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Percolation problems and phase transitions

A Coniglio†

Istituto di Fisica Teorica dell'Università, Mostra d'Oltremare pad. 19, Napoli, Italy

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Abstract. The solutions of the site percolation problem for some Bethe lattices of interacting spins are shown. For zero external field some arguments are given which predict for three-dimensional models $p_c < \frac{1}{2}$ and for planar models $p_c = \frac{1}{2}$ where p_c is the critical density of overturned spins for the percolation problem.

1. Introduction

The percolation problem has been studied for non-interacting systems mostly (for general reviews see Frisch and Hammersley 1963, Shante and Kirkpatrick 1971, Essam 1973). Kikuchi (1970) developed a method for finding approximate solutions, which applies also to interacting systems. The interest in studying the problem with interaction lies not only in generalizing the percolation problem to those systems for which the interaction cannot be neglected, but also because interacting systems may exhibit a phase transition. One can then ask if there is any connection between phase transition and percolation.

In § 2 of this paper we give the solution of the percolation problem for a particular class of models such as Bethe lattices with a ferromagnetic interaction. It is shown that spontaneous magnetization is always associated with an infinite cluster of 'up' and 'down' spins. On this basis, we give in § 3 some arguments which generalize this result to any other ferromagnetic system. It is shown that this implies, for such a system with zero external field, the relation $p_c \leqslant \frac{1}{2}$ for the critical probability, the equality referring to planar lattices.

2. Percolation problem for ferromagnetic systems: Bethe lattices

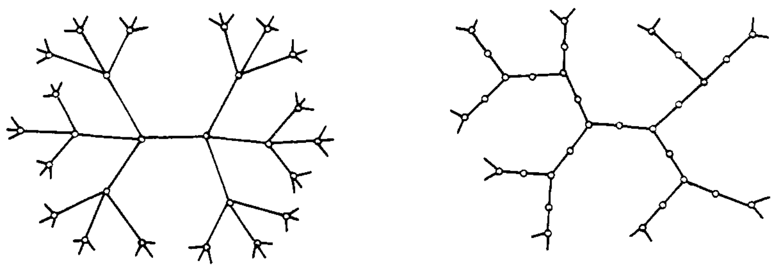
Let us begin by considering an Ising model. We introduce the usual variables $\mu = e^{-2mH/kT}$, $z = e^{-2J/kT}$ (see Domb 1960), J is the interaction between nearest-neighbour spins, T is the temperature, m is the magnetic moment of a single spin, H is the external magnetic field and k is the Boltzmann constant. The reduced magnetization is defined as $M = 1-2p(\mu, z)$ where $p(\mu, z)$ is the density of overturned spins, and also the probability that a given spin is 'down'.

Let $P_{\downarrow}(\mu, z)$ be the percolation probability, ie the probability that a given spin 'down' belongs to an infinite cluster of overturned spins and $S_{\downarrow}(\mu, z)$ be the mean cluster size

† Unità GNSM (Gruppo Nazionale di Struttura della Materia) del CNR.

of finite clusters of overturned spins. For $J = 0$ these quantities coincide with the usual percolation probability and mean cluster size in the site problem without interaction.

A closed-form solution of the percolation problem has not yet been found for the two-dimensional and three-dimensional lattices of principal interest. One can obtain appreciable insight by studying this problem for a class of models such as Bethe lattices. Examples of such lattices are given in figure 1.



(a) (b)

Figure 1. Examples of Bethe lattices: (a) simple Bethe lattice of coordination number $\sigma+1 = 4$; (b) decorated Bethe lattice derived from a simple Bethe lattice of coordination number $\sigma+1 = 3$ with the addition of an extra site on each bond.

The percolation problem for this class of model has already been solved by Fisher and Essam (1961) and Essam (1973) for a random distribution of overturned spins, ie $J = 0$.

