ON LONG-RANGE ORDER IN LOW-DIMENSIONAL LATTICE-GAS MODELS OF NEMATIC LIQUID CRYSTALS

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Abstract

The problem of the orientational ordering transition for lattice-gas models of liquid crystals is discussed in the low-dimensional case $d = 1, 2$. For isotropic short-range interactions, orientational long-range order at finite temperature is excluded for any packing of molecules on the lattice $Z^d$; on the other hand, for reflection-positive long-range isotropic interactions, we prove existence of an orientational ordering transition for high packing ($\mu > \mu_0$) and low temperatures ($\beta > \beta_c(\mu)$).

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The problem of long-range orientational order in models mimicking liquid crystalline (usually nematic) behaviour has been discussed at the rigorous level and in the framework of different interaction models, see, e.g., Ref. [1, 2, 3, 4]. In the following, we shall be considering cylindrically symmetric molecules, whose centres of mass belong to a $d-$dimensional space ($x \in \mathbb{Z}^d$, lattice models, or $x \in \mathbb{R}^d$, continuum models), and whose orientations are defined by $m-$component unit vectors $u \in S^{(m-1)} \subset \mathbb{R}^m$, $m \geq 2$.

For low-dimensional lattice models (i.e. dimension $d = 1, 2$) with isotropic short-range interactions, the Mermin-Wagner theorem entails absence of an orientational ordering transition taking place at finite temperature; a similar result was proven by Romerio for continuum fluids [1]. On the other hand, a two-dimensional lattice model with anisotropic interactions restricted to nearest neighbours can produce an ordering transition (also of the nematic type), see, e.g. Ref. [5], Ref. [6], Ch. 9, Example 9.22(2).

The proof of the existence of orientational order for continuum liquids is a rather complicated problem. In this connection we would like to mention Ref. [7], where the existence of a ferromagnetic phase transition is proven for a continuum fluid ($d \geq 2$) of classical particles carrying Ising-like spins and having suitable magnetic and non-magnetic interactions. The proof is based on the FKG- and GHS-inequalities, which make it possible to find a lower bound for the magnetization of the fluid in terms of that of a suitable spin system on a lattice; no such inequalities are known for $m \geq 3$.

The aim of the present note is to prove the existence of orientational ordering (at finite temperature) in low-dimensional lattice-gas models ($d = 1, 2$) [4] with isotropic long-range interactions of nematic symmetry, which therefore do not satisfy the hypotheses of the Romerio theorem [4].

In order to make contact with (nematic) liquid crystals, and following the standard phenomenology [8], we consider centrosymmetric molecules (sym-
metry \( D_{\infty h} \), and define the matrix
\[
Q^{\alpha \beta} = (u^\alpha u^\beta - \frac{1}{m} \delta_{\alpha \beta}), \quad \alpha, \beta = 1, 2, \ldots m;
\] (1)
then translationally invariant interactions between molecules can be expressed as
\[
V_{xy} = -a(|x - y|) \text{Tr}(Q_x \cdot Q_y) + g(|x - y|), \quad x, y \in R^d.
\] (2)

The Hamiltonian of the lattice-gas caricature of the nematic liquid crystal has the form [4]:
\[
H_{\Lambda}(\tilde{n}, \tilde{Q}) = -\frac{1}{2} \sum_{(x,y)} n_x n_y J_{xy} \text{Tr}(Q_x \cdot Q_y) + \frac{1}{2} \sum_{(x,y)} n_x n_y I_{xy} - \mu \sum_{x \in \Lambda} n_x,
\] (3)
where \((x, y) = \{x, y \in \Lambda : x \neq y\}\). In this context we can assume \(a(0) = g(0) = 0\).

