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Interacting dimers on the simple cubic lattice as a model for liquid crystals

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Abstract. We consider two lattice gas models where dimers are placed on the simple cubic lattice with an attractive interaction between collinear dimers. We prove (using reflection positivity and Peierls' argument) that at low enough temperatures both models exist in an ordered state where one or two of the three orientations are preferred. No attempt is made at deciding whether the ordered state actually has dimers of two orientations or only of one orientation. Both models have earlier been considered in the two-dimensional version and proved to exhibit ordering at low temperature.

1. Introduction

Hard rod models on a lattice have been used to discuss the types of partial ordering or mesomorphism which might occur in systems of long molecules. As discussed recently in the introduction to a paper by Heilmann and Lieb (1979), (hereinafter to be referred to as HL), one such class of models has the configuration of each lattice site completely specified in a given ordered state. HL then showed how to treat models of mesomorphic phases where alignment of long molecules occurs in the ordered state; the new aspect is that ordered lines can slide with respect to one another. The models postulate anisotropic, attractive interactions between rods; the interplay between such attractions and the hard core repulsion may well be an essential feature of the phenomenon of orientational ordering.

The present paper carries this line of reasoning further; as well as allowing relative sliding of stacks of rod-like molecules, ordered states will be given in which the planes are ordered, up to sliding where appropriate, but in which there is disorder between planes in the ground state.

One model treated is the generalisation of model I of HL to three dimensions; this is a monomer–dimer system which favours collinear alignment of dimers. The other is the three-dimensional extension of a soft dimer model introduced by Abraham and Heilmann (1975) (hereinafter referred to as AH); here straight configurations are favoured over bent ones, or chain termination. The treatment used here exploits Peierls' argument (for a review see, for instance, Griffith (1972)) and reflection positivity, recently exploited in this context by HL. A central feature of the application of the Peierls argument in the present article is that in three dimensions the relevant contours are made up of line segments rather than the usual sheets and polyhedra.

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The problem of the statistics of relative ordering, either of sliding or of orientation, has yet to be solved. As will probably become clear at the end of this paper, the problem bristles with difficulty.

2. Models

Both models can be viewed as dimer models on the simple cubic lattice (a dimer covers two vertices which are connected by an edge). Model I is the three-dimensional version of model I of HL; here the dimers are *hard* (i.e. a vertex is either empty or covered by at most one dimer) and there is a contribution $-a$ to the energy for each pair of neighbouring, collinear dimers and a contribution of zero for any other configuration. Model II is the three-dimensional version of the model considered in § 2 of AH, i.e. the dimers are softened to allow up to two dimers covering a vertex (but not more than one dimer on an edge of the lattice). The interaction is solely between dimers covering the same vertex; we shall change the notation compared to AH and introduce a contribution $-a$ to the energy if the overlapping dimers are collinear and a contribution $-b$ if they form an angle of 90°. Since we intend to use the grand canonical ensemble we include a chemical potential term $-\mu N_d$ to the Hamiltonian, writing N_d for the number of dimers.

We introduce a coordinate system such that the vertices of the lattice coincide with the points with integer coordinates (Z^3). We take as our domain Λ a box-shaped subset of size $2N \times 2M \times 2L$ with periodic boundary conditions:

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

and compute coordinates modulo $2N$, $2M$ or $2L$ onto the intervals $0 \leqslant x < 2N$, $0 \leqslant y < 2M$ and $0 \leqslant z < 2L$ whenever necessary. The conditions on Λ (even length and periodic boundary conditions) are necessary in order to have reflection positivity.

In the following we shall consider planes perpendicular to one of the coordinate axes; to be definite, let us assume that the plane is perpendicular to the z axis. We shall supply the plane with the cyclic boundary conditions introduced for Λ, i.e. x coordinates are calculated modulo $2N$ onto $0 \leqslant x < 2N$ and y coordinates modulo $2M$ onto $0 \leqslant y < 2M$. We shall be concerned about objects which are *connected in the plane*; this is defined in the usual transitive way by first defining when two objects are directly connected and then defining two objects to be connected if they are either directly connected or connected to the same third object, i.e. as a graph embedded in the plane. A *connected component* will be a set of objects which are not connected to any objects outside the set. A connected component is said to *extend infinitely in both directions in the plane* if one can find two loops in the corresponding graph, such that along one of the loops the net increase in the x coordinate is $2N$ (or $-2N$) and the net increase in the y coordinate is zero while along the other loop the increase in x is zero while the increase in y is $2M$ (or $-2M$). A connected component is said to *extend infinitely in one direction in the plane* if it does not extend infinitely in both directions, but one can find a loop in the graph, such that the net increase in at least one of the coordinates is different from zero. A connected component which neither extends infinitely in one direction nor in both directions is said to be *bounded in the plane.*

