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

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FINAL TECHNICAL REPORT. Nov 76 - Nov 79

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EUROPEAN RESEARCH OFFICE

United States Army

London NW1 England

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20. ABSTRACT

Many of the gaps in the scaling theory of percolation clusters for random systems have been filled during the past three years. These have led to a better understanding of the statistics of lattice animals, and of the nature of the percolation transition. Calculations have been undertaken to determine parameters which characterize the structure of the infinite percolating cluster. Investigations have been initiated of the properties of systems with correlated percolation (i.e. in which the probability of occupation of a given site influences its neighbours). Work has continued on high temperature expansions for the Ising and classical Heisenberg models in an attempt to remove the discrepancies with renormalization group calculations. Particular attention has been devoted to calculations in 4 dimensions because of the marginal significance of this dimension. Further investigations have been made of the statistical properties of a single polymer chain using the Domb-Joyce model, and of particular properties of self-avoiding walks.

TABLE OF CONTENTSPAGE NOS

1.	ABSTRACT	1
2.	INTRODUCTION AND SUMMARY	2
3.	APPENDICES	5

1. ABSTRACT

Many of the gaps in the scaling theory of percolation clusters for random systems have been filled during the past 3 years. These have led to a better understanding of the statistics of lattice animals, and of the nature of the percolation transition. Calculations have been undertaken to determine parameters which characterize the structure of the infinite percolating cluster. Investigations have been initiated of the properties of systems with correlated percolation (i.e. in which the probability of occupation of a given site influences its neighbours). Work has continued on high temperature expansions for the Ising and classical Heisenberg models in an attempt to remove the discrepancies with renormalization group calculations. Particular attention has been devoted to calculations in 4 dimensions because of the marginal significance of this dimension. Further investigations have been made of the statistical properties of a single polymer chain using the Domb-Joyce model, and of particular properties of self-avoiding walks.

2. INTRODUCTION AND SUMMARY

(a) Percolation

The theory of percolation has attracted increasing interest during the past 3 years, and there has been a rapid build up in the literature from research groups all over the world. The theory has now been applied to a variety of problems in solid state physics and chemistry. Particular progress has been made in the scaling theory of percolating clusters which has now reached a definitive stage¹, and has been applied with success to two and three dimensional systems. The research group at Watertown Arsenal (G. H. Bishop, G. D. Quinn and R. J. Harrison) has been in the forefront of these developments, and the principal investigator has acted in an advisory capacity to this group.

Our own group has continued to use the method of direct enumeration as a tool. The exponent δ_p has been estimated in three and higher dimensions (Appendix 1) and the general behaviour of bond percolation processes in d dimensions has been investigated (Appendix 2). A particular investigation was undertaken for the critical dimensions ($d = 6$) (Appendix 3). The closely related problem of lattice animals has also been investigated by this method (Appendices 4 and 5).

The Monte Carlo method has been used by the principal investigator in collaboration with Dr. E. Stoll of IBM Zurich to characterize the shapes and sizes of clusters arising in Ising systems (Appendix 6) and in percolating systems with and without correlations (Appendices 7 and 8). An important

¹ See e.g. D. Stauffer, "Scaling Theory of Percolation Clusters" Physics Reports, 54, 1 (1979).

conjecture was subsequently proved theoretically by A. Hankey². The degree of ramification was determined for finite and infinite clusters, and analogous results were derived independently for random percolation by the direct enumeration method (Appendix 9). A related problem of lattice animals and percolation with restricted valency was also dealt with by direct enumeration (Appendices 10 and 11).

Spin glasses constitute another random system of the percolation type, but their properties have proved to be extremely complex. Some observations on the nature of the singularity as deduced from series expansions are given in Appendix 12.

(b) Critical behaviour of many body systems

The series method is always more powerful when all the terms are consistent in sign since critical behaviour is directly related to asymptotic analysis of the coefficients. When the terms are inconsistent the Padé approximant has proved very useful, but the improvement with increasing numbers of terms is not systematic. Some investigators have used transformations to render the terms consistent in sign, but there has been no systematic method of generating these transformations. Such a method devised by C. J. Pearce (who was visiting the group for a year from Western Australia) is developed in Appendix 13.

