INTERMEDIATE PHASES IN MIXED NEMATIC/HEISENBERG SPIN-MODELS

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Abstract. We prove that in three or higher dimensions, an isotropic, ferromagnetic, nearest-neighbor O(N) perturbation of a nematic liquid crystal model (also having isotropic, nearest-neighbor interactions) has an intermediate phase. In this intermediate phase, the liquid crystal order parameter is non-zero but the spontaneous magnetization is zero while at low temperatures, these systems exhibit magnetization.

This paper concerns the (lattice) nematic liquid crystal model. Here, at each site i of a regular lattice, resides an $O(N)$ spin–variable, $\vec{s}_i$. (We will take $|\vec{s}_i| = 1$; for physical considerations, one focuses on $N = 2, 3$.) This variable, in some approximation, usually represents a rod–like molecule – or density thereof – that is symmetric about its center. Thus the spin–spin interaction boils down to the square of the usual Heisenberg term. Such models have been investigated mathematically in [AZ], [Z] where, in dimension $d \geq 3$, a low temperature phase was established. This phase, called the nematic phase, is characterized by the non–vanishing of the nematic order parameter, i.e. the matrix

$$\mathbb{Q}_i^{\alpha,\gamma} = s_i^\alpha s_j^\gamma - \frac{1}{N}\delta^{\alpha\gamma} \tag{1}$$

does not average to zero. Needless to say in these models the spins themselves have zero average at all temperatures.

Here we wish to consider a situation where the liquid crystal molecules have some asymmetry along the axis of the rod, that will become physically relevant at sufficiently low temperatures. For example, the "head" and "tail" ends of the molecules may have different interactions that tend to align the heads of the molecules, as was discussed in [LG]. Thus the natural model to consider is the standard liquid crystal model (e.g. as written down in [AZ])

Key words and phrases. Liquid crystal model, Classical Heisenberg model.

with the Hamiltonian perturbed by a Heisenberg term. This is precisely what was done in [LG] for the case of the two-dimensional $O(2)$ model.

Here, mostly for technical reasons, we will focus on $d \geq 3$. The techniques of reflection positivity and infrared bounds [FSS], [FILS] tell us that both the liquid crystal and the magnetic order parameters have associated temperatures, below which they are non-zero. The purpose of this paper is to show that these temperatures can be distinct, and consequently the existence of an intermediate phase with nematic order and no magnetic order. We will use a generalized graphical representation of the type discussed in [CM] to distinguish these temperatures.

The setup for this model in finite volume consists of a box $\Lambda \subset \mathbb{Z}^d$, $d \geq 3$, with bonds $\mathbb{B}$, and a "liquid crystal rod" (i.e., an $O(N)$ variable) centered at each site. The ends of the rod are antipodal points on the $(N-1)$–dimensional unit sphere S^{N-1} and the (matrix) observable for this molecule is $\mathbb{Q}_i^{\alpha,\gamma}$ as defined in Equ. (1). The unperturbed nematic interaction between two molecules at neighboring sites i and j is given by $-J\mathrm{Tr}[\mathbb{Q}_i\mathbb{Q}_j]$ with $J > 0$. The full Hamiltonian, including the Heisenberg perturbation that we consider is given by

$$\mathcal{H}_\Lambda(\vec{h}, \mathbb{K}) = -\sum_{\langle i,j\rangle \in \mathbb{B}} (J\mathrm{Tr}[\mathbb{Q}_i\mathbb{Q}_j] + \epsilon(\vec{s}_i \cdot \vec{s}_j)) - \sum_{i\in\Lambda}(\mathrm{Tr}[\mathbb{K}_i\mathbb{Q}_i] + \vec{h}_i \cdot \vec{s}_i) \tag{2}$$

with $\vec{s}_i \in S^{N-1}$, $\vec{h} \in \mathbb{R}^N$, and $\epsilon > 0$. The objects $\mathbb{K}_i$ are traceless $N \times N$ self-adjoint matrices:

