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PERCOLATION AND CRITICAL BEHAVIOUR IN MANY BODY SYSTEMS.(U)

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FINAL TECHNICAL REPORT

by

C. DOMB

November 1976

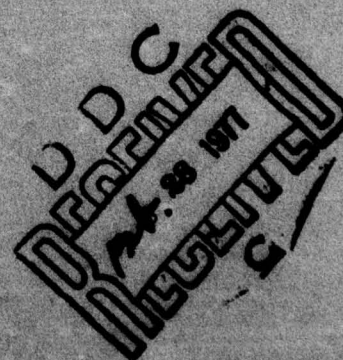
EUROPEAN RESEARCH OFFICE

United States Army

London NW1 England

Contract Number DAERO-76-G-003

King's College
Strand, WC2R 2LS
London



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20. ABSTRACT.

Earlier studies of percolation processes have been extended and the techniques applied to make a comprehensive study of the critical properties of random mixtures in three dimensions. Because of the theoretical interest, particularly in scaling theory, the investigation has been further extended to hyperdimensional mixtures and also to mixtures which are not random but determined by energetic considerations. The basic data has also been used for studies of the lattice gas model and the droplet model of condensation. A method of deriving series expansions for spin glasses has been developed. Thirteen appendices are attached to original copy of this Technical Report. All are available in the open scientific literature. Copies can also be obtained on request from controlling office.

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Appendix I

Percolation processes in two dimensions I.
Low-density series expansions.

Abstract The derivation of low-density series expansions for the mean cluster size in random site and bond mixtures on a two-dimensional lattice is described briefly. New data are given for the triangular, simple quadratic and honeycomb lattices and their matching lattices.

J.Phys.A: Math.Gen. 9, 87 (1976).

Appendix II

Percolation processes in two dimensions II.
Critical concentrations and the mean size index.

Abstract New series data are examined for the mean cluster size for site and bond mixtures in two dimensions. The critical concentration for the site problem on the simple quadratic lattice is estimated as $p_c = 0.593 \pm 0.002$ and on the honeycomb lattice as $p_c = 0.698 \pm 0.003$. It is concluded that the data are reasonably consistent with the hypothesis that the mean cluster size $S(p) = C(p_c - p)^{-\gamma}$ as $p \rightarrow p_c$ with γ a dimensional invariant, $\gamma = 2.43 \pm 0.03$ in two dimensions. Estimates of the critical amplitude C are also given.

J.Phys.A: Math.Gen. 9, 97 (1976).

Appendix III

Percolation processes in two dimensions III. High density series expansions.

Abstract The derivation of high density series expansions for the percolation probability and mean cluster size in random site and bond mixtures on a two-dimensional lattice is described. New data are given for the triangular, simple quadratic and honeycomb lattices.

J.Phys.A: Math.Gen. 9, 715 (1976).

Appendix IV Percolation processes in two dimensions IV. Percolation probability.

Abstract New series data are examined for the percolation probability $P(p)$ for site and bond mixtures in two dimensions. It is concluded that the data are reasonably consistent with the hypothesis that $P(p) = B(q_c - q)^\beta$ as $q \rightarrow q_c$ - with β a dimensional invariant, $\beta = 0.138 \pm 0.007$ in two dimensions. Estimates of the critical amplitude B are also given. Series data for the mean cluster size $S(p)$ in the high density region are examined and it is tentatively concluded that $S(p) = C'(q_c - q)^{-\gamma'}$ as $q \rightarrow q_c$ - and that the data are not inconsistent with the hypothesis $\gamma' = \gamma$.

J.Phys.A: Math.Gen. 9, 725 (1976).

Appendix V Percolation processes in three dimensions.

Abstract The derivation of low-density series expansions for the mean cluster size in random site and bond mixtures on a three-dimensional lattice is described briefly. New data are given for the face-centred cubic, body-centred cubic, simple cubic and diamond lattices. The critical concentration for the site problem is estimated as $p_c = 0.198 \pm 0.003$ (FCC), $p_c = 0.245 \pm 0.004$ (BCC), $p_c = 0.310 \pm 0.004$ (SC), $p_c = 0.428 \pm 0.004$ (D); for the bond problem as $p_c = 0.119 \pm 0.001$ (FCC), $p_c = 0.1785 \pm 0.002$ (BCC), $p_c = 0.247 \pm 0.003$ (SC), $p_c = 0.388 \pm 0.005$ (D). It is concluded that the data are reasonably consistent with the hypothesis that the mean cluster size $S(p) = C(p_c - p)^{-\gamma}$ as $p \rightarrow p_c$ - with γ a dimensional invariant, $\gamma = 1.66 \pm 0.07$ in three dimensions. Estimates of the critical amplitude C are also given.