Here we consider the same problem when the interaction among the spins is different from zero. In solving these models we make the usual assumption that edge effects are to be neglected as this leads to a physically realistic approximation, which is thermodynamically sound (see Domb 1960, Fisher and Essam 1961). Otherwise the models yield singularities of a quite different type (Eggarter 1974).

In a second paper we shall derive the general solutions for such models; here we shall give only the results for the simple Bethe lattices of coordination number $\sigma+1$. We find that

$$P_{\downarrow}(\mu, z) = P_{\downarrow}^{0}(a(\mu, z)) \tag{1}$$

$$S_{\downarrow}(\mu, z) = S_{\downarrow}^{0}(a(\mu, z)) \tag{2}$$

where $P_{\downarrow}^{0}(p)$ and $S_{\downarrow}^{0}(p)$ are respectively the percolation probability and the mean cluster size for the non-interacting Bethe lattices, which have already been calculated by Fisher and Essam (1961) and Essam (1973) and

$$a(\mu, z) = \frac{\mu_1}{\mu_1 + z} \tag{3}$$

where

$$\mu_1 = \mu\left(\frac{\mu_1 + z}{1 + \mu_1 z}\right)^{\sigma} \tag{4}$$

The density of overturned spins is given by

$$p = \frac{\mu_1(\mu_1 + z)}{\mu_1^2 + 2\mu_1 z + 1} \tag{5}$$

which is related to the reduced magnetization by

$$M(\mu, z) = 1-2p(\mu, z). \tag{6}$$

The critical behaviour of $P^0_\downarrow(p)$ and $S^0_\downarrow(p)$ is

$$\begin{aligned} P^0_\downarrow(p) &\sim p-p^0_c \qquad p \geqslant p^0_c \\ S^0_\downarrow(p) &\sim \frac{1}{|p-p^0_c|} \end{aligned} \tag{7}$$

where p^0_c is the critical probability of the Bethe lattices without interaction, and is given by

$$p^0_c = \frac{1}{\sigma}. \tag{8}$$

Equations (4)–(6) (Domb 1960) give the equation of state of the simple Bethe lattices. In the zero external magnetic field ($\mu = 1$) the system exhibits a spontaneous magnetization for $z \leqslant z_c = (\sigma-1)/(\sigma+1)$ which corresponds to the critical temperature. The equation $S^{-1}_\downarrow(\mu, z) = 0$ defines in the μ–z plane, a critical line of percolation points, $\mu_c = \mu_c(z)$. In the p–z plane the critical line is given by $p_c = p(\mu_c(z), z)$. For the Bethe lattices, from (2) and (8) the critical line of percolation points is given by

$$a(\mu, z) = \frac{1}{\sigma}$$

which together with equations (3) and (5) gives

$$p_c = \frac{1}{\sigma}\frac{\sigma^2 z^2}{(\sigma-1)^2+(2\sigma-1)z^2} \tag{9}$$

which coincides with the result found in a different way by Kikuchi (1970). We note that for all z, $p_c(z) \leqslant p^0_c$ as the attractive interaction facilitates the possibility of having an infinite cluster.

In figure 2 we have plotted p_c against z for $\sigma = 3$ The broken curve is

$$p(1^-, z) = \lim_{\mu\to 1^-} p(\mu, z);$$

z_c corresponds to the critical temperature in the order–disorder transition. The upper curve is $\mu_c(z)$, z_p corresponds to $\mu_c(z_p) = 1$; for $z < z_p$, $\mu_c > 1$ while $p_c < \frac{1}{2}$, which corresponds to instability. This means that for $z < z_p$ one can never reach the critical probability as this is larger than the density of overturned spins due to the spontaneous magnetization. At zero external field and $z < z_c$ the system of spins exhibits a degeneration in two states. Each state is characterized by a different value of the density of overturned spins $p(1^-, z)$ and $p(1^+, z)$ where 1^- and 1^+ mean that we have taken the limit $H \to 0^\pm$ respectively from positive and negative values. They satisfy the relation $p(1^-, z)+p(1^+, z) = 1$ and $0 \leqslant p(1^-, z) \leqslant \frac{1}{2}$. Also the percolation probability, for $z < z_c$ exhibits two values $P_\downarrow(1^-, z)$ and $P_\downarrow(1^+, z)$ corresponding to $p(1^-, z)$ and $p(1^+, z)$. Note that because of symmetry $P_\downarrow(\mu^{-1}, z) = P_\uparrow(\mu, z)$ where $P_\uparrow(\mu, z)$ is the probability that a given 'up' spin belongs to an infinite cluster of 'up' spins. In particular

