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Existence of an ordered phase for the repulsive lattice gas on the FCC lattice

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Abstract. It is proven by Peierls' argument in connection with reflection positivity that the lattice gas on the FCC lattice with nearest-neighbour repulsion (with interaction energy a) exists in an ordered state at low enough temperature provided the chemical potential, μ, satisfies $0 < \mu < 4a$, $4a < \mu < 8a$ or $8a < \mu < 12a$. This result immediately carries over to the antiferromagnetic Ising model and the lattice gas with nearest-neighbour exclusion on the FCC lattice, both of which will also exist in an ordered state under suitable circumstances. In particular, the existence of a phase transition at zero magnetic field is confirmed.

1. Introduction

It has earlier been proven that the lattice gas with nearest-neighbour repulsion on the simple cubic lattice (Dobrushin 1968), the body-centred cubic lattice (which follows by a trivial modification of the proof for the simple cubic lattice) and the diamond lattice (Heilmann 1974) exhibits a phase transition from an ordered to a disordered state. In all three cases the result follows from an application of Peierls' argument in the form originally introduced by Griffith (1964) and Dobrushin (1965). However, the nature of the ordered phase for the face-centred cubic lattice is more complicated, and one has to resort to contours which are made up of line segments (rather than surface segments) in spite of the three-dimensional nature of the problem. This problem has recently been solved by Abraham and Heilmann (1980) (to be referred to as AH) by application of reflection positivity (see Heilmann and Lieb (1979) (to be referred to as HL) and references therein). The present argument follows the argument of AH closely and the reader is referred to that paper for most of the details.

The antiferromagnetic Ising model with zero magnetic field had earlier been the subject of several articles. Danelian (1961) established the existence and nature of the partially ordered ground state. The existence of a phase transition from an antiferromagnetic to a disordered state was indicated by series expansions (Danelian 1961, Betts and Elliott 1969); a result which has recently been supported by Monte Carlo calculations (Phani *et al* 1979). Little seems to have been published about the behaviour at non-zero magnetic field (see, however, figure 5 in Domb (1974)).

In the following we shall adhere to the notation of the lattice gas and only give the results for the Ising model at the end.

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2. The model

We introduce a coordinate system such that the vertices of the FCC lattice coincide with the points with integer coordinates with even sum. The domain, Λ, is a box-shaped subset of size $2N \times 2M \times 2L$:

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

with cyclic boundary conditions i.e. x coordinates are calculated modulo $2N$ onto $0 \leq x < 2N$, y coordinates modulo $2M$ onto $0 \leq y < 2M$ and z coordinates modulo $2L$ onto $0 \leq z < 2L$ whenever necessary.

If we attach a copy of the two point space $\{0, 1\}$ to each vertex in Λ, then we can identify the set of all possible configurations of the repulsive lattice gas on Λ, $\mathscr{C}$, with $\{0, 1\}^{4NML}$, letting 1 correspond to an occupied vertex and 0 to an empty vertex. The set of all possible arrangements of particles on Λ which are consistent with the requirement of nearest-neighbour exclusion is denoted by $\mathscr{D}$; $\mathscr{D}$ is a subset of $\mathscr{C}$ which we describe by introducing a characteristic function, χ, defined for all $\xi \in \mathscr{C}$ by

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

If f is a function defined on $\mathscr{D}$, then we extend the function χf to a function on $\mathscr{C}$, just as in AH, by ($\xi \in \mathscr{C}$)

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

We shall call $\mathscr{C}$ the phase space for Λ for both lattice gases.