A dimer placed on the cubic lattice is identified by the position, in Cartesian coordinates, of its midpoint, i.e. for instance $(x+\frac{1}{2}, y, z)$ for the dimer which covers the vertices (x, y, z) and $(x+1, y, z)$. The set of all possible dimer positions is denoted by $\mathcal{B}$.

Sometimes $\mathscr{B}$ will be called the 'edges of Λ'. A *dimer arrangement* on Λ is an allowed configuration of dimers on the edges of Λ (whether a configuration is allowed or not might, of course, depend on the model). The set of all possible dimer arrangements on Λ (including the empty one) will be denoted $\mathscr{D}_{\mathrm{I}}$ (respectively $\mathscr{D}_{\mathrm{II}}$) for the two models or just $\mathscr{D}$ if we do not want to specify the model in a given context. If we attach a copy of the two-point space $\{0, 1\}$ to each dimer position in $\mathscr{B}$, then we can identify the set of all possible dimer configurations on Λ, $\mathscr{C}$, with $\{0, 1\}^{24\mathrm{NML}}$ by letting 1 correspond to the presence of a dimer and 0 to the absence of a dimer. We call $\mathscr{C}$ the phase space. $\mathscr{D}_{\mathrm{I}}$ and $\mathscr{D}_{\mathrm{II}}$ are subsets of $\mathscr{C}$ which we describe by introducing characteristic functions on $\mathscr{C}$ denoted χ_{I} and χ_{II} defined for all $\xi \in \mathscr{C}$ by ($i = \mathrm{I}$ or II):

$$\chi_i(\xi) = \begin{cases} 1 & \text{if} \quad \xi \in \mathscr{D}_i \\ 0 & \text{if} \quad \xi \notin \mathscr{D}_i. \end{cases} \tag{1}$$

Functions defined on $\mathscr{D}$ can, of course, be extended to functions on $\mathscr{C}$ in many ways. However, χf has a natural extension which we shall use in the following when necessary ($i = \mathrm{I}, \mathrm{II}$; $\xi \in \mathscr{C}$):

$$\chi_i f(\xi) = \begin{cases} f(\xi) & \xi \in \mathscr{D}_i \\ 0 & \xi \notin \mathscr{D}_i. \end{cases} \tag{2}$$

3. Reflection positivity

The reflection planes perpendicular to the x axis are defined as follows. Let j be an integer satisfying $0 \leqslant j < N$ and consider the pair of planes:

$$\begin{aligned} L^-{}_j &= \{(j+\tfrac{1}{2}, y, z) \colon y \in \mathbb{R}, z \in \mathbb{R}\} \\ L^+{}_j &= \{(j+N+\tfrac{1}{2}, y, z) \colon y \in \mathbb{R}, z \in \mathbb{R}\}. \end{aligned} \tag{3}$$

We define $\mathscr{B}^0{}_j$ as the dimer positions in $L^-{}_j \cup L^+{}_j$, $\mathscr{B}^+{}_j$ as dimer positions with x coordinates satisfying $j+1 \leqslant x \leqslant j+N$ and $\mathscr{B}^-{}_j$ as the dimer positions with x coordinates satisfying either $x \leqslant j$ or $j+N+1 \leqslant x$. Thus the set $\mathscr{B}$ is partitioned into three sets: $\mathscr{B}^0{}_j$, $\mathscr{B}^+{}_j$ and $\mathscr{B}^-{}_j$. The phase space $\mathscr{C}$ is partitioned similarly into $\mathscr{C}^0{}_j$, $\mathscr{C}^+{}_j$ and $\mathscr{C}^-{}_j$ (with $\mathscr{C}^0{}_j = \{0, 1\}^{8\mathrm{ML}}$ being the phase space corresponding to $\mathscr{B}^0{}_j$, etc). A point $\xi \in \mathscr{C}$ can be written as an ordered triplet, $\xi = (\xi^-{}_j, \xi^0{}_j, \xi^+{}_j)$ with $\xi^i{}_j \in \mathscr{C}^i{}_j$. By $F^+{}_j$ we denote the (complex-valued) functions on $\mathscr{C}$ which are independent of $\xi^-{}_j$; similarly $F^-{}_j$ denotes the functions on $\mathscr{C}$ which are independent of $\xi^+{}_j$. A function on $\mathscr{C}$ which depends only on $\xi^0{}_j$ is in both $F^+{}_j$ and $F^-{}_j$. The involution, θ_j, of Λ onto Λ is defined as the reflection:

