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Phase transition in a lattice gas with third nearest neighbour exclusion on a square lattice

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Abstract. The lattice gas problem with third nearest neighbour exclusion on a square lattice is shown to be equivalent to the problem of placing hard cross-shaped pentamers on the square lattice and the existence of a phase transition is proved by means of the Peierls argument.

1. Introduction

Peierls' argument has recently been applied successfully to prove phase transitions for a large class of repulsive lattice gas systems. A general treatment of Peierls' argument can be found in the review article by Griffiths (1972). Heilmann and Præstgaard (1973) have given a thorough discussion of the implications for repulsive lattice gases. The main feature of the argument is to prove that at sufficiently high fugacity the system will exist in several states (ie Gibbs' states, see Dobrushin 1968) which differ from each other only by spatial symmetry transformations. This is done by proving that if one fixes the boundary conditions of the system appropriately, one forces the whole system into a state which has a lower spatial symmetry than the model as such. At sufficiently low fugacity the system will always exist in a gas phase where the state of the system is independent of the boundary condition and has the full symmetry of the model. Consequently, one has a phase transition somewhere in between.

When one wants to apply Peierls' argument two kinds of problems arise. Some of these may be trivially solvable for some models.

Firstly one defines the pure states; a pure state is essentially a classification of the possible local structures, in the following we shall just call them states as no confusion seems possible. The local structure is given by the configuration of a volume element. In the lattice gas the volume element is often a single vertex. In the present case, however, it will also be necessary to include the configurations of the neighbouring vertices.

For a given configuration of the system each volume element is uniquely determined as belonging to a definite state (or possibly the contour between different states) and the configuration can now be associated with a system of contours separating the regions belonging to different states; knowledge of the system of contours should uniquely determine the configuration.

Secondly, one has to prove that the occurrence of a contour is unlikely. To do this one compares configurations with the contour in question to the configuration without the contour. This comparison is done with the aid of symmetry operations which interchange the local structures while mapping the model onto itself. The use of translation as a symmetry operation was introduced by Dobrushin (1965); the applicability of reflection, rotation and inversion as symmetry operations has recently been established by Heilmann (1974).

For the nearest neighbour exclusion on the square lattice, which divides into two sublattices A and B, the definition of local structures and contours is straightforward. A vertex in the A sublattice has A structure, when occupied, and B structure, when empty, and vice versa for a vertex in the B sublattice. Contours are drawn through the edges which separate vertices of opposite structure. When one has three sublattices as on the triangular lattice, the structure of an occupied vertex is still uniquely determined, while the structure of an empty vertex only is defined through the neighbouring occupied vertices and may not be uniquely given. This problem was resolved (Heilmann 1974) by including such vertices in the contour.

In this paper we consider the problem of third nearest neighbour exclusion on the square lattice as an example of a system where not even the structure of an occupied vertex is uniquely given without considering the configuration of the neighbouring vertices. Numerical calculations (Bellemans and Nigam 1967) indicate that the system has a phase transition.

2. The model

The model is the lattice gas model, the lattice is the square lattice and the particles are hard-core particles with third nearest neighbour exclusion, a configuration is shown in figure 1. The model also describes a system of hard pentamers on the square lattice as shown in figure 2, and in the following we shall refer to the model in terms of the pentamer system.

In the close-packed configuration all lattice points are covered by the pentamers and a region with one state is a region with close-packed pentamers. The structures of five different states are generated by translating one such ordered state on the square lattice by one unit. It is not possible to generate all the different states from each other by translation. In figure 3 two states are shown for which this is not the case. They can, however, be transformed to each other by a reflection in a diagonal line on the square lattice, a reflection that leaves the lattice invariant. The ten different states generated from each other by translation and reflection exhaust the possibilities.

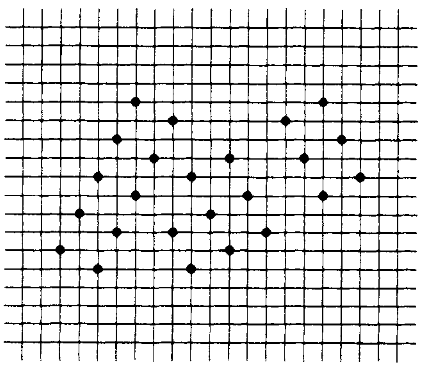

Figure 1. The configuration of a lattice gas with third nearest neighbour exclusion.

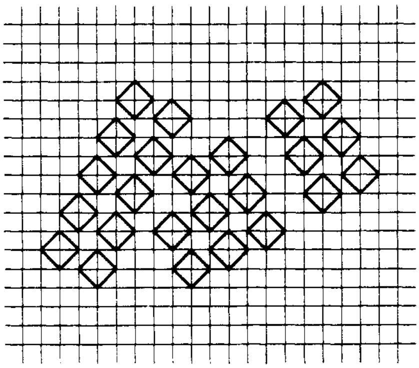

Figure 2. Hard pentamers on a square lattice in a configuration equivalent to the lattice gas configuration of figure 1.

