

Lattice Models for Liquid Crystals

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A problem in the theory of liquid crystals is to construct a model system which at low temperatures displays long-range orientational order, but not translational order in all directions. We present five lattice models (two two-dimensional and three three-dimensional) of hard-core particles with attractive interactions and prove (using reflection positivity and the Peierls argument) that they have orientational order at low temperatures; the two-dimensional models have no such ordering if the attractive interaction is not present. We cannot prove that these models do not have complete translational order, but their zero-temperature states are such that we are led to conjecture that complete translational order is always absent.

KEY WORDS: Lattice models; liquid crystals; phase transitions.

1. INTRODUCTION

Since the work of Onsager,⁽¹⁾ hard-rod models have been widely used to explain the existence of liquid crystals, especially the transition from an isotropic liquid phase to a liquid crystal. DiMarzio⁽²⁾ applied the Bethe-Guggenheim approximation to the model of hard rods of finite length on a cubic lattice, and showed that in this approximation one would obtain a phase with orientational ordering at sufficiently high density. It is doubtful, however, whether hard rods on a cubic lattice without any additional interaction do indeed undergo a phase transition (see de Gennes,⁽³⁾ in particular Fig. 2.6). The only rigorously known result is the absence of phase transitions for dimers (Heilmann and Lieb⁽⁴⁾).

It is possible to apply Peierls' argument to prove that hard rods on lattices

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undergo phase transitions when subjected to more artificial restrictions (Lebowitz and Gallavotti,⁽⁵⁾ Heilmann⁽⁶⁾) or to appropriate interactions between the rods (Runnels and Freasier,⁽⁷⁾ Heilmann and Præstgaard⁽⁸⁾). A characteristic of all these models, however, is that their ordered states have the configuration at every vertex completely specified. Thus, these states also have complete crystalline (i.e., translational) ordering and are not, therefore, like liquid crystals.

The purpose of this paper is to present five lattice models (defined in Section 2) which we believe have a phase transition from a liquid to a liquid crystal. (These results were announced in Ref. 17.) We shall prove that these models do have a phase transition from an isotropic to an anisotropic phase. At present we are not able to demonstrate rigorously that the anisotropic phase is not crystalline, but, in contrast to the above-mentioned cases, the proof of orientational ordering that we give does not imply that the anisotropic phase is crystalline. In the discussion at the end of this paper we shall give some additional arguments for the conjecture that the anisotropic phase of these models does not possess *complete translational ordering*. (Complete translational ordering means that translational invariance is broken in all directions, as in a crystal.) For model I it is possible to go a bit further. By combining the results of this paper with a Kirkwood-Salzburg equation analysis, it can be shown that the conjecture is true at sufficiently low temperature. A paper by Heilmann and Kjær⁽⁹⁾ will present the result.

In three of the models, dimers are placed on either a quadratic or a cubic lattice, while in the two other models the molecules are quadratic fourmers placed on a cubic lattice. In all five cases we include attractive forces which stabilize the anisotropic states without forcing the formation of a crystal. This combination of repulsive forces (i.e., steric hindrance) and attractive forces may be important for the formation of real liquid crystals.

In Section 3 we prove that these models possess a *reflection positivity*, a concept which goes back to the work of Osterwalder and Schrader⁽¹⁰⁾ in field theory and which has recently been used in lattice statistical mechanical models by Frohlich *et al.*⁽¹¹⁾ and Dyson *et al.*⁽¹²⁾ For the general theory of reflection positivity in statistical mechanics, see Ref. 18.

In Section 4 we show how reflection positivity can be used to prove that empty vertices are unlikely at high enough dimer fugacity and at low enough temperature. In Section 5 we define the contours which are needed for a Peierls argument⁽¹³⁾ and extend the argument of Section 4 to prove that contours are also unlikely. Finally, in Section 6 the results of Sections 4 and 5 are combined with Peierls' argument to give a simple proof of the existence of an anisotropic phase. The combination of Peierls' argument and reflection positivity was first used in field theory by Glimm *et al.*⁽¹⁴⁾ and in statistical mechanics by Frohlich and Lieb.⁽¹⁵⁾ Unfortunately, reflection positivity

cannot be extended (at least not at present) to systems in which the molecules are longer than dimers. Therefore the proof given here cannot be generalized to larger molecules, although we believe, of course, that the phase transition persists if the molecule length is increased from two to any larger value. All these models have the property of no ordering of any kind at high temperatures. This can be seen by standard high-temperature expansion methods. Therefore, all these models have a phase transition.

