Vertex models for the hard-square and hard-hexagon gases, and critical parameters from the scaling transformation

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D W Wood and M Goldfinch

Mathematics Department, University of Nottingham, Nottingham, UK

Abstract. In a general formulation of hard-core lattice gas models the hard-square and hard-hexagon models are expressed in terms of vertex models. It is shown that the hard-square gas is a 16-vertex model on the square lattice, and in one of its representations is equivalent to a lattice ramrod model first considered by Nagle. A lattice transformation of the hard-hexagon model generates a special case of the 64-vertex model on the triangular lattice. In these two reductions clear differences between these two hard-core models emerge, and it is probably not surprising that they exhibit quite different critical behaviour. It is also shown that the block-site scaling transformation can be used to provide an alternative computational scheme for obtaining accurate numerical estimates of critical point parameters for these models. The method is illustrated by calculations performed on the hard-square gas.

1. Introduction

Interest in the critical behaviour of hard-core lattice gas models has recently been revived by the work of Baxter and co-workers. Baxter and Tsang (1980) and Baxter *et al* (1980) have demonstrated that the corner transfer matrix formalism (Baxter 1978) can be applied to two-dimensional hard-core models to yield a very considerable extension of the earlier power-series expansions of Gaunt and Fisher (1965), and Gaunt (1967). In addition, Baxter (1980) has obtained the exact evaluation of the partition function of the two-dimensional gas of hard hexagons. An important outcome of this recent work is that the critical point exponents of the hard-square and hard-hexagon lattice gas models are quite different.

Both of these simple one-parameter models model the short-range repulsive forces which characterise all interatomic potentials; this is achieved by prohibiting simultaneous occupancy of a small extension of configuration space centred on each atom. This feature is present in the equilibrium structure of all atomic liquids, and is often thought to be a characteristic of the potential which dominates the nature of the melting transition. For a lattice gas this effect is accomplished by excluding any atomic configuration containing atoms simultaneously occupying nearest-neighbour lattice sites. In this sense the hard-square and hard-hexagon gases are precisely the same physical model, but in different lattice spaces, the simple quadratic and triangular lattices respectively. The quite different nature of these two phase transitions is somewhat worrying in terms of the general aims of this type of model building, which is

to unify transition phenomena under strong and common characteristics of interaction potentials. One purpose of the present paper is to examine these two models from a graph theoretical standpoint to see if the two lattice symmetries invoke differences between them. We find that this is indeed the case. The second purpose here is to present an alternative scheme for computing all of the critical parameters for such models.

In § 2 several mathematical equivalences between hard-core models and vertex models are established. In one such transformation the hard-hexagon gas is shown to be equivalent to a gas of hard and bent trimers on the quadratic lattice; however, both models can be transformed into types of ramrod models first introduced by Nagle (1968), and here clear differences emerge when the two model partition functions are considered as graph generating functions.

The general formulation of hard-core lattice problems which is given here leads naturally to the formulation of any such problem in terms of a transfer matrix. This makes it possible both to apply and to test the type of scaling transformation introduced by Nightingale (1976) as a reliable alternative method for computing any critical parameter for these models. The advantage of such an approach to these models could well be very considerable when consideration is given to extending the models to include additional potential features such as some form of short-range attraction. The jump from one to two parameters can severely inhibit the series expansion approach, where for example it may well increase the computing requirements by an order of magnitude, as for example in the corner transfer matrix method; in the method presented here this is much less the case. The use of the scaling transformation is presented in § 3, where some calculations are performed on the hard-square gas†. In our view these calculations show the scaling transformation to be very successful, and the method probably holds much promise for development and future work.

2. Expansions and vertex models

Consider any hard-core lattice gas where a simultaneous occupation of nearest-neighbour sites is excluded by an infinitely repulsive force, and where in addition the interatomic potential is zero for all separations beyond nearest-neighbour (nn) distances. For such models the grand partition function Ξ will be a function of the activity z of an occupied site. A low-density expansion of $\Xi(z)$ can be developed on an arbitrary lattice L_q (q is the nn coordination number) in terms of the embeddings of *all* the subgraphs $G \in L_q$. Using the site variables t_i (i labels the lattice site), where $t_i = 1(0)$ if an atom is present (absent) at a site i, $\Xi(z)$ can be written in the form

$$\Xi(z) = \sum_{\{t\}} \prod_{nn} (1 - t_i t_j) \prod_{i=1}^{N} z^{t_i}, \qquad (1)$$

where the summation is over the 2^N atomic configurations, and the first continued product extends over all nn pairs of lattice sites. In (1) the factor $(1 - t_i t_j)$ acts to annihilate atomic configurations in which nn sites i and j are simultaneously occupied.