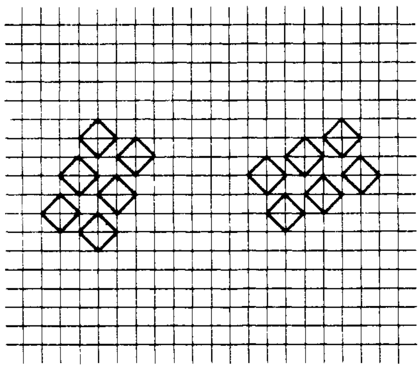

Figure 3. Two states that cannot be generated from each other by a translation on the lattice.

Consider the boundary of the system to have one fixed structure which we shall call the A structure. A different structure inside the boundary will, in general, be separated from the A structure by lattice points not covered by any particles. There is, however, the possibility that a particle can belong to two different structures as exemplified by the shaded pentamer in figure 4. The empty lattice points specify the configuration completely and a contour is now defined by tracing a curve through the empty points, a unit length of contour being a line segment between two adjacent empty points. In figure 5 the contour is seen to pass through a particle belonging to two structures; since such a particle can be considered to be part of the contour we do not need to assign it to a definite structure.

The contour separating the outer A structure from the structures inside is not a simple polygon; where different structures meet there is a possibility of branch points as seen in figure 5. The elimination of such a contour is described in detail in Heilmann and Præstgaard (1973).

The number of ways of continuing the contour is limited by the fact that adjacent empty points can only be separated by a certain distance, otherwise they will not be adjacent points, ie either there is an empty point between them or the space between

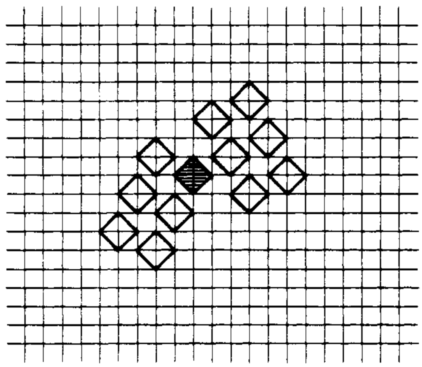

Figure 4. A configuration with a pentamer (shaded) belonging to two different states.

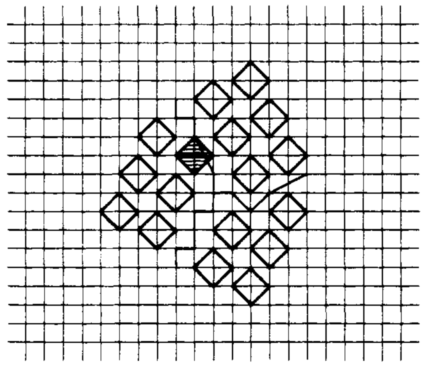

Figure 5. A contour with branch points which passes through a pentamer (shaded) belonging to two states.

them will be occupied with pentamers belonging to one structure. The possible contour segments in the positive quadrant are shown in figure 6.

The number of ways of drawing one contour segment is thus at most 35, and the number of ways of continuing a contour is thus bounded by

$$q = 1+35+\binom{35}{2}$$

where the possibilities of contour termination and branching are included.

The general theory behind the elimination of a contour using reflection symmetry is described in Heilmann (1974), where it is shown that Peierls' argument applies if the free energy of a contour segment can be made larger than a constant f_0:

$$\beta\epsilon - q > f_0$$

where ϵ is the lower bound on the energy of a contour segment. In the present case, where each particle covers five lattice points, we have $\epsilon = \mu/5$, where μ is the chemical potential of the particles.

We shall not go into any details about the rather complicated derivation leading to this result. However, it is necessary to consider one point. An important step is to transform the contours inside a region separately, ie reflect them in different lines of reflection. This might cause contours to cross each other after they have been reflected

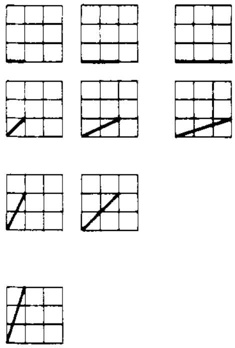

Figure 6. The possible contour segments in the positive quadrant.

in which case they are reflected in the same reflection line. In order to keep track of this, one has to keep track of the crossing points, and in this it was tacitly assumed that there was only one possible crossing point per unit step of contour. In the present case there are three possible crossing points for some of the contour segments. Rather than modifying the lengthy proof to include the possibilities of more than one crossing point, we shall just redefine a contour segment to be one third of the length considered so far. With the new definition of a segment, there can only be one crossing point and Peierls' argument will thus show a phase transition, if the inequality

$$\tfrac{1}{3}(\tfrac{1}{5}\beta\mu - q_0) > f_0$$

is fulfilled. We thus conclude that the system of hard pentamers on a square lattice has a phase transition, since it exists in an ordered phase for

$$\beta\mu > 15f_0 + 5q_0.$$

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