$$\mathbb{K}_i^{\alpha\gamma} = k_i^\alpha k_i^\gamma - \frac{1}{N}|\vec{k}_i|\delta^{\alpha\gamma}$$

where $\vec{k}_i$ is a vector like $\vec{h}_i$, with components $k_i^\alpha, \alpha = 1, \dots, N$. The external fields, $\mathbb{K} \equiv \mathbb{K}_i$ and $\vec{h} \equiv \vec{h}_i$ are for auxiliary purposes only and will not enter into the final results.

The partition function is given by

$$\mathcal{Z}_\Lambda(\vec{h}, \mathbb{K}) = \int d^{|\Lambda|}s \; e^{-\beta\mathcal{H}_\Lambda(\vec{h},\mathbb{K})} \tag{3}$$

where ds denotes the Haar measure on S^{N-1}. We let $\langle\cdot\rangle_{\Lambda;\vec{h},\mathbb{K}}$ denote the Gibbs measure corresponding to $\mathcal{Z}_\Lambda(\vec{h}, \mathbb{K})$.

Since we will be using reflection positivity to establish phase transitions, we first consider only periodic boundary conditions (cf. [FILS]). Thus, in the absence of spatially dependent external fields, the states we consider are translation invariant so the magnetization observable is equal to $\vec{s}_0$ and the nematic observable equal to $\mathbb{Q}_0$. The order parameters that we will consider are the infinite volume quantities $\langle\vec{s}_0\rangle_{0^+,0}$ and $\langle\mathbb{Q}_0\rangle_{0,0^+}$. In both cases, the zero field limit is taken with uniform external fields pointing along a particular axis.

Using the techniques in [FSS] and [FILS], we have first order phase transitions with respect to $\vec{h}$ and $\mathbb{K}$. Furthermore we have lower bounds on the transition temperatures for each order parameter. We will denote the lower bounds on the transition temperatures for $\langle \vec{s}_0 \rangle_{0^+,0}$ and $\langle \mathbb{Q}_0 \rangle_{0,0^+}$ by T_*^{spin} and T_*^{lc}, respectively. The actual transition temperatures (below which $\langle \vec{s}_0 \rangle_{0^+,0}$ and $\langle \mathbb{Q}_0 \rangle_{0,0^+}$ are non zero and above which they vanish) will be denoted by T_c^{spin} and T_c^{lc}. We summarize the current status in the following:

Proposition 1. *There is a first order phase transition in each variable $\vec{h}$ and $\mathbb{K}$ with $\langle \vec{s}_0 \rangle_{0^+,0}$ and $\langle \mathbb{Q}_0 \rangle_{0,0^+}$ the respective order parameters for these phase transitions. These quantities are non–zero when $T < T_*^{spin}$ and/or $T < T_*^{lc}$; here the lower bounds on the transition temperatures are related to the interaction constants by $T_*^{spin} \equiv 4\epsilon/[ND]$ and $T_*^{lc} \equiv 8J(N-1)/[N^2(N+1)D]$, where D is the constant in* [FILS]*:*

$$D \equiv (2\pi)^{-d} \int\limits_{\substack{|p_m| \leq \pi \\ m=1,\dots,d}} \left(\sum_{m=1}^{d} 1 - \cos p_m \right)^{-1} d^d p \,,$$

and d is the lattice dimension. Furthermore, the temperatures T_c^{spin} and T_c^{lc} are finite.

Proof. The temperatures T_*^{spin} and T_*^{lc} are obtained by the methods in section four of [FILS]; we will outline the derivation in [AZ] for T_*^{lc}.