On expanding the first product in (1) and summing over all configurations $\{t\}$, we generate the series expansion

$$\Xi(z) = (1+z)^N \left(1 + \sum_{G \in L_q} (-1)^l [G:l:p] u^p\right), \tag{2}$$

where $[G:l:p]$ is the number of embeddings of G which contains l edges and p vertices, and $u = z/(1+z)$. For the hard-square gas (2) generates the 'low z' expansion of Gaunt and Fisher (1965), but these authors formulated their expansion in terms of the direct emplacement of atoms on the lattice. The expansion in (2) was in fact generated by Gaunt and Fisher (see also Baxter *et al* 1980) as an Euler transformation $u = z/(1+z)$ to improve the convergence and general numerical analysis of their own series. Here (1) and (2) make it clear that the variable u has a graph theoretical significance and is a natural variable for *all* hard-core gas models.

The formulation in (1) has the advantage of being an algebraic basis for performing lattice transformations and for establishing transfer matrices (see § 3). Thus, for any lattice with a two-sublattice structure, we can define z_a and z_b as the activities on sublattices a and b, and write

$$\Xi(z_a, z_b) = \sum_{\{t_b\}} \sum_{\{t_a\}} \prod_{(a)} (1 - t_a t_{b_1})(1 - t_a t_{b_2}) \ldots (1 - t_a t_{b_q}) z_a^{t_a} \prod_{(b)} z_b^{t_b} \tag{3}$$

where an a-site has q nn b-sites and where $\Pi_{(a)}$, and $\Pi_{(b)}$ extend over all a- and b-sublattice sites respectively. The sums over each t_a variable can be done independently, and (3) becomes

$$\Xi(z_a, z_b) = \sum_{\{t_b\}} \prod_{(a)} [1 + (1 - t_{b_1})(1 - t_{b_2}) \ldots (1 - t_{b_q}) z_a] \prod_{(b)} z_b^{t_b}. \tag{4}$$

The atom occupancy variables on the b-sublattice can now be transformed into the hole occupancy variables $r_i = 1 - t_i$, whence

$$\Xi(z_a, z_b) = \sum_{\{r_b\}} \prod_{(a)} (1 + r_{b_1} r_{b_2} \ldots r_{b_q} z_a) \prod_{(b)} z_b^{1-r_b}. \tag{5}$$

If we construct a geometrical object out of the vertices $b_1, b_2, \ldots, b_q$ and call it a q-gon, then the first product in (5) is over all such q-gons in L_q, each containing one original a-site. The product in (5) can be expanded in the usual way and the sums over $\{r_b\}$ performed; here we make use of the fact that $r_i^m = r_i$. Thus a typical term in (5) relates to a graph containing n q-gons as a subgraph in L_q with, say, v vertices; this will yield a contribution to (5) of

$$[k:n:v] z_a^n (1 + z_b)^{N/2 - v} \tag{6}$$

where $[k:n:v]$ is the number of embeddings of a graph of type k composed of n q-gons. Thus

$$\Xi(z_a, z_b) = (1 + z_b)^{N/2} \sum_{n,k} [k:n:v] z_a^n (1 + z_b)^{-v}. \tag{7}$$

In the case of the hard-square gas the q-gon is the square of b-sites surrounding an a-site, and the expansion (7) is over all possible configurations of squares on a simple quadratic lattice of $N/2$ sites. This expansion was obtained by Gaunt and Fisher (1965) using a combinatorial argument, and can be used to relate high- and low-density expansions of the hard-square gas.

The hard-square gas can be formulated as a special case of a 16-vertex model on the square net. The construction is very simple and is illustrated in figure 1. In all of what follows we shall use the notation shown in figure 2 for the 16-vertex model, where the vertex states are denoted by graphs of solid and dotted lines (further references can be obtained from Lieb and Wu (1972), and Wood (1975)). Each site of the original lattice is located on an edge of the so-called super-lattice (also a square net) represented by the broken lines in figure 2. A 1 : 1 equivalence exists between the atomic configurations on the original lattice and the vertex configurations on the super-lattice through the representation $(t = 1) \equiv$ (solid line), and $(t = 0) \equiv$ (dotted line). Thus the sixteen vertex states are generated by the sixteen atomic configurations possible on the squares of the original lattice. The hard-core exclusion reduces the non-zero vertex weights to only seven; these are

$$\omega_1 = 1, \qquad \omega_3 = \omega_4 = z, \qquad \omega_9 = \omega_{10} = \omega_{11} = \omega_{12} = \sqrt{z}. \qquad (8)$$

