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# Hamiltonian formulation of site percolation in a lattice gas†

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**Abstract.** Site percolation in an interacting lattice gas is formulated as the limit of a random Potts' model. Explicit results are also given within a Bethe cluster approximation for near-neighbour interactions and percolation lengths.

## 1. Introduction

A well known formulation of random bond percolation theory is that of Kastelyn and Fortuin (1969). By formulating random bond percolation theory as a regular Potts' model continued to 'unphysical' values of $q$, the number of states per site in the Potts' model, their formulation permits the use of Hamiltonian methods in the random bond percolation problem, as opposed to less familiar generating function methods. The Hamiltonian formalism was, for example, exploited by Harris *et al* (1975), who applied renormalisation group and other techniques to the problem.

A Hamiltonian formulation for random site percolation was recently suggested by Giri *et al* (1977) and also by Kunz and Wu (1978), who use a Potts' model but with interactions between $z$ spins on a covering lattice, where $z$ is the coordination number of the original lattice. The point of this article is to discuss a different Hamiltonian formulation for site percolation and simultaneously generalise it to include the case of percolation in an interacting lattice gas. In addition, the results for percolation for both attractive and repulsive interactions will be derived within the Bethe cluster approximation, using the new formulation.

The advantage of the present formulation is its conciseness. (Compare it, for example, with Coniglio and Essam (1977).) Not surprisingly, it allows an unusually concise derivation of results within the Bethe cluster approximation. Of course, so long as only this level of approximation is desired, any one of the equivalent formulations of Kikuchi (1970), Odagaki (1975) or Coniglio (1975) can be used. However, it is hoped that the present formulation will be more generally useful.

It should be stressed, to avoid confusion, that the present problem is quite different from that of the more familiar problem of dilute magnets. In dilute Ising models, percolation and thermodynamic properties are of course intimately related; in fact, in the zero-temperature 'percolation limit', the calculation of thermodynamic properties becomes equivalent to that of the percolative properties. In the present problem one is asking a completely different question; namely, what are the percolative properties (such as critical site fraction) when the site random variables are no longer independent

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but are governed according to lattice gas statistics? In contrast to dilute magnets, the thermodynamic properties in the present problem are those of the lattice gas, or regular Ising model in a field, and do not reflect in any obvious fashion the percolation properties (such as the critical fraction) of the lattice gas. However, as will be shown, the converse is certainly not true.

The percolative properties of a lattice gas may be of interest when components of a percolative system interact and are not quenched but are free to equilibrate (spatially). One could also consider the case of a dilute magnet of magnetic and non-magnetic atoms, which is quenched from a finite temperature $T$. If the magnetic interactions are relatively weak, the percolative properties will correspond to the thermodynamic distributions in the binary alloy at $T$, which are not strictly random.

## 2. The random Potts model

The Hamiltonian of interest is

$$\mathcal{H} = -J_n \sum_{(nn)} n_i n_j - H_n \sum_i n_i - J \sum_{(nn)} n_i n_j (\delta_{\lambda_i \lambda_j} - 1) - H \sum_i (\delta_{\lambda_i 1} - 1). \tag{1}$$

Here, $J_n$ and $H_n$ are the near-neighbour interaction strength and chemical potential for the lattice gas, respectively; $n_i = 0$ or 1 is the lattice gas random variable, and $\lambda_i$ is the Potts' model random variable which can have any of $q$ different values: $1, 2, \ldots, q$. The random variables $n_i$ and $\lambda_i$ are both taken to be unquenched in the present case in contrast to dilute spin models, where $n_i$ is usually taken to be quenched†. Percolative properties in the lattice gas governed by $J_n$ and $H_n$ are recovered in the limits:

$$J \to \infty, \qquad q \to 1, \qquad H \to 0^+. \tag{2}$$

In order to give the precise relationships, one starts with the partition function for (1):

$$\begin{aligned} Z &= \mathrm{Tr}_{n,\lambda}\, \mathrm{e}^{-\beta\mathcal{H}} \\ &= \mathrm{Tr}_n \exp\Big[\beta\Big(J_n \sum n_i n_j + H_n \sum_i n_i\Big) \\ &\quad \times q^{(N-\sum_i n_i)} \sum_\gamma p^{R_\gamma} (1-p)^{L_\gamma} \prod_{\mathcal{G}(\gamma)} [1 + (q-1)\, \mathrm{e}^{-\beta H n_c}]. \end{aligned} \tag{3}$$