So, molecules live on the sites of the cubic sublattice \(\Lambda \subset Z^d\) with periodic boundary conditions, i.e.
\[
J_{xy} = \sum_{\{z \in Z^d; z=y(\text{mod} \Lambda)\}} a(|x - z|), \quad I_{xy} = \sum_{\{z \in Z^d; z=y(\text{mod} \Lambda)\}} g(|x - z|).
\]
A configuration is specified by a set of occupation numbers \(\{n_x = 0, 1; x \in Z^d\}\) and, for all \(\{x \in Z^d : n_x = 1\}\), by the configuration \(Q_x\) of the molecule at \(x \in Z^d\). The corresponding finite-volume Gibbs state is defined by
\[
\langle f \rangle_{\Lambda}(\beta, \mu) = \frac{\Xi_{\Lambda}(\beta, \mu)}{[\Xi_{\Lambda}(\beta, \mu)]^{-1}}
\] (4)
where \(\Xi_{\Lambda}\) is the partition function, \(d\nu\) is the \(O(m)\)-invariant probability measure induced by the Haar measure on the unit sphere in \(R^m\), see Eq. (1), and \(\tilde{n} \equiv \{n_x; x \in \Lambda\}, \tilde{Q} \equiv \{Q_x; x \in \Lambda\}\).

The chemical potential \(\mu\) governs the concentration (mean density) \(\rho(\beta, \mu) = \langle n_x \rangle_{\Lambda}\), of molecules on the lattice at the temperature \(\beta^{-1}\). The interaction term \(J_{xy} \text{Tr}(Q_x \cdot Q_y)\) involves both positional and orientational degrees of
freedom, and possibly produces orientational order, whereas $I_{xy}$ mimics a direct interaction between them (positional order).

Let $a(|x - y|)$ denote a short-range interaction ($SR$, i.e. finite-ranged or decreasing at least exponentially), or a long-range one with asymptotic behaviour $a(|x - y|) \sim |x - y|^{-(d + \sigma)}$, for $|x - y| \to \infty$, $\sigma > 0$. Then, in the limit $q \to 0$, the lattice Fourier transform of $J_{xy}$ is given by

$$
\hat{J}(0) - \hat{J}(q) \simeq \begin{cases} 
  c|q|^\sigma, & 0 < \sigma < 2 \\
  c|q|^2, & \sigma \geq 2, \text{ or } SR
\end{cases}
$$

(5)

where

$q \in \Lambda^* \equiv \{ q^\alpha = \frac{2\pi}{|\Lambda|^1/d} m_\alpha, \ m_\alpha = 0, \pm 1, \ldots, \pm (|\Lambda|^{1/d} - 1), \frac{1}{2} \leq \alpha \leq 1, 2, \ldots d \}$.

Then, since this interaction is $O(m)$–invariant, we have the following Proposition à la Mermin-Wagner, due to [9].

Proposition 2.1

Let $d = 1, 2, \sigma \geq 2$ (or let $a(|x - y|)$ define a $SR$ interaction), and let $g(|x - y|)$ be such that

$$
\sum_{y \in \mathbb{Z}^d} |g(|x - y|)| |x - y|^2 < +\infty.
$$

Then there is no orientational order at finite temperature, i.e.

$$
P(\beta, \mu) \equiv \lim_{|x - y| \to \infty} \lim_{\Lambda \to \mathbb{Z}^d} \langle Tr(D_x \cdot D_y) \rangle_{\Lambda} = 0,
$$

(6)

Here $D_x \equiv n_x \cdot Q_x$.

Proof

For any fixed configuration $\tilde{n}$ the limiting Gibbs state $\langle - \rangle(\beta, \tilde{n})$ is $O(m)$–invariant. In this case, the proof developed in [4] carries through verbatim for the $O(m)$–invariant interaction defined by (2) and corresponding to $U_{xy}(Q_x, Q_y)$ in Pfister’s notation [3]. Since the conditions both on $I_{xy}$ and $J_{xy}$ guarantee for the Hamiltonian (3) the equivalence of ensembles (see Ref. [10, 11]), one gets that the grand-canonical Gibbs state

$$
\langle f \rangle(\beta, \mu) = \int dK(\mu, \tilde{n}) \langle f \rangle(\beta, \tilde{n})
$$

