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Cluster size and shape in random and correlated percolation

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Abstract. A rigorous inequality between the pair correlation function and connectivity functions is proved for Ising model (correlated percolation). This relation shows that large correlations imply large connectivity. Such inequality becomes equality in the random percolation problem (infinite temperature). Other relations among susceptibility cluster size and perimeter are also derived which give information on the shape of the cluster for the random and correlated percolation problems.

1. Introduction

The percolation problem in a correlated system such as an Ising model has double interest: it generalises the percolation problem to more realistic systems, and allows a better understanding of the mechanisms of phase transitions. An exact solution of the correlated percolation problem for the Bethe lattice has been given by Coniglio (1975, 1976). Rigorous relations have been derived between "thermal" properties and 'connectivity' properties of the Ising model (Coniglio *et al* 1976, 1977). One of the most interesting consequences was that the critical point is also a percolation point in the two-dimensional Ising model. Rigorous cluster inequalities have been derived by Lebowitz and Penrose (1977). Numerical studies have been carried out by employing Monte Carlo techniques (Muller Krumbhaar 1974) or series expansion (Sykes and Gaunt 1976). The two-dimensional one-spin flip Ising model has been used to provide statistical data on Ising clusters (Domb *et al* 1975, Domb and Stoll 1977, Stoll and Domb 1978). In this paper we consider an Ising model and derive a simple relation between the spin–spin pair correlation function, the pair connectedness function p_{ij} (the probability that i and j belong to the same cluster) and t_{ij} (the probability that i belongs to a cluster and j to its perimeter). This relation shows that strong correlation has a large influence on the connectivity properties, namely one can show that divergence of the correlation length implies divergence of the connectedness length (linear dimension of a cluster). In § 3 we shall derive a relation between susceptibility, mean cluster size and mean cluster perimeter below and above the percolation threshold. A comparison with the recent Monte Carlo calculations of Stoll and Domb (1978) is performed, and the agreement with our theory is excellent. We shall consider the correlated case distinctly

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from the random case (temperature $T=\infty$) in which case all the inequalities that we derive become equalities. Preliminary results of this work have been presented at the IUPAP conference, Haifa 1977.

2. Correlations and connectivity properties

Consider a d-dimensional Ising model. Using the lattice gas terminology we shall associate a particle with a 'down' spin. Define a cluster as a maximal set of particles ('down' spins) connected by nearest neighbour bonds. The perimeter of a cluster is the set of empty sites ('up' spins) which are nearest neighbours to the particles belonging to that cluster. Let us introduce the following definitions:

$p=\langle\pi_i\rangle$ is the density of particles, where π_i is the lattice gas variable which is 1 or 0 depending on whether or not site i is occupied. The brackets stand for the usual thermal average with the Ising Hamiltonian.

$g_{ij}=\langle\pi_i\pi_j\rangle-\langle\pi_i\rangle\langle\pi_j\rangle$ is the density–density pair correlation function.

$p_{ij}[p_{ij}^{\infty}]$ is the pair connectedness function (Essam 1973) which is the probability that two sites i and j belong to the same finite $[\infty]$ cluster.

$t_{ij}[t_{ij}^{\infty}]$ is the probability that i belongs to a finite $[\infty]$ cluster and j to its perimeter.

Of course these quantities can be expressed as thermal averages of characteristic functions. For example $p_{ij}=\langle\gamma_{ij}\rangle$ where $\gamma_{ij}=1$ if i and j belong to the same finite cluster and $\gamma_{ij}=0$ otherwise. We shall prove the following:

Theorem: For any d-dimensional ferromagnetic Ising model with nearest neighbour ferromagnetic interaction at any temperature T and external magnetic field H we have

$$(1-p)(p_{ij}+p_{ij}^{\infty})-p(t_{ij}+t_{ij}^{\infty})\geqslant g_{ij}. \tag{1}$$

For $T=\infty$ (random case) relation (1) holds as an equality, namely

$$(1-p)(p_{ij}+p_{ij}^{\infty})-p(t_{ij}+t_{ij}^{\infty})=(1-p)p\delta_{ij} \tag{2}$$

where δ_{ij} is the usual Kronecker symbol which is 1 if $i=j$ and zero otherwise.

Those not interested in the details of the proof should go directly to § 3 where some consequences of (1) and (2) are derived.