We use matrices that have a single non–zero entry on or above the diagonal at (α, γ) to obtain all of the mixed-term bounds for Gaussian domination: $\mathcal{Z}_\Lambda(0, \mathbb{H}^{\alpha\gamma}) \leq \mathcal{Z}_\Lambda(0,0)$. We have N(N+1)/2 bounds (since there are that many elements on or above the diagonal of an $N \times N$ matrix). By summing these bounds and following the derivation in [FSS] and [FILS], we see that if

$$\langle Tr(\mathbb{Q}_0^2) \rangle - \frac{1}{4\beta} \frac{N(N+1)}{2} JD \geq 0 \tag{4}$$

there will be multiple phases, and thus for some ergodic state μ, $\mu(\mathbb{Q}_0) \neq 0$. This will happen if $T < [N(N+1)D]^{-1} 8J \langle \mathrm{Tr}(\mathbb{Q}_0^2) \rangle = [N(N+1)D]^{-1} 8J(N-1)/N$. The classic derivation (in [FSS]) results in the value for T_*^{spin}. Standard high temperature techniques ([S, V.1.3], Dobrushin's uniqueness theorem, or the method in [AC]) shows that the temperatures T_c^{spin} and T_c^{lc} are finite. $\square$

We will now employ a primitive graphical representation of our model to obtain an upper bound on the critical temperature T_c^{spin} for the magnetic order parameter. The goal of this paper is achieved if our upper bound lies below T_*^{lc} (which will be satisfied if ϵ is small).

Let us start this with some preliminary notation. As before, Let $\Lambda \subset \mathbb{Z}^d$ be a finite box with bonds $\mathbb{B}$. We define

$$\begin{aligned}
\mathcal{H}_\Lambda^{lc} &= -\sum_{\langle i,j\rangle\in\mathbb{B}} J\, Tr(\mathbb{Q}_i\mathbb{Q}_j)\,, \\
\mathcal{H}_\Lambda^{spin} &= -\sum_{\langle i,j\rangle\in\mathbb{B}} \epsilon\,(\vec{s}_i\cdot\vec{s}_j+1)\,, \\
\mathcal{H}_\Lambda &= \mathcal{H}_\Lambda^{lc}+\mathcal{H}_\Lambda^{spin}\,,
\end{aligned} \tag{5}$$

Here we allow arbitrary boundary conditions on $\partial\Lambda$ – but these will not enter into the notation. Observe that in the magnetic term, we have added a constant (which of course, has no physical consequences). To get our graphical representation, we write

$$\mathcal{Z}_\Lambda = \mathrm{Tr}[e^{-\beta\mathcal{H}_\Lambda}] = \mathrm{Tr}[e^{-\beta\mathcal{H}_\Lambda^{lc}}\prod_{\langle i,j\rangle\in\mathbb{B}} e^{\beta\epsilon(\vec{s}_i\cdot\vec{s}_j+1)}] \tag{6}$$

where the operation of "Tr" includes any special considerations that take place at the boundary. We expand the product in Equ.(6) associating each term in the expansion with a bond configuration $\omega \in \{0,1\}^{\mathbb{B}}$. In particular, for each $\langle i,j\rangle$ we must "choose" the term $(e^{\beta\epsilon\,(\vec{s}_i\cdot\vec{s}_j+1)}-1)$ or $+1$ which corresponds to $\omega_{\langle i,j\rangle}=1$ (occupied) or $\omega_{\langle i,j\rangle}=0$ (vacant) respectively. It is noted that the contribution from each term in the sum is positive. Thus the weights

$$V_\Lambda(\omega) = \int d^{|\Lambda|}s\; e^{-\beta\mathcal{H}_\Lambda^{lc}}\prod_{\langle i,j\rangle\in\omega}\left(e^{\beta\epsilon\,(\vec{s}_i\cdot\vec{s}_j+1)}-1\right) \tag{7}$$

when divided by the partition function may be interpreted as the probability of observing the configuration ω. We denote the associated probability measure by $v_\Lambda(-)$. We write $i \leftrightarrow \partial\Lambda$ if there is a path of occupied bonds in ω connecting the site i to $\partial\Lambda$, and $i \not\leftrightarrow \partial\Lambda$ if there is no such path connecting i to $\partial\Lambda$. Although the weights appear rather unwieldy it is straightforward to obtain *bounds* on certain probabilities. For example, we have