$$\theta_j \colon (x, y, z) \to (2j+1-x, y, z). \tag{4}$$

θ_j maps $\mathscr{B}^+{}_j$ onto $\mathscr{B}^-{}_j$ and $\mathscr{B}^-{}_j$ onto $\mathscr{B}^+{}_j$ while it is the identity on $\mathscr{B}^0{}_j$. It lifts to an involution of $\mathscr{C}$ onto $\mathscr{C}$ (which again is denoted by θ_j):

$$\theta_j \xi = \theta_j(\xi^-{}_j, \xi^0{}_j, \xi^+{}_j) = (\xi^+{}_j, \xi^0{}_j, \xi^-{}_j). \tag{5}$$

We shall also use the symbol θ_j for the involution on (complex-valued) functions on $\mathscr{C}$ defined by

$$\theta_j f(\xi) = \theta_j f(\xi^-{}_j, \xi^0{}_j, \xi^+{}_j) = f(\xi^+{}_j, \xi^0{}_j, \xi^-{}_j) \tag{6}$$

with a slight abuse of notation. Obviously

$$\theta_j F^+{}_j = F^-{}_j. \tag{7}$$

We now make a crucial observation; for models I and II the characteristic functions χ_{I} and χ_{II} can be factorised ($i = \mathrm{I}, \mathrm{II}$):

$$\chi_i = \chi^+{}_{i,j}\chi^-{}_{i,j} \tag{8}$$

where $\chi^+{}_{i,j} \in F^+{}_j$, $\chi^-{}_{i,j} \in F^-{}_j$, $\theta_i \chi^+{}_{i,j} = \chi^-{}_{i,j}$ ($\chi^+{}_{i,j}$ is the characteristic function on $\mathscr{C}^+{}_j \cup \mathscr{C}^0{}_j$ for model i). One should note that the factorisation (8) is not true in general; if the particles had been longer (for instance, trimers) then the factorisation would clearly not have been possible.

That model I has 'reflection positivity' (i.e. satisfies equation (12) below) follows from HL. That model II also has reflection positivity is even simpler; namely the Hamiltonian $H_{\mathrm{II}}(\xi)$ for model II can be written as the sum

$$H_{\mathrm{II}}(\xi) = h^+{}_{\mathrm{II},j}(\xi) + \theta_j h^+{}_{\mathrm{II},j}(\xi) \tag{9}$$

where $h^+{}_{\mathrm{II},j} \in F^+{}_j$.

The partition function Z is given by ($\beta = T^{-1}$, $i = \mathrm{I}, \mathrm{II}$):

$$Z_i = \sum_{\xi \in \mathscr{D}_i} \exp(-\beta H_i(\xi)). \tag{10}$$

If f is any (complex-valued) function on $\mathscr{D}$ then its expectation value $\langle f \rangle$ is given by ($i = \mathrm{I}, \mathrm{II}$)

$$\langle f \rangle_i = Z^{-1}{}_i \sum_{\xi \in \mathscr{D}_i} f(\xi) \exp(-\beta H_i(\xi)). \tag{11}$$

Reflection positivity implies that if f and g are complex valued functions on $\mathscr{D}$ and $f \in F^+{}_j$ and $g \in F^-{}_j$ then ($\bar{f}$ is the complex conjugate of f):

$$\langle \bar{f}(\theta_j f) \rangle \geqslant 0 \tag{12}$$

$$|\langle fg \rangle|^2 \leqslant \langle \bar{f}(\theta_j f) \rangle \langle \bar{g}(\theta_j g) \rangle. \tag{13}$$

Definition. In a given dimer arrangement $\xi \in \mathscr{D}$ a vertex is called a *bad vertex* in model I if it is not covered by a dimer and in model II if it is not covered by two collinear dimers. An edge is called a *bad edge* if at least one of the two vertices is a bad vertex or if in model I the vertices are covered by different dimers of which one is in the direction of the edge while the other is perpendicular to the edge. An elementary square of the cubic lattice (i.e. a square containing four vertices connected by four edges) is called a *bad square* if at least one of the four edges is bad. An elementary cube of the cubic lattice (i.e. a cube containing eight vertices connected by twelve edges and bounded by six elementary squares) is called a *bad cube* if at least one of the squares is a bad square. Vertices, edges, elementary squares and elementary cubes which are not bad are called *good.*