2. THE MODELS

In models I and II we place hard dimers on a (two-dimensional) quadratic lattice; i.e., a vertex of the lattice is either empty or covered by at most one dimer. A dimer covers two vertices that are connected by an edge. In model I there is a contribution $-a$ to the energy for each pair of neighboring, collinear dimers (see Fig. 1). In model II there is a contribution $-b$ to the energy for each edge of the lattice that has both its endpoints covered by dimers perpendicular to the edge (see Fig. 2).

In model III we place quadratic fourmers on a (three-dimensional) cubic lattice, again with the rule that a vertex is either empty or covered by at most one fourmer; a fourmer covers four vertices, which together constitute a minimal square of the cubic lattice, so that there are three orientations of fourmers altogether. An attractive energy $-a$ is included between coplanar fourmers that occupy two pairs of neighboring vertices in the cubic lattice (see Fig. 3). Model IV is identical to model III except that the energy is $-b$ for each edge that connects vertices covered by (distinct) coplanar fourmers (see Fig. 4).

Finally, model V is the three-dimensional version of model II, i.e., we

Fig. 1. A dimer arrangement on a subset of the square lattice. Uncovered vertices are shown as open circles. The attractive interactions corresponding to model I are shown as wavy lines.

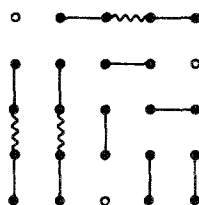
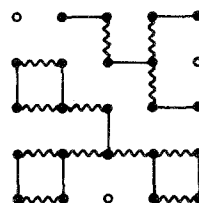


Fig. 2. The same as Fig. 1 but with the attractive interactions corresponding to model II shown as wavy lines.



place hard dimers on a cubic lattice and add $-b$ to the energy for each edge that connects vertices covered by parallel dimers perpendicular to the edge. Models II and V have been treated in the DiMarzio approximation by Cotter and Martire.⁽¹⁶⁾

In addition to the above-mentioned energies we also add a chemical potential term to the Hamiltonian (i.e., we use the grand canonical ensemble in which the particle number is not fixed):

$$-\mu N_d$$

where N_d is the number of particles (dimers or fourmers.)

For simplicity of exposition we confine our attention in the following sections to the two-dimensional systems; the extension to three dimensions is obvious and the relevant results will be stated at the end of the relevant sections.

In order to have a convenient notation we introduce a coordinate system in the plane of the quadratic lattice such that the vertices of the lattice are the points with integer coordinates (\mathbb{Z}^2). The reflection positivity only holds for finite systems if we have periodic boundary conditions and an even number of vertices in each direction; consequently we take as our domain Λ a rectangular subset of size $2N \times 2M$:

$$\Lambda = \{(x, y): x = 0, 1, \dots, 2N - 1, y = 0, 1, \dots, 2M - 1\}$$

and compute x -coordinates modulo $2N$ onto $0 \leq x < 2N$ and y -coordinates modulo $2M$ onto $0 \leq y < 2M$ whenever necessary, i.e., Λ is wrapped on a torus. (In three dimensions we take $0 \leq z < 2L$.)

A dimer placed on the quadratic lattice is identified by the position, in Cartesian coordinates, of its midpoint, i.e., $(x + 1/2, y)$ for the dimer that

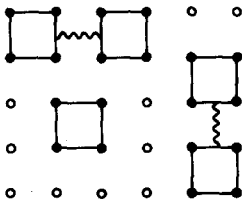


Fig. 3. An arrangement of coplanar fourmers. Uncovered vertices are shown as open circles. The attractive interactions corresponding to model III are shown as wavy lines.

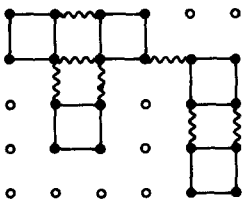


Fig. 4. The same as Fig. 3, but with the attractive interactions corresponding to model IV shown as wavy lines.

covers the vertices (x, y) and $(x + 1, y)$ and $(x, y + 1/2)$ for the dimer that covers (x, y) and $(x, y + 1)$. The former are called *horizontal dimers* and the latter *vertical dimers* in order to distinguish between the two possible orientations. The set of all possible dimer positions is denoted \mathcal{B} . Sometimes we will call \mathcal{B} the “edges of Λ .”

A dimer arrangement on Λ is an allowed configuration of dimers on the edges of Λ (i.e., without multiple occupancy of a vertex). The set of all possible dimer arrangements on Λ (including the empty one) will be denoted \mathcal{D} . A convenient way to describe \mathcal{D} is the following: To each of the $8NM$ possible dimer positions in \mathcal{B} one attaches a copy of the two point space $\{0, 1\}$ (i.e., a variable which is either zero or one). Then \mathcal{D} can be identified in a natural way with a subset of $\mathcal{C} = \{0, 1\}^{8NM}$, letting 1 correspond to the presence and 0 to the absence of a dimer. We call \mathcal{C} the *phase space* and introduce the characteristic function χ defined for all $\xi \in \mathcal{C}$ by

$$\chi(\xi) = \begin{cases} 1 & \text{if } \xi \in \mathcal{D} \\ 0 & \text{if } \xi \notin \mathcal{D} \end{cases} \tag{1}$$

with the above-mentioned identification between \mathcal{C} and dimer configurations being implicitly understood in (1).