3. Reflection positivity

We take the reflection planes to be perpendicular to one of the coordinate axes and passing through the vertices. More specifically, the reflection planes perpendicular to the x axis are given by (j is an integer satisfying $0 \leq j < N$)

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

The phase space, $\mathscr{C}$, is partitioned into the phase space for $L_j^- \cup L_j^+$, $\mathscr{C}^0_j$, the phase space for the vertices of Λ satisfying $j < x < j+N$, $\mathscr{C}^+_j$, and the phase space for the vertices satisfying either $x < j$ or $x > j+N$, $\mathscr{C}^-_j$, i.e. $\mathscr{C}^0_j = \{0, 1\}^{2ML}$, $\mathscr{C}^+_j = \{0, 1\}^{(2N-1)ML}$, and $\mathscr{C}^-_j = \{0, 1\}^{(2N-1)ML}$. 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 functions on $\mathscr{C}$ which are independent of ξ^-_j and by F^-_j we denote the functions on $\mathscr{C}$ which are independent of ξ^+_j. A function on $\mathscr{C}$ which depends only on ξ^0_j is in both F^+_j and F^-_j.

The involution, θ_j, of Λ onto Λ is defined as the reflection

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

θ_j lifts to an involution of $\mathscr{C}$ onto $\mathscr{C}$ (which again is denoted by θ_j); $\xi = (\xi^-{}_j, \xi^0{}_j, \xi^+{}_j) \in \mathscr{C}$:

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

Finally, θ_j is used for the involution on functions on $\mathscr{C}$ defined, with a slight abuse of notation, by

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

Obviously

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

We are now ready to state the conditions which imply that the models have reflection positivity. Let $\xi \in \mathscr{C}$; then we write $\nu(\xi)$ for the number of occupied vertices in ξ and $\eta(\xi)$ for the number pairs of nearest-neighbour vertices both of which are occupied in ξ. The Hamiltonian $H(\xi)$ for the lattice gas with nearest-neighbour repulsion can then be written as

$$H(\xi) = a\eta(\xi) - \mu\nu(\xi). \tag{8}$$

The grand canonical partition function is given by

$$Z_r = \sum_{\xi \in \mathscr{C}} \exp(-\beta H(\xi)) \tag{9}$$

for the repulsive lattice gas and by

$$Z_e = \sum_{\xi \in \mathscr{C}} \chi(\xi) \exp(\beta\mu\nu(\xi)) \tag{10}$$

for the lattice gas with nearest-neighbour exclusion. The Hamiltonians, $H(\xi)$ and $-\mu\nu(\xi)$, clearly can be written

$$H(\xi) = h^+(\xi) + \theta_j h^+(\xi) \tag{11}$$

$$-\mu\nu(\xi) = -\mu(\nu^+(\xi) + \theta_j \nu^+(\xi)) \tag{12}$$

where $h^+(\xi) \in F^+{}_j$ and $\nu^+(\xi) \in F^+{}_j$. We also have the factorisation

$$\chi(\xi) = \chi^+(\xi)[\theta_j \chi^+(\xi)] \tag{13}$$

where $\chi^+(\xi) \in F^+{}_j$ is the characteristic function on $\mathscr{C}^0{}_j \cup \mathscr{C}^+{}_j$ for the nearest-neighbour exclusion problem. The equations (11)–(13) are sufficient to ensure reflection positivity (see HL). If f is a function on $\mathscr{C}$ then its expectation value $\langle f \rangle$ is given by

$$\langle f \rangle_r = Z_r^{-1} \sum_{\xi \in \mathscr{C}} f(\xi) \exp(-\beta H(\xi)) \tag{14}$$

or

$$\langle f \rangle_e = Z_e^{-1} \sum_{\xi \in \mathscr{C}} \chi(\xi) f(\xi) \exp(\beta\mu\nu(\xi)) \tag{15}$$

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

$$\langle \bar{f}(\theta_j f) \rangle \geq 0 \tag{16}$$

$$|\langle fg \rangle|^2 \leq \langle \bar{f}(\theta_j f) \rangle \langle \bar{g}(\theta_j g) \rangle. \tag{17}$$