(7)
is also $O(m)$–invariant. Here $dK(\mu, \tilde{n})$ is the Kac-transformation kernel [10, 11]. For any pure state $\langle - \rangle(\beta, \mu)$, we get

$$
\lim_{|x-y| \to \infty} \langle Tr(D_x \cdot D_y) \rangle = (TrD_x)^2 = 0,
$$

where the last equality follows from the $O(m)$–invariance of the state (7). □

The presence of “holes” ($n_x = 0$) evidently disfavours the orientational order on $\lim_{\Lambda \uparrow \mathbb{Z}^d} M(\tilde{n})$. It is natural to guess that the order parameter $P(\beta, \tilde{n})$, and hence $P(\beta, \mu)$ are bounded by the order parameter of the lattice without “defects”, i.e. $\{n_x = 1; x \in \mathbb{Z}^d\}$, which corresponds to $\mu \to +\infty$. One can easily check this for particular cases of the lattice-gas Ising system (where $Tr(Q_x \cdot Q_y)$ is substituted by $\tau_x \cdot \tau_y$, $\tau_{x,y} = \pm 1$), or for the lattice-gas of plane rotators, due to the GHS inequalities. Hence, for these systems, the result (6) is a simple consequence of “pure system domination”: $P(\beta, \mu) \leq P(\beta, \mu = +\infty)$, and of the Mermin-Wagner theorem for the regular lattice $\mathbb{Z}^d$, $d = 1, 2$.

This result can be further strengthened: for $d = 1$ and $1 \leq \sigma \leq 2$, the absence of orientational order has also been proven for the lattice model(s) [Ref. [1], Ch. 9, Comment 9.34; Theorem 14’ in Ref. [12]; Refs. [13, 14]]. Notice that Romerio’s result [1] holds for $\sigma > 2$ but for a continuum model.

3

In contrast to the “no-go” Proposition 2.1, the proof of existence of orientational order at finite temperature ($P(\beta, \mu) > 0$) is a more delicate task. We are able to do this for long-range interactions which are reflection-positive with respect to reflections in planes without sites [12, 15].

From now on, let $g(|x-y|) = 0$ and let $a(|x-y|)$ correspond to the long-range interaction

$$
a(|x-y|) = b|x-y|^{-(d+\sigma)}, \; b > 0
$$

with $0 < \sigma < d$. First we note that, for (8) the asymptotic form of the Fourier transform (5) excludes a a “no-go” theorem à la Mermin-Wagner.

**Proposition 3.1**

For $d = 1, 2$ there exists a $\mu_0$ and, for every $\mu > \mu_0$ there exists a $\beta_c(\mu)$ such that $P(\beta, \mu) > 0$ for $\beta > \beta_c(\mu)$. This means that every limiting Gibbs state $\langle - \rangle = \lim_{\Lambda \uparrow \mathbb{Z}^d} \langle - \rangle_\Lambda$ has long-range orientational order.
Proof
The Proof is an adaptation to our case (I) of the line of reasoning developed in [4] for the case of the general matrix order parameter. By (I) one has $TrQ_x = 0$, i.e. $Tr \langle D_x \rangle_\Lambda = 0$. Then, by the $O(m)$-invariance of the state $\langle - \rangle_\Lambda$, one can deduce that $\langle D_x \rangle_\Lambda = 0$. Hence, $P(\beta, \mu) > Tr(\langle D_x \rangle^2) = 0$ will really mean existence of long-range orientational order.