The second line is obtained by now standard techniques (Kasteleyn 1969), where $N$ is the total number of sites and $p \equiv 1 - \mathrm{e}^{-\beta J}$ is the bond probability. Here, $\{\gamma\}$ is the set of ways one can introduce near-neighbour bonds on the *restricted* lattice where only those sites with $n_i = 1$ are considered present; $\mathcal{G}(\gamma)$ is the set of clusters present in one particular configuration $\gamma$; $R_\gamma$ and $L_\gamma$ are the number of bonds present and bonds missing, respectively, from the restricted lattice; and $n_c$ is the number of sites in the $c$th cluster in $\mathcal{G}(\gamma)$.

† An alternative formulation is possible if one uses quenched random variables. The site diluted Ising model is known to be equivalent to the site percolation problem in the 'percolation limit'. One need only distribute the quenched site variables $n_i$ according to lattice gas statistics. Such a formulation with quenched random variables can be brought into Hamiltonian form by using spin glass 'replica methods'. See, for example, Stephen and Giri (1978).

In the limit of $J \to +\infty$, $p$ tends to unity, and only the maximally connected configuration $\gamma_m$ contributes. The quantity

$$x_f = \frac{1}{N}\left\langle \sum_{c \in \mathcal{G}(\gamma_m)} n_c \right\rangle = \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{N}\frac{1}{1-q}\frac{\partial}{\partial y} \ln Z \tag{4}$$

where $y = \beta H$, therefore represents the fraction of sites in finite clusters. In the above, the brackets denote the thermodynamic average

$$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}_n \, \mathrm{e}^{-\beta \mathcal{H}_l} \mathcal{O}}{\mathrm{Tr}_n \, \mathrm{e}^{-\beta \mathcal{H}_l}}$$

where

$$\mathcal{H}_l = -J_n \sum_{(nn)} n_i n_j - H_n \sum_i n_i$$

is the lattice gas Hamiltonian. The fraction of sites which are part of the infinite cluster is therefore

$$\tilde{P}(x, \beta J_n) = x - x_f \tag{5}$$

where $x$ is the density

$$x = \left\langle \sum_i n_i \right\rangle \Big/ N.$$

The mean square cluster size is also given by

$$S = \frac{1}{N}\left\langle \sum_{c \in \mathcal{G}(\gamma_m)} n_c^2 \right\rangle = \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{N}\frac{1}{q-1}\frac{\partial^2}{\partial y^2} \ln Z. \tag{6}$$

The pair connectedness $C_{ij}$, the probability that $i$ and $j$ lie within the same finite cluster, can be defined in a manner similar to $S$, by introducing inhomogeneous fields $y_i$ at each site. The relation is

$$C_{ij} = \lim_{\substack{J\to\infty \\ q\to 1 \\ \{y_i\}\to 0^+}} \frac{1}{q-1}\frac{\partial}{\partial y_i}\frac{\partial}{\partial y_j} \ln Z. \tag{7}$$

Thus, by calculating the partition function for the general Hamiltonian and then taking appropriate limits, site percolation properties of the lattice gas are automatically generated. Random site percolation is of course obtained for the special case $J_n = 0$.