It is clear that the 16-vertex model in (8) generates configurations of rigid linear rods of arbitrary lengths in both horizontal and vertical directions, where no two rods can intersect $(\omega_2 = 0)$. This vertex model is in fact a *lattice gas* of such rods, and was considered by Nagle (1968) in a general discussion of weak graph expansions under the title of a 'lattice ramrod model'. Nagle speculated that such a model might have a phase transition similar to the lattice gas of hard squares!
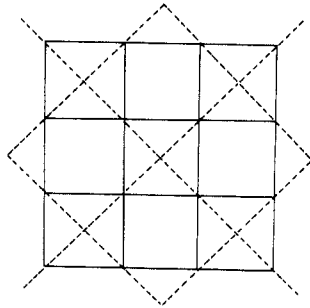
Figure 1. The vertex configurations of the 16-vertex model.
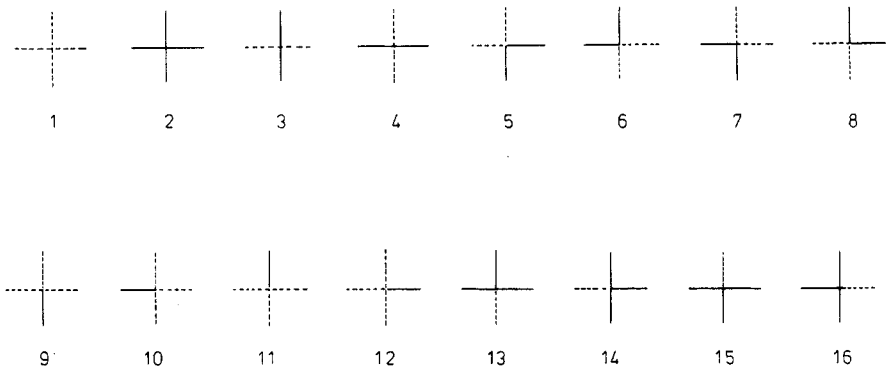
Figure 2. Each vertex configuration of the super-lattice (dotted lines) can be defined by the 16 possible atomic configurations of the four surrounding vertices of the original lattice.

It is interesting to consider Fisher's super-exchange model of a lattice gas (Fisher 1963) in relation to the vertex model (8). The general super-exchange model includes nn exclusion on the square lattice, but in addition the atoms can interact over next-nearest-neighbour (nnn) distances, *but* only those formed in alternate squares (the white squares on a chess board say). Using the same notation as in (1), the partition function for this model is in the form

$$\Xi(z, x) = \sum_{\{t\}} \prod_{(ab)} (1 - t_a t_b) \prod_{(aa')} x^{t_a t_{a'}} \prod_{(bb')} x^{t_b t_{b'}} \prod_{(a)} z^{t_a} \prod_{(b)} z^{t_b} \tag{9}$$

where (ab) runs over all nn pairs, (aa') and (bb') run over all nnn pairs in 'white' squares, and $x = \exp(-\beta\epsilon)$ where ϵ is the interaction potential at nnn distances. If the white squares are chosen to be the squares in figure 1 containing the vertices of the super-lattice, then the super-exchange lattice gas can be seen to be the 16-vertex model with vertex weights,

$$\omega_1 = 1, \qquad \omega_3 = \omega_4 = xz, \qquad \omega_9 = \omega_{10} = \omega_{11} = \omega_{12} = \sqrt{z}, \tag{10}$$

and contains the monomer dimer problem at $x = 0$. Fisher showed that (9) can be transformed into an Ising model in zero field under the transformation

$$\exp(4K) = 1 + 4z \qquad (K = \beta J) \tag{11}$$

for the special case $x = 2$, at which point (9) can be written in the form

$$\Xi(z) = \sum_{\{t\}} \prod_{(ab)} (1 - t_a t_b) \prod_{(aa')} (1 + t_a t_{a'}) \prod_{(bb')} (1 + t_b t_{b'}) \prod_{(a)} z^{t_a} \ldots \prod_{(b)} z^{t_b}. \tag{12}$$

Fisher's treatment of the super-exchange model is in terms of a rather complicated spin decoration transformation, and involves redundant many-body terms. Here we investigate the general vertex model (10) in terms of the theory of Gaaf and Hijmans (1975), which is a very compact scheme for investigating the structure of any arbitrary 16-vertex model. Any such model can be reduced to a standard model which has only ten independent parameters, and these have an invariance property which allows all of the equivalent forms of a given model to be generated by a group of linear transformations. In particular, the standard model allows for a classification of a given model in terms of well known subclasses of the general model. Following this scheme through for (10), the partition function of the original model is expressed first in terms of 16 new parameters in the form

$$Z = Z(w_0, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{W}) \tag{13}$$

where in the case of (10) the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ are

$$\boldsymbol{u} = \boldsymbol{v} = (\tfrac{1}{2}\sqrt{z}, 0, \tfrac{1}{4}) \tag{14}$$

and the matrix $\boldsymbol{W}$ is given by

$$\boldsymbol{W} = \begin{pmatrix} 0 & 0 & \tfrac{1}{2}\sqrt{z} \\ 0 & 0 & 0 \\ \tfrac{1}{2}\sqrt{z} & 0 & \tfrac{1}{4}(1 - 2xz) \end{pmatrix}. \tag{15}$$

In terms of the new parameters $\boldsymbol{u}$, $\boldsymbol{v}$ and $\boldsymbol{W}$, all equivalent forms of (10) are generated by the set of 3×3 orthogonal linear transformations R_s and R_t, where

$$Z(w_0, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{W}) = Z(w_0, R_s^{-1}\boldsymbol{u}, R_t^{-1}\boldsymbol{v}, R_s^{-1}\boldsymbol{W}R_t). \tag{16}$$