Using the translational invariance of $\langle - \rangle_\Lambda$, we get

$$c_\Lambda = |\Lambda|^{-2} \sum_{(x,y)} \langle Tr(D_x D_y) \rangle_\Lambda = Tr \langle D_x^2 \rangle_\Lambda - |\Lambda|^{-1} \sum_{p \in \Lambda^* \{0\}} Tr \langle \tilde{D}_p \cdot \tilde{D}_{-p} \rangle_\Lambda,$$

(10)

where

$$\tilde{D}_p = |\Lambda|^{-1/2} \sum_{x \in \Lambda} \exp(-ipx) D_x.$$

Thus, in order to prove that $P(\beta, \mu) > 0$, it suffices to verify that

$$c(\beta, \mu) \equiv \lim_{\Lambda \uparrow \mathbb{Z}^d} \text{inf} \, c_\Lambda > 0.$$

(11)

The upper bound on $Tr \langle \tilde{D}_p \tilde{D}_{-p} \rangle_\Lambda$ for $p \in \Lambda^* \{0\}$ results from the Infrared Bound [12, 15]

$$\langle Tr(\tilde{D}_p \tilde{D}_{-p}) \rangle_\Lambda \leq \frac{\text{const}}{\beta \hat{J}(0) - \hat{J}(p)} \sim |p|^{-\sigma}, \text{ for } p \to 0$$

(12)

which holds true for the reflection-positive interaction (9), due to the chessboard estimate proving the gaussian domination; see Refs. [5, 16] for a review. Therefore, the sum over $\Lambda^* \{0\}$ divided by $|\Lambda|$ (see (10)) can be estimated in the limit $\Lambda \uparrow \mathbb{Z}^d$ from above by the integral

$$I_{d, \sigma}(\beta) = \frac{\text{const}}{\beta} \int_{[-\pi, +\pi]^d} d^d p \big[\hat{a}(0) - \hat{a}(p)\big]^{-1} < \infty, \; 0 < \sigma < d.$$

(13)

In order to get the lower bound of the first term of (10), $Tr \langle D_x^2 \rangle_\Lambda = \langle n_x^2 \rangle_\Lambda Tr(Q_x^2) = \frac{m-1}{m} \langle n_x \rangle_\Lambda$, we again use the chessboard estimate [12, 15]:

$$\langle 1 - n_x \rangle_\Lambda \leq [\prod_{y \in \Lambda} (1 - n_y)]^{1/|\Lambda|}.$$

(14)

Then one gets

$$\langle n_x \rangle_\Lambda \geq 1 - [\prod_{y \in \Lambda} (1 - n_y)]^{1/|\Lambda|}.$$

(15)
According to (4) the last term in (15) is equal to 
\[ Z \Lambda(\beta, \mu) \Bigl( -\frac{1}{|\Lambda|} \Bigr) \]. To get a lower bound on the partition function \( Z \Lambda(\beta, \mu) \), we choose a \( \overline{D} \in \text{supp } \nu \) and a neighbourhood \( \mathcal{N}_\epsilon \) of \( \overline{D} \) such that

\[ \text{Tr}(D_1 \cdot D_2) > (1 - \epsilon)\text{Tr}(\overline{D}^2) > 0, \]  

(16)

for some \( \epsilon > 0 \) and for every \( D_1, D_2 \in \mathcal{N}_\epsilon \). Then for configurations \( \Delta^{(\epsilon)} \equiv \{ D_x : D_x \in \mathcal{N}_\epsilon, x \in \Lambda \} \), we get by (16) that

\[ n_x = 1; \quad x \in \Lambda \]  

and

\[ -H(\mu, Q) = \frac{1}{3} \sum_{(x,y)} J_{xy} + \mu |\Lambda| \geq \beta \bigl((1 - \epsilon)\text{Tr}(Q^2)\hat{a}(0) + \mu\bigr) \cdot |\Lambda|. \]  

(17)

Therefore, upon restricting the integration in the partition function to configurations \( \Delta^{(\epsilon)} \), we obtain

\[ [Z(\beta, \mu)]^{-1/|\Lambda|} \leq \nu(\mathcal{N}_\epsilon)^{-1} \exp\{ -\beta[(1 - \epsilon)\text{Tr}(Q^2)\hat{a}(0) + \mu]\}, \]  