3. REFLECTION POSITIVITY

We first introduce the reflection lines: Let j be an integer satisfying $0 \leq j \leq N - 1$ and consider the pair of “vertical” lines in the plane

$$\begin{aligned} L_j^- &= \{(j + \frac{1}{2}, y) : y \in \mathbb{R}\} \\ L_j^+ &= \{(j + N + \frac{1}{2}, y) : y \in \mathbb{R}\} \end{aligned} \tag{2}$$

Let \mathcal{B}_j^0 be the (horizontal) dimer positions that are in $L_j^- \cup L_j^+$ (i.e., $\mathcal{B}_j^0 = \{(x, y) : x = j + 1/2 \text{ or } j + N + 1/2, y = 0, 1, \dots, 2M - 1\}$) and let \mathcal{B}_j^+ (resp. \mathcal{B}_j^-) be the dimer positions to the right of L_j^- and to the left of L_j^+ (resp. to the right of L_j^+ or the left of L_j^-). The dimer positions \mathcal{B} are thus partitioned into three sets, \mathcal{B}_j^0 , \mathcal{B}_j^+ , and \mathcal{B}_j^- , where the first set contains $4M$ points and the two latter contain $2M(2N - 1)$ points each. The phase space \mathcal{C} is then given by

$$\mathcal{C} = \mathcal{C}_j^0 \times \mathcal{C}_j^+ \times \mathcal{C}_j^-$$

where $\mathcal{C}_j^0 = \{0, 1\}^{4M}$ corresponds to the dimer configurations on \mathcal{B}_j^0 , etc.

There is a natural involution θ_j of Λ onto Λ obtained by reflection

$$\theta_j : (x, y) \rightarrow (2j + 1 - x, y) \tag{3}$$

The reflection θ_j maps \mathcal{B}_j^+ onto \mathcal{B}_j^- and \mathcal{B}_j^- onto \mathcal{B}_j^+ , while it is the identity on \mathcal{B}_j^0 . It lifts to an involution of \mathcal{C} onto \mathcal{C} mapping \mathcal{C}_j^+ onto \mathcal{C}_j^- and \mathcal{C}_j^- onto \mathcal{C}_j^+ and leaving \mathcal{C}_j^0 invariant. We shall use θ_j as a symbol for all these maps.

We also consider the natural action of θ_j as an involution on (complex-valued) functions on \mathcal{C} . If f is such a function, then $\theta_j f$ is the function given by

$$(\theta_j f)(\xi) = f(\theta_j \xi), \quad \xi \in \mathcal{C} \tag{4}$$

By \mathcal{F}_j^+ we denote the functions that depend only on the \mathcal{C}_j^0 and \mathcal{C}_j^+ coordinate, i.e., a point $\xi \in \mathcal{C}$ is a triplet $\xi = (\xi^-, \xi^0, \xi^+)$ with $\xi_j^i \in \mathcal{C}^i$, and $f \in \mathcal{F}_j^+$ if $f(\xi^-, \xi^0, \xi^+)$ is independent of ξ^- . Similarly \mathcal{F}_j^- denotes the functions that are independent of \mathcal{C}_j^+ . Clearly $\theta_j \mathcal{F}_j^+ = \mathcal{F}_j^-$. A function that depends only on \mathcal{C}_j^0 is in both \mathcal{F}_j^+ and \mathcal{F}_j^- .

Lemma 1. Let $f \in \mathcal{F}_j^+$. Then

$$S = \sum_{\xi \in \mathcal{C}} \overline{f(\xi)} (\theta_j f)(\xi) \geq 0$$

Proof. Write $\xi \in \mathcal{C}$ as $\xi = (\xi^-, \xi^0, \xi^+)$. Then $f(\xi^-, \xi^0, \xi^+) = g(\xi^0, \xi^+)$

and

$$S = \sum_{\xi^0 \in \mathcal{C}_j^0} \sum_{\xi^- \in \mathcal{C}_j^-} \sum_{\xi^+ \in \mathcal{C}_j^+} \overline{g(\xi^0, \xi^+)} g(\xi^0, \xi^-)$$

