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Random-bond Potts models on hypercubic lattices: high-temperature series expansions*

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We derive high-temperature series expansions for the free energy and the susceptibility of random-bond q-state Potts models on hypercubic lattices using a star-graph expansion technique. This method enables the exact calculation of 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 allows us to scan large regions of the (p, d) parameter space for any value of q. For the bond-diluted 4-state Potts model in three dimensions we present first results for the critical temperature as a function of p as obtained from the analysis of susceptibility series up to order 18.

1. INTRODUCTION

Systematic series expansions for statistical models defined on a lattice are a well-known method to study phase transitions and critical phenomena [1]. They provide an useful complement to large-scale numerical simulations, in particular for quenched, disordered systems where the average over the different disorder realizations is numerically very time consuming. To this end we developed further the method of "star-graph expansion" which allows us to take the disorder average on the level of individual graphs exactly and apply it to Potts models with a bimodal quenched distribution of ferromagnetic couplings.

Depending on the dimension d and the number of states q, 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 ($d = 2$, $q = 2$). At first-order transitions, randomness softens the transitions. For $d = 2$ even infinitesimal disorder induces a continuous transition [2], whereas for $d = 3$, $q > 2$ a tricritical point at a finite disorder strength is expected [3].

In this note we report on an ongoing large-scale project to study this area using series expansions. After a brief outline of the method used for generating the series we concentrate on first results of analyses of the resulting susceptibility series for the bond-diluted 4-state Potts model in three dimensions (3D).

2. MODEL AND STAR-GRAPH EXPANSION METHOD

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

$$Z = \sum \exp\left(\beta \sum_{\langle ij \rangle} J_{ij} \delta(S_i, S_j)\right), \qquad (1)$$

where $\beta = 1/k_B T$ is the inverse temperature, $S_i = 1, \ldots, q$ and $\delta(.,.)$ is the Kronecker symbol. Quenched disorder averages are taken over an uncorrelated bimodal distribution of the form

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

which can include spin glasses ($R = -1, p = 1/2$), random-bond ferromagnets ($0 < R < 1$) and bond dilution ($R = 0$) as special cases. Other

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distributions can, in principle, also be considered with our method.

The method of star-graph expansion allows one to obtain high-temperature series expansions up to order N for appropriate quantities, e.g. the free energy $\log Z$ and the inverse susceptibility $1/\chi$, on infinite lattices by calculating the partition function and two-point correlators on all doubly connected ("star") graphs with up to N links and counting the embedding numbers of those graphs with respect to the lattice geometry. The advantage of this expansion method is that quenched averages over the coupling distribution can be calculated on the level of individual graphs.

The partition function and correlation functions $M_{nm} \equiv \langle q\delta(S_n, S_m) - 1\rangle$ for each graph are calculated symbolically in the cluster representation

$$M_{nm} \propto \sum_{C_{nm}} q^{l+c} \left(\prod_{\langle ij\rangle \in C} v_{ij} \right) \left(\prod_{\langle ij\rangle \notin C} (1 - v_{ij}) \right). \quad (3)$$

Here $v_{ij} = (e^{\beta J_{ij}} - 1)/(e^{\beta J_{ij}} - 1 + q)$, 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 [4] such that two consecutive clusters in the sum (3) differ by exactly one (added or deleted) link. This allows to speed up the calculation considerably by re-using every term in the sum for the calculation of the next one. All calculations were carried out on Pentium Linux farms and on a T3E.

3. 3D 4-STATE POTTS MODEL WITH BOND DILUTION

In the follwoing we shall focus on the bond-diluted 4-state Potts model in three dimensions which exhibits in the pure case a strong first-order transition. The expected softening to a second-order transition beyond a tricritical point at some finite disorder strength has recently been verified in Monte Carlo (MC) simulations [5] (for a MC study of the 3D *site*-diluted 3-state Potts model see [6]).

