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Computer Physics Communications 147 (2002) 435–438

Computer Physics Communications

www.elsevier.com/locate/cpc

High-temperature series expansions for random-bond Potts models on $\mathbb{Z}^d$

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Abstract

We use a star-graph expansion technique to compute high-temperature series for the free energy and susceptibility of random-bond q-state Potts models on hypercubic lattices. This method allows us to calculate quenched disorder averages for arbitrary uncorrelated coupling distributions. Moreover, we can keep the disorder strength p as well as the dimension d as symbolic parameters. This enables scans over large regions of the (p, d) parameter space for any value of q. For the bond-diluted Ising model ($q = 2$) in three dimensions we present first results for the critical temperature and exponent γ obtained from the analysis of susceptibility series up to order 19.

PACS: 64.60.Cn; 05.50.+q; 05.70.Jk; 64.60.Fr

Keywords: High-temperature series expansions; Star graphs; Quenched random disorder; Bond-diluted Ising model

1. Introduction

Despite considerable efforts in the past few years there are still many open problems in the physics of disordered systems. One alternative to large-scale numerical simulations are systematic series expansions. Such expansions for statistical models defined on a lattice are a well-known method to study phase transitions and critical phenomena [1]. The extension of this method to disordered systems [2] demands the development of new graph theoretical and algebraic algorithms.

To this end we developed further the method of "star-graph expansion" which allows one to take the disorder average on the level of individual graphs, and apply it to Potts models with a bimodal quenched distribution of ferromagnetic couplings.

Depending on dimension d and number of states q the pure Potts models show first- or second-order phase transitions. According to the Harris criterion one expects in the second-order case either the appearance of a new random fixed point ($d = 2$, $q = 3, 4$ and $d = 3$, $q = 2$) or logarithmic corrections to the pure fixed point ($d = 2$, $q = 2$). The latter system has been successfully studied using high-temperature series in [3].

At first-order transitions, randomness softens the transitions. For $d = 2$ even infinitesimal disorder induces a continuous transition [4], whereas for $d = 3$, $q > 2$ a tricritical point at a finite disorder strength is expected [5].

In this note we report on an ongoing large-scale project to study this area using series expansions. We concentrate on the first, most laborious step, the

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0010-4655/02/$ – see front matter
PII: S0010-4655(02)00321-1

generation of high-temperature series to high order, and present first results of analyses of the resulting susceptibility series for the bond-diluted Ising model in three dimensions (3D).

2. Model

The q-state Potts model on arbitrary graphs G with arbitrary coupling constants J_{ij} assigned to the nearest-neighbor links $\langle ij\rangle$ of G is defined by its partition function

$$\begin{aligned} Z &= \sum_{\{S_i\}} \exp(-\beta H), \\ H &= -\sum_{\langle ij\rangle} J_{ij}\delta(S_i, S_j), \end{aligned} \tag{1}$$

where $\beta = 1/k_{\mathrm{B}}T$ is the inverse temperature, $S_i = 1,\ldots,q$ and $\delta(.,.)$ is the Kronecker symbol. Quenched disorder averages are done using an uncorrelated bimodal distribution of the form

$$P(J_{ij}) = (1-p)\delta(J_{ij}-J_0) + p\delta(J_{ij}-RJ_0), \tag{2}$$

which can include spin glasses ($R=-1$, $p=\frac{1}{2}$), random-bond ferromagnets ($0<R<1$) and bond dilution ($R=0$) as special cases. Other distributions can, in principle, also be considered with our method.