For each ξ^0

$$\sum_{\xi^+ \in \mathcal{C}_j^+} g(\xi^0, \xi^+) = \sum_{\xi^- \in \mathcal{C}_j^-} g(\xi^0, \xi^-)$$

so $S \geq 0$. ■

We now turn our attention to the dimer arrangement space $\mathcal{D} \subset \mathcal{C}$ and to the Hamiltonian H of the dimer system. If f is any (complex-valued) function on \mathcal{D} , it can be extended to a function on \mathcal{C} in many ways. However, χf , where χ is given by (1), has a natural extension, i.e.,

$$(\chi f)(\xi) = \begin{cases} f(\xi), & \xi \in \mathcal{D} \\ 0, & \xi \notin \mathcal{D} \end{cases} \tag{5}$$

χ itself can be written as

$$\chi = \chi_j^- \chi_j^+$$

with $\chi_j^+ \in \mathcal{F}_j^+$, $\chi_j^- = \theta_j \chi_j^+$, and χ^\pm take on the values 1 or 0.

The Hamiltonians discussed in Section 2 can all be written in the following canonical way: For $\xi = (\xi^-, \xi^0, \xi^+) \in \mathcal{D}$, $\xi^i \in \mathcal{C}_j^i$,

$$H(\xi) = k(\xi^0) + h(\xi^0, \xi^+) + (\theta_j h)(\xi^0, \xi^-) - \sum_i g_i(\xi^0, \xi^+) (\theta_j g_i)(\xi^0, \xi^-) \tag{6}$$

$h(\xi^0, \xi^+)$ [resp. $(\theta_j h)(\xi^0, \xi^-)$] is the interaction energy (including the chemical potential) of all the dimers on $\mathcal{B}_j^+ \cup \mathcal{B}_j^0$ [resp. $\mathcal{B}_j^- \cup \mathcal{B}_j^0$]. Here $-k(\xi^0)$ is the interaction energy (if any) of the dimers on \mathcal{B}_j^0 together with their chemical potential. The term k is included in H in order that the energy of \mathcal{B}_j^0 not be counted twice. The only relevant fact about these functions is that they are real. The sum in (6) is the interaction of the dimers on \mathcal{B}_j^+ with those on \mathcal{B}_j^- . The functions g_i are real and nonnegative; the minus sign in front of the summation expresses the fact that the interaction is *attractive*. The minus sign is crucial. The sum on i will have $4M$ terms in the simple nearest neighbor case, but for the purpose of the following Theorem 2 it could have more terms if more than nearest neighbor term were present.

The partition function of the system of interacting dimers at the temperature $T = \beta^{-1}$ is given by

$$Z = \sum_{\xi \in \mathcal{D}} \exp[-\beta H(\xi)] \tag{7}$$

If f is any (complex-valued) function on \mathcal{D} , then its expectation value is

$$\langle f \rangle = Z^{-1} \sum_{\xi \in \mathcal{D}} f(\xi) \exp[-\beta H(\xi)] \tag{8}$$

Theorem 2. Let f be a (complex-valued) function on \mathcal{D} and $f \in \mathcal{F}_j^+$. Then

$$\langle \bar{f}(\theta_j f) \rangle \geq 0$$

Proof. For $\xi \in \mathcal{D}$ let $G(\xi) = \exp[-\beta H(\xi)]$. Consider $\bar{G} = \chi G$ as a function on \mathcal{C} [see (5)]. Clearly $\bar{G} = G_j^+ G_j^- G_j'$, where

$$\begin{aligned} G_j^+(\xi^-, \xi^0, \xi^+) &= \chi_j^+(\xi^0, \xi^+) \exp\{-\beta[\frac{1}{2}k(\xi^0) + h(\xi^0, \xi^+)]\} \\ G_j^- &= \theta_j G_j^+ \\ G_j' &= \chi(\xi) \exp\left[\beta \sum_i g_i(\xi^0, \xi^+) (\theta_j g_i)(\xi^0, \xi^-)\right] \end{aligned}$$

and $G_j^+ \in \mathcal{F}_j^+$. We can make a power series expansion of the exponential in G_j' and thereby obtain for \bar{G} a sum of terms, each with a positive coefficient. Each term is clearly of the form

$$\chi(\xi) \mu(\xi^0, \xi^+) (\theta_j \mu)(\xi^0, \xi^-) = \rho(\xi^0, \xi^+) (\theta_j \rho)(\xi^0, \xi^-)$$

where $\rho = \chi_j^+ \mu$. Thus, \tilde{G} is a sum (with positive coefficients) of terms of the form $\phi(\xi^0, \xi^+)(\theta, \phi)(\xi^0, \xi^-)$ with $\phi \in \mathcal{F}_j^+$ and ϕ real. Theorem 2 now follows from Lemma 1. ■

Corollary 3. Let f and g be (complex-valued) functions on \mathcal{D} with $f \in \mathcal{F}_j^+$ and $g \in \mathcal{F}_j^-$. Then

$$|\langle fg \rangle|^2 \leq \langle \tilde{f}(\theta, f) \rangle \langle \tilde{g}(\theta, g) \rangle$$

Proof. Standard Schwarz inequality. ■

Corollary 3 is the desired goal of this section. For Models I and II the decomposition of H in the form (6) holds for every $j = 0, 1, \dots, N - 1$ and also for every pair of horizontal lines through the center of the vertical edges and separated by a distance M .