We have paid some attention to series expansions for the Ising model in 4 dimensions since this is the marginal

² A. Hankey, J.Phys.A 17 L49-55 (1978).

dimension for renormalization group calculations. This work is described in appendices 14, 15. Other work extending the Ising series in 2 and 3 dimensions is described in Appendix 16, and corresponding work on the classical vector model in Appendix 17. The need for more terms is shown by Appendices 18 and 19 which show how conclusions on the value of the critical exponent γ with the present terms available still depend on the method of analysis used.

Appendix 20 investigates in more detail a generalized form of lattice-lattice scaling which has been suggested previously by others. The asymptotic behaviour of the b_n coefficients in the Mayer series for the condensation of a gas was a subject of much discussion in the early days of the theory of condensation and was never successfully resolved. Much more information can be obtained from lattice gas expansions, and this behaviour is analysed in Appendix 21.

(c) Polymers

Earlier work on the application of universality to the expansion factor of a polymer chain because of excluded volume has been successfully completed, and is described in Appendix 22. A diagrammatic expansion of the virial series is developed in Appendix 23.

The star graph expansion method is successfully applied to the problem of generating self-avoiding walks in 3 dimensions (Appendix 24) and in 4 dimensions (Appendix 25). The problem of self-avoiding walks in a finite slab is considered in Appendix 26; and that of a self-avoiding walk attached to a surface in Appendix 27.

3. APPENDICES

Appendix 1

Percolation exponent δ_p for lattice dimensionality $d \geq 3$

Abstract Series expansions are used to study the exponent δ_p for site and bond percolation problems on three-dimensional lattices. Our results, which include $\delta_p = 5.0 \pm 0.8$, are discussed in relation to scaling theory and universality.

To test Toulouse's conjecture regarding the critical dimensionality ($d_c = 6$) for percolation processes, a similar analysis is attempted for the site problem on simple hypercubic lattices of dimensionality $4 \leq d \leq 7$.

Appendix 2

Bond percolation processes in d dimensions

Abstract We study bond percolation processes on a d -dimensional simple hypercubic lattice. 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 fourth order, respectively. The zeroth-order terms are the Bethe approximations. The critical probability p_c is found to have the expansion, probably asymptotic,

$$p_c = \sigma^{-1} (1 + 2\frac{1}{2}\sigma^{-2} + 7\frac{1}{2}\sigma^{-3} + 57\sigma^{-4} + \dots) ,$$

while the cluster growth parameter λ can be expanded as

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

where λ_B is the Bethe approximation for λ .

We also present series data for the mean cluster size and the cluster growth function for $d = 4$ to 7. Numerical analysis suggests that the critical dimension d_c for bond percolation is $d_c = 6$, as it seems to be for the site problem. The evidence also supports the conjecture that the value of a particular critical exponent in a given dimension is the same for both bond and site processes.

Appendix 3

Percolation theory at the critical dimension

Abstract Corrections to scaling at the critical dimension have been calculated from the ϕ^3 field theory. Numerical calculations based upon series expansions for the mean cluster size in percolation theory are shown to be consistent with an asymptotic behaviour of the type found for the susceptibility in the $n = 0$ limit of the ϕ^3 model.

Appendix 4

On the asymptotic number of lattice animals in bond and site percolation

Abstract A recently proposed asymptotic form, due to Domb, for the total number of bond and site animals of size n , has been investigated numerically. It is found to fit the available data better than simpler forms previously assumed. The critical parameters entering into the asymptotic form are estimated for a number of two- and three-dimensional lattices, and conclusions are drawn about their lattice and dimensional dependence. In particular, the cluster growth parameter λ is estimated with a higher degree of precision than that previously attained.

Appendix 5

Lower bounds on the numbers of lattice animals

Abstract Rigorous lower bounds on the connective constants for site and bond animals have been derived for d -dimensional simple hypercubic lattices. These bounds establish for arbitrary d that the connective constants for site and bond animals are strictly greater than the connective constant for self-avoiding walks.

