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LETTER TO THE EDITOR

A test of scaling near the bond percolation threshold†

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Abstract. The bond percolation problem is studied by the Monte Carlo method on a two-dimensional square lattice of 2×10^6 bonds. Through the inclusion of a ghost field h, we obtain the generating function (the percolation analogue of the Gibbs free energy), percolation probability (the analogue of the spontaneous magnetisation), and mean cluster size ('isothermal susceptibility') as functions of two 'thermodynamic' variables, $\epsilon \equiv (p_c-p)/p_c$ and h. We discuss the non-trivial problems associated with the identification of the singular parts of these functions. We demonstrate that scaling holds for all three 'thermodynamic' functions within a rather large 'scaling region'.

1. Introduction

The percolation problem has received increasing attention recently. One reason for this interest is that it provides a testing ground for theories of phase transitions and critical phenomena. A second reason is that it is a good model for a variety of physical phenomena, including conduction in disordered materials and the gelation of polymers (for reviews of the subject, see, e.g., Frisch and Hammersley 1963, Shante and Kirkpatrick 1971, Essam 1972). A third reason stems from the correspondence to the $Q\to1$ limit of the Q-state Potts model (Kasteleyn and Fortuin 1969).

The scaling hypothesis is of particular interest since it aids in the understanding of the equation of state near the critical point (Essam and Gwilym 1971). However, the study of scaling for the percolation probem has been limited in large part to the cluster size distribution function (Stauffer 1975a,b, 1976, Flammang 1977, Reynolds *et al* 1977, Stauffer and Jayaprakash 1978, Wolff and Stauffer 1978), and the lattice animals (Stauffer 1978, Reich and Leath 1978, Leath and Reich 1978, Stoll and Domb 1978).

Here we study the equation of state for the percolation analogue of thermodynamic functions. In particular, we numerically confirm scaling for the two-dimensional square bond percolation problem using the Monte Carlo method. We also present the actual scaling forms of these functions graphically. Except for $d=1$, no previous work has given this information, possibly because of the difficulty in separating the scaling (or singular) part of the 'thermodynamic' functions from the remainder‡.

† This work forms a portion of the PhD thesis of HN to be submitted to the Department of Physics, Harvard University.

‡ For $d=1$, the percolation problem can be solved exactly, and hence the scaling hypothesis can be directly tested (Reynolds *et al* 1977, Klein *et al* 1978, Stauffer and Jayaprakash 1978).

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The percolation analogue of the Gibbs free energy is the mean number of finite clusters per site, denoted by $G(\epsilon, h)$, where $\epsilon \equiv (p_c - p)/p_c$ (p and p_c being, respectively, the bond occupation probability and its critical value), and h is the probability that a lattice site is connected to the 'ghost' site via the occupation of a 'ghost' bond. There is a correspondence, as $Q \to 1$, to the dimensionless parameters J and H of the Potts model, $1-p = \exp(-J)$ and $1-h = \exp(-H)$, where J is the nearest-neighbour exchange integral and H is the external magnetic field (Kasteleyn and Fortuin 1969, Essam and Gwilym 1971). Thus the percolation analogue of the free energy may be written as (Reynolds *et al* 1977)

$$G(\epsilon, h) = \sum_{s \geqslant 1}{}' \langle n_s(\epsilon) \rangle_{h=0} (1-h)^s \tag{1}$$

where $\langle n_s(\epsilon) \rangle_{h=0}$ is the mean number of s-site clusters per site in the absence of the ghost bonds; the prime denotes the fact that the summation extends only over the finite clusters.

The analogue of spontaneous magnetisation is $P(\epsilon, h)$, the probability that an (occupied) site belongs to the infinite cluster,

$$P(\epsilon, h) = 1 - \sum_{s \geqslant 1}{}' s \langle n_s(\epsilon) \rangle_{h=0} (1-h)^s. \tag{2}$$

The analogue of the isothermal susceptibility is $S(\epsilon, h)$, the mean number of sites contained in a finite cluster,

$$S(\epsilon, h) = \frac{\sum'_{s \geqslant 1} s^2 \langle n_s(\epsilon) \rangle_{h=0} (1-h)^s}{\sum'_{s \geqslant 1} s \langle n_s(\epsilon) \rangle_{h=0} (1-h)^s}. \tag{3}$$

In the subsequent sections, we shall first rephrase the scaling hypothesis for these three functions and then: (*a*) discuss the method of extracting their singular parts; and (*b*) exhibit the Monte Carlo results that confirm the scaling hypothesis.