One can readily extend the above formulation to cases where the pairwise interactions $J_n$ and $J$ extend beyond near neighbours. Thus the continuum limit can be considered. In particular, in a problem where the percolation or connectivity length extends beyond near neighbours, one simply assigns a non-zero $J$ between each pair of sites $(i, j)$ which are to be considered 'connected' when filled and then takes the limit $J \to \infty$ for each such $J$ in the final formulae. The percolation length, or range of $J$, can of course be different from the interaction length, or range of $J_n$.

## 3. The Bethe cluster approximation

The above Hamiltonian formulation will be used here to derive results within the Bethe cluster approximation. One can proceed for $J_n > 0$ and outside the two-sublattice region for $J_n < 0$ by taking a single cluster consisting of a central site and its near neighbours. The effects of the rest of the lattice will be represented by fields $H'_n$ and $H'$, analogous to $H_n$ and $H$, respectively, but which act in place of them on the near neighbours. Their values are determined by the usual translational invariance assumptions

$$x \equiv \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{\partial \ln Z_C}{\partial y_n} = \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{z} \frac{\partial \ln Z_C}{\partial y'_n} \tag{8}$$

where $y_n = \beta H_n$, $y'_n = \beta H'_n$, $z$ is the coordination number, and $Z_C$ is the 'partition function' for the finite Bethe cluster. Similarly

$$x_f \equiv \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{1-q} \frac{\partial}{\partial y} \ln Z_C = \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{z} \frac{1}{1-q} \frac{\partial}{\partial y'} \ln Z_C \tag{9}$$

where $y = \beta H$ and $y' = \beta H'$. Thus, the joint lattice gas and percolation problem is reduced to evaluating $Z_C$, which is straightforward. It is given by

$$\begin{aligned} Z_C = {} & q[q + \exp(y'_n) + (q-1)\exp(y'_n - y')]^z \\ & + \exp(y_n)[q + \exp(\beta J_n + y'_n) + (q-1)\exp(\beta J_n + y'_n - \beta J - y')]^z \\ & + (q-1)\exp(y_n - y)[q + \exp(\beta J_n + y'_n - \beta J) \\ & + \exp(\beta J_n + y'_n - y') + (q-2)\exp(\beta J_n + y'_n - \beta J - y')]^z. \end{aligned} \tag{10}$$

For completeness, the thermodynamic properties are discussed first. The equation (8) for $x$ becomes

$$x = \frac{\exp(y_n)[1 + \exp(\beta H_n + y'_n)]^z}{[1 + \exp(y'_n)]^z + \exp(y_n)[1 + \exp(\beta J_n + y'_n)]^z}. \tag{11}$$

However, the self-consistency condition (the second equality of (8)) can be written as

$$\frac{[1 + \exp(y'_n)]^{z-1}}{[1 + \exp(\beta J_n + y'_n)]^{z-1}} = \exp(y_n - y'_n) \tag{12}$$

so that

$$x = \frac{1}{1 + \exp[(y_n - z y'_n)/(z-1)]}. \tag{13}$$

Equations (12) and (13) can of course be solved to eliminate $y'_n$ and thus obtain the standard equation of state.

Analogous equations for $x_f$ can be obtained from (9). Namely, one has

$$x_f = \frac{\exp(y_n - y)[1 + \exp(\beta J_n + y'_n - y')]^z}{[1 + \exp(y'_n)]^z + \exp(y_n)[1 + \exp(\beta J_n + y'_n)]^z} \tag{14}$$

where it is understood that $y$ shall be set to $0^+$ at the end of the calculation. The self-consistency condition from (9) is written

$$\frac{[1+\exp(y'_n)]^{z-1}}{[1+\exp(\beta J_n + y'_n - y)]^{z-1}} = \exp(y_n - y - y'_n + y'). \tag{15}$$