Lemma 2. *Let $\{e_1,e_2,\dots,e_n\}$ denote a given set of edges. Then in any boundary condition, the probability that all of these edges are occupied, $v_\Lambda(e_1{=}1,e_2{=}1,\dots,e_n{=}1)$, is bounded above by $(e^{2\beta\epsilon}-1)^n$.*

Proof. This is an elementary observation:

$$\begin{aligned}
v_\Lambda(e_1{=}1,e_2{=}1,\dots,e_n{=}1) &= \sum_{\substack{\omega:\omega(e_m)=1\\ m=1,\dots,n}} \mathcal{Z}_\Lambda^{-1}\int d^{|\Lambda|}s\; e^{-\beta\mathcal{H}_\Lambda^{lc}}\prod_{\langle i,j\rangle\in\mathbb{B}}\left(e^{\beta\epsilon\,(\vec{s}_i\cdot\vec{s}_j+1)}-1\right)^{\omega\langle i,j\rangle} \\
&\le \left(e^{2\beta\epsilon}-1\right)^n v_\Lambda(e_1{=}0,e_2{=}0,\dots,e_n{=}0) \\
&\le \left(e^{2\beta\epsilon}-1\right)^n .
\end{aligned} \tag{8}$$

It is noted that the inequality in Equ.(8) is independent of boundary conditions. □

Theorem 3. *Let T_0^{spin} be defined by* $\exp\{2\epsilon/T_0^{spin}\} - 1 = 1/[2d-1]$*. Then for* $T > T_0^{spin}$*, the spontaneous magnetization for the system defined by the Hamiltonian in Equ.(2) (at zero external fields) is zero.*

Proof. Let Λ be a finite box as above and let $\langle\cdot\rangle_\Lambda^*$ be the finite-volume Gibbs measure using the Hamiltonian $\mathcal{H}_\Lambda$ in Equ.(2) (at zero external field) with boundary conditions $*$ and the temperature dependence suppressed. Then, by well known arguments (cf. [S, ch. III.3]) the spontaneous magnetization is bounded above by $\sup_* \langle s_0^1\rangle_\Lambda^*$. Thus it is sufficient to show that for large Λ, this quantity is small in any boundary condition.

Let us write, according to the preliminary steps of the graphical representation, the identity

$$\langle s_0^1\rangle_{\Lambda,\beta}^* = \sum_{\omega\in\{0,1\}^{\mathbb{B}}} \mathcal{Z}_\Lambda^{-1} \int d^{|\Lambda|}s \; e^{-\beta\mathcal{H}_\Lambda^{lc}} \, s_0^1 \prod_{\langle i,j\rangle\in\omega} \left(e^{\beta\epsilon\,(\vec{s}_i\cdot\vec{s}_j+1)} - 1\right). \tag{9a}$$

We claim that for any configuration ω such that $0 \not\leftrightarrow \partial\Lambda$, the corresponding term in Equ.(9) vanishes.

To see this let $C_0(\omega)$ denote the connected cluster of the origin in the configuration ω. If $C_0(\omega)$ does not touch the boundary, then the integrals of all of the $\vec{s}_k$, $k \in C_0(\omega)$ are performed with respect to the full Haar measure. Now consider the change of variables $\vec{s}_k \mapsto -\vec{s}_k$, $k \in C_0(\omega)$. Obviously if i and j are both in $C_0(\omega)$, then the term $\vec{s}_i\cdot\vec{s}_j$ is unaffected. Further, since each spin component s_i^α appears quadratically in $\mathcal{H}_\Lambda^{lc}$ these terms are also invariant (regardless of whether or not $i \in C_0(\omega)$). On the other hand, this transformation negates the s_0^1 that sits in front and hence the whole term cancels out.