2. Scaling hypothesis

In analogy to the thermal scaling hypothesis for the Gibbs free energy, we postulate that $G(\epsilon, h)$ contains a singular part, G_{sing}, that is asymptotically a generalised homogeneous function (GHF) in ϵ and h near the critical point $\epsilon = h = 0$ (Hankey and Stanley 1972, Essam and Gwilym 1971),

$$G_{\text{sing}}(\lambda^{a_\epsilon} \epsilon, \lambda^{a_h} h) = \lambda G_{\text{sing}}(\epsilon, h). \tag{4a}$$

The percolation exponents β, γ, and δ defined by the relations $P(\epsilon, 0) \sim |\epsilon|^\beta$, $S(\epsilon, 0) \sim |\epsilon|^{-\gamma}$ and $P(0, h) \sim h^{1/\delta}$ are directly expressible in terms of the scaling powers a_ϵ and a_h,

$$\beta = (1-a_h)/a_\epsilon, \qquad \gamma = (2a_h - 1)/a_\epsilon, \qquad \delta = a_h/(1-a_h). \tag{4b}$$

Since equation (4*a*) leads to the scaling expressions

$$G_{\text{sing}}(\epsilon, h) = h^{1/a_h} G_{\text{sing}}\left(\frac{\epsilon}{h^{a_\epsilon/a_h}}, 1\right) \tag{5a}$$

$$G_{\text{sing}}(\epsilon, h) = |\epsilon|^{1/a_\epsilon} G_{\text{sing}}\left(\operatorname{sgn} \epsilon, \frac{h}{|\epsilon|^{a_h/a_\epsilon}}\right), \tag{5b}$$

equations (4*b*) and (5) give the asymptotic behaviour

$$G_{\text{sing}}(\epsilon = 0, h) \sim h^{1+1/\delta} \tag{6a}$$

$$G_{\text{sing}}(\epsilon, h = 0) \sim |\epsilon|^{\beta(\delta+1)}. \tag{6b}$$

Similarly, for the first derivative of G_{sing} with respect to h,

$$G^{(1)}_{\text{sing}}(\epsilon, h) = h^{(1-a_h)/a_h} G^{(1)}_{\text{sing}}\left(\frac{\epsilon}{h^{a_\epsilon/a_h}}, 1\right), \tag{7a}$$

$$G^{(1)}_{\text{sing}}(\epsilon, h) = |\epsilon|^{(1-a_h)/a_\epsilon} G^{(1)}_{\text{sing}}\left(\text{sgn } \epsilon, \frac{h}{|\epsilon|^{a_h/a_\epsilon}}\right) \tag{7b}$$

and further, for the second derivative,

$$G^{(2)}_{\text{sing}}(\epsilon, h) = h^{(1-2a_h)/a_h} G^{(2)}_{\text{sing}}\left(\frac{\epsilon}{h^{a_\epsilon/a_h}}, 1\right) \tag{8a}$$

$$G^{(2)}_{\text{sing}}(\epsilon, h) = |\epsilon|^{(1-2a_h)/a_\epsilon} G^{(2)}_{\text{sing}}\left(\text{sgn } \epsilon, \frac{h}{|\epsilon|^{a_h/a_\epsilon}}\right). \tag{8b}$$

Here $G^{(n)}_{\text{sing}}$ denotes $(\partial^n/\partial h^n)G_{\text{sing}}(\epsilon, h)$.

In order to obtain the singular part, G_{sing}, from the total G, we consider the following. Since

$$P(\epsilon, h) = 1 + (1-h)G^{(1)}(\epsilon, h), \tag{9a}$$

and since

$$G^{(1)}_{\text{sing}}(\epsilon = 0, h) \sim h^{1/\delta} \sim P(\epsilon = 0, h), \tag{9b}$$

$$G^{(1)}_{\text{sing}}(\epsilon, h = 0) \sim |\epsilon|^{\beta} \sim P(\epsilon, h = 0), \tag{9c}$$