3. Star-graph expansion method

Graphs constitute a partially ordered set under the "subgraph" relation. Therefore, for every function $F(G)$ defined on the set of graphs exists another function $W_F(G)$ such that for all graphs G

$$F(G) = \sum_{g\subseteq G} W_F(g), \tag{3}$$

and this function can be calculated recursively via

$$W_F(G) = F(G) - \sum_{g\subset G} W_F(g). \tag{4}$$

This gives for an infinite (e.g., hypercubic) lattice

$$F\big(\mathbb{Z}^d\big) = \sum_G \big(G:\mathbb{Z}^d\big) W_F(G), \tag{5}$$

where $(G:\mathbb{Z}^d)$ denotes the weak embedding number of the graph G in the lattice [6]. Let G be a graph with an articulation vertex where two star subgraphs $G_{1,2}$ are glued together. Then $W_F(G)$ vanishes if $F(G) = F(G_1) + F(G_2)$. It is easy to see that the free energy $\log Z$ has this property and it can be proved [2] that the inverse susceptibility $1/\chi$ has it, too, even for arbitrary inhomogeneous couplings J_{ij}. This restricts the sum in Eq. (5) to a sum over star graphs. The linearity of Eqs. (3)–(5) enables the calculation of quenched averages over the coupling distribution on the level of individual graphs. The resulting recipe for the susceptibility series is:

- Graph generation and embedding number counting;
- Calculation of $Z(G)$ and
  $$M_{nm}(G) = \mathrm{Tr}\big(q\delta(S_n,S_m)-1\big)\mathrm{e}^{-\beta H(\{J_{ij}\})}$$
  for all graphs;
- Disorder average
  $$N_{nm}(G) = [M_{nm}/Z]_{P(J)};$$
- Subgraph subtraction
  $$W_\chi(G) = \sum_{n,m}(N^{-1})_{nm} - \sum_{g\subset G} W_\chi(g);$$
- $1/\chi = \sum_G (G:\mathbb{Z}^d) W_\chi(G)$.

Implementing this program, we classified for the first time all star graphs up to order 19 and calculated their embedding numbers for d-dimensional hypercubic lattices (up to order 17 for arbitrary d, order 18 and 19 for dimensions $\leqslant 4$). The embedding count uses a refined version of the algorithm by Martin [6] employing optimized hash tables for collision testing.

For the symbolic calculations we developed a C++ template library using an expanded degree-sparse representation of polynomials and series in many variables. The open source library GMP is used for the arbitrary-precision arithmetics.

The partition function and correlation functions for each graph are calculated in the cluster representation,

$$M_{nm} \propto \sum_{C_{nm}} q^{l+c}\Bigg(\prod_{\langle ij\rangle\in C} v_{ij}\Bigg)\Bigg(\prod_{\langle ij\rangle\notin C}(1-v_{ij})\Bigg). \tag{6}$$

Here $v_{ij} = (\mathrm{e}^{\beta J_{ij}}-1)/(\mathrm{e}^{\beta J_{ij}}-1+q)$, the sum goes over all clusters $C_{nm}\subseteq G$ in which the vertices n and m are connected, l is the number of links of the cluster and c the number of connected components.

The clusters are enumerated by Gray codes [7] such that two consecutive clusters in the sum (6) differ by exactly one (added or deleted) link. This results in a considerable speed-up of the calculations by re-using every term in the sum for the calculation of the next one.

Our longest series, up to order 19, are obtained for the case of bond dilution where (2) simplifies to

$$P(J_{ij}) = (1-p)\delta(J_{ij} - J_0) + p\delta(J_{ij}), \tag{7}$$

since in this case the disorder average for a series is most easily done via

$$\left[v_1^{n_1} \dots v_k^{n_k}\right]_{P(J)} = (1-p)^k v_0^{n_1+\dots+n_k}. \tag{8}$$

All calculations were carried out on Pentium Linux farms and on a T3E.

4. Example: bond-diluted Ising model in three dimensions

The 3D disordered Ising model has been extensively studied both by field theoretical and numerical methods. The Monte Carlo simulations using site dilution in [8] affirm the expectation that a new random fixed point with $\gamma = 1.342(5)(5)$ arises between the pure one ($p = 0$) and the percolation threshold. A comprehensive compilation of this and other Monte Carlo results can be found in [9], showing a wide scatter in the critical exponents of different groups, presumably due to large crossover effects.

