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# Renormalisation group study of a lattice model of the isotropic-nematic transition

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**Abstract.** The isotropic-nematic transition is studied using the Lebwohl-Lasher lattice model of liquid crystal behaviour. The details of the transition are investigated using the Migdal-Kadanoff potential moving version of the real space renormalisation group. The method gives good results when applied to the closely related Heisenberg model of ferromagnetism. A second-order transition is predicted, in disagreement with mean field and some computer simulation results.

## 1. Introduction

Fluids consisting of anisotropic molecules can under some circumstances at low temperatures form a phase in which the molecules possess angular but no spatial order. This phase—the simplest liquid crystal phase—is known as the nematic phase (Chandrasekhar 1977). The simplest fluid for which such a transition can take place consists of molecules which have uniaxial symmetry. The order parameter for the transition is a tensor (the Saupe ordering matrix)

$$S_{ij} = \frac{1}{2} \langle 3 \hat{n}_i(\Omega) \hat{n}_j(\Omega) - \delta_{ij} \rangle_{\text{molecules}} \quad (1)$$

where  $\Omega$  is the direction of the molecule,  $\hat{n}(\Omega)$  is a unit vector in that direction, and  $\hat{n}_i(\Omega) = \hat{n}(\Omega) \cdot \hat{e}_i$ , and  $\hat{e}_i$  is a unit vector in the  $i$  direction. In the absence of an external field

$$S_{ij} = \frac{1}{2} \bar{P}_2 (3 \hat{l}_i \hat{l}_j - \delta_{ij}) \quad (2)$$

where  $\hat{l}$  is the liquid crystal director (a unit vector) and axis of symmetry for molecule directions, and

$$\bar{P}_2 = \langle P_2(\cos \theta) \rangle_{\text{molecules}} \quad (3)$$

where  $\cos \theta = \hat{l} \cdot \hat{n}(\Omega)$ .

About 25 years ago Maier and Saupe (1958, 1959, 1960) enunciated a mean field theory of the nematic phase. This theory is an analogue of the van der Waals theory of the liquid-vapour transition and assumes that the orientationally ordering forces are long range. It was rather successful, except in the immediate region of the nematic-isotropic transition. The nematic phase diagram should be universal, which is not the case precisely. However, the main discrepancies between the Maier-Saupe theory and experiment were as follows. The order parameter susceptibility above the

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phase transition is predicted to behave as

$$\chi \propto (T - T^*)^{-1}; \quad (4)$$

$T^*$  is a temperature below the nematic-isotropic transition at  $T_{NI}$ . This does correspond to observed behaviour; however, whereas in the Maier-Saupe theory  $t^* = (T_{NI} - T^*)/T^* \sim 10\%$ , experimentally  $t^* \sim 0.2\%$ . Another notable discrepancy is the entropy jump per particle  $\Delta S_{NI}$  at the first-order phase transition; typically Maier-Saupe overestimates this by a factor of ten, as compared with experiment.

A number of reasons have been proposed to explain why the Maier-Saupe theory fails to explain the details of the nematic-isotropic transition. It has been pointed out that it is the short-range details of molecular shape, rather than long-range intermolecular dispersion forces, which govern the phase transition. However, as we and others have shown (Sluckin and Shukla 1983), using modern perturbation theory of liquids, the predicted details of the transition are relatively robust against changes in the form of the potential. Others have shown that a mean field theory of the nematic phase of biaxial molecules can predict smaller  $t^*$  and  $\Delta S_{NI}$ , and even predict a second-order nematic-isotropic transition (Mulder and Ruijgrok 1982), observing that an important feature of nematogenic fluid molecules is precisely their biaxiality.