we conclude

$$G^{(1)}_{\text{sing}}(\epsilon, h) \sim P(\epsilon, h). \tag{10}$$

From equations (9) and (10) we may write

$$G^{(1)}(\epsilon, h) = G^{(1)}_{\text{reg}}(\epsilon, h) + G^{(1)}_{\text{sing}}(\epsilon, h) \tag{11}$$

with

$$G^{(1)}_{\text{reg}}(\epsilon, h) = -\frac{1}{1-h}, \tag{12a}$$

$$G^{(1)}_{\text{sing}}(\epsilon, h) = \frac{1}{1-h} P(\epsilon, h). \tag{12b}$$

Therefore, asymptotically we have for the leading terms,

$$G^{(1)}_{\text{reg}}(\epsilon, h) \simeq -1, \tag{13a}$$

$$G^{(1)}_{\text{sing}}(\epsilon, h) \cong P(\epsilon, h). \tag{13b}$$

(We note that equations (13) hold with equals signs if the scaling hypothesis (4) is written in terms of ε and H.) The singular part of the mean cluster size $S(\epsilon, h)$ is

$$G^{(2)}_{\text{sing}}(\epsilon, h) = \frac{\partial}{\partial h} G^{(1)}_{\text{sing}}(\epsilon, h) \sim G^{(2)}(\epsilon, h). \tag{14}$$

Moreover, upon integration of $G^{(1)}_{\text{sing}}(\epsilon, h)$ (see equations (13)), we obtain

$$G_{\text{sing}}(\epsilon, h) = G(\epsilon, h) + h - f(\epsilon) \tag{15}$$

where $f(\epsilon)$ is a suitable regular function of ϵ only,

$$f(\epsilon) = \sum_{i=0}^{\infty} a_i \epsilon^i. \tag{16a}$$

In fact, since $G_{\text{sing}}(\epsilon, h=0) \sim \epsilon^{2-\alpha}$ where $2 < 2-\alpha < 3$, terms of $O(\epsilon^3)$ are already dominated by G_{sing}. Thus, we only need to keep the first three terms of $f(\epsilon)$ in order to cancel the regular part of G in equation (14), i.e. $f(\epsilon) = a_0 + a_1\epsilon + a_2\epsilon^2$. We further approximate $f(\epsilon)$ as

$$f(\epsilon) \cong a_0 + a_1\epsilon \tag{16b}$$

neglecting the ϵ^2 term. This is done in analogy to the one-dimensional case and the Cayley tree, where a_2 is indeed zero†. We note that $a_0 = G(\epsilon = 0, h = 0)$, from equation (15), where Temperley and Lieb (1971) have given an exact expression for $G(\epsilon = 0, h = 0)$. We find $a_0 = 0{\cdot}09875$, about 1% higher than the Temperley–Lieb value of $0{\cdot}0980_7$. We therefore have one parameter, a_1, with which to achieve the best data collapsing from our Monte Carlo data (cf equation (5)).

We note that the above discussion is completely general, and not restricted to the square bond problem. In particular, the extension to the site percolation problem may be done readily in complete analogy to the present work.

3. Monte Carlo results

We have undertaken detailed Monte Carlo studies of the three moments of $G(\epsilon, h)$, focusing on the scaling properties (5), (7) and (8). Here we present only the most significant results pertaining to the demonstration that 'thermodynamic' functions scale. The full results of our investigation, including a discussion of the functional forms of these scaling functions, will be reported in a subsequent publication.

In particular, we give here our bond percolation results on a 1000×1000 square lattice with free boundaries. In all, 960 configurations are generated with a total of 64 different probabilities in increments ranging from 0·001 to 0·025. The bond probabilities range from 0·275 to 0·7, and the h field ranges from 0·01 to 0·1. In order to estimate p_c, we study the function $g(\epsilon) \equiv \Sigma''_{s \geqslant 1} s^2 \langle n_s(\epsilon) \rangle_{h=0}$ where the largest cluster is omitted from the summation for all p both below and above p_c. We find that $g(\epsilon)$ decreases even more sharply than $S(\epsilon, h = 0)$ just above p_c, and this fact makes it possible to estimate p_c very accurately (Hoshen and Kopelman 1976)‡.