A bad cube has an alternative characterisation: given a cube S_i let the restriction $\xi \downharpoonright S_i$ for $\xi \in \mathscr{D}_j$, $j = \mathrm{I}, \mathrm{II}$, specify the state on all edges either in, or incident on, S_i. Then 'S_i is good' means $\xi \downharpoonright S_i$ must be compatible with an overall ground state of the model.

An elementary cube may be identified by its midpoint, i.e. a vertex in a cubic lattice obtained by shifting the original lattice by $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$; we shall call this lattice the *shifted*

cubic lattice and supply it with the cyclic boundary conditions corresponding to Λ. If r is a vertex of the shifted cubic lattice, then we define Q_r as the function on $\mathcal{D}$ which is 1 on the dimer arrangements where the cube at r is bad and 0 on the dimer arrangement where the cube at r is good (note that Q_r depends on the model). If A is a non-empty collection of (distinct) cube midpoints and $|A|$ is the number of elements in A, then we have analogously to the lemma of § 5 of HL that (assuming $\mu + a > 0$)

$$\left\langle \prod_{r \in A} Q_r \right\rangle^{1/|A|} \leqslant 8\, \mathrm{e}^{-\beta\alpha} \tag{14}$$

where

$$\alpha_{\mathrm{I}} = \tfrac{1}{8}[\mu + a - \max\{0, \mu\}] \tag{15a}$$

$$\alpha_{\mathrm{II}} = \tfrac{1}{4}[\mu + a - \max\{0, \mu + b, \tfrac{1}{2}\mu\}] \tag{15b}$$

(in model II we have assumed $b < a$).

4. Peierls' argument

In a dimer arrangement two bad cubes are said to be directly connected if they have an elementary square in common (i.e. if they are connected by an edge in the shifted cubic lattice). In the following we shall use the word *contour* to mean *planar, self avoiding polygon* on the shifted cubic lattice, such that all the vertices visited by the walk correspond to bad cubes, i.e. a contour is a planar connected set of bad cubes which may be connected to other bad cubes. We shall call a contour *long* if the polygon extends infinitely in one or both directions in the plane; otherwise it is called *short.*

Lemma 1. Let P_{LC} be the function on $\mathcal{D}$ which is one on arrangements with at least one long contour and zero on arrangements without long contours. If $24\, \mathrm{e}^{-\beta\alpha} < 1$ then

$$\langle P_{\mathrm{LC}} \rangle \leqslant 8(ML(24\, \mathrm{e}^{-\beta\alpha})^{2N} + NL(24\, \mathrm{e}^{-\beta\alpha})^{2M} + NM(24\, e^{-\beta\alpha})^{2L})(1 - 24\, \mathrm{e}^{-\beta\alpha})^{-1}. \tag{16}$$

Proof. Let us consider the contribution from contours in a plane perpendicular to the z axis and such that the net increase in x is at least $2N$. This contour has to cross the line $x = \frac{1}{2}$ in at least one point; there are $2M$ vertices to choose in between. If we pick one of them as a starting point for the contour, then the following vertices can at most be added in three different ways. Since the length is at least $2N$ and there are $2L$ planes perpendicular to the z axis then it follows from equation (14) that the contribution to $\langle P_{\mathrm{LC}} \rangle$ from long contours in 'the x direction' in planes perpendicular to the z axis is at most

$$4ML(24\, \mathrm{e}^{-\beta\alpha})^{2N}(1 - 24\, \mathrm{e}^{-\beta\alpha})^{-1}.$$

The lemma follows by taking all the possible 'orientations' of long contours into account.

The lemma implies that if $24\, \mathrm{e}^{-\beta\alpha} < 1$, then dimer arrangements with long contours can be neglected in the infinite-volume limit at the cost of a mild restriction on how this limit is taken.

We shall consider good cubes to be connected if they have an edge in common. With this definition one has for obvious topological reasons the following lemma.

Lemma 2. In dimer arrangements with no long contours, in each plane of the shifted cubic lattice there is a connected component of good cubes which extends infinitely in both directions.