In particular if $R_s^{(0)}$ and $R_t^{(0)}$ transform W to the diagonal form $W^{(0)}$, and correspondingly u and v to $u^{(0)}$ and $v^{(0)}$, then the transformed vertex weights $\omega_i^{(0)}$ have the symmetry given by

$$\omega_5^{(0)} = \omega_6^{(0)}, \qquad \omega_7^{(0)} = \omega_8^{(0)}, \qquad \omega_9^{(0)} = \omega_{15}^{(0)}, \qquad \omega_{10}^{(0)} = \omega_{16}^{(0)},$$

$$\omega_{11}^{(0)} = \omega_{13}^{(0)}, \qquad \omega_{12}^{(0)} = \omega_{14}^{(0)}. \tag{17}$$

The condition that the original model is equivalent to a general 8-vertex model is that the standard vectors $u^{(0)}$ and $v^{(0)}$ lie along one (and the same) of the axes. $R_t^{(0)}$ obtained from (15) transforms u and v in (14) to yield

$$u^{(0)} = v^{(0)} = \{(z+\lambda_1)/2(z+4\lambda_1^2)^{1/2}, 0, (z+\lambda_2)/2(z+4\lambda_2^2)^{1/2}\} \tag{18}$$

where $\lambda_{1,2}$ are the two non-zero eigenvalues of W. Thus for (10) to be a general 8-vertex model, one of the eigenvalues of W must be $-z$; the *only* point at which this is possible is at $x = 2$, at which point the model is a free fermion model (Fan and Wu 1970), and the critical point is

$$z_c = (1+\sqrt{2})/2. \tag{19}$$

All the other cases of (10) are transformed into versions of the 16 vertex model; the standard model has the vertex weights

$$\omega_1^{(0)} = (1+2xz)/4 + (z+\lambda_2)/(z+4\lambda_2^2)^{1/2} + \lambda_2 \tag{20}$$

$$\omega_2^{(0)} = (1+2xz)/4 - (z+\lambda_2)/(z+4\lambda_2^2)^{1/2} + \lambda_2 \tag{21}$$

$$\omega_3^{(0)} = \omega_4^{(0)} = (1+2xz)/4 - \lambda_2 \tag{22}$$

$$\omega_5^{(0)} = \omega_6^{(0)} = \omega_7^{(0)} = \omega_8^{(0)} = \lambda_1 \tag{23}$$

$$\omega_9^{(0)} = \omega_{10}^{(0)} = \ldots = \omega_{16}^{(0)} = (z+\lambda_1)/2(z+4\lambda_1^2)^{1/2}. \tag{24}$$

Finally we note that in the special case of the hard-square gas ($x = 1$) an equivalent 16-vertex model form of the problem is given by the expansion (2), which is generated by the vertex weights

$$\omega_1 = 1+z, \qquad \omega_2 = z, \qquad \omega_3 = \omega_4 = \ldots = \omega_8 = -z,$$

$$\omega_9 = \omega_{10} = \omega_{11} = \omega_{12} = iz, \qquad \omega_{13} = \omega_{14} = \omega_{15} = \omega_{16} = -iz. \tag{25}$$

It is interesting to note in passing that the hard-core model (1) on the Kagomé lattice is simply the monomer dimer problem on the hexagonal lattice. The construction is shown in figure 3, where the hexagonal lattice is superimposed onto the Kagomé lattice. Under the equivalence ($t = 1(0)$, Kagomé) = (solid (dotted) line, hexagonal), the hard-square gas on the Kagomé lattice is a special case of the 8-vertex model on the hexagonal lattice (Wu 1974), where the non-zero weights are

$$ \tag{26}$$
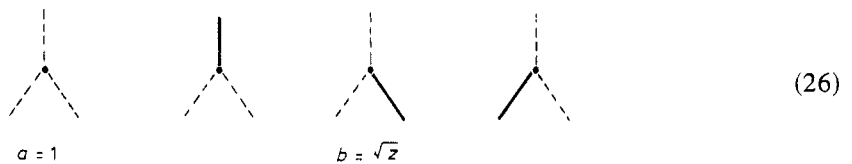
This is the monomer dimer problem on the hexagonal lattice, and is known not to have a phase transition (Heilmann and Lieb 1972). In this respect the same 'physical' models
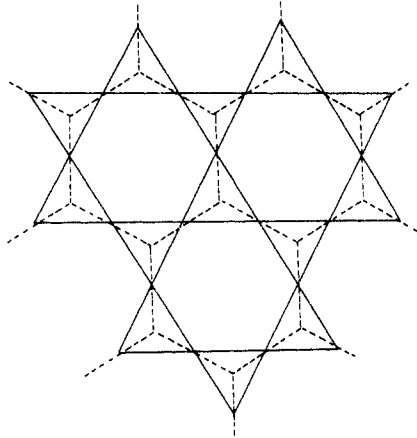
Figure 3. The hexagonal lattice superimposed onto the Kagomé lattice. The eight possible atomic configurations on a triangle define the vertex states of the hexagonal lattice.

