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LETTER TO THE EDITOR

A lattice model of liquid crystals with matrix order parameter

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Abstract. A lattice model with full rotational invariance is proposed for describing nematic liquid crystals. Orientational long-range order at low temperature is proved using the infrared bound method.

An actual problem of the theory of liquid crystals is to construct models exhibiting at sufficiently low temperature orientational long-range order (LRO), which should however not be accompanied by positional LRO in all space directions. Such is the experimentally observed behaviour, and a phenomenology based on the Landau theory is by now well developed (de Gennes 1974, ch 3, Pikin 1981). The simplest case is the transition from an isotropic to a nematic liquid phase. Onsager (1949) argued that the ordering could be explained as an excluded volume effect, i.e. it should be sufficient to assimilate the molecules to hard rods without any further interaction. Following this idea, various models, typically polymer models on a lattice, have been proposed. Though approximate treatments indicate the appearance of an oriented phase at high density (di Marzio 1961; further references in de Gennes 1974, ch 2.2), this is questionable, in view of the rigorously established fact that the simplest model of this kind, the monomer–dimer system, has no phase transition (Heilmann and Lieb 1972). However, it has been recently proved that, when switching on suitable attractive forces between dimers, the monomer–dimer model exhibits an oriented phase at low temperature, and thereby strong arguments (though no formal proof) have been given in favour of the absence of positional order (Heilmann and Lieb 1979, Abraham and Heilmann 1980). This kind of lattice model still has the highly unphysical feature of *a priori* allowing the molecules to point only along a finite number of directions defined by the underlying lattice.

Another line of thought originates with Maier and Saupe (1959, 1960). For liquids consisting of long non-chiral (i.e. identical to their reflected images) molecules without permanent dipole moment, they attribute the nematic transition to the dispersion forces (arising as the second-order perturbation terms of the pure Coulomb interaction), which favour alignment of the long molecular axes, while the form of the molecule (excluded volume effect) should play a secondary role. Their calculation of the dipole–dipole part of the dispersion force gives the following expression for the intermolecular potential (see also Blinc and Žekš 1974, Blinc *et al* 1974):

$$V_{ij} = -a(|\boldsymbol{r}_i - \boldsymbol{r}_j|)P_2(\cos\theta_{ij}), \qquad 0 < a(r) \sim r^{-6} \qquad (r \to \infty), \tag{1}$$

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where r_i, r_j are the positions of the two molecules, θ_{ij} is the angle between their long axes and P_2 is the second Legendre polynomial. The interaction (1) is manifestly rotational invariant. For this interaction supplemented with a hard core condition, Romerio (1978) proved the absence of ordering in one and two dimensions†. For higher dimensions the model has been treated only within the mean field approximation (Maier and Saupe 1959, 1960, Blinc *et al* 1974), which provides the generally accepted phenomenological description of the nematics in terms of a matrix order parameter (Pikin 1981).

In the note we propose a new lattice model of a nematic liquid crystal, which is the lattice variant of the Maier–Saupe model, and prove for it orientational LRO at low temperature. Keeping in mind that matrices are adequate objects for describing the nematic phase, we shall define for every molecule with long axis along the unit vector d the matrix

$$Q^{\alpha\beta} = d^{\alpha}d^{\beta} - \tfrac{1}{3}\delta_{\alpha\beta} \qquad (\alpha, \beta = 1, 2, 3) \tag{2}$$

and transcribe the interaction (1) in terms of these matrices as

$$V_{ij} = -\tfrac{2}{3}a(|\boldsymbol{r}_i - \boldsymbol{r}_j|)\,\mathrm{Tr}(\boldsymbol{Q}_i\boldsymbol{Q}_j). \tag{3}$$

More generally, the state space of a molecule is taken as the set, M, of all real symmetric 3×3 matrices, $\boldsymbol{Q}$, with $\mathrm{Tr}\,\boldsymbol{Q} = 0$; the rotation group O(3) acts on M as $\boldsymbol{Q} \mapsto \boldsymbol{R}\boldsymbol{Q}\boldsymbol{R}^{-1}$ ($\boldsymbol{R} \in \mathrm{O}(3)$); an O(3)-invariant probability measure, ν, is given on M such that

$$\nu(\{0\}) = 0, \qquad \int \mathrm{d}\nu(\boldsymbol{Q})\exp[k\,\mathrm{Tr}(\boldsymbol{Q}^2)] < \infty \qquad \forall k > 0. \tag{4}$$

(For instance, in order to describe uniaxial molecules, for which Q is given by equation (2), ν should be taken as the unique O(3)-invariant probability measure concentrated on $\{\boldsymbol{Q} \in M\colon \mathrm{Tr}(\boldsymbol{Q}^2) = \frac{2}{3},\ \mathrm{Tr}\,(\boldsymbol{Q}^3) = \frac{2}{9}\}$.)