Proof: Consider a box Λ with fixed boundary conditions. All the quantities defined before will now be labelled with a suffix Λ. The following identity holds:

$$\langle\pi_i\pi_j\rangle_\Lambda=p_{ij,\Lambda}+\sum_A\langle\lambda_{ij}^A\pi_j\rangle_\Lambda \tag{3}$$

$p_{ij,\Lambda}$ is the pair connectedness defined in the box Λ which in the limits of infinite Λ gives

$$\lim_{\Lambda\to\infty}p_{ij,\Lambda}=p_{ij}+p_{ij}^{\infty}. \tag{4}$$

The sum is over all the clusters A:

$$\lambda_{ij}^A=\begin{cases}1 & \text{if } i\in A \text{ and } j\notin A\,U\,\partial A\\ 0 & \text{otherwise}\end{cases}$$

given two sites i and j we also have

$$\langle\pi_i\rangle_\Lambda = p_{ij,\Lambda} + t_{ij,\Lambda} + \sum_A \langle\lambda_{ij}^A\rangle_\Lambda \tag{5}$$

which expresses the fact that given a particle at site $i(\langle\pi_i\rangle_\Lambda)$ any site j can belong to the same cluster as i $(p_{ij,\Lambda})$ or to its perimeter $(t_{ij,\Lambda})$ or neither of the two $(\Sigma_A \langle\lambda_{ij}^A\rangle_\Lambda)$.

From (3) and (5) we have

$$g_{ij,\Lambda} = \langle\pi_i\pi_j\rangle_\Lambda - \langle\pi_i\rangle_\Lambda\langle\pi_j\rangle_\Lambda$$

$$= (1-p)p_{ij,\Lambda} - pt_{ij,\Lambda} + \sum_A (\langle\lambda_{ij}^A\pi_j\rangle_\Lambda - \langle\lambda_{ij}^A\rangle_\Lambda\langle\pi_j\rangle_\Lambda). \tag{6}$$

The last sum in (6) is zero for $T=\infty$ (no correlation).

Taking into account that

$$\lim_{\Lambda\to\infty} t_{ij,\Lambda} = t_{ij} + t_{ij}^\infty \tag{7}$$

from (4) and (6) in the limit $\Lambda\to\infty$ we recover the second part (2) of the theorem. To prove the first part of the theorem we need to prove that the last sum in (6) is less than or equal to zero. In fact we can write for any cluster A: $i\in A, j\notin AU\ \partial A$

$$\lambda_{ij}^A = \pi^A(1-\pi)^{\partial A} \tag{8}$$

where

$$\pi^A = \prod_{K\in A} \pi_K \qquad (1-\pi)^{\partial A} = \prod_{K\in\partial A} (1-\pi_K)$$

$$\langle\lambda_{ij}^A\pi_j\rangle_\Lambda = \frac{\langle\lambda_{ij}^A\pi_j\rangle_\Lambda}{\langle\lambda_{ij}^A\rangle_\Lambda}\langle\lambda_{ij}^A\rangle_\Lambda = \frac{\langle(1-\pi)^{\partial A}\pi_j\rangle_\Lambda}{\langle(1-\pi)^{\partial A}\rangle_\Lambda}\langle\lambda_{ij}^A\rangle_\Lambda \tag{9}$$

where the last identity is based on equation (8) and the Markovian property of the Ising model (for more details see Coniglio *et al* 1977). Using the FKG inequalities (Fortuin *et al* 1971)

$$\langle(1-\pi)^{\partial A}\pi_j\rangle_\Lambda \leqslant \langle(1-\pi)^{\partial A}\rangle_\Lambda\langle\pi_j\rangle_\Lambda. \tag{10}$$

From (9) and (10) it follows that

$$\langle\lambda_{ij}^A\pi_j\rangle_\Lambda - \langle\lambda_{ij}^A\rangle_\Lambda\langle\pi_j\rangle_\Lambda \leqslant 0. \tag{11}$$

From (6) and (11) in the limit $\Lambda\to\infty$ the first part of our theorem (1) follows.

3. Cluster size and shape

In this section we wish to derive some consequences of our theorem. An immediate consequence of (1) is that the correlation length is always less than or equal to the connectedness length which represents the linear dimension of a cluster. This means that if the correlation length is infinite, the connectedness length is also infinite, which shows that regions which are highly correlated are also highly connected. The converse is not true.