For the three three-dimensional models on a lattice $2N \times 2M \times 2L$ we have, by a similar argument, reflection positivity (i.e., the analog of Corollary 3) for reflection through pairs of planes separated by N or M or L .

4. A LOWER BOUND ON THE DIMER DENSITY

As the first application of reflection positivity we shall show how a useful upper bound on the density of empty vertices can be obtained. In the two-dimensional case let $(x, y) \in \Lambda$ be a vertex and let $P_{(x,y)}$ be the projection onto the configurations in which there is no dimer on (x, y) , i.e., for $\xi \in \mathcal{D}$

$$P_{(x,y)} = \begin{cases} 0 & \text{if there is a dimer on } (x, y) \text{ in } \xi \\ 1 & \text{if there is no dimer on } (x, y) \text{ in } \xi \end{cases} \tag{9}$$

In conformity with the convention in Section 3, $P_{(x,y)}$ should really be thought of as a function on the bonds incident on (x, y) . By translational invariance

$$1 - 2\rho = \langle P_{(x,y)} \rangle$$

is independent of (x, y) (ρ is the dimer density).

If, in Corollary 3, we take $f = P_{(x,y)}$ and $g = 1$ (assuming $j + 1 \leq x \leq j + N$) we obtain ($w = 2j + 1 - x + 2N$)

$$\langle P_{(x,y)} \rangle^2 \leq \langle P_{(x,y)} P_{(w,y)} \rangle \langle 1 \rangle$$

so that

$$1 - 2\rho = \langle P_{(x,y)} \rangle \leq \langle P_{(x,y)} P_{(w,y)} \rangle^{1/2}$$

Our goal in the next theorem is to extend this argument to every vertex in Λ , not just two. The advantage of this is clear: instead of having to estimate

$\langle P_{(x,y)} \rangle$, i.e., the expectation value of a local quantity, we need only estimate the expectation value of a global quantity, which is much easier.

Theorem 4. Let T be the set of projections of the form $P = P_{z_1} P_{z_2} \dots P_{z_k}$, where z_1, z_2, \dots, z_k are distinct vertices in Λ and $1 \leq k \leq 4NM$; $|P| = k$. Then

$$\max_{P \in T} \langle P \rangle^{1/P} = \langle \hat{P} \rangle^{1/4MN}$$

where $\hat{P} = \prod_{z \in \Lambda} P_z$. In particular

$$1 - 2\rho \leq \langle \hat{P} \rangle^{1/4MN} \tag{10}$$

Proof. Define $f(P) = \langle P \rangle^{1/|P|}$ for $P \in T$ and $f(I) = 1$. (Here, I is the unit operator, i.e., the unit function on configurations, $|I| = 0$.) Let $t \subset T$ be the set of P 's that maximize $f(P)$. If θ is a reflection operator and $P \in T$, then we can write $P = QR$, where $Q \in \mathcal{F}^-$ and $R \in \mathcal{F}^+$. Now, Q or R might be I , but not both; Q and R belong to T except if they are I . Let $\tilde{Q} = \theta Q$, $\tilde{R} = \theta R$; then $|\tilde{Q}| = |Q|$, $|\tilde{R}| = |R|$, and $|Q| + |R| = |P|$. By Corollary 3

$$\langle P \rangle^2 \leq \langle Q\tilde{Q} \rangle \langle R\tilde{R} \rangle$$

so

$$f(P) \leq f(Q\tilde{Q})^{|Q|/|P|} f(R\tilde{R})^{|R|/|P|} \tag{11}$$

This holds even if $R = I$. From (11) we see that if $R \neq I$, $P = QR$, and $P \in t$, then $R\tilde{R} \in t$ also. Let P be any element in t (t cannot be empty since T is finite) and suppose that $P_{(x,y)}$ is a factor in P . Reflect in the vertical line through $(x + 1/2, y)$, then in the line through $(x + 3/2, y)$, then in the line through $(x + 5/2, y)$, etc. In this way we eventually obtain a $P' \in t$ containing a horizontal chain of P_z 's of length $2N$ (namely $P_{(i,y)}$, $i = 0, 1, \dots, 2N - 1$). If we then reflect P' in the horizontal lines with ordinates $y + 1/2, y + 3/2, y + 5/2$, etc., we eventually obtain $\hat{P} \in t$. ■