J.Phys.A: Math.Gen. 9, 1705 (1976).

Appendix VI The percolation probability for the site problem on the face-centred cubic lattice.

Abstract The percolation probability for the site problem on the face-centred cubic lattice is investigated by series methods. It is concluded that $P(p)$ vanishes near the critical point like $(p - p_c)^\beta$ with $\beta = 0.42 \pm 0.06$.

J.Phys.A: Math.Gen. 9, L43 (1976).

Appendix VII Percolation processes in two dimensions V. The exponent δ_p and scaling theory.

Abstract By introducing a notional field variable λ into the percolation problem, a function $P_c(\lambda)$ is defined whose Ising analogue is the magnetic field variation of the magnetization along the critical

isotherm. Series expansions are used to study the critical behaviour of $P_c(\lambda)$, characterized by an exponent δ_p , for both site and bond percolation problems on the more common two-dimensional lattices. We conclude that δ_p is a dimensional invariant and estimate $\delta_p = 18.0 \pm 0.75$.

It appears that $\delta_p = 18$, $\gamma_p = \frac{23}{7}$, $\beta = \frac{1}{7}$ is the simplest set of rational exponents which is most consistent with the available data and which satisfies the scaling law $\gamma_p = \beta_p(\delta_p - 1)$ exactly.

J.Phys.A: Math.Gen. 9, 1109 (1976).

Appendix VIII Percolation processes in d-dimensions.

Abstract Series data for the mean cluster size for site mixtures on a d-dimensional simple hypercubical lattice are presented. Numerical evidence for the existence of a critical dimension for the cluster growth function and for the mean cluster size is examined and it is concluded that $d_c = 6$.

Exact expansions for the mean number of clusters $K(p)$ and the mean cluster size $S(p)$ in powers of $1/\sigma$ where $\sigma = 2d - 1$ and $p < p_c$ are derived through fifth and third order, respectively. The zeroth-order terms are the Bethe approximations.

The growth parameter λ is found to have the expansion

$$\lambda = \lambda_B(1 - \frac{1}{2}\sigma^{-1} - 2\sigma^{-2} - \dots)$$

where λ_B is the value of λ in the Bethe approximation. Similarly the critical probability p_c can be expanded in inverse powers of σ as

$$p_c = \sigma^{-1} + \frac{1}{2}\sigma^{-2} + \frac{3}{4}\sigma^{-3} + \frac{20}{3}\sigma^{-4} + \dots$$

Although these expansions are probably only asymptotic, they yield good approximations even when $d = 3$.

J.Phys.A: Math.Gen. 9, 798 (1976).

Appendix IX A note on the mean size of clusters in the Ising model

Abstract The derivation of series expansions for the mean size of finite clusters in the Ising model is described briefly. From an analysis of low temperature series it is concluded that for a two-dimensional lattice in zero magnetic field the mean size probably diverges at the Ising

critical temperature, T_c , as $(T_c - T)^{-\theta}$, with $\theta = 1.91 \pm 0.01$. It appears therefore that $\theta > \gamma' = 1.75$ the corresponding Ising susceptibility exponent. For a three-dimensional lattice it is tentatively concluded that the mean size diverges at some temperature $T^* < T_c$.

J.Phys.A: Math.Gen. 9, 836 (1976).

Appendix X

Lattice animals and percolation

Abstract A brief analysis is undertaken of the statistics of lattice animals (connected clusters) of n cells, and the results are applied to the site percolation problem. Recent proposals by Stauffer and Leath are examined, and an alternative interpretation is offered of the relation between percolation critical exponents and cluster statistics.

J.Phys.A: Math.Gen. 9, L141 (1976).