The molecules live on the sites of the cubic lattice $\boldsymbol{Z}^3$. A configuration is specified by the location of the molecules, i.e. by a function $\boldsymbol{Z}^3 \ni x \mapsto n_x \in \{0, 1\}$ and, for all x with $n_x = 1$, by the state, $\boldsymbol{Q}_x \in M$, of the molecule at x. Molecules interact according to equation (3); with every molecule we associate a chemical potential μ. Thus, for a parallelepiped $\Lambda \subset \boldsymbol{Z}^3$ with periodic boundary conditions, the energy of a configuration $(\boldsymbol{n}, \boldsymbol{Q}) = \{(n_x, \boldsymbol{Q}_x)\colon x \in \Lambda\}$ is

$$H_\Lambda(\boldsymbol{n}, \boldsymbol{Q}) = -\sum_{\{x,\,y\}\subset\Lambda} J_{xy}n_xn_y\,\mathrm{Tr}(\boldsymbol{Q}_x\boldsymbol{Q}_y) - \mu\sum_{x\in\Lambda} n_x \tag{5}$$

where $J_{xy} = \frac{3}{2}\sum_{\{z\in\boldsymbol{Z}^3\colon z = y\,(\mathrm{mod}\,\Lambda)\}} a(|x - z|)$. The corresponding Gibbs state is defined by

$$\langle f\rangle_\Lambda = Z_\Lambda^{-1}\sum_{\{n_x = 0,\,1\colon x\in\Lambda\}}\int\prod_{\{x\in\Lambda\colon n_x = 1\}}\mathrm{d}\nu(\boldsymbol{Q}_x)\exp[-\beta H_\Lambda(\boldsymbol{n}, \boldsymbol{Q})]f(\boldsymbol{n}, \boldsymbol{Q}) \tag{6}$$

where Z_Λ is the partition function.

One could, alternatively, give up considering explicitly the occupation numbers n_x and instead, using as new variables $\boldsymbol{D}_x = n_x\boldsymbol{Q}_x$, modify the *a priori* measure on M to $\mathrm{d}\nu_0 = \mathrm{d}\nu + \delta_0$, where δ_0 is the unit mass at $\boldsymbol{0} \in M$. Equation (5) becomes

$$H_\Lambda(\boldsymbol{D}) = -\sum_{\{x,\,y\}\subset\Lambda} J_{xy}\,\mathrm{Tr}(\boldsymbol{D}_x\boldsymbol{D}_y) - \mu\sum_{x\in\Lambda}[1 - \delta_0(\{\boldsymbol{D}_x\})]. \tag{5'}$$

† For finite-range interactions, but relaxing the hard core condition up to superstability, Shlosman (1979) proved the rotational invariance of the Gibbs states for $d = 1, 2$.

Proposition. Let $a(|x|)$ $(x \in \boldsymbol{Z}^3)$ be given either by $\alpha\delta_{|x|,1}$, or by $a|x|^{-\gamma}$ $(\gamma > 3)$, with a a positive constant. Then, there exists $\mu_0 (<0)$ such that, for every $\mu > \mu_0$, one can find a $\beta(\mu)$, such that for $\beta > \beta(\mu)$ every limit point $\langle \cdot \rangle$ of the states $\langle \cdot \rangle_\Lambda$ has orientational† LRO, i.e.

$$\lim_{|x-y|\to\infty} \mathrm{Tr}\langle \boldsymbol{D}_x \boldsymbol{D}_y \rangle > \mathrm{Tr}(\langle \boldsymbol{D}_x \rangle^2) = 0. \tag{7}$$

The proof is an application of the infrared bounds, which hold because the interactions we choose are reflection positive with respect to the reflections in planes without sites (Fröhlich 1978, Fröhlich *et al* 1978). We shall only sketch the main steps.

First, the state $\langle \cdot \rangle_\Lambda$ satisfies

$$\langle \boldsymbol{D}_x \rangle_\Lambda = 0. \tag{8}$$

Indeed, $\langle \boldsymbol{D}_x \rangle_\Lambda \in M$ and can be diagonalised by a rotation $R \in \mathrm{O}(3)$. Thus, applying R to all $\boldsymbol{D}_y$, $y \in \Lambda$, and exploiting the O(3) invariance of $\langle \cdot \rangle_\Lambda$, one concludes that $\langle \boldsymbol{D}_x \rangle_\Lambda$ is in fact diagonal. One sees analogously, by considering rotations which permute the coordinate axes, that $\langle \boldsymbol{D}_x^{\alpha\alpha} \rangle_\Lambda$ does not depend on α. As $\mathrm{Tr}\,\langle \boldsymbol{D}_x \rangle = 0$, we obtain (8).