4. Peierls' argument for $0<\mu<4a$

Definitions. In a given configuration $\xi \in \mathscr{C}$, an elementary tetrahedron (i.e. four vertices all of which are each other's nearest neighbours) is called a *good tetrahedron* if precisely one of the four vertices is occupied; otherwise it is called a *bad tetrahedron.* The midpoints of the elementary tetrahedrons form a simple cubic lattice with edge length one and vertices at the points in $\mathbb{R}^3$ with half-integer coordinates. In the following, when we refer to the SC lattice we shall mean this lattice. Again referring to a specific configuration, $\xi \in \mathscr{C}$, a vertex of the SC lattice is called *bad* if the corresponding tetrahedron is bad; an edge of the SC lattice is called *bad* if at least one of the two vertices on which it is incident is bad; similarly, *bad squares* and *bad cubes* are defined as elementary squares, respectively elementary cubes, of the SC lattice which contains at least one bad vertex. Vertices, edges, elementary squares and elementary cubes which are not bad are called good, i.e. good edges, good squares and good cubes contain only good vertices.

The crucial implication of reflection positivity is that bad cubes are unlikely. If r is an elementary cube of the SC lattice, for example identified by its midpoint (which is a point in Z^3), then we define Q_r as the function on $\mathscr{C}$ which is one on configurations where the cube r is bad and zero on configurations where it is good.

The following lemma is analogous to the lemma in § 5 of HL and is proved the same way.

Lemma. Let A be a non-empty collection of distinct elementary cubes and let $|A|$ be the number of elements in A. If $0<\mu<4a$ for the lattice gas with nearest-neighbour repulsion, then

$$\max_{A\neq\varnothing}\left\langle\prod_{r\in A} Q_r\right\rangle^{1/|A|} \leqslant \sqrt{2}\,\mathrm{e}^{-\beta\alpha} \tag{18}$$

where

$$\alpha=(\mu-\max\{0,2\mu-4a\})/64. \tag{19}$$

For the nearest-neighbour exclusion equation (18) holds, with

$$\alpha=\mu/64. \tag{20}$$

Proof. The elementary cubes of the SC lattice are divided into eight equivalence classes such that the midpoints of all the cubes of a class form a simple cubic lattice with lattice spacing 2. In that way each vertex of the SC lattice belongs to one cube from each equivalence class. If B is the set of all the cubes from one of the classes then it follows from reflection positivity by the 'checker board' estimate (see HL) that

$$\max_{A\neq\varnothing}\left\langle\prod_{r\in A} Q_r\right\rangle^{1/|A|} \leqslant \left\langle\prod_{r\in B} Q_r\right\rangle^{1/8|B|}. \tag{21}$$

Strictly speaking, the right-hand side should be maximised over the eight equivalence classes since they are not identical (except for translation) in the present case. However, the way the following estimate is made makes it immaterial which class is chosen.

In the following we only refer explicitly to the nearest-neighbour repulsion, the case of nearest-neighbour exclusion following trivially. We have from equation (14)

$$\left\langle\prod_{r\in B} Q_r\right\rangle_r = Z_r^{-1}\sum_{\xi\in\mathscr{C}}\left(\prod_{r\in B} Q_r(\xi)\right)\mathrm{e}^{-\beta H(\xi)}. \tag{22}$$

Clearly

$$Z \geq e^{\beta\mu NML}. \tag{23}$$

A bound on the terms in the sum in equation (22) can be obtained as follows. A vertex in the FCC lattice belongs to eight elementary tetrahedra and an edge in the FCC lattice belongs to two tetrahedra. This implies that the Hamiltonian can be written as a sum of the energies of elementary tetrahedra if in the energy of a tetrahedron we include $-\mu/8$ for each occupied vertex and $a/2$ for each pair of occupied vertices, i.e. the energy of a tetrahedron with $0, 1, 2, 3$ and 4 occupied vertices is respectively 0, $-\mu/8$, $(-2\mu+4a)/8$, $(-3\mu+12a)/8$ and $(-4\mu+24a)/8$. If all the cubes in B are bad then each vertex of the SC lattice (each tetrahedron of the FCC lattice) belongs to precisely one bad cube; therefore, at least one-eighth of the tetrahedra ($=NML$ tetrahedra) are bad and the energy of such a configuration is larger than $-7\mu NML/8 - NML\max\{0, (-2\mu+4a)/8\}$ if $0<\mu<4a$. The lemma then follows from the fact that the number of elements in $\mathscr{C}$ is 2^{4NML}.