Appendix XI

Metastability and spinodals in the lattice gas model

Abstract The droplet model of condensation as developed by Fisher is modified to take account of: (a) ramified clusters whose surface/volume ratio tends to a finite limit as the number n of consistent molecules becomes large; (b) the excluded volume interactions between clusters. It is found that the interactions change the position of the first singularity in the activity series so that it no longer coincides with the phase boundary but is located beyond it. A thermodynamic metastable state can then be defined as in the classical Gibbs picture. At sufficiently low temperatures compact clusters (i.e. those in which the surface/volume ratio tends to zero for large n) dominate and give rise to an essential singularity. Near the critical temperature ramified clusters dominate and give rise to a spinodal line with a branch point singularity. Critical behaviour can be explained in terms of ramified clusters alone.

J.Phys.A: Math.Gen. 9, 283 (1976).

Appendix XII

Mean number of clusters for percolation processes in two dimensions

Abstract We use a transformation suggested recently by Zwanzig and Ramshaw on the series expansion for the mean number of clusters in the square bond and triangular site percolation problems. The new series are smooth and well behaved, and we estimate critical exponents and amplitudes. A value of -0.668 ± 0.004 is found for the exponent α_p , which is close to the rational fraction $-2/3$.

J.Phys.A: Math.Gen. 9, L137 (1976).

Appendix XIII Series expansions for a spin-glass model

Abstract Series expansions are investigated for a spin-glass Ising model with nearest-neighbour interactions J which can be randomly positive or negative. For the high-temperature phase the following conclusions result:- (i) the free energy has a singularity at about $w = \mu^{-1/2}$ ($w = \tanh \beta J$) (where μ is the self-avoiding walk limit), (ii) the magnetic susceptibility corresponds to uncoupled spins, (iii) the second derivative of susceptibility is simply related to the susceptibility of the standard Ising model and has a singularity at $w = w_c^{1/2}$ (where w_c refers to the standard model). Higher derivatives can be dealt with similarly. The low-temperature phase is more difficult to deal with because of the degeneracy of the lowest energy state. Further investigation is needed to decide whether the experimentally observed singularities correspond to the above, or arise as discontinuities from the meeting of the two phases.

J.Phys.A: Math.Gen. 9, L17 (1976).

1. ABSTRACT

Earlier studies of percolation processes have been extended and the techniques applied to make a comprehensive study of the critical properties of random mixtures in two and three dimensions. Because of the theoretical interest, particularly in scaling theory, the investigation has been further extended to hyperdimensional mixtures and also to mixtures which are not random but determined by energetic considerations. The basic data has also been used for studies of the lattice gas model and the droplet model of condensation. A method of deriving series expansions for spin glasses has been developed.

2. INTRODUCTION AND SUMMARY

An investigation has been made into the derivation of series expansions required for a study of random mixtures of sites on a lattice and extensive series data derived. For two and three dimensional lattices the data have been used to elucidate the percolation probability and critical behaviour. This work is reported in detail in Appendices I-VI. We have examined the close formal analogy between percolation processes and the ferromagnetic Ising model and made a special study of the critical exponent δ_p and scaling (Appendix VII). Because of the recent suggestion by Toulouse and Pfeuty that percolation processes should exhibit a critical dimension ($d_c = 6$) we have investigated random mixtures on the system of hypercubic lattices. From an analysis of data in series form we have concluded that they are consistent with the hypothesis (Appendix VIII). We have extended the study of the mean size of clusters in the Ising model initiated recently by Coniglio. Series expansions of useful length have been obtained and analysed and some conclusions drawn (Appendix IX).

We have made an analysis of the statistics of connected clusters (lattice animals) and investigated the relation between percolation critical exponents and cluster statistics (Appendix X). These investigations have been extended and applied to study the theory of metastability and spinodals in the lattice gas model (Appendix XI). To analyse some series expansions which have hitherto proved difficult to interpret we have developed a method based on a transformation suggested recently by Zwanzig and Ramshaw (Appendix XII).

The behaviour of spin-glasses with randomly competing ferromagnetic

and antiferromagnetic interactions (but no long-range magnetic order) has given rise to a number of theoretical investigations recently. We have found it possible to develop series expansion techniques for this problem. This work is reported in Appendix XIII.