Appendix 6

Shape and size of clusters in the Ising model

Abstract The cyclomatic number of a cluster is introduced as a measure of its degree of compactness or ramification. Using Monte Carlo data for a two-dimensional Ising model, estimates are given of the average number of spins and the average number of cycles per cluster as a function of temperature. The results are related to the Whitney polynomial studied recently by Temperley and Lieb. An exact calculation by these authors at the critical temperature enables the pattern of behaviour in the critical region to be conjectured.

Appendix 7

Monte Carlo studies of two-dimensional percolation

Abstract A one-spin flip Ising model is used to provide data on cluster statistics for random and Ising percolation. The concentration p is controlled by the magnetic field. At sufficiently high temperatures the system corresponds to random percolation, and the theoretical formula $s/n = (1-p)/p$ is verified for large clusters at critical concentration p_c (s = number of boundary sites). It is also found that the relation is accurately satisfied for all percolating clusters when $p > p_c$ but not for Ising percolation at temperature $2T_c$. For random percolation with $p > p_c$ the finite n -clusters are found to follow an asymptotic decay of the form $\exp(-b(p)n^{1/2})$ in accord with theory.

Appendix 8

Shape and size of two-dimensional percolation clusters with and without correlations

Abstract The statistical analysis previously used for the temperature behaviour of clusters for the Ising model is applied to Monte Carlo samples of percolation clusters. Three cases are considered: (a) positive correlation ($T = 2T_c$ ferromagnetic); (b) random ($T = \infty$); (c) negative correlation ($T = 2T_c$ antiferromagnetic). It is found that the exponents which characterise the decay of the cluster-size distributions do not depend on correlation. These distributions can be fitted over their whole range by assuming that percolation critical exponents are independent of correlation, but the scaling functions which then result do depend on correlation. Statistical parameters which are related to the compactness or ramification of clusters change smoothly with correlation. However, some features of negative correlation are significantly different in behaviour.

Appendix 9

Aspects of the structure of the infinite cluster in site percolation

Abstract In this paper we present the results of preliminary investigations into the structure of the infinite cluster in site percolation theory. It is shown how series expansions, for quantities defined as site and bond valency, respectively, may be derived. The series are used to obtain a measure of the degree of ramification of the infinite cluster, and techniques for obtaining a free energy series for the infinite cluster in a site-dilute ferromagnet are discussed.

Appendix 10

Percolation with restricted valence

Abstract We have enumerated exactly the square lattice site animals with vertex degree less than or equal to three and with up to fourteen sites in the cluster. Using series analysis techniques estimates have been made of the location, exponent and amplitude of the principal singularity in the animal generating function for maximum vertex degree $v = 2, 3$ and 4 . We have shown rigorously that the dominant singularity in the generating function must have a different exponent for $v = 2$ than for $v = 3$ and the numerical results suggest that the generating function diverges with an exponent of $\frac{4}{3}$ for $v = 2$ but logarithmically for both $v = 3$ and $v = 4$.

Appendix 11

Restricted valence site animals on the triangular lattice

Abstract Exact values of the numbers of connected clusters of n sites, each site having valence no larger than v , are presented for the triangular lattice for $v = 2, 3, 4$ and 5 for small values of n . Assuming a plausible asymptotic form for the

dependence of these numbers on n and ν we show, using series analysis techniques, that the exponent characterising the dominant singularity in the generating function has the same value for all $\nu \geq 3$ but a different value for $\nu = 2$.

Appendix 12

Nature of the singularity in a spin-glass model

Abstract High temperature series expansions are developed for the specific heat of a random bond Ising model of a spin glass for standard two- and three-dimensional lattices. Padé approximant analysis of the series indicates the absence of any singularity on the positive real axis. The solution for the Bethe lattice is investigated using results obtained previously for the Mattis random site model. It is concluded that the high temperature partition function and all its derivatives with respect to magnetic field have no singularity at the transition temperature. This behaviour may also extend to lattice models.