$$P_\downarrow(1^+, z) = P_\uparrow(1^-, z). \tag{10}$$

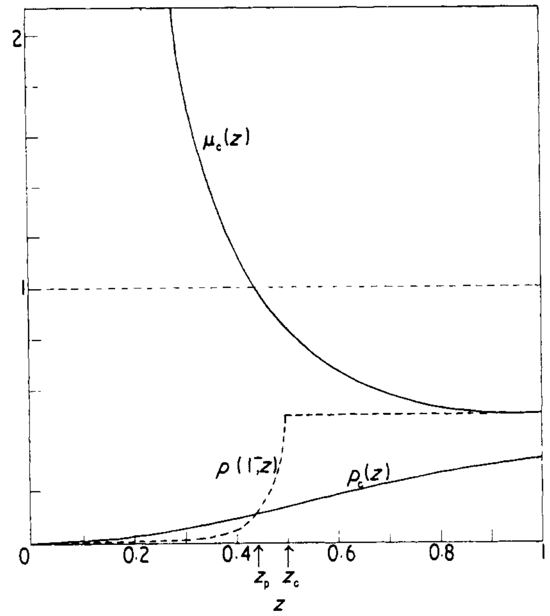


Figure 2. The upper full curve is $\mu_c(z)$, the critical value of μ characterizing the percolation points, against z; the broken curve is $p(1^-, z)$, the density of overturned spins for $\mu = 1^-$. The lower full curve is $p_c(z)$, the critical density of overturned spins. The percolation point z_p corresponding to $\mu_c = 1$ is coincident with the value of z for which $p(1^-, z)$ and $p_c(z)$ intersect. All the curves refer to the simple Bethe lattice of coordination number $\sigma + 1 = 4$.

Analogously we define $S_\downarrow(1^-, z)$, $S_\downarrow(1^+, z)$ and $S_\uparrow(1^-, z)$ where

$$S_\downarrow(1^+, z) = S_\uparrow(1^-, z).$$

In order to understand the connection between the critical point in the order–disorder transition and the percolation point, we have analysed two models at zero magnetic field, the simple Bethe lattice of coordination number 4 (figure 1(*a*)) for which the critical probability with zero interaction is $p_c^0 = \frac{1}{3} < \frac{1}{2}$ and the decorated lattice of coordination number 3 (figure 1(*b*)) for which $p_c^0 = \sqrt{\frac{1}{2}} > \frac{1}{2}$. In figures 3(*a*) and (*b*) we have plotted $P_\downarrow(1^-, z)$ and $P_\uparrow(1^-, z) = P_\downarrow(1^+, z)$ against z. In the same figures we have also plotted $S_\downarrow(1^-, z)$ and $S_\uparrow(1^-, z) = S_\downarrow(1^+, z)$ against z.