An elementary cube, of course, belongs to three perpendicular planes of the shifted cubic lattice. A good cube which in all three planes belongs to the connected component of good cubes which extends infinitely in both directions is called a *really good cube.* Other cubes (including bad cubes) are denoted *not really good cubes.* If r is a vertex of the shifted cubic lattice, then we define Q'_r as the function on $\mathscr{D}$ which is zero when there are no long contours and the cube at r is really good and one when there is a long contour or the cube at r is not really good.

Theorem 3.

$$\langle Q'_r \rangle \leqslant \langle P_{LC} \rangle + P_{RG} \tag{17}$$

$$P_{RG} = \tfrac{1}{6}[\gamma^3 + 4\gamma^2(1-\gamma)](1-\gamma)^{-2} \tag{18}$$

$$\gamma = 576\, \mathrm{e}^{-2\beta\alpha}. \tag{19}$$

Proof. The first term in (17) corresponds to the occurrence of a long contour; the second term is a standard estimate on the probability of having a contour of bad cubes which surrounds r. The number of contours of length l surrounding r is estimated as follows. The plane can be chosen in three ways; a contour of length l can be formed in less than $4\cdot 3^{l-2}/2l$ ways and be placed 'around' r in at most $(l/4+1)^2$ ways (the contour is a walk on the same lattice as the lattice on which r is chosen; consequently r may be on the contour). Together that gives

$$\tfrac{1}{12}3^l(l+4)^2/2l \leqslant \tfrac{1}{12}3^l(l+4)$$

since $l \geqslant 4$. The value for P_{RG} then follows from equation (14) and the fact that l is even.

If we consider really good cubes to be connected whenever they have an edge in common and cubes which are not really good to be connected whenever they have an elementary square in common, then lemma 2 would still hold if we replaced 'long contours' with 'long contours of not really good cubes' and 'good cubes' with 'really good cubes'. Consequently, we want the following lemma which bounds the probability of 'long contours of not really good cubes'.

Lemma 4. Let P_{NRG} be the function on $\mathscr{D}$ which is zero if each plane of the shifted cubic lattice has a connected component of really good cubes which extends infinitely in both directions and is one otherwise. If $96\cdot 4\, \mathrm{e}^{-\beta\alpha} < 1$ then

$$\langle P_{NRG} \rangle \leqslant 8(ML{\gamma_1}^{2N} + NL{\gamma_1}^{2M} + NM{\gamma_1}^{2L})(1-\gamma_1)^{-1} \tag{20}$$

$$\gamma_1 = 96\cdot 4\, \mathrm{e}^{-\beta\alpha}. \tag{21}$$

Proof. Once we have established the number of ways in which we can continue a 'contour of not really good cubes' (called an *NRG contour* in the following), then the inequality (20) follows by the same argument as lemma 1. If the not really good cubes of our NRG contour are surrounded by a contour in the plane, then we might just follow that contour around from the entry point to the exit point of the NRG contour. For each bad cube in the contour we can (as usual) continue to three different cubes and each time we can choose that cube to be bad or good but surrounded by a contour in one

of the two perpendicular planes. This gives an extra factor 3 or a total factor of 9 per bad cube in the plane.

For a contour perpendicular to the plane we count as follows. We choose a bad cube (with unspecified position so far) to start from; the next bad cube can be placed in four different positions and each of the following bad cubes in three positions. When the position chosen is identical to the position of the first cube, then this contour is finished, i.e. at a cost of an extra factor three we obtain the information on the length of this particular contour. Assume that the length is l; then we have so far collected a factor $(\frac{4}{3})3^l$. However, any cube might have been chosen as starting point and we can go around the contour in both directions; this reduces the number of different contours by a factor $1/2l$. Next we have to choose one of the interior cubes as the place where our NRG contour enters; as in the proof of lemma 3 we can choose between at most $(l/4+1)^2$ cubes. Finally, we have to choose an exit point of the NRG contour; this has to be a cube in the plane of the NRG contour which is a neighbour of one of the not really good cubes surrounded by the contour just placed. There are at most l such cubes of which one can be excluded because it is the point of entry. As explained in the caption to figure 1, we might need more than one exit point; therefore we include a factor 4^{l-1} to account for the possibility that each of the candidates might or might not be used (in the latter case we also have to choose the orientation of the plane of the next contour). In all we have collected a factor

$$12^l(l/4+1)^2/6l$$

for the possibilities of continuing the NRG contour with a piece surrounded by a contour of length l, including the decision on the length of this particular contour and the position and orientation of the continuation. The length l is even and at least eight, since otherwise all the cubes inside the contour are bad and we might have considered this part of the NRG contour as consisting of bad contours in the plane. For l even (and positive) we have

$$12^l(l/4+1)^2/6l \leqslant 12^l(961/366)^{l/244}.$$

This concludes the proof of the lemma.