Once the lemma has been established it follows from the arguments of § 4 of AH that the structure of 'really good cubes' dominates provided $17 \cdot 1\, e^{-\beta\alpha} < 1$, and the only remaining problem is the analysis of the structure of the configurations where the really good cubes dominate.

5. The ordered state for $0<\mu<4a$

The FCC lattice can be divided into four simple cubic lattices with the lattice spacing two, such that each elementary tetrahedron of the FCC lattice has one vertex from each sublattice. We shall number the four simple cubic lattices from one to four and characterise the good tetrahedron by the number of the lattice to which the occupied vertex belongs; a good vertex of the SC lattice (of tetrahedra midpoints) is characterised according to the tetrahedron. As in AH we find that a good edge (of the SC lattice) is of type one (same structure at both vertices) or of type two (different structure at the two vertices); in the latter case the possibilities are limited by the fact that the two tetrahedra which correspond to the two vertices (of the SC lattice) have two vertices (of the FCC lattice) in common. For the good squares (of the SC lattice) we have (as in AH) that either all the edges are of type one or two parallel edges are of type two and the other two of type one (note that one vertex of the FCC lattice is common to all four tetrahedra of an elementary square of the SC lattice, four vertices are each common to two tetrahedra and the remaining four vertices of the four tetrahedra (each of which only belongs to one tetrahedron) all belong to the same SC sublattice). Finally, a good cube either has twelve edges of type one or four parallel edges of type two and eight edges of type one.

This is precisely the same result as in AH; therefore, we can draw the same conclusion. Either all the edges of the really good cubes are of type one, which implies that all the good tetrahedra corresponding to the vertices of these cubes have the same structure, i.e. one of the four SC sublattices of the FCC lattice is occupied and the other three are empty (except for the occurrences of disorder which have a low probability), or one of the three coordinate axes is special (let us say the x axis) in the sense that the edges of the really good cubes which are perpendicular to the x axis must be of type one while the edges which are parallel to the x axis can be of type two; if one of these edges is of type two, then all the parallel edges of the really good cubes whose midpoints have the same x coordinate must also be of type two; furthermore, it follows from the special structure of the present problem that the spacing between planes perpendicular to the x axis and passing through edge midpoints of edges of type two (when they belong to the really good cubes) must be an even integer. In this case in the ordered structure (which dominates the configurations) every second plane of the FCC lattice perpendicular to the x axis is totally empty, while the other planes have half of the vertices (all belonging to the same SC sublattice) occupied and the other half of the vertices are empty, i.e. two of the SC sublattices are totally empty while the other two have some vertices occupied, the occupied vertices of a given sublattice being in planes perpendicular to the x axis (or the y or the z axis).

At absolute zero ($\beta = \infty$) it follows from an entropy consideration that the state is one where two of the SC sublattices are empty and the other two partly occupied, the choice between the two occupied sublattices being a random choice for each plane common to the two sublattices (and perpendicular to a coordinate axis). However, as soon as the temperature is larger than zero we are faced with the same predicament as in AH; most likely, the occurrences of defects will single out a particular choice for the relative ordering between neighbouring occupied planes, but we can say nothing about what actually happens.

6. The case $4a<\mu<8a$

The essential change from the case $0<\mu<4a$ is that a *good tetrahedron* is now an elementary tetrahedron with precisely two occupied vertices, while all other configurations correspond to a *bad tetrahedron*.