(1) on the Kagomé and simple quadratic lattices are radically different; the simple quadratic lattice model is known to have a phase transition (Dobrushin 1968). It is immediately obvious that the two vertex models (26) and (8), when viewed as graph generating functions on their respective lattices, generate quite different classes of graph, and it would appear that the differences in lattice symmetry have undermined the original modelling idea, in a way which cannot happen in, say, the Ising model lattice gas.

We now show that a very similar effect appears when we reduce the hard-hexagon gas to a vertex model. Consider (1) on the triangular lattice. We can perform a partial trace in the manner of (4) over the sites denoted by an open circle in figure 4. This will in effect remove all of the bonds incident at such sites, thus leaving the Kagomé lattice denoted by the heavy lines in figure 4. On taking the partial trace, we find that the partition function can be expressed in the form

$$\Xi(z) = \sum_{\{t\}} \prod_{nn} (1 - t_i t_j) \prod_h f_h(t_1, t_2, \ldots t_6, z) \prod_i z^{t_i}. \tag{27}$$

In (27) the first product is over all nn pairs in the Kagomé lattice, the second product is over all of the hexagonal holes (the decimated sites of the original lattice) of the Kagomé lattice and the third product runs over the sites of the Kagomé lattice. The functions f_h are defined on the site variables of each hexagonal hole (here denoted by $t_1, t_2, \ldots, t_6$) and are given by

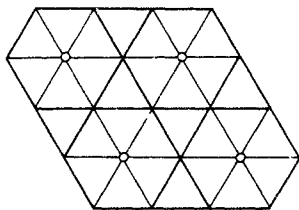$$f_h = 1 + (1 - t_1)(1 - t_2) \ldots (1 - t_6)z. \tag{28}$$

Figure 4. The partial trace in (27) is taken over the sites denoted by the open circles.

Now we can place a vertex of a new triangular lattice at the centre of each hexagonal hole, as illustrated in figure 5; on making the usual equivalence ($t = 1(0)$, Kagomé) = (solid (dotted) line, triangular) the 64 atomic configurations on each hexagonal hole
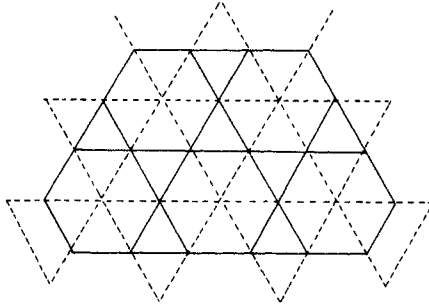

Figure 5. The vertex states of the triangular lattice sites are defined by the 64 possible atomic configurations on the surrounding hexagons of the Kagomé lattice.

generate the 64 vertex states of the 64-vertex model on the triangular lattice. On writing (27) in the form

$$\Xi(z) = \sum_{\{t\}} \prod_h F_h, \tag{29}$$

where, following the scheme of (28),

$$F_h = (1 - t_1 t_2)(1 - t_2 t_3) \ldots (1 - t_6 t_1) f_h z^{(t_1 + t_2 + \cdots + t_6)/2}, \tag{30}$$

we see that the 64 vertex weights are given by the values of F_h. The gas of hard hexagons is then equivalent to the following special case of the 64-vertex model where the *non-zero* weights are
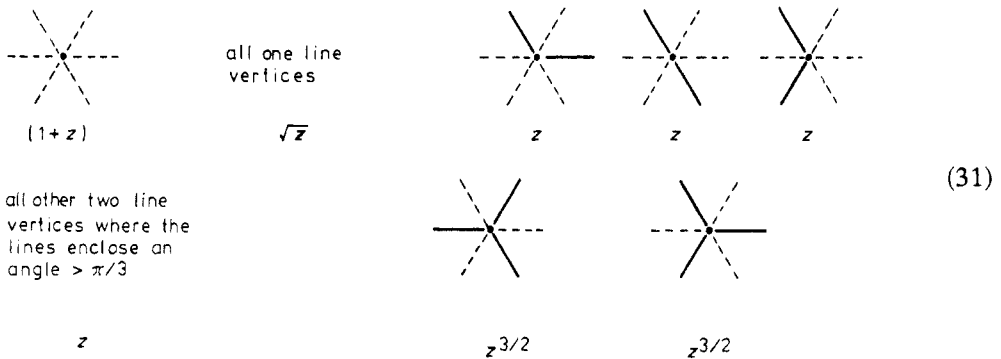
We can now see that the vertex model of (31) is *not* simply a generalisation of the previous ramrod model (8) to the triangular lattice. It is in fact quite different. The partition function of (31) will generate closed loops (polygon subgraphs) because of the bends which are allowed in the degree-two vertices. The two allowed degree-three vertices will also generate classes of graphs which are excluded in (8). Thus, from a graph theoretical viewpoint, the 'physical' models (1) on the square net and triangular lattices are very different types of graph generating function; this is again the effect of

differences in lattice symmetry, and on this basis alone it might be anticipated that the two models would exhibit quite different types of transition.