Appendix 13

Transformation methods in the analysis of series for critical properties

Abstract During the past twenty years, considerable use has been made of conformal transformations as an aid to series analysis in the study of critical phenomena; however, there has been no evident systematic approach to the task of choosing the most suitable transformation for a given series. In this review we discuss the theory of transformations and provide such a rational and systematic method of approach. The purpose of transformation is to map the singularity of interest (usually the critical point) significantly closer to the origin than any other singularity, so that it dominates the later coefficients of the series; extrapolation methods based on Darboux's theorems may then be employed. We show that, for series likely to arise in thermodynamics, it is always possible to find transformations which achieve this purpose. We provide a set of conditions, which should be satisfied by any transformation function, to ensure straightforward and valid analysis, and we then discuss the basic types of transformation and their selection in practice. In the final sections, we illustrate the approach with some important examples, and show that it leads to transformed series which are much smoother than those previously obtained.

Appendix 14

The critical isotherm of the four-dimensional Ising model

Abstract The critical isotherm of the Ising model for the four-dimensional simple hypercubic lattice is studied using a high-field expansion through μ^{15} . The series for the magnetisation

is analysed for singularities of the asymptotic form $E(1-\mu)^{1/3} |\ln(1-\mu)|^p$, predicted by renormalisation group theory. Good convergence is obtained for values of p around $1/3$ (the renormalisation group prediction) and we estimate $p = 0.30 \pm 0.05$. Assuming $p = 1/3$, the critical amplitude E is estimated to be 0.896 ± 0.02 .

Appendix 15

Susceptibility and fourth-field derivative of the spin- $\frac{1}{2}$ Ising model for $T > T_c$ and $d = 4$

Abstract We investigate the spin- $\frac{1}{2}$ Ising model with nearest-neighbour interactions on the four-dimensional simple hypercubic lattice. High-temperature series expansions are studied for the zero-field susceptibility χ_0 and the fourth field derivative of the free energy $\chi_0^{(2)}$ up to order v^{17} . The series are analysed for singularities of the form $t^{-q} |\ln t|^p$ where t is the reduced temperature. For χ_0 it is found that $p = 0.33 \pm 0.07$ when $q = 1$, in good agreement with the prediction $p = 1/3$, $q = 1$ of renormalisation group theory. The critical temperature is estimated to be $v_c^{-1} = 6.7315 \pm 0.0015$. Results for $\chi_0^{(2)}$ are more slowly convergent but are not inconsistent with the renormalisation group prediction $p = 1/3$, $q = 4$.

Appendix 16

Extended high temperature low field expansions for the Ising model

Abstract High temperature low field expansions are derived from the free energy of the Ising model for several two- and three-dimensional lattices. These represent a considerable advance on earlier work. Expansions for the four-dimensional hypercubic lattice are also presented.

Appendix 17

Extension of the high-temperature, free-energy series for the classical vector model of ferromagnetism in general spin dimensionality

Abstract In this paper we present the results of a study of the free energy and specific heat of the classical vector model of ferromagnetism. High-temperature series for the free energy are presented as far as the 12th term in general spin dimensionality (D) and the 13th term for the case $D = 3$. The techniques used to derive these series are discussed in some detail. The general series is shown to reduce to that for the Ising model for $D = 1$, and to agree with the expansion of the exact result for the spherical model for the case $D = \infty$. The cases $D = 2$ and $D = 3$ correspond to the classical planar and classical Heisenberg models, respectively. We demonstrate that our general series reproduces previous results for both of these models, with the exception of a small disagreement with the calculated 11th terms of Ferer et al (1971, 1973).

In addition, our general series extends the series for each of these models by one term, and our independent work for $D = 3$ provides one further term. We present the results of a ratio analysis of the series for $D = 2$ and $D = 3$, comparing previous work with our additional results. Although we are able to make predictions of both the critical point and the critical exponent, we conclude that further terms for the susceptibility series are required in order to refine the estimate of the critical point. We compare our estimate of the exponent α for $D = 2$ with the determination (Muller et al 1976) of the exponent α for the λ transition in liquid helium II, finding striking agreement.