For small values of z we only have infinite clusters of 'up' spins. $P_\uparrow(1^-, z)$ starts with its maximum value at $z = 0$ and then decreases as $p(1^-, z)$ is an increasing function of z; at $z = z_p$ corresponding to $p_c = p(1^-, z_p) < \frac{1}{2}$ the mean cluster size of finite clusters of overturned spins diverges. The behaviour of $P_\downarrow(1^-, z)$ is quite clear. It is zero for $z < z_p$. For $z_p < z < z_c$ it is an increasing function of z, since z is a rapidly increasing function of $p(1^-, z)$. For $z > z_c$ $P_\downarrow$ $(1^-, z)$ becomes equal to $P_\uparrow(1^-, z)$, and decreases, since as z increases, $p(1^-, z)$ remains always equal to $\frac{1}{2}$, while the distribution of 'up' and 'down' spins becomes always more random. $P_\downarrow(1^-, z)$ will go to zero depending on whether or not $p_c^0 \gtrless \frac{1}{2}$. This is easily explained if one considers that

$$P_\downarrow(1^-, 1) = P_\downarrow^0(p = \tfrac{1}{2}).$$

Note that as a consequence of this fact, the model of figure 3(*b*) for which $p_c^0 > \frac{1}{2}$ exhibits a second percolation point at $z = z_{p'} > z_c$.

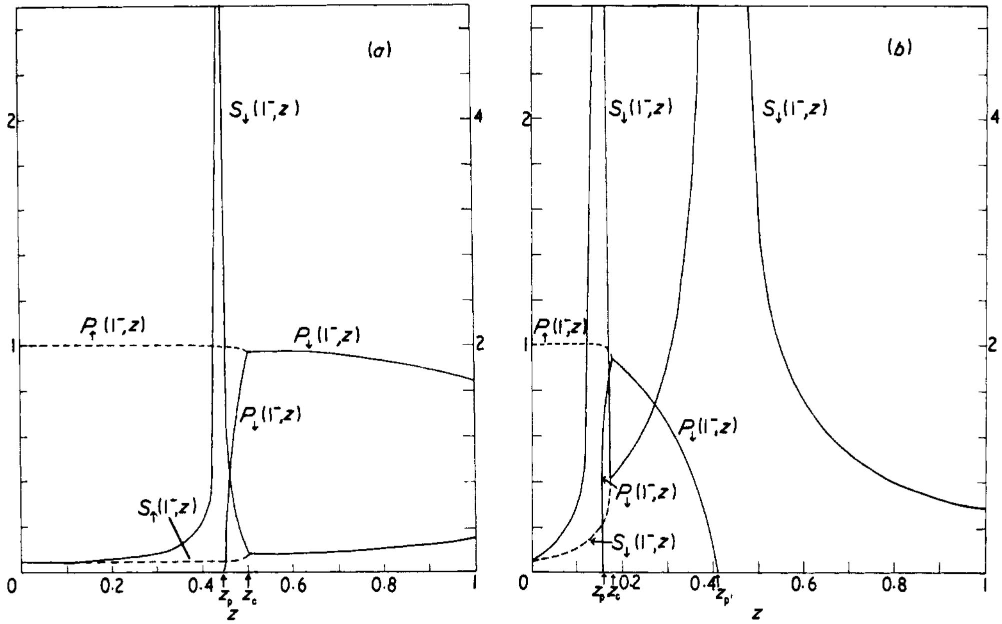


Figure 3. The broken curves are $P_\uparrow(1^-, z)$ and $S_\uparrow(1^-, z)$, respectively, the probability that a given 'up' spin belongs to an infinite cluster of 'up' spins and the mean cluster size of finite clusters of 'up' spins for $\mu = 1^-$. $P_\downarrow(1^-, z)$ and $S_\downarrow(1^-, z)$ are the same quantities for 'down' spins. For $z > z_c$, $P_\uparrow(1^-, z) = P_\downarrow(1^-, z)$ and $S_\uparrow(1^-, z) = S_\downarrow(1^-, z)$. The percolation point is the value of z where $P_\downarrow(1^-, z)$ goes to zero and $S_\downarrow(1^-, z)$ diverges. On the left is the scale of $P_\uparrow(1^-, z)$ and $P_\downarrow(1^-, z)$, on the right the scale of $S_\uparrow(1^-, z)$ and $S_\downarrow(1^-, z)$. (*a*) refers to the simple Bethe lattice of coordination number $\sigma + 1 = 4$; (*b*) refers to the decorated Bethe lattice of figure 1(*b*). Note that this model exhibits two percolation points.