A rather intriguing equivalence between the hard-hexagon gas and a 16-vertex model on the simple quadratic lattice is illustrated by the construction in figure 6, where
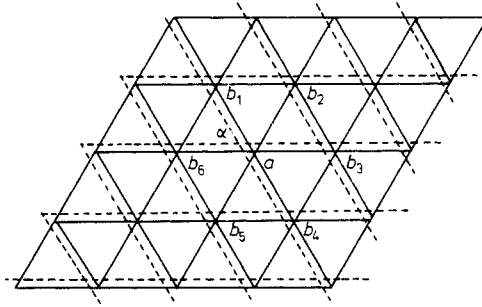

Figure 6. The square lattice superimposed onto the triangular lattice in such a way that each triangular lattice site lies within one square of the simple quadratic lattice.

a square lattice has been superimposed onto the triangular lattice in such a way that every site of the triangular lattice is enclosed by a square of the square net. If a site such as 'a' in figure 6 is occupied by an atom, the exclusion prohibits the occupancy of sites $b_1, b_2, \ldots, b_6$. Now if we place the vertex configuration ω_5 on the square lattice site 'α' corresponding to 'a', and repeat this decoration for all such sites which are occupied, we recover the vertex configurations of a 16-vertex model where the only non-zero weights are

$$\omega_1 = 1 \qquad \omega_5 = z \qquad \omega_{10} = 1 \qquad \omega_{11} = 1 \tag{32}$$

If in the model (32) a particular vertex is in the configuration ω_5, then there are six neighbouring vertices (four nn and two nnn) which cannot be in this same configuration; this is in 1 : 1 correspondence with the nn exclusion of the atomic model. We can think of the ω_5 vertices as representing a triatomic molecule, which is hard in the sense that none of the three atoms can be superimposed onto an atom of another molecule. Thus the gas of hard hexagons is equivalent to a gas of bent trimers held in a fixed orientation on the simple quadratic lattice, and the thermodynamics of this system are of course given by Baxter's recent exact solution (Baxter 1980). In his work on the weak graph expansion, Nagle (1968) also speculated that 'objects' longer than dimers would probably undergo a proper phase transition.

3. The scaling transformation

The most accurate calculations of the critical point parameters of the hard-square lattice gas are those recently obtained by Baxter *et al* (1980), who developed very long

power-series expansions for various thermodynamic functions of the model. Dowson (1979) has recently completed a detailed investigation into the scaling transformation approach of Nightingale (1976) over a wide range of spin lattice models, in terms of it being a serious alternative method of providing accurate numerical estimates of critical point parameters. We show here that the scaling transformation can be used to determine the critical parameters of hard-core lattice gas models with a high degree of accuracy.

The basis of the method is the simple site-block scaling transformation of Kadanoff *et al* (1967), which in the thermodynamic limit can be represented in the form

$$b^d \beta f(\beta) = g(\beta) + \beta' f(\beta') \qquad (\beta = 1/kT) \qquad (33)$$

where $f(\beta)$ and $f(\beta')$ are the appropriate free energies per site and per block respectively, and b is the spacial rescaling factor. In (33) $g(\beta)$ is the so-called regular part of the free energy (for further details see Niemeijer and van Leeuwen (1976)), and β and β' are the site and block inverse temperatures respectively. The corresponding scaling relation for the correlation length ξ is

$$\xi(\beta) = b\xi(\beta'); \qquad (34)$$

thus if $\beta = \beta' = \beta^*$ is a solution of (34), $\xi(\beta^*)$ is either 0 or infinity, and β^* is either the true critical point or a trivial fixed point of the system. The critical exponent of the correlation length ν is given by

$$b^{1/\nu} = (\partial \beta'/\partial \beta)_{\beta = \beta^*}. \qquad (35)$$

The scaling transformation of Nightingale (1976) aims to achieve a sequence of approximations of increasing accuracy to both (33) and (34) by using *finite* lattice systems of N and N' sites ($b^d N' = N$) in which correlation lengths ξ_N and $\xi_{N'}$ can be defined, and where (34) becomes

$$\xi_N(\beta) = b\xi_{N'}(\beta'). \qquad (36)$$

Now if a solution to (36) exists in the form $\beta = \beta' = \beta^*$, ξ_N and $\xi_{N'}$ do not have to be zero or infinity. For systems of increasing size, (36) must approach (34) in the thermodynamic limit; hence it may be hoped that sequences $\beta^*(b)$ obtained from (36) and $\nu(b)$ from (35) will converge to the true critical values of the model. On the square net lattice the finite systems N and N' can be chosen to be two strips of $N = mL$ and $N' = nL(n < m)$ sites. Here the N' system represents the block system, and thus