Using translation invariance, one has

$$c_\Lambda \equiv |\Lambda|^{-2} \sum_{x,\, y \in \Lambda} \langle \mathrm{Tr}(\boldsymbol{D}_x \boldsymbol{D}_y) \rangle_\Lambda = |\Lambda|^{-1} \mathrm{Tr}\langle \hat{\boldsymbol{D}}_0^2 \rangle_\Lambda$$

$$= \mathrm{Tr}\langle \boldsymbol{D}_x^2 \rangle_\Lambda - |\Lambda|^{-1} \sum_{\{p \in \Lambda^* : p \neq 0\}} \mathrm{Tr}\langle \hat{\boldsymbol{D}}_p \hat{\boldsymbol{D}}_{-p} \rangle_\Lambda \tag{9}$$

where Λ^* is the Fourier dual of Λ and $\hat{\boldsymbol{D}}_p = |\Lambda|^{-1/2} \Sigma_{x \in \Lambda} \mathrm{e}^{-\mathrm{i}px} \boldsymbol{D}_x$. In order to prove equation (7), it is sufficient to show that $\liminf_{\Lambda \nearrow \boldsymbol{Z}^3} c_\Lambda > 0$, which is done by providing suitable lower and upper bounds on the first and, respectively, second term in the RHS of equation (9).

The upper bound on $\mathrm{Tr}\langle \hat{\boldsymbol{D}}_p \hat{\boldsymbol{D}}_{-p} \rangle_\Lambda$ for $p \neq 0$ is obtained in the usual way from the reflection positivity (Fröhlich *et al* 1978):

$$\langle \mathrm{Tr}(\hat{\boldsymbol{D}}_p \hat{\boldsymbol{D}}_{-p}) \rangle_\Lambda \leqslant \text{constant}/[\beta(\hat{J}(0) - \hat{J}(p))] \tag{10}$$

where $\hat{J}$ is the Fourier transform of J. Under our assumption, the function on the RHS is bounded by an integrable function, so its sum over Λ^* divided by $|\Lambda|$ converges for $\Lambda \nearrow \boldsymbol{Z}^3$ to $(\text{constant}/\beta) \int \mathrm{d}^3 p\, (\hat{a}(0) - \hat{a}(p))^{-1}$.

The lower bound on $\langle \mathrm{Tr}(\boldsymbol{D}_x^2) \rangle_\Lambda$ is obtained by chessboard estimates as follows. Let $\chi_x^{(\varepsilon)}$ be the indicator of the event $\{\mathrm{Tr}(\boldsymbol{D}_x^2) < \varepsilon\}$. Then

$$\langle \mathrm{Tr}(\boldsymbol{D}_x^2) \rangle_\Lambda \geqslant \varepsilon (1 - \langle \chi_x^{(\varepsilon)} \rangle_\Lambda). \tag{11}$$

By chessboard estimates

$$\langle \chi_x^{(\varepsilon)} \rangle_\Lambda \leqslant \left[\left\langle \prod_{y \in \Lambda} \chi_y^{(\varepsilon)} \right\rangle_\Lambda \right]^{1/|\Lambda|}$$

so we have to bound from above the probability that $\mathrm{Tr}(\boldsymbol{D}_y^2) < \varepsilon$ at all sites $y \in \Lambda$. The energy of such a configuration is majorised using $|\mathrm{Tr}(\boldsymbol{D}_x \boldsymbol{D}_y)| \leqslant [\mathrm{Tr}(\boldsymbol{D}_x^2)\, \mathrm{Tr}(\boldsymbol{D}_y^2)]^{1/2} < \varepsilon$,

† Let us stress that equation (7) does not imply 'positional' LRO, which should mean $\lim_{|x-y|\to\infty} [\langle n_x n_y \rangle - \langle n_x \rangle \langle n_y \rangle] > 0$.

which gives

$$-H_\Lambda(\boldsymbol{D}) \leqslant \varepsilon \sum_{\{x,y\}\subset\Lambda} J_{xy} + \mu\theta(\mu)|\Lambda| = [\varepsilon\|a\| + \mu\theta(\mu)]|\Lambda|, \tag{12}$$

where $\theta(\mu) = 1$ for $\mu \geqslant 0$ and $=0$ otherwise, and $\|a\| = \frac{3}{2}\sum_{x\in\mathbf{Z}^3} a(|x|)$.