Nevertheless we do not believe that biaxiality is a crucial feature; rather we believe, mainly as a result of computer simulation studies on fluids of uniaxial molecules, that the observed small  $t^*$  and  $\Delta S_{NI}$  are universal features of the phase transition. It is often useful, when studying the phase transition properties of a system, to study a similar but simpler system in the same *universality class*, which will exhibit the same generic behaviour in the neighbourhood of the phase transition. Lebwohl and Lasher (1972) have introduced a lattice model of a liquid crystal, with Hamiltonian

$$H_{LL} = -\varepsilon_0 \sum_{\langle ij \rangle} P_2(\cos \Omega_{ij}) \quad (5)$$

where at each site  $i$  on a prescribed three-dimensional lattice (in our case a simple cubic lattice) lies a rigid rotator whose state is defined by a unit vector  $\hat{n}_i(\theta_i, \phi_i)$  the direction in which it points. The sum runs over nearest-neighbour pairs on the lattice. Following the usual convention  $\theta_i$  and  $\phi_i$  represent the polar and azimuthal angles respectively, so that the three components of  $\hat{n}$  are  $\sin \theta_i \cos \phi_i$ ,  $\sin \theta_i \sin \phi_i$  and  $\cos \theta_i$ . In this representation the angle between neighbouring vectors is given by

$$\hat{n}_i \cdot \hat{n}_j = \cos \Omega_{ij} = \cos \theta_i \cos \theta_j + \sin \theta_i \sin \theta_j \cos(\phi_i - \phi_j) \quad (5a)$$

and  $P_2(\cos \Omega_{ij})$  is the second Legendre polynomial. This Hamiltonian undergoes an isotropic-nematic transition.

Monte Carlo studies of the Lebwohl-Lasher model given results for  $\Delta S_{NI}$  and  $t^*$  in line with experimental results on real liquid crystal systems; for this reason we believe the two systems are in the same universality class. The mean field theory of the Lebwohl-Lasher model is, identically, the Maier-Saupe theory. More sophisticated mean field theories, using larger clusters in the spirit of Kikuchi and Bethe-Peierls, have been attempted (Sheng and Wojtowicz 1976, van der Haegen *et al* 1980). There is an improvement in the calculated values of  $t^*$  and  $\Delta S_{NI}$ , as indicated in table 1. Nevertheless,  $t^*$  and  $\Delta S_{NI}$  are not well described by current mean field theories. Mean field theories ignore fluctuations and always overestimate  $T_c$ . It seems likely that if these fluctuations were taken into account, the discrepancies between theory and

**Table 1.** The Lebwohl-Lasher model (simple cubic lattice).

	Monte Carlo <sup>a</sup>	Mean field (Maier-Saupe)	Two-cluster mean field <sup>b</sup>	Four-cluster mean field <sup>c</sup>
$T_{NI}/\varepsilon_0$	1.127	1.321	1.160	1.142
$\bar{P}_{2NI}$	0.27	0.43	0.39	0.35
$\Delta S_{NI}$	0.07	0.55	0.33	
$t^*$	$\sim 0.002$	0.092	0.054	0.038

<sup>a</sup> Luckhurst and Simpson 1982,<sup>b</sup> Sheng and Wojtowicz (1976).<sup>c</sup> Van der Haegh *et al* (1980).

simulation (and implicitly experiment) could be resolved, in particular the dramatic overestimates of  $t^*$  and  $\Delta S_{NI}$ .

We have carried out what is, as far as we know, the first non-mean-field treatment of the Lebwohl-Lasher model. We have exploited similarities between the Lebwohl-Lasher model and the Heisenberg model of ferromagnetism, and have brought to bear upon the liquid crystal problem techniques developed in the study of the magnetic problem. José *et al* (1977) pioneered a particular real space renormalisation group (RG) approach to the study of the two-dimensional XY model, based on the bond-moving scheme of Migdal (1975) and Kadanoff (1976). This was generalised by Jayaprakash *et al* (1978) to apply to the XY and Heisenberg models in three dimensions. We have essentially carried over this method to study the Lebwohl-Lasher model.

## 2. Renormalisation group analysis of the Lebwohl-Lasher model

We study the reduced Hamiltonian

$$\mathcal{H}_2 = -\frac{H_{LL}}{k_B T} = K \sum_{\langle ij \rangle} P_2(\cos \Omega_{ij}) \quad (6)$$

whereas by contrast Jayaprakash *et al* (1978) studied a reduced Hamiltonian

$$\mathcal{H}_1 = K \sum_{\langle ij \rangle} P_1(\cos \Omega_{ij}) = K \sum_{\langle ij \rangle} \cos \Omega_{ij} \quad (7)$$

where we emphasise that  $x = P_1(x)$ , the first Legendre polynomial.