† For the $d = 1$ bond problem G_{sing} calculated according to (15) with $f(\epsilon) = 0$ ($a_0 = a_1 = a_2 = 0$) is asymptotically,

$$(\epsilon^2 + \epsilon h + h^2)/(\epsilon + h).$$

This gives $G_{\text{sing}}(\epsilon = 0, h) \sim h$, $G_{\text{sing}}(\epsilon, h = 0) \sim \epsilon$, leading to $\delta = \infty$, $\alpha = 1$. For the Cayley tree bond problem, $a_1 = \frac{1}{2}(1 + 1/\sigma) = 1 - G(\epsilon = 0, h = 0)$, $a_0 = \frac{1}{2}(1 - 1/\sigma) = G(\epsilon = 0, h = 0)$ and $a_2 = 0$ give $G_{\text{sing}}(\epsilon = 0, h) \sim h^{3/2}$, $G_{\text{sing}}(\epsilon, h = 0) \sim \epsilon^3$ leading to $\delta = 2$, $\alpha = -1$ where $\sigma + 1$ is the site coordination number. We note that the Cayley tree result does not reduce to the $d = 1$ result as $\sigma \to 1$. This gives yet another example of the non-equivalence of $d = 1$ and Cayley tree $\sigma \to 1$ limit (Stauffer and Jayaprakash 1978).

‡ The function $g(\epsilon)$ behaves much the same as $S(\epsilon, h = 0)$ below p_c, but it is significantly smaller than $S(\epsilon, h = 0)$ above p_c because the denominator in the expression for $S(\epsilon, h = 0)$ decreases rapidly from unity as p increases (equation (3)).

Once p_c is determined in this manner, we take the largest cluster for $p > p_c$ to be the 'infinite' cluster. In other words, the summation extends over *all* clusters for $p < p_c$, and over *all but the largest* cluster for $p > p_c$. We compute the moments $\Sigma'_{s\geq 1} s^k (1-h)^s \langle n_s(\epsilon)\rangle_{h=0}$ for $k = 0$, 1, and 2, by using the cluster distribution data first at a zero ghost field, and then by putting in the factor of $(1-h)^s$ exactly. Alternatively, we could have randomly generated the ghost bonds as well as the lattice