3. Considerations for two- and three-dimensional systems

We have found that for zero external magnetic field, the critical probability p_c is always less than $\frac{1}{2}$ not only for those models for which $p_c^0 \leqslant \frac{1}{2}$ but also for the $\sigma = 2$ decorated lattice for which $p_c^0 > \frac{1}{2}$.

We want to give a plausibility argument which shows for a general ferromagnetic lattice in zero external magnetic field that $p_c \leqslant \frac{1}{2}$. Let us first show that a lattice system with spontaneous magnetization must exhibit an infinite cluster. In fact suppose that there are no infinite clusters. Divide the system in regions much larger than the mean cluster size, so that every region can be a good sample of the whole system, and much larger than the coherence length, so that correlations among regions can be neglected. If we have a distribution of clusters of 'up' spins and 'down' spins in one region with a given probability, the same distribution with reversed spins must occur in another region with the same probability. As a consequence the net magnetization will be zero.

If we now assume $p_c > \frac{1}{2}$ we get

$$P_\downarrow(1^-, z) = 0 \qquad \text{for any } z$$

and (11)

$$P_\uparrow(1^+, z) = 0 \qquad \text{for } z > z_{p'}$$

where $z_{p'} < z_c$ and is such that $p(1^+, z_{p'}) = p_c > \frac{1}{2}$. As a consequence, for all $z \in [z_{p'}, z_c]$ where the spontaneous magnetization is different from zero, we get $P_\downarrow(1^-, z) = 0$ and from (10), $P_\uparrow(1^-, z) = 0$, which, together with equation (11) implies the absence of an infinite cluster of either 'up' or 'down' spins. But this contradicts the argument given before that spontaneous magnetization can only exist if an infinite cluster is present. Therefore, in conclusion, for a ferromagnetic lattice with zero external magnetic field, $p_c \leqslant \frac{1}{2}$.

An interesting application of this result could be made to planar lattices. Harris (1960) and Fisher (1961) proved that for any two-dimensional site percolation problem $p_c \geqslant \frac{1}{2}$ when the distribution of particles or overturned spins is random. If one can extend the validity of this theorem to interacting spins, then the relation $p_c \geqslant \frac{1}{2}$ combined with the previous one $p_c \leqslant \frac{1}{2}$ leads to the conclusion that for any planar lattice with ferromagnetic interaction and zero external magnetic field, $p_c = \frac{1}{2}$, ie at zero external magnetic field the critical point in the order–disorder transition and the percolation point coincide. This result is verified rigorously for the triangular lattice, not only in the random distribution (Sykes and Essam 1964a) but also in the interacting case (Essam 1973).

Series expansions on the square lattice with $H = 0$ also seem to exhibit $p_c = \frac{1}{2}$ (M F Sykes and D S Gaunt, private communication).

What can be said for the three-dimensional lattices? Series expansions (Essam 1973) give strong evidence (Sykes and Essam 1964b) that in the random distribution for all the three-dimensional lattices studied $p_c^0 < \frac{1}{2}$.

The presence of a ferromagnetic interaction, as shown on the Bethe models, tends to reduce the value of the critical probability. We should expect that for a three-dimensional lattice $p_c < \frac{1}{2}$ and a behaviour for the percolation probability and mean cluster size of the type shown in figure 3(*a*). Series expansions for some three-dimensional lattices, with a ferromagnetic interaction (M F Sykes and D S Gaunt, private communication) and a Monte Carlo method calculation on the simple cubic lattice (Müller-Krumbhaar 1974) show that $p_c < \frac{1}{2}$ for zero external magnetic field.

In conclusion we have given some results for the percolation problem on Bethe lattices with ferromagnetic interactions. These results suggest some conjectures for two- and three-dimensional lattices, whose rigorous validity would be worthy of further investigation.

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