It is convenient to employ a Fourier-Legendre transform

$$\exp[KP_2(\cos \Omega_{ij})] = \sum_{l=0}^{\infty} f_l P_l(\cos \Omega_{ij}). \quad (8)$$

In practice we truncate at  $l = 20$ , but all results are sensibly insensitive to this truncation.

The RG transformations involve potential-moving and decimation steps. The advantage of the representation (8) is that it incorporates in a very simple way the effect of decimation along a one-dimensional chain of atoms. We can see this by considering a chain of three spins, and decimating over the middle spin. Then

$$\frac{1}{4\pi} \int d\Omega_2 \exp[KP_2(\cos \Omega_{12}) + KP_2(\cos \Omega_{23})] = \sum_{l=0}^{\infty} f_l^d P_l(\cos \Omega_{13}). \quad (9)$$

One may easily verify that  $\{f_l^d\}$  in (9) are given by the simple formula

$$f_l^d = R_d(\{f_l\}) = f_l^2 / (2l + 1). \quad (10)$$

For an infinite chain (10) constitutes the renormalisation group transformation for a change in length scale of a factor of two. The set  $\{f_i\}$  characterises the initial Hamiltonian, and the set  $\{f_i^d\}$  describes the renormalised Hamiltonian after the degrees of freedom at alternative sites have been integrated out. The Migdal-Kadanoff scheme essentially bootstraps this result, which is exact in one dimension, to three dimensions (Burkhardt 1982). We may most easily visualise how this is carried out using the potential-moving viewpoint of Kadanoff.

Let us denote interactions between neighbouring sites by  $K_x$ ,  $K_y$  and  $K_z$ , depending on whether the bonds are along the  $x$ ,  $y$  or  $z$  axes. The RG transformation involving a length scale change of two takes place in three steps.

(1) Alternate  $K_y$  and  $K_z$  bonds are moved parallel to themselves by one lattice spacing. One now decimates over alternate spins in the  $x$  direction which are now only connected by bonds in the  $x$  direction to just two other sites.

(2) Alternate  $K_x$  and  $K_z$  bonds are moved parallel to themselves and an analogous decimation along the  $y$  axis performed.

(3) Alternate  $K_x$  and  $K_y$  bonds are moved, and one decimates along the  $z$  direction.

At the end of the last step we arrive at a lattice with lattice spacing twice that of the original lattice and renormalised nearest-neighbour interactions.

If we let  $R_b$  denote the bond-moving operation and initially suppose that the interaction is isotropic and characterised by a set of Fourier-Legendre coefficients  $\{f_i\}$ . Then after the three steps characterised above, the renormalised interactions along the  $x$ ,  $y$  and  $z$  axes are given respectively by

$$R_x(\{f_i\}) = R_b R_b R_d(\{f_i\}) \quad (11a)$$

$$R_y(\{f_i\}) = R_b R_d R_b(\{f_i\}) \quad (11b)$$

$$R_z(\{f_i\}) = R_d R_b R_b(\{f_i\}). \quad (11c)$$

For an initially isotropic Hamiltonian, the renormalised interactions  $R_x$ ,  $R_y$ ,  $R_z$  are not, however, equal. We describe below a procedure which chooses one of these three recursion relations.

The bond-moving operation for a nearest-neighbour interaction of the form given in (6) or (7) is simply effected by replacing  $K$  by  $2K$ . Equivalently, in the Fourier-Legendre representation, the bond-moving operation is given by

$$R_b\{f_i\} = \{f_i^b\} \quad (12a)$$

with

$$f_i^b = \sum_{l_1, l_2} f_{l_1} f_{l_2} \langle l_1 l_2 00 | l_1 l_2 l_0 \rangle^2 \quad (12b)$$

where  $\langle l_1 l_2 00 | l_1 l_2 l_0 \rangle$  is a Clebsch-Gordan coefficient in the usual notation (Brink and Satchler 1968, p 136ff). If the interaction is exactly of the form of (6) or (7) then (12) is simply equivalent to replacing  $K$  by  $2K$ , but it is not limited to nearest-neighbour interactions of this form. Indeed, the decimation operation does change the form of the interaction in detail, and so the form (12b) is essential. After each decimation operation we normalise the  $\{f_i\}$  so as to ensure that

$$\sum_{l=0}^{\infty} f_l = 1. \quad (13)$$

This normalisation is preserved by the bond-moving operation. Its significance is that

unimportant numerical constants, generated in decimation, are ignored, and the zero of the interaction energy is taken to be the state for which neighbouring spins are parallel (for  $\mathcal{H}_1$ ) a parallel or antiparallel (for  $\mathcal{H}_2$ , in which these configurations are energetically degenerate).