(18)

and, as a consequence of (15), one gets

\[ \text{Tr}(D_x^2) \geq \frac{2}{3} \bigl[1 - \frac{1}{\nu(\mathcal{N}_\epsilon)} \exp\{ -\beta[(1 - \epsilon)\text{Tr}(Q^2)\hat{a}(0) + \mu]\}\bigr] \equiv L(\beta, \mu). \]  

(19)

Combining (13) with (19), we obtain the following estimate for (11):

\[ c(\beta, \mu) \geq L(\beta, \mu) - I_{\delta, \sigma}(\beta). \]  

(20)

Now one immediately sees that for

\[ \mu > \mu_0 \equiv -(1 - \epsilon)\text{Tr}(Q^2)\hat{a}(0), \]  

there exists a \( \beta_c(\mu) \) such that

\[ L(\beta_c(\mu), \mu) = I_{\delta, \sigma}(\beta), \]  

where \( 0 < \sigma < 1, \quad d = 1 \) and \( 0 < \sigma < 2, \quad d = 2 \). Hence, for \( \beta \)\( \beta_c(\mu) > \mu_0 \) we get \( c(\beta, \mu) > 0 \). According to Eqs. (10), (11), this means that \( P(\beta, \mu) > 0 \) in the named \( (\beta, \mu) \) domain, i.e. in any pure limiting Gibbs state \( \langle D_x \rangle = \langle Q_x \rangle \neq 0 \): thus the \( O(m) \) symmetry is broken, which means long-range orientational order. \( \square \)

Notice that the sign of \( a(|x - y|) \) plays an important role in the existence theorem, but not in its absence counterpart.

Moreover, the following corollaries can be obtained, by the same line of reasoning as in the preceding propositions.
Corollary 1.
Consider the ferromagnetic (lattice gas) counterpart of the present model, i.e. whose orientation-dependent two-body interaction reads

$$V_{xy} = -a(|x - y|)(u_x \cdot u_y). \quad (21)$$

Then, under the same hypotheses on $a(|x - y|)$ and $g(|x - y|)$, one can prove absence or existence of an ordering transition, respectively.

Corollary 2.
Let $m = 3$, and let the orientation-dependent two-body interaction have the general form

$$V_{xy} = -a(|x - y|)P_L(u_x \cdot u_y), \quad (22)$$

for an arbitrary positive integer $L$; owing to the addition theorem for spherical harmonics, the Legendre polynomial can be written as

$$P_L(u_x \cdot u_y) = \omega_L Tr(W^{(L)}_{x} \cdot W^{(L)}_{x}), \quad (23)$$

where $W^{(L)}$ denote real multipole tensors of rank $L$ constructed in terms of components of $u_x$ and $u_y$, respectively, and $\omega_L$ is an appropriate positive normalization factor, so that $Tr(W^{(L)}_{x} \cdot W^{(L)}_{x}) = 1/\omega_L$. Then, under the same hypotheses on $a(|x - y|)$ and $g(|x - y|)$, one can prove absence or existence of an ordering transition, respectively, for arbitrary $L$. Even values of $L$ define lattice-gas models of nematic liquid crystals, and the result proven in Ref. [4] and for $d = 3$ can be similarly generalized.

In conclusion, we would like to point out that the present note yields a partial answer to questions proposed in [1] as open problems. We have shown that long-range interactions violating conditions (2.5) of Ref. [1] (cf. (9)) can produce long-range orientational order in low-dimensional lattice models of nematic liquid crystals. The problem of the possible existence of long-range orientational order for continuum models remains open.

Another open problem which can be formulated in the framework of this lattice model (3) concerns existence of long-range positional order, i.e.

$$\lim_{|x - y| \to +\infty} [\langle n_x \cdot n_y \rangle - \langle n_x \rangle \langle n_y \rangle] > 0,$$

when $g(|x - y|) \geq 0$, repulsion which crudely mimics excluded-volume effects for nematic molecules.
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