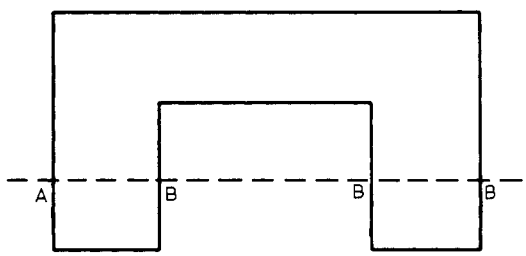

Figure 1. Let the full line represent a contour and the broken line a perpendicular plane. If an NRG contour in that plane enters somewhere along the part A–A, then it has to leave again at the part A–A (otherwise the NRG contour would not be connected in the plane). Let us now suppose that further along the same NRG contour we enter the contour drawn at the part B–B; then we have to choose a new exit point at that part, but the bad cubes have already been counted once. Therefore, we do not get any additional bad cubes to counterweigh the extra 'entropy'. The only remedy is to decide on any other exit point when the contour is included at its first entrance.

Consequently, if $96{\cdot}4\,e^{-\beta\alpha} < 1$, then the dimer arrangements on which P_{NRG} is one can be neglected in the infinite-volume limit. The only problem left is to analyse the structure of the arrangements on which P_{NRG} is zero.

A good vertex can be classified according to the direction of the dimer(s) which cover(s) it as having x, y or z structure. Similarly, a good edge may classify as having xx, yy, zz, xy, yx, xz, zx, yz or zy structure, giving the structure of the two terminal vertices with the vertex with the lowest coordinate first. If a good edge has xx, yy or zz structure then it is said to be of *type 1*, otherwise it is said to be of *type 2*. The following statements arise by realising that any other conceivable structure is impossible. If a good edge is of type 2, then the direction of the edge has to be perpendicular to the directions of the structure of the terminal vertices. A good square either has four good edges of type 1 or two good edges of type 2 which are parallel and have the same structure. A good cube either has 12 good edges of type 1 or four good edges of type 2 which are parallel and have the same structure.

From the last statement is follows that, in a connected component of good cubes in a plane of the shifted cubic lattice, the edges perpendicular to the plane are either all of type 1 or all of type 2 and have the same structure. The same is, of course, true for a connected component of really good cubes. If $P_{\mathrm{RNG}} = 0$ then any two perpendicular planes of the shifted cubic lattice have at least one really good cube in common. Consequently, if $P_{\mathrm{NRG}} = 0$ then either all the really good cubes have only edges of type 1 and all the vertices of the really good cubes have the same structure, or one of the three coordinate axes is special in the sense that in any plane of the cubic lattice perpendicular to this direction, all the vertices of the really good cubes have the same structure and the direction of the structure is one of two directions parallel to the plane, but different planes can have a different structure (in fact, both directions have to occur in order to single out the direction).

5. Regions of disorder

For model I it is easy to see that one can apply the theory of Ruelle (1963) to prove that the Kirkwood–Salsburg equations have a unique solution with clustering properties of the correlation functions (Ruelle 1964) if the temperature is high enough and/or the chemical potential is small enough (i.e. negative enough).

The same method can be applied to model II if one uses the rewriting to a trimer model introduced by Abraham and Heilmann (1972). We shall, however, follow the analysis of AH, since this yields the following additional results.

Theorem 5. In model II if $b > a$ (favouring of bend configurations over stretched), then there is no phase transition.

Proof. The proof essentially follows the argument given in § 3 by AH, i.e. we rewrite the model as a monomer–dimer model and use the method by Heilmann and Lieb (1972) to prove absence of phase transition. However, certain technical points have to be changed. Nevertheless, the reader might well prefer not to read the rest of this section.