We find it convenient to work with a parameter

$$K_{\text{eff}} = \frac{1}{3} \sum_{l=0}^{\infty} f_l \left. \frac{dP_l(x)}{dx} \right|_{x=1}. \quad (14)$$

For an interaction of the form of (6)  $K_{\text{eff}} = K$ . We find that the set of coefficients  $\{f_l^d\}$ , as defined in (10), along with the normalisation (13), leaves the form of  $\mathcal{H}_2$  almost unchanged. Consequently the single parameter  $K_{\text{eff}}$  serves exceedingly well to characterise the set  $\{f_l^d\}$ .

This is a greatly simplifying feature in the application of the Migdal-Kadanoff scheme. We find that bond-moving performed by calculating  $K_{\text{eff}}$  from (14) and doubling it, gives very nearly the same results as by employing the whole machinery of Clebsch-Gordan coefficients embodied in (12).

With this perspective we return to the renormalised interactions  $R_x, R_y, R_z$  described in (11). Some reflection shows that the fixed points of  $R_x, R_y, R_z, K_x^*, K_y^*, K_z^*$ —are in the ratio 1:2:4, although the different recursion relations (11) give rise to the same critical exponents. In general for a Migdal-Kadanoff transformation with scale change  $b$ , there will be three fixed points, related by the ratios 1:  $b$ :  $b^2$ . In some applications it is possible to work in the limit  $b \rightarrow 1$ , when the three critical values of  $K^*$  converge to a single value close to that given by the middle recursion relation (11b). In this spirit we chose recursion relation (11b) as the canonical RG transformation.

It turns out to be much simpler computationally to follow the parameter  $K_{\text{eff}}$  under RG flows, than to follow the full set  $\{f_l\}$ ; one then only uses the Fourier-Legendre representation in the decimation step. We present results for  $\mathcal{H}_1$  using this procedure, and compare them to the results of Jayaprakash *et al* (1978), who use the full flows of  $\{f_l\}$ ; for all purposes the results are very similar. Consequently we feel confident in merely following the parameter  $K_{\text{eff}}$  when iterating  $\mathcal{H}_2$  under the RG flows. The crucial difference between  $\mathcal{H}_1$  and  $\mathcal{H}_2$  is that the Fourier-Legendre representation of  $\mathcal{H}_2$  admits only terms of even  $l$ . The RG trajectories exhibit a non-trivial fixed point  $K^* = 0.58$ ; for  $K < K^*$ ,  $K_{\text{eff}}$  reaches a high-temperature fixed point at  $K_{\text{eff}} = 0$ ,  $f_l = \delta_{l0}$ , and for  $K > K^*$  the  $\{f_l\}$  reach a low-temperature fixed point.

A thermal exponent  $\lambda_T$  at the transition may be defined either by diagonalising the matrix  $\partial f_l / \partial f_j$ , and taking the largest eigenvalue  $\varepsilon$ , or by putting

$$\partial K'_{\text{eff}} / \partial K \Big|_{K^*} = \varepsilon = 2^{\lambda_T} \quad (15)$$

where  $K' = R_y(K)$ . Both procedures give rise to the same results within the accuracy quoted. We find  $\lambda_T = 0.85$ , whereas for  $\mathcal{H}_1$ ,  $\lambda_T = 0.86$ .

### 3. Effect of an ordering field

We have also calculated the effect of adding an ordering field perturbation to the Hamiltonian, which now becomes

$$\mathcal{H}'_2 = K \sum_{\langle ij \rangle} P_2(\cos \Omega_{ij}) + V \sum_{\langle i \rangle} P_2(\cos \theta_i). \quad (16)$$

This is analogous to the magnetic field perturbation discussed by Jayaprakash *et al* (1978).