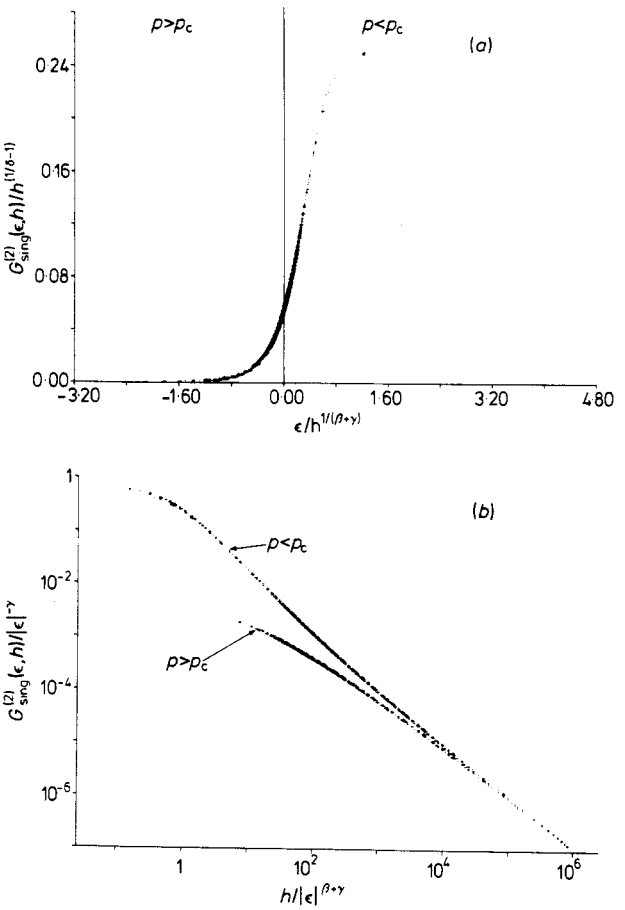

Figure 1. Monte Carlo data for $G^{(2)}_{\text{sing}}(\epsilon, h)$, the singular part of mean cluster size, which is the analogue for the percolation problem of the isothermal susceptibility of a ferromagnet. The lattice size is 1000×1000, and each data point represents the average value over 15 configurations (i.e. 15 Monte Carlo realisations). There are 63 different values of $p(\neq p_c)$ in the range $0{\cdot}275 \leq p \leq 0{\cdot}7$ and 10 values of h in the range $0{\cdot}01 \leq h \leq 0{\cdot}1$; hence there are a total of 630 Monte Carlo data points. However, data points that are clearly outside the scaling region are not plotted. (*a*) Scaling of $G^{(2)}_{\text{sing}}(\epsilon, h)$ with respect to h (equation (5*a*)). For $0{\cdot}275 \leq p \leq 0{\cdot}375$, only those points that correspond to $h = 0{\cdot}01$ are plotted, while, for all other values of p, h ranges from 0·01 to 0·1. Thus, there are 585 points on this plot altogether (285 below and 300 above p_c). (*b*) Scaling of $G^{(2)}_{\text{sing}}(\epsilon, h)$ with respect to $|\epsilon|$ (equation 6*b*)). For $0{\cdot}575 \leq p \leq 0{\cdot}7$, only those points that correspond to $h = 0{\cdot}01$ are plotted, while, for all other values of p, h ranges from 0·01 to 0·1. There are 576 points on the plot (330 below and 246 above p_c). One method we use to obtain an approximate bound on C_+ of equation (17*b*) is to extrapolate the upper branch of this plot horizontally toward $h \to 0$.

bonds. We also note that, since we deal with macroscopic quantities (i.e. summed over s), fluctuations in cluster size distributions have little effect. Moreover, the presence of non-zero h helps diminish the spurious boundary effects of very large clusters since the factor $(1-h)^s$ attenuates contributions from large clusters significantly.

In the manner described above we estimate the critical bond probability p_c to be $0{\cdot}500 \pm 0{\cdot}002$ in excellent agreement with the known exact result of $0{\cdot}5$. We also find the critical exponents $\beta = 0{\cdot}146 \pm 0{\cdot}02$ and $\gamma = 2.29 \pm 0{\cdot}01$ consistent with the estimates of $\beta = 0{\cdot}138 \pm 0{\cdot}007$ and $\gamma = 2{\cdot}43 \pm 0{\cdot}03$ previously calculated using the series methods (Sykes *et al* 1976a, b).