The city which replaces a vertex is built up as follows. Each of the six external edges is incident on a separate vertex with monomer weight zero; these six vertices are called the outer vertices and denoted $+x$, $-x$, $+y$, $-y$, $+z$ and $-z$ after the direction of the external edge. Next we have three vertices called the inner vertices and denoted 1, 2

and 3; they all have monomer weight m. Finally, we have two centre vertices denoted 4 and 5; 4 has monomer weight m', and 5 has monomer weight zero. All of the outer vertices are connected to all the inner vertices with edges with weights a_1, a_2 or a_3; vertices $+x$ and $-x$ are connected to vertex i with weight a_i $(i = 1, 2, 3)$; vertices $+y$ and $-y$ are connected to vertex i with weight a_{i+1} for $i = 1, 2$ and with weight a_1 for $i = 3$; vertices $+z$ and $-z$ are connected to vertex i with weight a_3 for $i = 1$ and with weight a_{i-1} for $i = 2, 3$. The three inner vertices are mutually connected by edges with weight w, they are all connected to vertex 4 by edges with weight u and to vertex 5 by edges with weight 1.

Following AH we have the following conditions on the parameters (f is an extra factor included for each city):

$$e^{\beta(a+\mu)} = 2(a_1a_2 + a_2a_3 + a_1a_3)m'f \tag{22a}$$

$$e^{\beta(b+\mu)} = (a_1^2 + a_2^2 + a_3^2 + a_1a_2 + a_2a_3 + a_1a_3)m'f \tag{22b}$$

$$e^{\frac{1}{2}\beta\mu} = 2(a_1 + a_2 + a_3)(u + mm')f \tag{22c}$$

$$1 = 3(m'w + 2mu + m^2m')f. \tag{22d}$$

It is again relatively easy to see that if $a < b$, one can always find strictly positive (real) values of the five edge weights, a_1, a_2, a_3, u and w, which satisfy these four equations.

The only remaining step is to prove that the lemma of AH holds in the present case. We shall do this by indicating the changes in the proof of AH. The contribution from linear polymers of length $n+2$ is bounded by

$$6|e^{\beta\mu}|(|e^{\beta(a+\mu)}| + 4|e^{\beta(b+\mu)}|)^n(n+2)/2 \tag{23a}$$

while the contribution from closed polygons of length $n+2$ is bounded by

$$(|e^{\beta(a+\mu)}| + 4|e^{\beta(b+\mu)}|)^n. \tag{23b}$$

We define η by

$$\xi = \eta/(|e^{\beta(a+\mu)}| + 4|e^{\beta(b+\mu)}|) \tag{24}$$

and have

$$\hat{S}(\xi) = \frac{|e^{\beta\mu}|}{(|e^{\beta(a+\mu)}| + 4|e^{\beta(b+\mu)}|)^2} \frac{6\eta^2 - 3\eta^3}{(1-\eta)^2} + \eta^4/(1-\eta). \tag{25}$$

Equations (9) of AH are replaced by

$$3|m'w + 2mu + m^2m'|\,|f|$$

$$\geqslant 2|m'|\,|f|\frac{\alpha}{\eta}\left(1 + \frac{\eta^4}{1-\eta} + \frac{|a_1 + a_2 + a_3|^2|u + mm'|^2}{\alpha^2|m'|^2} \frac{6\eta^2 - 3\eta^3}{(1-\eta)^2}\right) \tag{26}$$

$$\alpha = |a_1^2 + a_2^2 + a_3^2 + a_1a_2 + a_2a_3 + a_1a_3| + |a_1a_2 + a_2a_3 + a_1a_3|. \tag{27}$$

The rearrangement leads to the following sufficient inequality:

$$3|m^2|\,|m'|\left(1 - 2\frac{2\eta - \eta^2}{(1-\eta)^2} \frac{|a_1 + a_2 + a_3|^2}{\alpha}\right)$$

$$> 6|m|\,|u| + |m'|[3|w| + (2\alpha/\eta)(1 + \eta^4(1-\eta)^{-1})]$$

$$+ 6[|u|^2/|m'| + 2|u|\,|m|]\frac{2\eta - \eta^2}{(1-\eta)^2} \frac{|a_1 + a_2 + a_3|^2}{\alpha}. \tag{28}$$

Since

$$|a_1+a_2+a_3|/\alpha \leqslant 1 \tag{29}$$

for all (not necessarily real) choices of a_1, a_2 and a_3, then we end up with the same condition on η as in AH to ensure that

$$1-2\frac{2\eta-\eta^2}{(1-\eta)^2}\frac{|a_1+a_2+a_3|^2}{\alpha}>0$$

and we have thus established that the lemma of AH also holds in the three-dimensional case.