The Migdal-Kadanoff scheme is ambiguous in its treatment of ordering fields; following Jayaprakash *et al* we have moved the fields with the bonds along the  $y$  axis. The bond-moving transformation merely takes  $V$  to  $2V$ . The decimation transformation generates terms nonlinear in  $V$ , but these may be neglected near the fixed point  $K = K^*$ ,  $V = 0$ .

We can see how decimation affects  $V$  by considering a chain of three spins as in (9). Then, to linear order in  $V$ , the new interaction after decimation is

$$\begin{aligned} & \frac{1}{4\pi} \int d\Omega_2 \exp[KP_2(\cos \Omega_{12}) + KP_2(\cos \Omega_{23})] \\ & \quad \times [1 + VP_2(\cos \theta_1) + 2VP_2(\cos \theta_2) + VP_2(\cos \theta_3)] \\ & = \frac{1}{4\pi} \int d\Omega_2 \sum_{l_1=0}^{\infty} f_{l_1} P_{l_1}(\cos \Omega_{12}) \sum_{l_3=0}^{\infty} f_{l_3} P_{l_3}(\cos \Omega_{23}) \\ & \quad \times [1 + VP_2(\cos \theta_1) + 2VP_2(\cos \theta_2) + VP_2(\cos \theta_3)]. \end{aligned} \quad (17)$$

A renormalised value of  $V$  may be obtained by noting that if  $\Omega_{13} = 0$ , from the normalisation (13) the resulting interaction should be of the form  $1 + 2V_d P_2(\cos \theta_1)$ . The resulting integrals on the right-hand side of (17) can now be carried out, using the closure relations: (Brink and Satchler 1968, pp 145-6)

$$P_l(\cos \Omega_{ij}) = \sum_m C_l^m(\cos \Omega_i) C_l^{-m}(\cos \Omega_j) \quad (18a)$$

$$[(2l+1)/4\pi]^{1/2} C_l^m(\cos \Omega_{ij}) = Y_l^m(\cos \Omega_{ij}) \quad (18b)$$

$$(4\pi)^{-1} \int P_{l_1}(\cos \Omega) P_{l_2}(\cos \Omega) P_l(\cos \Omega) d\Omega = [1/(2l+1)] |\langle l_1 l_2 00 | l_1 l_2 l 0 \rangle|^2 \quad (18c)$$

we obtain (for  $\Omega_{13} = 0$ )

$$\begin{aligned} & \sum_l \frac{f_l^2}{2l+1} [1 + 2VP_2(\cos \Omega_1)] + 2V \sum_{l_1 l_2} \frac{1}{3} f_{l_1} f_{l_2} \langle l_1 l_2 00 | l_1 l_2 l 0 \rangle P_2(\cos \Omega_1) \\ & = f_0^d [1 + 2V_d P_2(\cos \Omega_1)]. \end{aligned} \quad (19)$$

We may now make use of the relation (12b) to write the total renormalised ordering field  $V'$ , after bond-moving and decimation steps<sup>†</sup>, in the linear approximation, as

$$V' = 4V(1 + f_2^{bb}/5f_0^{bb}) \quad (20)$$

where  $f_l^{bb} = (f_l^b)^b$ .

The order field exponent at the transition  $\lambda_v$  is thus given by

$$(\partial V'/\partial V)_{K^*} = 2^{\lambda_v} = 4(1 + f_2^{*bb}/5f_0^{*bb}) \quad (21)$$

where  $\{f_l^*\}$  are evaluated at the fixed point.

<sup>†</sup> There is a misprint in equation (11) of Jayaprakash *et al* (1978), which should read

$$2^{\lambda_m} = 4[1 + \tilde{f}_1^b/\tilde{f}_0^b(2l+1)].$$

We recall that mean field theory predicts a nematic–paranematic critical point near  $T = T_{NI}$  for  $V \sim 0.05$  (Fan and Stephen 1970, Wojtowicz and Sheng 1974, Palfy-Muhoray and Dunmur 1983).

Our results for fixed points and critical exponents are displayed in table 2.