Now, from (13), (14) and (15) it follows that one can write the percolation probabilty as

$$\tilde{P}(x) = x(1-Q^z) \tag{16}$$

where

$$Q = \exp\left(\frac{1}{z(z-1)}y - \frac{1}{z-1}y'\right).$$

From (12) and (15) one can derive the equation

$$Q = (1-\hat{x})\exp(-y/z) + \hat{x}Q^{z-1}\exp(-2y/z) \tag{17a}$$

where

$$\hat{x} = \frac{1}{1+\exp(-\beta J_n - y'_n)}. \tag{17b}$$

These results for $\tilde{P}$ and $Q$ are similar in form to those previously obtained for random site percolation. If one sets $J_n = 0$ and $y = 0$, then $x = \hat{x}$ and (16) and (17) become the equations for random site percolation (Fisher and Essam 1961).

Expressions for the percolation threshold can be given directly. First, Equations (12) and (13) can be solved for $\exp(-y'_n)$:

$$\exp(-y'_n) = \frac{1-2x+[(1-2x)^2+4\exp(\beta J_n)(1-x)x]^{1/2}}{2x}. \tag{18}$$

The percolation threshold from (17) is known by analogy to the random case (Fisher and Essam 1961) to be located at

$$(\hat{x})^* = (z-1)^{-1}. \tag{19}$$

Equation (19) can be rewritten, using (17$b$) and (18), in the form

$$x^* - \frac{z-1}{(z-2)^2\exp(\beta J_n)+2z-3}. \tag{20}$$

Equation (20) was first derived by Kikuchi (1970), and is valid outside the two-phase region (except in a metastable sense) for $J_n > 0$ and outside the sublattice ordering region for $J_n < 0$.

Because of the absence of a more obvious relation between percolation and thermodynamics of the lattice gas, it is interesting to note that the percolation threshold $x^*$ for $J_n > 0$ plotted as the full curves for $z = 6$ and $z = 12$ in figure 1 occurs to the left of the spinodal (chain) curves which mark the limit of stability of the metastable phase. The other set of curves with long–short dashes marks the coexistence line; $T_r$ is the reduced temperature, in units of the critical temperature for the repulsive case.

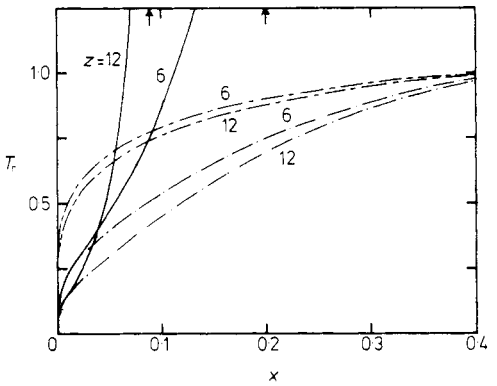


**Figure 1.** The percolation threshhold $x^*$ (full curves) for attractive interaction $J_n > 0$. The long–short dashed curves show the coexistence line; the chain curves the spinodal. The arrows denote the high temperature asymptotes for the two coordination numbers $z$.

One can derive an equation for the spinodal $\partial y_n/\partial x = 0$ for comparison to (20):

$$x_{\text{spinodal}} = \frac{1}{2} \pm \frac{1}{2}\left(1 + \frac{4(z-1)}{(z-2)^2[1-\exp(\beta J_n)]}\right)^{1/2}. \tag{21}$$

A comparison shows that for $z > 2$, $x_{\text{spinodal}} > x^*$, at least for the Bethe lattice. If this relation is correct in general, then the line for the threshold $x^*$ cannot penetrate the unstable region. Presumably, then, an extension of the two-dimensional Monte Carlo results of Odagaki *et al* (1975) to include values of $T_r$ between 2 and 1 should actually show a zero slope for the threshhold $dx^*/dx = 0$ at $x = 1/2$.