The remaining part of the argument is the same as in AH.

6. Higher dimensions

It is natural to ask whether there is an immediate generalisation from three dimensions to higher dimensions. The answer is that the arguments of §§ 3 and 4 as far as the proof of lemma 4 is concerned are essentially independent of the number of dimensions if the dimensionality is at least 3; only some of the numerical constants are changed. However, the arguments presented at the end of § 4 break down as soon as we move on to four dimensions.

Since in four dimensions we have two directions perpendicular to any plane, then we can create good squares where all four edges are of type 2 (by alternating between the two perpendicular directions); we can also create a good square with three different directions present (the two perpendicular directions at one vertex each and one of the parallel directions at two neighbouring vertices). We can continue to construct a good 3D cube where all four directions are present as shown in figure 2 and finally, we can construct a good 4D cube where again all four directions are present as shown in table 1. If or e let this 4D cube manifold by reflection in the planes of the 4D simple cubic lattice, then one obtains a configuration where the 4D cubic lattice is covered by infinitely long rods of all four orientations in equal proportions; it seems possible to create 'ground states' with the four directions present in any relative proportions. Therefore, our proof will not yield an ordered phase with certain directional preferences; although it might yield a low-temperature phase with some kind of limitations on the possible disorder.

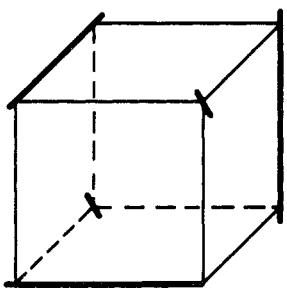

Figure 2. The figure shows a good three-dimensional cube in a four-dimensional space, where all four directions are represented at the vertices (the directions are shown as bold lines).

Table 1. The table shows a good four-dimensional cube in a four-dimensional space with all four directions represented.

Vertex (x_1, x_2, x_3, x_4)	Direction	Vertex (x_1, x_2, x_3, x_4)	Direction
(0, 0, 0, 0)	1	(0, 0, 0, 1)	1
(1, 0, 0, 0)	1	(1, 0, 0, 1)	1
(0, 1, 0, 0)	3	(0, 1, 0, 1)	3
(1, 1, 0, 0)	4	(1, 1, 0, 1)	4
(0, 0, 1, 0)	4	(0, 0, 1, 1)	4
(1, 0, i, 0)	2	(1, 0, 1, 1)	2
(0, 1, 1, 0)	3	(0, 1, 1, 1)	3
(1, 1, 1, 0)	2	(1, 1, 1, 1)	2

In fact, our investigations indicate that in four dimensions the degeneracy of the 'ground state' increases as some constant to the linear dimensions of Λ or to the square of the linear dimensions of Λ, i.e. the system has no residual entropy. We shall not pursue the problems further; after all we believe the real world to be three dimensional and we have made the points we want to make: the treatment of higher dimensions is not trivial and the difference between three and four dimensions is so large that attempts to reach the three-dimensional world by an expansion from the four-dimensional world must be considered futile.

7. Conclusion

We have demonstrated that both models have a phase transition from a low-temperature state with some orientational order to a high-temperature gas-like state with no order. The state at absolute zero ($\beta = \infty$) will single out one of the coordinate directions; in any plane of the cubic lattice perpendicular to this direction all vertices will have the same orientation which will be one of the two directions in the plane; there will be no correlation between the preferred direction in different planes.

However, as soon as we move to non-zero temperatures the picture might change. We, of course, still expect there to be a direction such that in each plane perpendicular to this direction most of the vertices will have the same direction, which will be one of the two directions in the plane. But now we might very well find a strict correlation between the preferred direction in different planes; the most obvious possibilities are that the structure is the same in all planes or that the structures in neighbouring planes are perpendicular, but more complicated patterns could also be perceived. The cause for the possible ordering is the occurrence of defects. It is possible that, for instance, identical structures dominating neighbouring planes will make the occurrence of defects more favourable than opposite structures will (either through the energy or the entropy associated with these defects). Since any preference will give a contribution to the free energy which increases proportionally to the area of the plane while the contribution from the random choice of the structure of next plane is an addition of ln(2) to the entropy independent of the size of the system, then the preference will always win in the infinite-volume limit. We shall abstain from suggesting any conjectures on what actually happens.

In model I we expect the same lack of translational order as HL suggested in the two-dimensional case.

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