$$b = m/n. \qquad (37)$$

Now if the correlation length for each system is determined in the limit $L \to \infty$, (36) takes the form

$$\xi_{m,\infty}(\beta) = b\xi_{n,\infty}(\beta'). \qquad (38)$$

The form of (1) and the various vertex models of § 2 make it easy to establish a transfer matrix for the hard-core lattice gas models. Our purpose here is to test this method for the hard square gas, where we consider a hard-square gas on an $m \times L$ lattice (m even) and define a symmetric transfer matrix T between neighbouring columns of m sites. The matrix T is readily obtained from the form of (1), and is given by

$$T(t:\tau) = \prod_{i=1}^{m} (1 - t_i t_{i+1}) \prod_{j=1}^{m} (1 - \tau_j \tau_{j+1}) \prod_{i=1}^{m} (1 - t_i \tau_i) z^{\frac{1}{2}\Sigma(t_i + \tau_i)} \qquad (39)$$

where t and τ are the m site variables on neighbouring columns, and cyclic boundary conditions are imposed. The dimension of T is less than $2^m \times 2^m$ because of the exclusion contained in (39); thus, for $m = 2$, T is given by

$$T = \begin{pmatrix} 1 & \sqrt{z} & \sqrt{z} \\ \sqrt{z} & 0 & z \\ \sqrt{z} & z & 0 \end{pmatrix} \tag{40}$$

and the dimensions of T for strips of even width from 4 to 12 are 7, 18, 47, 123, and 322 respectively (see table 1).

Table 1. Estimates of the critical activity $z_c(m, n)$ and the critical exponent $\nu(m, n)$ obtained from the solutions to (47) and (48) by using the transfer matrices (39) and those of the vertex model (8). The corresponding results for Fisher's super-exchange gas ($x = 2$ in (10)) are also shown for comparison and are adapted from the results of Nightingale (1976).

From T in (39)			From the vertex model (10)			Fisher's super-exchange gas		
(m, n)	$z_c(m, n)$	$\nu(m, n)$	(m, n)	$z_c(m, n)$	$\nu(m, n)$	(m, n)	$z_c(m, n)$	$\nu(m, n)$
4, 2	4·1011	1·1613	3, 2	3·4494	0·9203	4, 3	1·1511	0·9442
6, 4	3·8536	1·0585	4, 3	3·6576	0·9500	5, 4	1·1798	0·9644
8, 6	3·8166	1·0278	5, 4	3·7348	0·9740	6, 5	1·1930	0·9772
10, 8	3·8057	1·0158	6, 5	3·7650	0·9858	7, 6	1·1991	0·9845
12, 10	3·8013	1·0098	7, 6	3·7783	0·9913	8, 7	1·2021	0·9888
						9, 8	1·2038	0·9915
						10, 9	1·2048	0·9933
Exact	3·7962†						1·2071	1

† The series result of Baxter *et al* (1980).

The correlation function $\langle t_0 t_r \rangle$ of two sites spacially separated by r lattice units along one row of the $m \times L$ system can be determined from the eigenvalues and eigenvectors of T (see Fisher and Burford 1967). In the limit $L \to \infty$ the result is

$$\langle t_0 t_r \rangle = \sum_j (\lambda_j / \lambda_1)^r (\varphi_1 \cdot t_0 \varphi_j)^2, \tag{41}$$

where $\lambda_1 > \lambda_2 > \lambda_3 \dots$ are the eigenvalues, and φ_j are the eigenvectors of T, which for (41) to hold must be symmetric, and

$$(\varphi_1 \cdot t_0 \varphi_j) = \sum_k \varphi_1(k) t_0(k) \varphi_j(k), \tag{42}$$

where k indexes the components of the eigenvectors and $t_0(k)$ is the value of t_0 in the configuration k (implicit in the ordering of T). The density is simply the first term in (41) where

$$\rho = (\varphi_1 \cdot t_0 \varphi_1). \tag{43}$$

If we carry out this calculation for the $2 \times L$ lattice using (40), we obtain

$$\langle t_0 t_r \rangle - \rho^2 = \left(\frac{(1+z) - g}{(1+z) + g} \right)^r \frac{z}{2g} + \left(\frac{-2z}{(1+z) + g} \right)^r \frac{(z-1) + g}{8g} \tag{44}$$

where

$$g = [(1+z)^2 + 4z]^{1/2}. \tag{45}$$

In the limit of maximum packing, we obtain the expected result

$$\lim_{z \to \infty} \langle t_0 t_r \rangle = (-1)^r \tfrac{1}{4} + \tfrac{1}{4} \tag{46}$$

yielding zero correlations for sites on different sublattices.