Other inequalities relating spontaneous magnetisation and percolation probability have been derived elsewhere (Coniglio *et al* 1976, 1977). We want to derive a relation between cluster perimeter size and susceptibility. Let us consider first the case in which we are below the percolation threshold $p < p_C$. In this case (1) and (2) holds with $p_{ij}^{\infty} = t_{ij}^{\infty} = 0$. If we sum (1) and (2) over i we obtain

$$(1-p)\bar{n} - p\bar{s} \geqslant \chi/p, \qquad \forall T \tag{12}$$

$$(1-p)\bar{n} - p\bar{s} = 1-p \qquad T = \infty \tag{13}$$

where

$\bar{n} = p^{-1} \sum_i p_{ij}$ is the mean cluster size (Essam 1973)

$\bar{s} = p^{-1} \sum_j t_{ij}$ is the mean cluster perimeter

$\chi = \sum_i g_{ij}$ is the susceptibility.

Equation (13) has been derived independently by Leath (1976). For the two-dimensional Ising model (12) gives very interesting results. In fact it has been proved by Coniglio *et al* (1976) that for such a model, for $H = 0$, $T \geqslant T_C$ there are no infinite clusters ($p < p_C$). Therefore we can apply (12). Consequently at T_C the mean cluster size diverges faster than or equal to the susceptibility. This implies that the critical point is also a percolation point (see also Coniglio 1975, Coniglio *et al* 1977). Another interesting result of (12) and (13) is that if one considers the left hand side of (12) as an index of the compactness of the clusters, then one can deduce that the compactness of clusters increases from random (13) to correlated percolation (12). This result is in agreement with the Monte Carlo calculations of Domb and Stoll (1977) where the index of compactness was defined in a different way.

Let us now consider the case $p > p_C$. If we sum (1) and (2) over j we will find divergences due to the infinite cluster. In order to avoid such difficulties we consider an ideal box Λ whose origin if j and sum over $i \in \Lambda$. (We point out that here we are not considering a finite system as we have done in § 2. We consider an infinite system and sum (1) and (2) over a finite region Λ of the space.) From (12) and (13) we then obtain:

$$p_f(1-p)\bar{n}_\Lambda + p_\infty(1-p)\bar{n}_\Lambda^\infty - pp_f\bar{s}_\Lambda - pp_\infty\bar{s}_\Lambda^\infty \geqslant \chi_\Lambda, \qquad \forall T \tag{14}$$

$$p_f(1-p)\bar{n}_\Lambda + p_\infty(1-p)\bar{n}_\Lambda^\infty - pp_f\bar{s}_\Lambda - pp_\infty\bar{s}_\Lambda^\infty = (1-p)p, \qquad T = \infty \tag{15}$$

where $p_f[p_\infty]$ is the density of particles included in finite $[\infty]$ clusters

$$\bar{n}_\Lambda = \overline{n \cap \Lambda} = p_f^{-1} \sum_{i \in \Lambda} p_{ij}; \qquad \bar{n}_\Lambda^\infty = \overline{n^\infty \cap \Lambda} = p_\infty^{-1} \sum_{i \in \Lambda} p_{ij}^\infty$$

$$\overline{s_\Lambda} = \overline{s \cap \Lambda} = p_f^{-1} \sum_{i \in \Lambda} t_{ij}; \qquad \bar{s}_\Lambda^\infty = \overline{s^\infty \cap \Lambda} = p_\infty^{-1} \sum_{i \in \Lambda} t_{ij}^\infty$$

$\bar{n}_\Lambda^\infty$ diverges in the limit $\Lambda \to \infty$. In the case $T = \infty$, $d = 2$, it can be proved (Russo 1978) that $\bar{n}$ and $\bar{s}$ are finite for $p \neq p_C$. We suppose that this is true for any d and T. If then we divide (14) and (15) by $\bar{n}_\Lambda^\infty$ in the limit $\Lambda \to \infty$ we obtain

$$\frac{\bar{s}^\infty}{\bar{n}^\infty} \leqslant \frac{1-p}{p}, \qquad \forall T \tag{16}$$

$$\frac{\bar{s}^{\infty}}{\bar{n}^{\infty}}=\frac{1-p}{p}, \qquad T=\infty \tag{17}$$

where

$$\frac{\bar{s}^{\infty}}{\bar{n}^{\infty}}=\lim_{\Lambda\to\infty}\frac{\bar{s}_{\Lambda}^{\infty}}{\bar{n}_{\Lambda}^{\infty}}.$$