A lower bound on Z_Λ is obtained by choosing a $\bar{\boldsymbol{D}} \in \operatorname{supp}\nu$ and a neighbourhood $V_{\varepsilon'}$ of $\bar{\boldsymbol{D}}$, such that

$$\operatorname{Tr}(\boldsymbol{D}'\boldsymbol{D}'') > \operatorname{Tr}(\bar{\boldsymbol{D}}^2)(1-\varepsilon') > 0, \qquad \forall \boldsymbol{D}', \boldsymbol{D}'' \in V_{\varepsilon'}. \tag{13}$$

For configurations $\{\boldsymbol{D}_x\}$ such that $\boldsymbol{D}_x \in V_{\varepsilon'}$ for all $x \in \Lambda$, we have

$$-H_\Lambda(\boldsymbol{D}) \geqslant \operatorname{Tr}(\bar{\boldsymbol{D}}^2)(1-\varepsilon') \sum_{\{x,y\}\subset\Lambda} J_{xy} + \mu|\Lambda| = [(1-\varepsilon')\operatorname{Tr}(\bar{\boldsymbol{D}}^2)\|a\| + \mu]|\Lambda|. \tag{14}$$

Restricting integrations only to such configurations, we obtain

$$Z_\Lambda^{1/|\Lambda|} \geqslant \nu(V_{\varepsilon'}) \exp\{\beta[(1-\varepsilon')\operatorname{Tr}(\bar{\boldsymbol{D}}^2)\|a\| + \mu]\}. \tag{15}$$

Using these estimates in the expression for $\langle \Pi_y \chi_y^{(\varepsilon)} \rangle_\Lambda$, we have

$$\langle \chi_x^{(\varepsilon)} \rangle_\Lambda \leqslant \frac{1+\nu(\chi^{(\varepsilon)})}{\nu(V_{\varepsilon'})} \exp\{-\beta[\|a\|(\operatorname{Tr}(\bar{\boldsymbol{D}}^2)(1-\varepsilon') - \varepsilon) + \mu\theta(-\mu)]\}. \tag{16}$$

One sees that for $\mu > \mu_0 = -\|a\| \max_{\bar{\boldsymbol{D}}\in\operatorname{supp}\nu} \operatorname{Tr}(\bar{\boldsymbol{D}}^2)$, $\langle \chi_x^{(\varepsilon)} \rangle_\Lambda \to 0$ for $\beta \to \infty$, uniformly in Λ, and introducing this into equation (11), that $\langle \operatorname{Tr}(\boldsymbol{D}_x^2) \rangle_\Lambda$ is bounded away from zero.

Using these estimates in equation (9), we obtain $c_\Lambda \geqslant$ constant > 0 for $\mu > \mu_0$ and $\beta > \beta(\mu)$, with μ_0, $\beta(\mu)$ independent of Λ, whence the assertion follows.

According to equation (7), the matrix $\langle \boldsymbol{D}_x \rangle = \langle \boldsymbol{Q}_x \rangle$ should be non-zero in a pure phase, so it plays the role of the order parameter. On the other hand, at high temperature, LRO is absent: $\operatorname{Tr}\langle \boldsymbol{D}_x \boldsymbol{D}_y \rangle$ decays to zero in the same weighted summability sense as the interaction (see e.g. Gross (1979) for a very general result of this kind).

We believe that at least its full O(3)-invariance makes the model look physically more realistic than the interacting dimer model. Technically, the model seems to be more manageable than the dimer models. For instance, it allows in principle an application of the renormalisation group techniques. Our proof of LRO works for long-range forces with power fall-off, instead of only the nearest-neighbour interactions allowed for dimers by Heilmann and Lieb (1979) and Abraham and Heilmann (1980).

On the other hand, our approach almost completely neglects excluded volume effects; in fact, it takes them into account only via the lattice. These would appear with the wrong sign in the Hamiltonian and would destroy its reflection positivity. We have no proof of the absence of positional LRO, either. However, we conjecture that every limit state $\langle \cdot \rangle$ when restricted only to the variables $\{n_x\}$ is clustering, at least for large μ and β where orientational LRO appears. Intuitively this should be the case, because in this regime the typical Q-configurations vary slowly in space, which results in effective attraction between molecules; so, as far as $\{n_x\}$ are concerned, the model should behave as a lattice gas with attractive interactions at high μ.

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