Thus we are left with the more restrictive sum

$$\langle s_0^1\rangle_{\Lambda,\beta}^* = \mathcal{Z}_\Lambda^{-1} \sum_{\omega:0\leftrightarrow\partial\Lambda} \int d^{|\Lambda|}s \; e^{-\beta\mathcal{H}_\Lambda^{lc}} \, s_0^1 \prod_{\langle i,j\rangle\in\mathbb{B}} \left(e^{\beta\epsilon\,(\vec{s}_i\cdot\vec{s}_j+1)} - 1\right). \tag{9b}$$

Since $|s_0^1| \le 1$, we see that

$$|\langle s_0^1\rangle_{\Lambda,\beta}^*| \le v_\Lambda(0 \leftrightarrow \partial\Lambda) \tag{10}$$

(where on the right hand side we suppress in our notation any dependence on boundary conditions).

At this point all we need is a Peierls' argument. Any configuration ω with $0 \leftrightarrow \partial\Lambda$ must have a connected path of occupied bonds (a self–avoiding *walk*) between the origin and the boundary. Let R denote the distance between the origin and the boundary. If $\{e_1, e_2, \dots, e_S\}$ (with $S \ge R$) is one such walk, let $\mathcal{W}(e_1, e_2, \dots, e_S)$ denote the event that all these edges are occupied. Using the result of Lemma 2 we have

$$
\begin{aligned}
v_\Lambda^*(0 \leftrightarrow \partial\Lambda) &\le \sum_{\substack{\text{all walks, } S\ge R\\ \mathcal{W}(e_1,e_2,\dots,e_S)}} v_\Lambda^*(\mathcal{W}(e_1,e_2,\dots,e_S)) \\
&\le \sum_{\substack{\text{all walks, } S\ge R\\ \mathcal{W}(e_1,e_2,\dots,e_S)}} \left(e^{2\beta\epsilon}-1\right)^S \\
&\le C\left(e^{2\beta\epsilon}-1\right)^R (2d-1)^R
\end{aligned}
\tag{11}
$$

for some constant C independent of R that is finite if $(e^{2\beta\epsilon}-1)(2d-1)<1$.

Since these arguments are uniform in $|\Lambda|$ and independent of boundary conditions it follows immediately that when $(e^{2\beta\epsilon}-1)(2d-1)<1$, the spontaneous magnetization vanishes. □

Remark. Improved values for T_0^{spin} can be obtained in a couple of ways. First, rather trivially, quantity $(2d-1)$ can be replaced by the connectivity constant for the d–dimensional square lattice. On the basis of a little more effort, it can be established that the measures $v_\Lambda(-)$ are dominated by independent (Bernoulli) measures with parameter $p = 1 - e^{-2\beta\epsilon}$. This may be derived by going to a full blown Edwards-Sokal measure [ES] along with an associated cluster algorithm. Then, at each bond step, regardless of the spin configuration, one notices that the maximum bond probability can never exceed $1 - e^{-2\beta\epsilon}$. The upshot is that the improved T_0^{spin} satisfies $1 - \exp\{-2\epsilon/T_0^{spin}\} = p_c(d)$ where $p_c(d)$ is the bond percolation threshold for the d–dimensional lattice.

Corollary. *If $d \ge 3$ and ϵ/J is sufficiently small (depending on N and d) there is an intermediate phase where the magnetization is zero and the nematic order parameter is positive.*

Proof. To demonstrate the above, we need only find a "window" between T_*^{lc} and T_0^{spin}. Since, (for fixed N and d) the former scales with J and the latter with ϵ (for $\epsilon \ll 1$) the desired result follows. □

Remark. A detailed analysis of the minimal requirements on ϵ/J will appear in the forthcoming [Ca].

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