Table 2.

	Heisenberg model ( $\mathcal{H}_1$ )			Lebwohl-Lasher model ( $\mathcal{H}_2$ )
	(A)	(B)	(C)	
$K_C$	0.692 <sup>(a)</sup>	0.41	0.449	0.583 (0.887 ± 0.003)
$\lambda_T$	1.35 <sup>(b)</sup>	0.86	0.86	0.85
$\lambda_V$	2.49 <sup>(b)</sup>	2.55	2.58	2.59

(A) High-temperature series 'exact' results; <sup>(a)</sup> Betts (1977), <sup>(b)</sup> Jasnow and Wortis (1978).

(B) Jayaprakash *et al* (1978), using full  $\{f_i\}$  RG flows.

(C) This work, using  $K_{eff}$  flows.

The figure in parentheses is a value from a Monte Carlo simulation (Luckhurst and Simpson 1982). For a first-order transition  $\lambda_T = \lambda_V = 3$ .

#### 4. Concluding remarks

Our work predicts that  $\mathcal{H}_2$  has a second-order phase transition similar to that of  $\mathcal{H}_1$ . The transition temperature for  $\mathcal{H}_2$  is predicted to be lower than that for  $\mathcal{H}_1$  and this feature of the prediction is in line with exact results. Indeed from table 2 it can be seen that the ratio of the predicted critical temperature to the actual critical temperature is the same for  $\mathcal{H}_1$  and  $\mathcal{H}_2$  using comparable procedures. The thermal exponent  $\lambda_T$  is given poorly for  $\mathcal{H}_1$  by the Migdal-Kadanoff procedure; we cannot be surprised if  $\lambda_T$  is not well predicted for  $\mathcal{H}_2$  either. But the order parameter exponent is given well for  $\mathcal{H}_1$ , and hence we might expect good results for  $\mathcal{H}_2$ —at least the trends ought to be correct. Nevertheless, our prediction for the order of the phase transition is in disagreement with the predictions of the Maier-Saupe theory as well as computer simulations. There is, however, a strong size dependence of the nature of the transition, and small (1000 particle) simulations do not distinguish, for this system, the order of the transition.

The discrepancy between computer simulations and our results cannot be resolved within the Migdal-Kadanoff approximation employed in this study. Further investigations, using improved theoretical and computation techniques, are highly desirable.

The failure of the Migdal approximation to illuminate the nature of the nematic-isotropic transition is disappointing, but nevertheless there may be some significance in our results. There have been speculations that in  $d$ ,  $2 < d < 3$ , the nematic-isotropic transition would become second order. We expect that, by the Mermin-Wagner theorem (Mermin and Wagner 1966),  $d = 2$  is the lower critical dimension of the nematic phase. The Migdal approximation, on the other hand, is a 'realisable approximation', in the sense that it is an exact solution of a different problem. In our case the problem is one with Hamiltonian given by (5) on a fractal (Mandelbrot 1977), self-similar, lattice (Burkhardt 1982) with Hausdorff-Besicovitch dimension  $d = 3$ , but with topological dimension  $D_T = 1$ . Clearly the Migdal approximation assumes that the topological dimension (=1 + dimension of a cut which divides the system into two) is an irrelevant variable; this is evidently not the case, but the error is consistent with



the rather cavalier essays into fractional dimensions made by RG trail blazers in the early days. It seems that in calculating  $\lambda_T$  the system is, for some as yet unexplained reason, more interested in  $D_T$  than in  $d$ , whereas for  $\lambda_V$ ,  $d$  is the controlling variable. It seems that although the speculations of a critical dimension dividing a first- and second-order regions for the nematic-isotropic transition are a little difficult to pin down, nevertheless in a *realisable* model which is in some sense a compromise between one and three dimensions, there is a second-order nematic-isotropic transition, which is almost first order as far as the order parameter  $\bar{P}_2$  (conjugate to  $V$ ) is concerned, but does *not* have this property as far as the entropy  $S$  (conjugate to  $T$ ) is concerned. There is at least some echo here of the Monte Carlo results of table 1, which show a large discontinuity in  $\bar{P}_2$ , but a very small discontinuity in  $S$ .

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