In figures 2 and 3, the probability $P \equiv \tilde{P}/x$ that a particle is part of an infinite cluster is plotted for $z = 6$ and 12, respectively. The full curves give percolation at equilibrium, calculated in the two-phase region under the coexistence curve by assuming macroscopic phase separation and using the 'lever rule' to compute amounts of the two phases. For comparison, the broken curves give percolation of the single metastable phase. If these lines are extended into the unstable region by solving (12)–(17) there, no

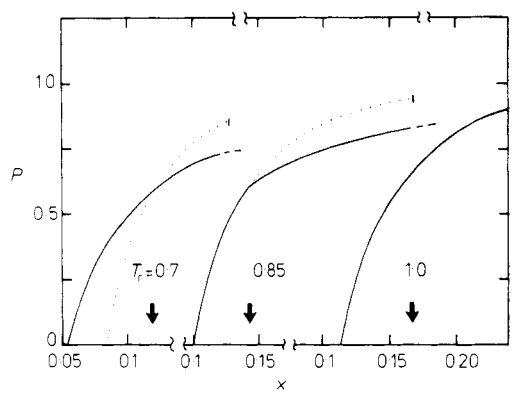


**Figure 2.** For $z = 6$ and attractive interaction, the full curves represent the probability $P$ that a particle is in an extensive cluster under equilibrium conditions, with phase separation if necessary. The dotted curve is the behaviour in the metastable phase.

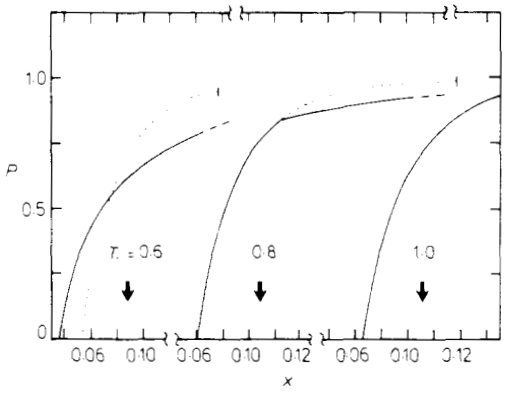


**Figure 3.** As in figure 2, but for $z = 12$.

anomalies in $P$ reflecting the instability directly are found. In addition, no anomalies are found in $P$ for $T_r = 1$ for $x$ in the vicinity of the critical point.

## 4. The region of sublattice ordering for $J_n < 0$

The Bethe cluster method can be extended to the region of sublattice, or 'antiferromagnetic', ordering for repulsive $J_n < 0$ by the method of assuming inequivalent A and B sublattices. The new self-consistency conditions involve a 'partition function' $Z_A$ for an A site surrounded by B sites:

$$Z_A = Z_C(H_n \to H_{nA}, H'_n \to H'_{nA}, H' \to H'_A)$$

and one for the converse situation

$$Z_B = Z_C(H_n \to H_{nB}, H'_n \to H'_{nB}, H' \to H'_n).$$

The combined equations of state and self-consistency conditions become

$$\begin{aligned} x_A &= \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{\partial}{\partial y_{nA}} \ln Z_A = \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{z} \frac{\partial}{\partial y'_{nB}} \ln Z_B \\ x_B &= \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{\partial}{\partial y_{nB}} \ln Z_B = \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{z} \frac{\partial}{\partial y'_{nA}} \ln Z_A. \end{aligned} \tag{22}$$

One should remember that $H'_{nA}$ and $H'_A$ act on the neighbours of A sites which are in the B sublattice.

In addition the finite cluster fraction is obtained from

$$\begin{aligned} x_{fA} &= \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{1-q} \frac{\partial}{\partial y} \ln Z_A \\ &= \lim_{\substack{J\to\infty \\ q\to 1 \\ y\to 0^+}} \frac{1}{z} \frac{1}{1-q} \frac{\partial}{\partial y'_B} \ln Z_B \end{aligned} \tag{23}$$

with an analogous equation for $x_{fB}$, where $x_{fA}$, for example, is the probability that an A site is in a finite cluster. The percolation probability $P$ is again given by (5) with

$$x \equiv \tfrac{1}{2}(x_A + x_B), \qquad x_f \equiv \tfrac{1}{2}(x_{fA} + x_{fB}).$$

In computing the above percolation probability $P$, adjacent particles are of course considered connected even though they are in different sublattices.