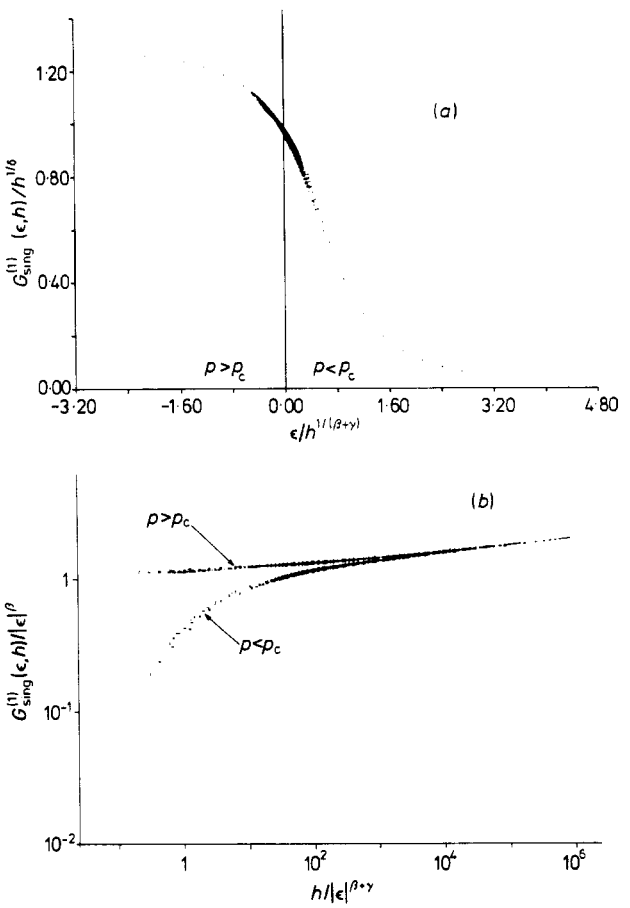

Figure 2. Monte Carlo data for $G^{(1)}_{sing}(\epsilon, h)$, the percolation probability, which is the analogue of the magnetisation function of a ferromagnet. (*a*) Scaling of $G^{(1)}_{sing}(\epsilon, h)$ with respect to h (equation (7*a*)). For $0{\cdot}275 \leqslant p \leqslant 0{\cdot}4$ and $0{\cdot}575 \leqslant p \leqslant 0{\cdot}7$, only those points that correspond to $h = 0{\cdot}01$ are plotted, while for all other values of p, h ranges from $0{\cdot}01$ to $0{\cdot}1$. There are 522 points on the plot (276 below and 246 above p_c). This figure may be compared with the analogous plot for a Heisenberg magnet, figure 2 of Milošević and Stanley (1972). They show remarkable similarities both in scale and in shape.

(*b*) The second form of scaling of $G^{(1)}_{sing}(\epsilon, h)$ (equation (7*b*)). For all values of p ($0{\cdot}275 \leqslant p \leqslant 0{\cdot}7$), h ranges from $0{\cdot}01$ to $0{\cdot}1$. All 630 points are plotted (330 below and 300 above p_c). One method we use to obtain an estimate of B of equation (17*a*) is to extrapolate the upper branch ($p > p_c$) horizontally toward $h \to 0$.

Our estimates are obtained from the slopes of the straight lines fitted to the log–log plots of $P(\epsilon, h=0)$ and $S(\epsilon, h=0)$ against ϵ. The series estimates were used to obtain the scaling functions for G_{sing}, $G^{(1)}_{\text{sing}}$, and $G^{(2)}_{\text{sing}}$. Since $G^{(2)}_{\text{sing}}$ diverges at the critical point as the mean size of finite clusters tends to infinity, we expect the singular behaviour of $G^{(2)}_{\text{sing}}$ to appear more clearly than that of $G^{(1)}_{\text{sing}}$ or G_{sing}, whose singular behaviour may be masked until we come very close to the critical point.

On this basis we first studied $G^{(2)}$, which by equation (14) should equal $G^{(2)}_{\text{sing}}$ without any subtraction. This function shows the scaling behaviour (equation (8)) very well (see figures 1(*a*) and 1(*b*)). Figures 2(*a*) and 2(*b*) show the scaling of the singular part of the first moment (equations (7)). Figures 3(*a*) and 3(*b*) show the scaling of the singular part G_{sing} of the full 'Gibbs free energy', using equations (15) and (16*b*) with