The correlation length $\xi_{m,\infty}$ of the correlation function defined on the sites of one sublattice can be obtained in the usual way (Fisher and Burford 1967; see also Dowson (1979)), and now (38) can be established in the form

$$m \ln[\lambda_1(m)/|\lambda_2(m)|] = n \ln[\lambda_1(n)/|\lambda_2(n)|] \qquad (m, n \text{ even}) \tag{47}$$

where $\lambda_{1,2}(m)$, and $\lambda_{1,2}(n)$ are the largest and next largest (in modulus) eigenvalues of the transfer matrices of the $m \times L$ and $n \times L$ systems respectively. Equation (47) is of course established numerically and a solution for $z_c(m, n)$ (the approximation to the critical point from (47)) is found by iteration. At $z_c(m, n)$ both $\xi_{m,\infty}$ and $\xi_{n,\infty}$ are numerically differentiated to determine the exponent estimate $\nu(m, n)$ given by

$$b^{1/\nu(m,n)} = \frac{1}{b}\left(\frac{\partial \xi_m}{\partial z}\right) \Big/ \left(\frac{\partial \xi_n}{\partial z}\right) \qquad (z = z_c(m, n)). \tag{48}$$

An alternative transfer matrix for the hard-square gas can be formed either by using the vertex model (8) or the form (5) for $\Xi(z)$ (they are equivalent). If we use (5), then

$$\Xi(z) = \sum_{\{t\}} \prod_s (1 + r_1 r_2 r_3 r_4 z) z^{\sum t_i} \tag{49}$$

where the product is over all the squares of the lattice, and r_1, r_2, r_3 and r_4 are the hole occupation variables at the vertices of a typical square. We can write (49) in the form

$$\Xi(z) = \sum_t \prod_s (1 + z)^{r_1 r_2 r_3 r_4} \prod_i z^{t_i} \tag{50}$$

and it is now a simple matter to define a transfer matrix between neighbouring columns of an $m \times L$ lattice. Both sets of transfer matrices have been used to form estimates of the critical activity z_c, and the exponent ν, which we assume is related to the exponent α by the scaling relation $d\nu = 2 - \alpha$, where α is the exponent in

$$(\rho_c - \rho) \sim (z_c - z)^{1-\alpha}. \tag{51}$$

The results of these calculations are shown in table 1, where we have also included a sample of Nightingale's results for the Ising model, which are here adapted to show the equivalent results for the super-exchange lattice gas at $x = 2$ in (10). The final result for z_c obtained by Baxter *et al*, using 24 terms in the expansion of the order parameter, is

$$z_c = 3 \cdot 7962 \pm 0 \cdot 0001. \tag{52}$$

The (12, 10) result for z_c in table 1 is only $0 \cdot 1\%$ away from this value. Baxter *et al* obtained the following result for the exponent α:

$$\alpha = 0 \cdot 09 \pm 0 \cdot 05. \tag{53}$$

There is good reason to suppose that the approach of the sequences $z_c(m, m - k)$ and $\nu(m, m - k)$ to the true critical values will be monotonic; this is the case in Nightingale's

calculations on the Ising model, which were performed using the analytic form of the solutions of Onsager for $m \times \infty$ strips. If we assume monotonic convergence for *both* of the sequences given in table 1, then we arrive at the conclusion that

$$-0 \cdot 0196 < \alpha < 0 \cdot 0174 \tag{54}$$

and this conflicts with the series result (53). It is tempting to conclude that the transition is Ising-like with the exact values $\nu = 1$ and $\alpha = 0$.

The method here can of course be used to determine the value of any thermodynamic function at the critical point. All of the thermodynamic properties of $m \times \infty$ strips can be found from $\lambda_1(m)$ and its derivatives at z_c. As an example, if we use $z_c(10, 8)$ in table 1 and $\lambda_1(10)$, we find that the critical density ρ_c and critical pressure βP_c are

$$\rho_c(m = 10) = 0 \cdot 3681 \tag{55}$$

and

$$\beta P_c(m = 10) = 0 \cdot 7951. \tag{56}$$

The series estimate of Baxter *et al* for ρ_c is $0 \cdot 368 \pm 0 \cdot 001$ and the series result of Gaunt and Fisher (1965) for the critical pressure is $0 \cdot 792 \pm 0 \cdot 005$.

4. Summary

We have shown that the hard-square lattice gas can be expressed as a special case of the 16-vertex model on the square net lattice, one form of which is identical to the lattice ramrod model originally considered by Nagle (1968). When a lattice transformation is performed on the hard-hexagon gas, a special case of the 64-vertex model on the triangular lattice emerges. In a graph theoretical sense, the two lattice symmetries invoke significant differences between these two hard-core lattice gas models when their respective partition functions are seen as graph generating functions.

Using the hard-square lattice gas as an example, we have shown how the scaling transformation of Nightingale (1976) can be employed as an alternative and accurate method of calculating all of the critical point parameters for these models. Our attempts to determine the correlation length exponent for atomic correlations on one sublattice seem to indicate Ising model values for the critical exponents.

Acknowledgments

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