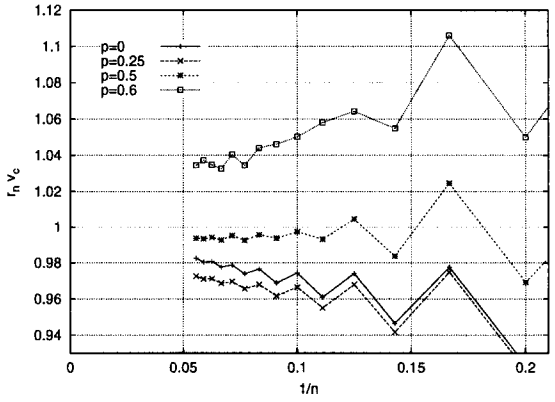

Figure 1. Ratio approximants for different dilutions p vs. $1/n$.

We obtained high-temperature series expansions for the susceptibility up to order 18 with coefficients given as polynomials in the disorder strength p. For such a series in two variables, the method of partial differential approximants should be well suited. Up to date, however, the only application of this method to a tricritical point [7] used a test series of order 50 generated from an exactly solvable model. In our case, it was unable to give conclusive results. Therefore, we confined ourselves to the analysis of single-parameter series for selected values of p.

A high-temperature series alone is not sufficient to localize a first-order transition point where the correlation length remains finite. In analysing series by ratio, Padé or differential approximants, the approximant will provide an analytic continuation of the thermodynamic quantities beyond the transition point into a metastable region on a pseudo-spinodal line with a singularity $T_c^* < T_c$ and effective "critical exponents" at T_c^*.

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

$$r_n = \frac{a_n}{a_{n-1}} = v_c^{-1} \left(1 + \frac{\gamma - 1}{n}\right). \quad (4)$$

Figure 1 shows these ratios for different values of p. In order to make them visually comparable,

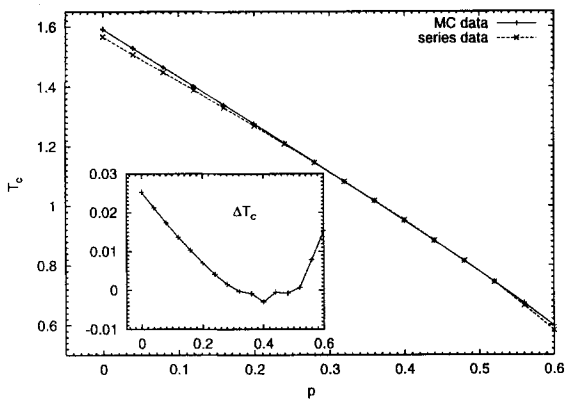

Figure 2. Critical temperature for different dilution p as obtained from MC simulations [5] and DLog-Padé series analyses. The inset shows the difference between the two estimates.

they are 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 $p = 0.7512$ (where T_c goes to 0) the series is clearly ill-behaved, related to the $\exp(1/T)$ singularity expected there. Besides that, the slope ($\propto \gamma - 1$) is increasing with p, changing from $\gamma < 1$ to $\gamma > 1$ around $p = 0.5$.

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. Figure 2 compares the critical temperature, estimated from an average of 25-30 Padé approximants for each value of p,[1] with the results of recent MC simulations [5]. For small p, in the first-order region, the series underestimates the critical temperature. As explained above, this is an estimate not of T_c but of T_c^*. Between $p = 0.3$ and $p = 0.5$, the estimates confirm, within errors, the MC results, indicating that now both methods see the same second-order transition. Beyond $p = 0.5$, the scatter of different Padé approximants increases rapidly, related to the crossover to the percolation point.

[1]Notice that "p" in the present notation corresponds to "$1 - p$" in Ref. [5].

4. CONCLUSIONS

We have implemented a comprehensive toolbox for generating and enumerating star graphs as required for high-temperature series expansions of quenched, disordered systems. Monte Carlo simulations of systems with quenched disorder require an enormous amount of computing time because many realizations have to be simulated for the quenched average. For this reason it is hardly possible to scan a whole parameter range. Using high-temperature series expansions, on the other hand, one can obtain this average exactly. Since the relevant parameters (degree of disorder p, spatial dimension d, number of states q, etc.) can be kept as symbolic variables, the number of potential applications is very large.

Here we only presented a preliminary analysis of the 3D bond-diluted 4-state Potts model. The phase diagram confirms recent Monte Carlo results and, by comparing with the numerical data, we also see signals for the onset of a second-order transition at finite disorder strength.

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