Appendix 18

The critical exponent γ for the three-dimensional Ising model

Abstract Estimates for the critical exponent γ for the initial susceptibility of the three-dimensional spin- $\frac{1}{2}$ Ising model are summarised. There is a discrepancy between estimates based on high-temperature series expansions and those obtained using renormalisation group theory. High-temperature series estimates for γ are reviewed and re-examined using some new data. It is tentatively concluded that a small discrepancy still appears to exist and that further work is needed to resolve it.

Appendix 19

The exponent γ for the spin- $\frac{1}{2}$ Ising model on the face-centred cubic lattice

Abstract The high-temperature, zero-field susceptibility series of the spin- $\frac{1}{2}$ Ising model on the face centred cubic lattice is analysed assuming the asymptotic form $A_1 t^{-\gamma} + A_2 t^{-\gamma+1} + B t^{-\gamma+\Delta_1}$ where t is the reduced temperature.

Good convergence is obtained for $\gamma = 1.241$ and $\Delta_1 = 0.496$, the values predicted by renormalisation group theory. Attempts to fit the series coefficients with $\gamma = 1.25$ and $B = 0$, do not prove as successful. The amplitudes A_2/A_1 and B/A_1 are estimated.

Appendix 20

A generalised form of extended lattice-lattice scaling and its relationship to the scaled equation of state with applications to the Ising model

Abstract A natural generalisation of lattice-lattice scaling is suggested which holds exactly for the second most singular amplitudes for the Ising model on the triangular, honeycomb, square and Kagomé lattices. In general, this scaling theory requires three scaling parameters, g , n and m , but includes extended lattice-lattice scaling as the special case of $m = n$. The generalised form of lattice-lattice scaling does not seem to be applicable to the three-dimensional

Ising model. The connections between lattice-lattice scaling, its extension and generalisation, and the critical equation of state including correction terms are established and discussed.

Appendix 21

Behaviour of the Mayer cluster sums, b_n , for the Ising lattice-gas

Abstract The high-field polynomials $L_n(u)$ (or equivalently the Mayer b_n coefficients) for the spin $S = \frac{1}{2}$ Ising model with nearest-neighbour ferromagnetic interactions (or equivalently the simple lattice-gas) have been studied for a variety of two and three dimensional lattices. We find that (a) the leading zero of $L_n(u)$ on the positive real u axis always corresponds to a temperature T_1 greater than the critical temperature T_c , and approaches T_c as $n \rightarrow \infty$ like $1/n^{1/\Delta}$, where Δ is the usual gap exponent. In addition, (b), $L_n(u)$ appears to have exactly $n-1$ zeros in the physical interval $(u_c, 1)$ corresponding to $T_c < T < \infty$.

Result (a) appears to be rather general since it holds for a variety of other Ising systems including those (I) with longer-ranged interactions, (II) with spin $S > \frac{1}{2}$, and (III) on Bethe lattices of coordination numbers $q = 2$ (linear chain) and (IV) $q = 3$. Result (b), on the other hand, is not generally valid when $S > \frac{1}{2}$ although it does seem to apply for all the other systems studied.

Appendix 22

Polymer chain statistics and universality I

Abstract A brief summary is given of the concept of universality in the theory of critical phenomena. The concept is applied to random walks and self-avoiding walks on lattices corresponding to the $n = -2$ and $n = 0$ universality classes. The Domb-Joyce model of a random walk on a lattice with a δ function interaction of strength w is identified with crossover behaviour w serving as a crossover parameter. Exact enumerations are undertaken of the mean-square end-to-end length (R_N^2) for the Domb-Joyce model for a number of three-dimensional lattices. Using the smoothness postulate of Griffiths, estimates are obtained of the asymptotic behaviour of the expansion factor $\alpha^2 = (R_N^2)/N$ in the range $0.5 < w < 1$. By combining these with exact virial coefficients for small w the range is extended to $w = 0$. The two-parameter approximation which assumes that α^2 is a function of $wN^{1/2}$ is satisfied with maximum errors of 2 or 3%. The two-parameter function which has been the subject of much discussion by polymer theorists is estimated and an empirical formula is proposed.