Next we use Theorem 4 to obtain an upper bound on $1 - 2\rho$. Let E_0 be the energy of a close-packed configuration with the lowest possible energy and ϵ_0 be the corresponding energy per vertex (i.e., $\epsilon_0 = E_0/4NM$ in two dimensions and $\epsilon_0 = E_0/8NML$ in three dimensions); then we have the following result:

Theorem 5

$$1 - 2\rho \leq \exp(\beta\epsilon_0)$$

Proof. By considering only a term with energy E_0 in Z [Eq. (7)], we find $Z \geq \exp(-\beta E_0)$. If \hat{P} is as in Theorem 4, then the numerator in (8) for $\langle \hat{P} \rangle$

contains only the term with no dimers; this term is one. Thus $\langle P \rangle = Z^{-1}$ and Theorem 5 follows from Theorem 4. ■

The following are the values of ϵ_0 in the five models mentioned in Section 2:

$$\begin{aligned} \epsilon_0(\text{I}) &= -\mu/2 - a/2, & \epsilon_0(\text{II}) &= -\mu/2 - b \\ \epsilon_0(\text{III}) &= -\mu/4 - a/2, & \epsilon_0(\text{IV}) &= -\mu/4 - b \\ \epsilon_0(\text{V}) &= -\mu/2 - 2b \end{aligned} \quad (12)$$

Clearly, if μ and a (resp. b) are chosen such that $\epsilon_0 < 0$, then $1 - 2\rho$ goes to zero as $T \rightarrow 0$, i.e., all vertices become occupied by dimers.

5. ESTIMATES FOR THE PROBABILITY OF BAD SQUARES

In the previous section reflection positivity was used to provide an upper bound for the probability of empty vertices. Here we extend the argument to somewhat more complex events called "bad squares." These estimates will be used in the next section, where a Peierls-type argument will be given to show that there is long-range order at low temperatures.

In two dimensions, let S_z denote an elementary square of the lattice centered at $z = (l + 1/2, m + 1/2)$, $0 \leq l < 2L$, $0 \leq m < 2M$, and consisting of the four vertices (l, m) , $(l + 1, m)$, $(l, m + 1)$, and $(l + 1, m + 1)$. Henceforth, for simplicity, we will assume L and M are even. There are four classes of squares, labeled σ_{ee} , σ_{eo} , σ_{oe} , σ_{oo} , according as l (resp. m) is even or odd, and there are ML squares in each class.

The extensions to three dimension is obvious. S_z is then a "cube" of six vertices centered at $(l + 1/2, m + 1/2, n + 1/2)$ with $0 \leq l < 2L$, $0 \leq m < 2M$, $0 \leq n < 2N$. The L , M , and N are assumed to be even. There are eight equivalence classes: $\sigma_{eee}, \dots, \sigma_{ooo}$ with LMN cubes in each.

Fix z and consider a configuration ξ . We say that S_z is "bad" if and only if ξ restricted to S_z is not compatible with a ground state. Specifically this means: S_z is bad if and only if there is one or more empty vertice on S_z or else the dimers (resp. fourmers) on the vertices of S_z are not all of the same orientation. [Note: The dimers (fourmers) on S_z refer to all the dimers (fourmers) incident on the vertices of S_z , including those that connect vertices of S_z to some other vertex.]

Let Q_z be the projection onto configurations in which S_z is "bad." Thinking of Q_z as a function on dimer configurations (in two dimensions), the support of Q_z is the 12 bonds connected to S_z . The three-dimensional analogue is obvious.

If A denotes a nonempty subset of square (cube) midpoints, and $|A|$ the number of its elements, let

$$g = \max_{A \neq \emptyset} \left\langle \prod_{z \in A} Q_z \right\rangle^{1/|A|} \tag{13}$$

Our aim is to show that $g \rightarrow 0$ as $\beta \rightarrow \infty$ (exponentially fast, in fact), uniformly in L and M . We will show:

Lemma. If Q_z is the projection onto a bad square (resp. cube) centered at z and if g is given by (13), then

$$g \leq c e^{-\beta\alpha}$$

with $c = \{4 \text{ (in 2 dim.)}, 8 \text{ (in 3 dim.)}\}$ and $\alpha > 0$. Here α depends on the model and its parameters and is given by the following (note $\alpha > 0$ as long as $\epsilon_0 < 0$):

- model 1 $\alpha = \frac{1}{4}[\mu + a - \max(0, \mu)]$
- model 2 $\alpha = \frac{1}{4}[\mu + 2b - \max(0, \mu + b)]$
- model 3 $\alpha = \frac{1}{8}[\mu + 2a - 1/4 \max(0, \mu) - 1/4 \max(0, 3\mu + 4a)]$
- model 4 $\alpha = \frac{1}{8}[\mu + 4b - 1/4 \max(0, \mu) - 1/4 \max(0, 3\mu + 8b)]$
- model 5 $\alpha = \frac{1}{8}[2\mu + 8b - \frac{1}{2} \max(0, 3\mu + 10b) - \frac{1}{2} \max(0, \mu + 2b)]$