Recently Stoll and Domb (1978) by means of Monte Carlo calculations have found that both (16) and (17) are well verified except from a few discrepancies of (17) near p_C. The reason for such discrepancies is due to the fact that their result is valid only for finite systems while (17) is valid only for infinite systems. In fact since near p_C the size of the finite clusters becomes relevant their contribution (17) cannot be neglected compared to the size of the spanning cluster. We will show later how to take them into account (20). Relation (17) has also been derived independently by Kunz and Souillard (1978), Stauffer (1978) and Hankey (1978). We want to show for the random case how to relate the contribution of the finite clusters in (15) to $\mathrm{d}p_{\infty}/\mathrm{d}p$. Let us consider the following relation:

$$p_f=\sum_{n,s} M(n,s)p^n(1-p)^s \tag{18}$$

where $M(n, s)$ is the number of distinct cluster of n sites and perimeters which contain the origin. If we take the derivative of (18) with respect to p we have

$$p(1-p)\frac{\mathrm{d}p_f}{\mathrm{d}p}=(1-p)p_f\bar{n}-pp_f\bar{s} \tag{19}$$

for $p<p_C$ $\mathrm{d}p_f/\mathrm{d}p=1$ and (19) gives equation (13). In fact this is the way it was obtained by Leath (1976). For $p>p_C$

$$\frac{\mathrm{d}p_f}{\mathrm{d}p}=1-\frac{\mathrm{d}p_{\infty}}{\mathrm{d}p}$$

which near p_C behaves as $|p-p_C|^{\beta_p-1}$ where β_p is the critical index of the percolation probability. From (15) and (19) we have

$$p(1-p)\frac{\mathrm{d}p_{\infty}}{\mathrm{d}p}=\lim_{\Lambda\to\infty}(p_{\infty}(1-p)\bar{n}_{\Lambda}^{\infty}-pp_{\infty}\overline{s_{\Lambda}^{\infty}}). \tag{20}$$

Since $\mathrm{d}p_{\infty}/\mathrm{d}p\geqslant 0$, for very large but finite Λ near p_C we have

$$\frac{\overline{s_{\Lambda}^{\infty}}}{\overline{n_{\Lambda}^{\infty}}}\geqslant\frac{1-p}{p}$$

in agreement with the Monte Carlo data of Stoll and Domb (1978).

In conclusion one of the main goals of this paper was to characterise the pair correlation function in terms of geometrical properties. In this sense it could be very interesting either to improve the inequality or to find a non-trivial lower bound for the pair correlation function in terms of 'connectivity' functions. Relations between mean cluster size, mean cluster perimeter and susceptibility have been derived from the basic relations (1) and (2). Such relations are equalities in the random case ($T=\infty$) but inequalities in the correlated case ($T\neq\infty$). It would be interesting to obtain equalities also for the correlated case at least near $T=\infty$ by means of series expansion.

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References

Coniglio A 1975 *J. Phys. A: Math. Gen.* **8** 1773–9
—— 1976 *Phys. Rev.* B **13** 2194–3207
Coniglio A, Nappi C R, Peruggi F and Russo L 1977 *J. Phys. A: Math. Gen.* **10** 205–218
—— 1976 *Commun. Math. Phys.* **51** 315–323
Domb C, Schneider T and Stoll E 1975 *J. Phys. A: Math. Gen.* **8** L90–4
Domb C and Stoll E 1977 *J. Phys. A: Math. Gen.* **10** 1141–1149
Essam J W 1973 *Phase Transitions and Critical Phenomena* vol 2 ed C Domb and M S Green (NY: Academic) pp 197–270)
Fortuin C M, Kastleyn P W and Ginibre J 1971 *Commun. Math. Phys.* **22** 89–103
Hankey A 1978 *J. Phys. A: Math. Gen.* **11** L49–56.
Kunz H and Souillard B 1978 *J. Stat. Phys.* **19** 77–106
Lebowitz J L and Penrose O 1977 *J. Stat. Phys.* **16** 321–337
Leath P L 1976 *Phys. Rev.* B **14** 5055–66
Muller Krumbhaar H 1974 *Phys. Lett.* **50**A 27–8
Reich G R and Leath P L 1978 *J. Phys. C: Solid State Phys.* **11** 1155–68
Russo L 1978 *Z. Wahrsch.* **43** 39–48
Stoll E and Domb C 1978 *J. Phys. A: Math. Gen.* L57–61
Stauffer, D 1975 *J. Phys. C: Solid State Phys.* **8** L172
—— 1978 *J. Stat. Phys.* **18** 125
Sykes M F and Gaunt D S 1976 *J. Phys. A: Math. Gen.* **9** 2131–7