The new equations (22) and (23) do not simplify in a significant way and will not be discussed in detail. However, for completeness it is possible to give an equation for the *lines* of critical points found at zero staggered field, $H_{ns} \equiv \frac{1}{2}(H_{nA} - H_{nB}) = 0$, which are indicated for $z = 6$ and $z = 12$ by the chain curves in figure 4. This equation is

$$x_{crit} = \frac{1}{2}\left[1 \pm \left(\frac{(z-2)^2/z^2 - \exp(\beta J_n)}{1 - \exp(\beta J_n)}\right)^{1/2}\right] \tag{24}$$

for $J_n < 0$. The interior of the dome-shaped regions in figure 4 is the region of sublattice order.

A numerical solution of (22) and (23) shows that sublattice order is important for near-neighbour connectivity. The percolation threshold $x^*$ given by the full curves of

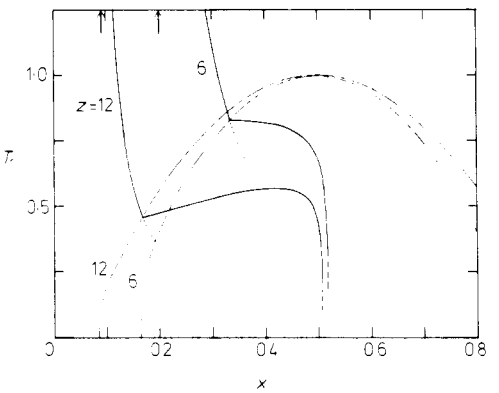


**Figure 4.** The percolation threshhold $x^*$ (full curve) for repulsive interaction for different $z$. The broken curves indicate the region of two sublattice ordering.

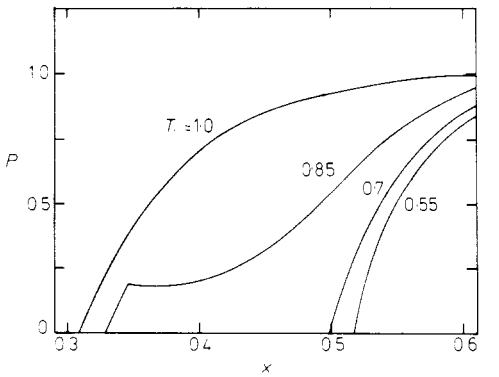


**Figure 5.** A plot of $P$ for repulsive interaction and $z = 6$, showing non-monotonic behaviour due to sublattice ordering.

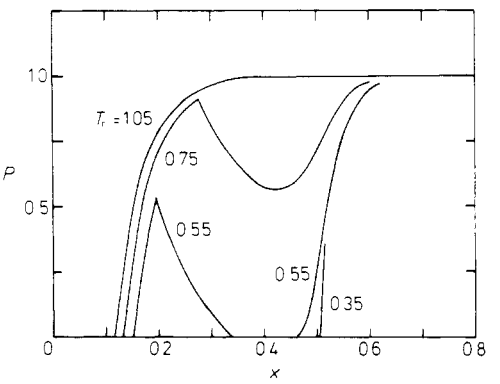


**Figure 6.** As in figure 5, but for $z = 12$.

figure 4 shows a sharp break at the bicritical point marking the point of entry into the region of sublattice order. The detailed behaviour of $P(x) = \tilde{P}(x)/x$ is shown in figures 5 and 6.

## 5. Conclusions

A new, concise formulation of percolation in an interacting lattice gas has been discussed and applied to the Bethe lattice. General effects on percolation due to lattice gas ordering have been discussed briefly, including new results in the region of sublattice ordering.

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