In the literature many different series analysis techniques have been discussed which all have their merits and drawbacks [10]. Our high-temperature series expansions for the susceptibility up to order 19 are given with coefficients as polynomials in p, $\chi(v) = \sum_n a_n(p)v^n$. Therefore it should be well-suited for the method of partial differential approximants [11] which was successfully used to analyze series with an anisotropy parameter describing the crossover between 3D Ising, Heisenberg and XY behaviour. But this method was unable to give conclusive results. Therefore we confined ourselves to the analysis of single-parameter series for selected values of p.

The ratio method assumes that the expected singularity of the form $\chi(v) \sim A(v_c - v)^{-\gamma}$ is the nearest to the origin. Then the consecutive ratios of series coefficients behave asymptotically as

$$r_n = \frac{a_n}{a_{n-1}} = v_c^{-1}\left(1 + \frac{\gamma - 1}{n}\right). \tag{9}$$

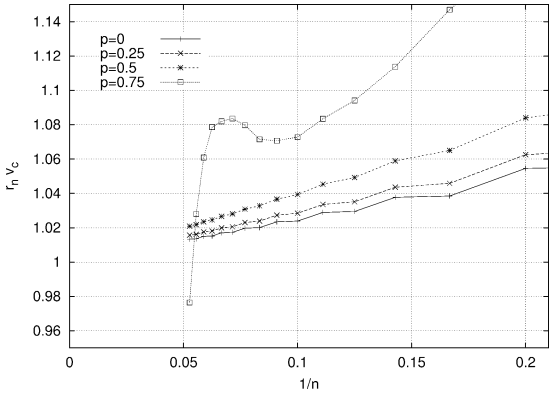

Fig. 1. Ratio approximants for different dilutions p vs. $1/n$.

Fig. 1 shows these ratios for different values of p. In order to make them visually comparable, they are (except for $p = 0.75$) normalized by their respective critical couplings v_c. For small p they show the typical oscillations related to the existence of an antiferromagnetic singularity at $-v_c$. Near the percolation threshold at $p = p_c = 0.7512$ (where T_c goes to 0, v_c to 1) the series is clearly ill-behaved, related to the $\exp(1/T)$ singularity expected there. Besides that, the slope (related to γ) is increasing with p.

The widely used DLog-Padé method consists in calculating Padé approximants to the logarithmic derivative of $\chi(v)$. The smallest real pole of the approximant is an estimation of v_c and its residue gives γ. The results presented in Table 1 are the averages of 45–55 Padé approximants for each value of p, with the error in parentheses indicating the standard deviation. The scattering of the Padé approximants increases with p, getting again inconclusive near the percolation threshold. The critical exponent γ, as provided by this method, varies with the disorder strength.

More sophisticated analysis methods, such as inhomogeneous differential approximants or the methods [12] M1 and M2, especially tailored to deal with confluent singularities as one would expect in a crossover situation, give essentially the same results.

Table 1
Transition points $v_c = \tanh(\beta_c J_0/2)$ and critical exponents γ for different dilutions p as obtained from DLog-Padé approximants

p	v_c	γ
0	0.21813(1)	1.2493(7)
0.075	0.23633(1)	1.2589(8)
0.15	0.25788(1)	1.2714(8)
0.225	0.28382(1)	1.2873(10)
0.3	0.31566(2)	1.305(4)
0.375	0.35557(5)	1.329(4)
0.45	0.40743(10)	1.365(6)
0.525	0.4772(2)	1.400(10)
0.6	0.576(1)	1.435(60)

5. Conclusion

We have implemented a comprehensive toolbox for generating and enumerating star graphs as required for high-temperature series expansions of quenched, disordered systems. Since the relevant parameters (degree of disorder p, spatial dimension d, number of states q, etc.) are kept as symbolic variables, the number of potential applications is very large. Here we have only presented a preliminary analysis of the 3D bond-diluted Ising model. The results obtained so far leave three possibilities: the series are still much too short to cope with the expected crossover effects, the critical parameters are p-dependent or the series analysis is seriously hampered by logarithmic corrections [13].

Acknowledgements

Support by DFG grant No. JA 483/17-1 and partial support from the German-Israel-Foundation under grant No. I-653-181.14/1999 is gratefully acknowledged.

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