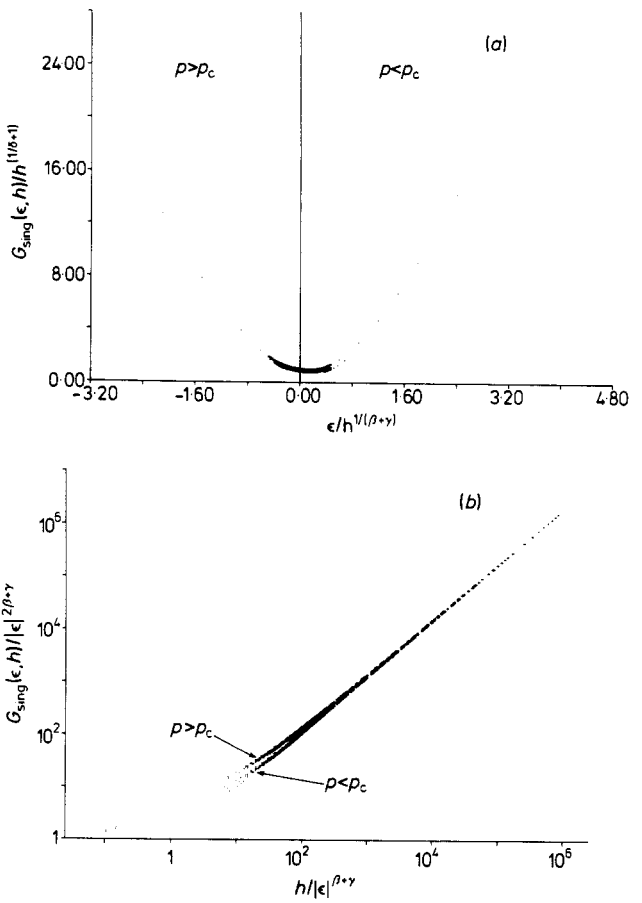

Figure 3. Monte Carlo data for $G_{\text{sing}}(\epsilon, h)$, the analogue of the Gibbs potential. $G_{\text{sing}}(\epsilon, h)$ is estimated using equations (15) and (16*b*) with $a_0 = 0{\cdot}098747$, $a_1 = 0{\cdot}5$, and $a_2 = 0$. The possible existence of a small quadratic term a_2 does not seem to affect this plot significantly for the range of h we use. (*a*) Scaling of $G_{\text{sing}}(\epsilon, h)$ with respect to $|\epsilon|$ (equation (8*a*)). For $0{\cdot}275 \leq p \leq 0{\cdot}4$ and $0{\cdot}575 \leq p \leq 0{\cdot}7$, only those points that correspond to $h = 0{\cdot}01$ are plotted, while, for all other values of p, h ranges from 0·01 to 0·1. There are 522 points on the plot (276 below and 246 above p_c). (*b*) The second form of scaling of $G_{\text{sing}}(\epsilon, h)$ (equation (8*b*)). There are 522 points on the plot (276 below and 246 above p_c) and they correspond to the same values of p and h as in (*a*).

$a_0 = 0{\cdot}098747$, $a_1 = 0{\cdot}5$. The value of $a_1 = 0{\cdot}5$ in equation (16*b*) is found to give the best data collapsing for equations (5). This contrasts, for example, with $a_1 = 0$ for $d = 1$, and with $a_1 = \frac{1}{2}(1 + 1/\sigma)$ for the Caley tree of coordination number $\sigma + 1$.

We have also found that these data collapsing methods show much less sensitivity to the values of critical exponents than to the location of p_c, (Sur *et al* 1976). In fact, we have varied p_c, β, and γ in order to see the change in the degree of data collapsing and we have found that, although sensitivity for p_c is fairly high (to within 0·01 or 2% of p_c itself), the sensitivity for β and γ is very low (typically 20% for the combinations appearing in equations (5), (7), and (8)). We also note that $B = 1{\cdot}39 \pm 20\%$ and $C_+ \sim 0{\cdot}168 \pm 20\%$, $C_- \sim 0{\cdot}0068 \pm 20\%$ where B is the amplitude of $P(\epsilon, h = 0)$,

$$P(\epsilon, h = 0) = B(p - p_c)^{\beta}, \qquad p > p_c \tag{17a}$$

and C_+ and C_- are those of mean size $S(\epsilon, h = 0)$ below and above p_c respectively,

$$S(\epsilon, h = 0) = \begin{cases} C_+(p_c - p)^{-\gamma}, & p < p_c \\ C_-(p - p_c)^{-\gamma}, & p > p_c. \end{cases} \tag{17b}$$

These values were obtained from the intercepts of the straight lines fitted to the log–log plots of $P(\epsilon, h = 0)$ and $S(\epsilon, h = 0)$ against ϵ. We have an independent check on the bounds of the values C_+ and B by extrapolating the scaling plots of figures 1(*b*) and 2(*b*) to $h \to 0$, and they are in agreement with the values quoted above. On the other hand, Sykes *et al* (1976a, b) found $B = 1{\cdot}545 \pm 0{\cdot}004$ and $C_- \sim 0{\cdot}07$ (order of magnitude estimate) using high-density series expansions, and $C_+ = 0{\cdot}134 \pm 1\%$ using low-density series expansion. Thus we have $C_+/C_- = \mathrm{O}(10)$ whereas Sykes *et al* found $C_+/C_- = \mathrm{O}(1)$. We also observe that the discrepancy is mainly in C_-, where Sykes *et al* use a particularly poorly behaving high-density series. Wolff and Stauffer (1978) also noted, from their $n_s(\epsilon)$ scaling argument, that $C_+/C_- = 180 \pm 20\%$ for the square site problem, while Sykes *et al* gave the order of magnitude estimate of 3·9; Wolff and Stauffer also found that the discrepancy is mainly in the value of C_-.

4. Conclusion

In summary, we have discussed the scaling forms of 'thermodynamic' functions for percolation in general, and demonstrated that the scaling hypothesis holds for the square bond problem for ϵ and h at least in the range $\epsilon \lesssim 0{\cdot}1$, $h \lesssim 0{\cdot}1$. More detailed study of the size of the critical region will be published in a separate article.

Acknowledgments

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