Proof. As a preliminary step, let $Q(A) = \prod_{z \in A} Q_z$. Write $Q(A) = Q_{ee}(A)Q_{eo}(A)Q_{oe}(A)Q_{oo}(A)$ [in three dimensions $Q(A) = Q_{eee}(A) \cdots Q_{ooo}(A)$]. Here

$$Q_{ee}(A) = \prod_{z \in A \cap \sigma_{ee}} Q_z$$

and so forth. Let j denote the subscript (eo), etc. Since $Q_j(A) \leq 1$, $\langle Q(A) \rangle \leq \langle Q_j(A) \rangle$ for any j . There is at least one j such that $|A_j| \geq |A|/4$ ($|A|/8$ in three dimensions). Thus,

$$g \leq \max\{\langle Q(A) \rangle^{1/4|A|} : \emptyset \neq A \subseteq \sigma_{ee}\} \tag{14}$$

(resp. $8|A|$ in three dimensions). In other words, (14) says that at the expense of a factor of 4 we can restrict attention to A 's such that all squares are in the same equivalence class. The arbitrary choice of σ_{ee} is based on the symmetry with respect to the class.

There are LM (resp. LMN) possible pairs of reflection lines (planes). Of these there are $LM/4$ (resp. $LMN/8$) which carry an S_z into an S_z (and Q_z into Q_z) provided $z \in \sigma_{ee}$. In two dimensions these are the lines $\{(l + 1/2, y) : l \text{ odd}, y \in \mathbb{R}\}$ and $\{(x, m + 1/2) : m \text{ odd}, x \in \mathbb{R}\}$. Thus, by the same reasoning as for the empty vertex estimate (Section 4), a maximizing A for (14) is $A = \sigma_{ee}$, i.e., $Q(A)$ is the projection onto configurations in which every (ee)

square is bad. Then $|A| = LM$. (In three dimensions $A = \sigma_{eee}$, $|A| = LMN$). Let E be the minimum energy under the condition that every (ee) square is bad. Then

$$g \leq (\#e^{-\beta E})^{1/4LM} / e^{-\beta \epsilon_0}$$

(resp. $8LMN$ in three dimensions), since $Z \geq \exp(-4\beta LM \epsilon_0)$ (resp. $8LMN$).

Here $\#$ is the total number of possible configurations. In two dimensions $\# \leq 2^{8LM}$ since every edge has a dimer, or it does not. ($\# \leq 2^{24LMN}$ in three dimensions).

The lemma is proved if we show $E/4LM$ (resp. $E/8LMN$) $- \epsilon_0 \equiv \alpha > 0$. Specifically,

$E \geq -[\mu + a + \max(0, \mu)]LM$	model 1
$\geq -[\mu + 2b + \max(0, \mu + b)]LM$	model 2
$\geq -[\mu + 2a + 1/4 \max(0, \mu) + 1/4 \max(0, 3\mu + 4a)]LMN$	model 3
$\geq -[\mu + 4b + 1/4 \max(0, \mu) + 1/4 \max(0, 3\mu + 8b)]LMN$	model 4
$\geq -[2\mu + 8b + \frac{1}{2} \max(0, 3\mu + 10b) + \frac{1}{2} \max(0, \mu + 2b)]LMN$	model 5

We give the proof for model 1. The reader can easily do the other cases. The energy for a configuration ξ can be thought of as a sum of vertex energies, namely 0 (for an empty vertex), $-\frac{1}{2}\mu$ for a dimer with an unsaturated end (absence of a wiggly line in the figures), and $-\mu/2 - a/2$ for a dimer with a saturated end. Now every vertex in Λ belongs to exactly one square in σ_{ee} . The total vertex energy of a bad square is not less than 0 (all empty), $-\mu/2$ (three empty), $-\mu - a$ (two empty), $-3\mu/2 - a$ (one empty), $-2\mu - a$ (none empty). Thus, this square energy is not less than $-\mu - a - \max(0, \mu)$, and this leads to the E given above. ■

6. THE PEIERLS ARGUMENT FOR LONG-RANGE ORDER

In Section 5 we showed that the probability of finding k bad squares at arbitrary locations is not greater than g^k , with $g = c \exp(-\beta\alpha)$. Both α and c depend on the model, but $\alpha < 0$ (since $\epsilon_0 < 0$ by hypothesis). Thus $g \rightarrow 0$ as $\beta \rightarrow \infty$. We will use this information in a Peierls-type argument to prove that if a dimer (fourmer) is placed at a fixed vertex (say $z = 0$), then the probability of finding a dimer of the same orientation at a vertex $z \neq 0$ is greater than $1/2$ for large β , uniformly in z .