Instead of equation (23) we use

$$Z \geqslant \exp[\beta NML(2\mu - 4a)] \tag{24}$$

and find that the lemma holds with α given by

$$\alpha = (2\mu - 4a - \max\{\mu, 3\mu - 12a\})/64. \tag{25}$$

The structure of the configurations where the really good cubes dominate has already been described by Danelian (1961); however, it might still be of value to obtain this result with the notation used in § 5, which is rather different from that of Danelian. The good tetrahedra are characterised according to which of the sublattices the two occupied vertices belong to (six possibilities). This is most conveniently done by pointing an arrow from the midpoint of the edge (of the tetrahedron) which connects the two empty vertices towards the midpoint of the edge which connects the two occupied vertices. These arrows will be parallel or antiparallel to one of the coordinate axes. Characterising a good vertex of the SC lattice (of tetrahedra midpoints) according to the tetrahedron, we find that a good edge (of the SC lattice) is of type one (parallel or antiparallel arrows at the two vertices) or of type two (perpendicular directions of the two arrows).

As before, the fact that the two tetrahedra which correspond to the endpoints of an edge of the SC lattice have two vertices (of the FCC lattice) in common limits the possibilities for the good edges. If the two common vertices (of the FCC lattice) are either both occupied or both empty, then the arrows of the two tetrahedra are antiparallel and in the direction of the corresponding edge of the SC lattice, i.e. the edge is necessarily of type one. If only one of the two common vertices (of the FCC lattice) is occupied, then both arrows must be perpendicular to the corresponding edge of the SC lattice and the edge can either be of type one or type two; if it is of type one, then the arrows have to be parallel.

It is now easily seen that a good square (of the SC lattice) either has all four edges of type one or two parallel edges of type two and the other two of type one and the arguments of AH and § 5 apply. In the order state we have one coordinate directions such that in each of the perpendicular planes of the FCC lattice we have perfect antiferromagnetic ordering of the corresponding square lattice, while we can say nothing about the relative ordering of planes separated by a distance two.

7. The case $8a<\mu<12a$

The normal symmetry between occupied and empty vertices in a lattice gas with pair interactions (Gallavotti *et al* 1967) implies that if $8a<\mu<12a$ and the temperature is low enough, then we have an ordered state which is equivalent to the one described above for $0<\mu<4a$ except that the roles of occupied and empty vertices are interchanged and

$$\alpha=(3\mu-12a-\max\{2\mu-4a, 4\mu-24a\})/64. \tag{26}$$

8. The Ising model

It follows from the equivalence between the lattice gas and the Ising model (Lee and Yang 1952) that for the antiferromagnetic Ising model on the FCC lattice with nearest-neighbour interaction J for parallel spins and $-J$ for antiparallel spins and magnetic field H one will have an ordered state at low enough temperature if $4J<|H|<12J$ or $|H|<4J$. The structure will be the same as for the lattice gas with the empty vertices playing the role of spin up and the occupied vertices playing the role of spin down. The value of α will be

$$\alpha=(-|H|+8J-\max\{-2H+12J, -4J\})/32 \tag{27}$$

for $4J<|H|<12J$ and

$$\alpha=(-|H|+4J)/32 \tag{28}$$

for $|H|<4J$.

We have thus established the existence of three different ordered phases for the antiferromagnetic Ising model (as well as for the repulsive lattice gas) on the FCC lattice. It should be noticed that for $H=\pm 4J$, which are the values which separate the different ordered phases at $T=0$, one has a residual entropy. This can be seen as follows. The energy can, as stated above, be considered as the sum of contributions from the elementary tetrahedra. An elementary tetrahedron with three spins up and one down contributes $-H/4$, while a tetrahedron with two spins up and two spins down contributes $-J$. If $H=4J$ then the two contributions are equal and the lowest possible. Consequently, if we divide the FCC lattice into four SC lattices (with lattice spacing two) and fix the spins of two of the SC sublattices to be up while the third SC sublattice has all spins down, then each of the spins of the fourth SC sublattice may be chosen independently to be either up or down, and we will in any case have a configuration with the ground-state energy if $H=4J$, i.e. the residual entropy per site is at least $\frac{1}{4}\ln 2$.

The most natural conjecture about the phase diagram therefore appears to be that the disordered phase extends all the way down to $T = 0$ for $H = \pm 4J$ and that the only possible phase transitions are between one of the ordered phases and the disordered phase.

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