Appendix 23

Virial expansion for a polymer chain: the two parameter approximation

Abstract A complete diagrammatic expansion is developed for the Domb-Joyce model of an N-step chain, with an interaction w which varies between 0 and 1. Simple rules are given for obtaining the diagrams. The correspondence between these diagrams and appropriate generating functions permits computation of the coefficients of the series $\alpha_N^2(w) = 1 + k_1 w + k_2 w^2 + \dots$, where $\alpha_N^2(w)$ is the expansion factor of the mean square end-to-end length of the chain. The dominant term in N of each of the first three k_i is shown to be identical for the three cubic lattices and for the Gaussian continuum model, with the exception of a scale factor h_0 . Retention of only this dominant term yields a 'two-parameter' expansion equivalent to that of Zimm (1946), Fixman (1955) and others. Diagrams are classed either as ladder or as non-ladder graphs. The ladder graph contributions are summed by using functional relations of Domb and Joyce (1972). The non-ladder contributions for the first three coefficients are computed individually, thereby yielding results for k_1 , k_2 and k_3 in terms of the 'universal' parameter $z = h_0 N^{1/2} w$. The terms k_1 and k_2 agree with previous computations for the Gaussian model but k_3 differs slightly.

Appendix 24

Self-avoiding walks on the face-centred cubic lattice

Abstract The generating function $C(x)$ for the number of self-avoiding walks on the face-centred cubic lattice is extended by two terms to order 14. The series coefficients are analysed for a singularity of the form $A_1 t^{-\gamma} + A_2 t^{-\gamma+1} + B t^{-\gamma+\Delta_1}$ with $t = 1 - \mu x$, where μ is the connective constant. Two cases of interest are studied, (a) $\gamma = 1\frac{1}{2}$, $B = 0$ as conjectured in earlier work on series expansions and (b) $\gamma = 1.1615$, $\Delta_1 = 0.465$ as predicted by renormalisation group (RG) calculations. It is found that the series coefficients are better fitted to the RG predictions (b).

Appendix 25

Self-avoiding walks on the hyper face-centred cubic lattice in four dimensions

Abstract The star graph expansion method for calculating high temperature susceptibility series for the Ising model has been extended to the polymer problem. The generating function for self-avoiding walks on the four-dimensional face-centred cubic lattice has been calculated to ninth order. The series coefficients are analysed for singularities of the form $t^{-1} |\ln t|^p$, predicted by renormalisation group calculations. Good convergence is obtained for values of p in the vicinity of $p = \frac{1}{2}$, (the renormalisation group prediction) and we esti-

mate $p = 0.24 \pm 0.03$. The critical point (connective constant for the polymer problem) is found to be 22.072 ± 0.004 .

Appendix 26

Self-avoiding walks in a slab of finite thickness: a model of steric stabilisation

Abstract The technique of exact enumeration coupled with series analysis has been used to study the behaviour of the properties of long self-avoiding walks on a square lattice slab as the thickness (D) of the slab is varied. Scaling arguments due to Daoud and de Gennes predict the variation of mean-square end-to-end distance and of free energy with D . Our results are consistent with these scaling predictions for the mean-square end-to-end distance, but suggest that the free-energy crossover exponent is closer to unity than the value ($1/3$) predicted by scaling.

Appendix 27

Some tests of scaling theory for a self-avoiding walk attached to a surface

Abstract We have defined analogues of the surface and layer susceptibilities of a semi-infinite magnetic system for the self-avoiding walk model of a polymer attached to a surface. Surface scaling relations between exponents appearing in the magnetic problem, as well as a recent renormalisation group exponent relationship, should apply to the self-avoiding walk case and we have generated extensive series expansions of the analogues of these susceptibilities for the square and simple cubic lattices. Our analyses of these series show that surface scaling holds for the self-avoiding walk problem in both two and three dimensions but that the renormalisation group argument gives incorrect values of the exponents in two dimensions.