We will assume that the reader is familiar with the Peierls argument and will explain only the novel features for our liquid crystal models. In particular, we assume familiarity with the nonessential technical problems arising from the use of periodic boundary instead of free boundary conditions (contours that run around the torus), and that as $L, M, N \rightarrow \infty$ one needs a condition

such as $\min(L, M, N)/\log \max(L, M, N) \rightarrow \infty$. It is also well known, and easy to prove, that our definition of long-range order implies other definitions of phase transitions, such as the existence of at least two Gibbs states or the existence of a spontaneous polarization or the discontinuity of the derivative free energy/unit volume with respect to an external polarizing field at zero field. References 15 and 18 can be consulted about some of these points.

With a dimer (fourmer) fixed at 0, we will show that the probability of *not* having an identically oriented object at $z \neq 0$ is less than 1/2 for large β .

Call the object (dimer or fourmer) at 0 an *h-object* (e.g., a horizontal dimer in models 1 and 2). Let ξ be a configuration with an *h-object* at 0 and no *h-object* at z . A *plus vertex* is defined as one which (a) has an *h-object* and (b) belongs to at least one good (i.e., not bad) square (cube). Otherwise, the vertex is said to be *minus*.

Let Λ^* be the lattice of midpoints of squares in Λ together with the usual notion of nearest neighbor points. Two points in Λ^* are said to be connected if and only if there is a connected path from one to the other. Squares in Λ are said to be connected if and only if their midpoints are connected in Λ^* .

Suppose that in ξ there are two nearest neighbor vertices, one of which is plus and the other minus. They have two squares (resp. four cubes) in common, *all of which must be bad*. The midpoints of these two squares (resp. four cubes) can be connected by a line (resp. square) which we call a *piece of contour*.

Now we refer to the usual Peierls argument for the Ising model. Since the origin is plus and z is minus, there is a closed contour γ in Λ^* separating the two points. On one side of the contour there are plus vertices and on the other side there are minus vertices.

As we saw above, every vertex of the contour (in Λ^*) is the midpoint of a bad square. Hence

$$\text{Prob}(\gamma) < g^{|\gamma|}$$

with $|\gamma|$ being the length (area) of γ .

We sketch the remainder of the Peierls argument: There must be a closed contour surrounding 0 or surrounding z . If P is the probability that there is no *h-object* at z , we then have

$$P \leq 2 \sum_{|\gamma| \geq 4} g^{|\gamma|} 3^{|\gamma|} (|\gamma|/4)^2$$

in two dimensions, and with a similar expression in three dimensions. $P \rightarrow 0$ as $\beta \rightarrow \infty$. Here $3^{|\gamma|}$ is an upper bound for the number of contours of length $|\gamma|$ and $(|\gamma|/4)^2$ is an upper bound to their area, i.e., to the number of ways they can be placed to enclose a given point.

7. CONCLUSION

We have demonstrated that at low enough temperatures (and not too negative a chemical potential) each of the five models presented in Section 2 will exist in a phase where one of the two (three) possible orientations is preferred over the other. The question of a possible positional ordering remains open. We conjecture that long-range positional ordering does not occur, for the following reasons (as exemplified for model I): Presumably, if there is no positional ordering for large β , there is none for any β . In the ground state all dimers are of one orientation, say horizontal. Thus, for large β , the system is like a product of uncorrelated one-dimensional systems because there is no interaction among the rows unless defects are present. These we have shown to be rare for large β . Along a column there is not likely to be long-range ordering because in one dimension any defects, however rare, will destroy ordering. However, this argument leads us to expect that the (finite) correlation lengths will be very different in the direction of the dimers and in the orthogonal direction, the former tending to infinity as $\beta \rightarrow \infty$.

A similar argument applies to the two fourmer models when one considers the ordering of fourmer positions among planes parallel to the preferred orientation of the planes of the fourmers. However, the situation is quite different if one considers possible ordering within a plane. The attractive interaction in model III clearly favors a complete ordering within a plane and it is easy to prove by Peierls' argument that the two-dimensional version (where one only has fourmers of one orientation) does exist in a completely ordered phase at low enough temperatures. This effect would be expected to carry over to the three-dimensional model, in which case it raises the intriguing question of whether the model can exist in six different phases.

In model IV the attractive interaction is designed to allow "sliding" of a row of fourmers relative to a neighboring row in the same plane and one would not expect the two-dimensional version to exhibit a phase transition (Nisbet and Farquhar⁽¹⁹⁾). This two-dimensional problem has not yet been resolved, however.

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