature in the two-dimensional liquid crystal. The critical properties of the system below the Kosterlitz-Thouless transition temperature are controlled by the zero temperature fixed point. We may define a critical exponent λ_t characterising the instability of the fixed point with respect to the changes in the effective temperature of the system as follows:

$$dT'/dT = 2^{\lambda_t}. \tag{10}$$

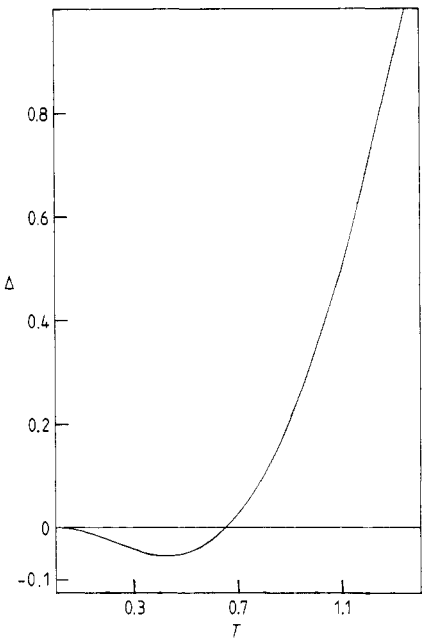

Figure 2. Plot of Δ (the change in the effective temperature of the system under a renormalisation group scale change by a factor 2) against the effective temperature.

The zero temperature fixed point is approached infinitely slowly corresponding to $\lambda_t = 0$ and the correlation length exponent $\nu = \infty$.

In order to examine the stability of the fixed points under crystalline symmetry breaking fields, we add to the Hamiltonian (1) a perturbation of the term of the form $h_p \cos p\theta$, $p = 0, 2, 4, 5$. In the linear order in h_p the renormalised Hamiltonian acquires a term of the form $h'_p \cos p\theta$ where

$$h'_p = 2\left(1 + \frac{I_{p/2}(2/T)}{I_0(2/T)}\right) h_p. \tag{11}$$

An exponent λ_p corresponding to the perturbation h_p may be defined by the equation

$$dh'_p/dh_p = 2^{\lambda_p} \qquad p = 2, 4, 6. \tag{12}$$

The exponents λ_t, λ_2, λ_4 and λ_6 for the fixed points $T^* = 0$ and $T^* = 0.647$ are listed in table 1. A positive value of the exponent means that the critical behaviour associated with the fixed point is unstable with respect to the corresponding perturbation.

Table 1. Fixed points and eigenvalues characterising their instability.

T^*	0	0.647	$\frac{1}{4}\pi$
λ_t	0	0.43	0
λ_2	2.0	1.86	1.87
λ_4	2.0	1.55	1.50
λ_6	2.0	1.27	0.87

The reader may wish to compare the foregoing analysis of the liquid crystal system with that of Jose *et al* [5] for the two-dimensional XY magnet. The two calculations are very similar owing to the fact that the input Fourier-Bessel coefficients are very similar for the two problems†. The behaviour of the isotropic liquid crystal is similar to the behaviour of the isotropic XY magnet at twice the temperature of the liquid crystal. The liquid crystalline order is unstable to symmetry breaking perturbations $\cos p\theta$ with $p = 2, 4, 6$. In the Migdal-Kadanoff approximation the XY magnetic order is also unstable to perturbations with $p = 1, 2, 3, 4, 6$. However, Jose *et al* have suggested that the Migdal-Kadanoff approximation does not treat vortex excitations adequately and the result of this approximation for λ_p in the XY model is suspect for $p = 4$ and 6. These authors have suggested that the Migdal-Kadanoff approximation may be relied upon insofar as to note that the critical behaviour of the XY model is in the same universality class as the Villain model [7] but the Villain model can be analysed without recourse to the Migdal-Kadanoff approximation. When this is done a sharp vortex unbinding transition is found at $T_c = \frac{1}{2}\pi$ (where, as in the calculation of Jose *et al* based solely on the Migdal-Kadanoff approximation, there is no sharp transition temperature corresponding to the Thouless-Kosterlitz transition). The perturbations with $p = 1, 2, 3, 4$ remain relevant below T_c ($p = 4$ becomes marginal at the transition temperature) but the $p = 6$ perturbation becomes irrelevant over a finite range of temperature below the Kosterlitz-Thouless transition temperature.

The remarks of Jose *et al* on the inadequacy of the Migdal-Kadanoff approximation to treat vortices in the XY model also apply in the case of the Lebwohl-Lasher model. However, in our case, the effective temperature parameter T' serves better to characterise the system. There is some arbitrariness in choosing a single parameter to characterise the effective temperature of the system. For example, we could choose

$$T'' = \tfrac{1}{2} \sum_{m=-\infty}^{+\infty} f_m(1/T) \left(\sum_{m=-\infty}^{+\infty} m^2 f m(1/T) \right)^{-1}. \tag{13}$$

If the interaction is initially the Lebwohl-Lasher interaction, i.e. the f_m are given by equation (5), we have $T'' = T$, just as $T' = T$. The parameter T'' is a straightforward generalisation to the liquid crystal case of the effective temperature used by Jose *et al* for the XY model. The parameter T'' fails to yield a fixed point characterising the Kosterlitz-Thouless transition, although, as in the case of the XY model it does give an indication that the critical behaviour of the Lebwohl-Lasher model may be in the same universality class as the Villain-like model in which the Fourier-Bessel coefficients of the pair interaction are given by equation (6). This feature of the Lebwohl-Lasher model is, of course, also brought out by the T' description of the system. The T' description has the advantage that it gives a sharp transition temperature and does not suffer from the problems of numerical analysis that T'' has at low temperatures. In order to calculate T' we need only three coefficients but in order to calculate T'' we need an infinite series of coefficients which converges very slowly at low temperatures.

We have also calculated analytically the properties of the Lebwohl-Lasher model when the couplings are given by the low temperature limit, i.e. equation (6). We find

† The Migdal-Kadanoff(MK) approximation also gives qualitatively similar results for the Heisenberg magnet and the Lebwohl-Lasher model of a liquid crystal in three dimensions. This makes the straightforward application of the MK approximation to the three-dimensional liquid crystal model suspect. (See [6] for a discussion of this problem.) However, in the present two-dimensional case, the results of the approximation are qualitatively correct in view of the Monte Carlo simulations of the Lebwohl-Lasher model.

that a vortex unbinding transition takes place at $T_c = \frac{1}{4}\pi$ which is close to the transition temperature $T^* = 0.647$ found by the Migdal-Kadanoff transformation. Below T_c, we find that all crystalline symmetry breaking fields are relevant with eigenvalues given by

$$\lambda_p = 2 - (p^2/8\pi)T. \tag{14}$$

The values of λ_p at $T_c = \frac{1}{4}\pi$ are listed in table 1 for comparison with the corresponding values obtained by the Migdal-Kadanoff approximation. It is seen that in the Migdal-Kadanoff approximation as well as in the other low temperature analysis of the Lebwohl-Lasher model the nematic ordered state is unstable to every crystalline symmetry breaking field. We feel that this may be a possible explanation for the failure (so far) to fabricate thin nematic films in the laboratory which are stable against rupture.

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