Disorder-driven phase transitions of the large $q$-state Potts model in three dimensions

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Abstract. – Phase transitions induced by varying the strength of disorder in the large-$q$ state Potts model in 3d are studied by analytical and numerical methods. By switching on the disorder the transition stays of first order, but different thermodynamical quantities display essential singularities. Only for strong enough disorder the transition will be soften into a second-order one, in which case the ordered phase becomes non-homogeneous at large scales, while the non-correlated sites percolate the sample. In the critical regime the critical exponents are found universal: $\beta/\nu = 0.60(2)$ and $\nu = 0.73(1)$.

Real materials are generally three-dimensional and contain some sort of quenched disorder, whose effect on the properties of the phase transition is an intensively studied question. If the phase transition in the non-random system is of second order, relevance or irrelevance of disorder can be decided due to the Harris criterion [1] and also perturbative field-theoretical calculations are possible [2]. For first-order transitions in the pure system, however, we have only a more limited knowledge. In 2d any amount of continuous disorder is sufficient to soften the transition into a second-order one [3, 4], which is studied in detail numerically [5–7]. In 3d, however, there is no such a rigorous criterium. Here experimental work [8] and numerical simulations [9–11] show that for strong enough disorder the phase transition becomes second order. In the numerical work mostly the $q = 3$—and 4-state Potts models were studied by Monte-Carlo simulations, both by site [9,10] and bond dilutions [11].

In the present work we revisit the problem of the effect of disorder at first-order phase transitions in 3d and address mainly such questions which have not been treated previously. We consider the disorder as realized by random ferromagnetic bonds, which contains as a limiting case the bond dilution. The problem we investigate is the Potts model in the large-$q$ limit, which allows us to make partially analytical calculations and in this way to shed light on
the physical mechanism responsible of the softening of the transition. We have also performed extensive numerical calculations, in which exact results on large finite samples are averaged over disorder. In particular, we addressed the question of universality of the second order transition and the location of the tricritical point.

We start to define the Hamiltonian of the q-state Potts model [12]:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \delta(\sigma_i, \sigma_j)$$

(1)

in terms of the Potts-spin variables, $\sigma_i = 0, 1, \cdots, q - 1$, at site $i$ and the summation runs over nearest neighbors of a simple cubic lattice. The ferromagnetic couplings, $J_{ij} > 0$, can take two values, $J_1 = J(1 + \delta)$ and $J_2 = J(1 - \delta)$ with equal probability [13]. The strength of disorder is $\delta$ and the dilute model is recovered for $\delta = 1$. As usual for the random model we calculate disorder averages of the free energy and the correlation function.

For a given realization of disorder the partition function is given in the random cluster representation [14]:

$$Z = \sum_{G} q^{\ell(G)} \prod_{ij \in G} [q^{\beta J_{ij}} - 1]$$

(2)

where the sum runs over all subset of bonds, $G$, $c(G)$ stands for the number of connected components of $G$ and we use the reduced temperature [7], $T \to T \ln q = O(1)$ and its inverse as $\beta \to \beta/\ln q$. In the large-$q$ limit, where $q^{\beta J_{ij}} \gg 1$, the partition function can be written as

$$Z = \sum_{G \leq E} q^{\phi(G)}, \quad \phi(G) = c(G) + \beta \sum_{ij \in G} J_{ij}$$

(3)

which is dominated by the largest term, $\phi^* = \max_G \phi(G)$, and the degeneracy of the optimal set $G^*$ is likely to be one. Thus the study of the large-$q$ state Potts model is reduced to an optimization problem, whose solution (for a given realization of disorder) depends on the temperature. The free-energy per site is proportional to $\phi^*$ and given by $-\beta f = \phi^*/N$, where $N$ stands for the number of sites of the lattice. From the point of view of magnetization and the correlation function the largest connected cluster of the optimal set, $C$, plays a crucial role. The magnetization, $m$, is given by the fraction of sites in $C$, and its disorder average is $m > 0$ in the ordered phase, $T < T_c$. In the disordered phase, $T > T_c$, $C$ has a finite linear extent, $\xi < \infty$, which is proportional to the average correlation length in the system. At the phase-transition point, $T = T_c$, if the transition is of second order, $C$ is a fractal and its fractal dimension, $d_f$, is related to the magnetization scaling dimension, $x_m$, as $d = d_f + x_m$. Here $x_m$ can be expressed by the standard critical exponents as $x_m = \beta/\nu$. On the contrary, if the transition is of first order there is phase coexistence at $T = T_c$ and the correlation length is finite. This type of formalism has been used by us previously in 2d [7], and we refer to this work for a detailed presentation of the method.

The solution of the problem is the simplest for the non-random model, $\delta = 0$, when there are only two homogeneous optimal sets. For $T < T_c(0)$ it is the fully connected diagram with a free-energy: $-\beta N f = 1 + N \beta J z$ ($z = d = 3$ is the connectivity of the lattice) and for $T > T_c(0)$ it is the empty diagram with $-\beta N f = N$. Consequently the transition point is located at: $T_c(0) = J z / (1 - 1/N)$ and the latent heat is $\Delta e / T_c(0) = 1$.

Introducing disorder into the system, $\delta > 0$, new type of non-homogeneous optimal diagrams will appear close to $T_c(0)$. Let us consider first $T > T_c(0)$, where the new optimal set contains connected clusters of linear size, $l$, embedded into the empty diagram. Here we refer to the treatment of this problem in 2d [7] when close to $T = T_c(0)$ the excess quantities
over the homogeneous optimal sets are i) a bulk term due to disorder fluctuations, $\Delta f_\alpha$, and ii) an interface term due to missing bonds, $\Delta f_\alpha \sim \beta J S$, where the size of the interface is $S \sim l^d - 1$. For Gaussian fluctuations $\Delta f_\alpha^2 \sim \delta^2 V^{1/2}$, where $V \sim l^d$ is the volume of the cluster. Consequently for $d \leq 2$ normal fluctuations of disorder will lead to the creation of clusters of arbitrary size and for any weak disorder there is no phase coexistence and the transition is of second order [3].

On the contrary for $d > 2$, clusters are created only due to extreme fluctuations, when say the cluster consists of only strong bonds, thus $\Delta f_\alpha^+ \sim \beta J \delta (V - c S)$, where $c = O(1)$ is a geometrical factor. The existence of such large cluster is exponentially rare, its density is given by $-\ln \rho_+ \sim V - c S$. For a small $\delta$ only large clusters can be formed and we obtain the possible size from the condition, $\Delta f_\alpha^+ \geq \Delta f_\alpha$, as $l \geq l_+ (\delta) \sim 1/\delta$ [16]. Finally, the free energy of the non-homogeneous optimal set relative to the empty graph is given by the sum of contribution of the possible clusters:

$$-\beta N f_+ \simeq N + N \sum_{l \geq l_+ (\delta)} (\Delta f_\alpha^+(l) - \Delta f_\alpha(l)) \rho_+(l),$$

and it is dominated by the contribution with $l = l_+ (\delta)$.

A similar analysis can be performed for $T < T_c (0)$, when the new inhomogeneous optimal set is obtained from the fully connected graph by creating clusters of isolated sites. In this case a cluster of size, $l$, has $V + c S$ weak bonds, a bulk gain of $\Delta f_\alpha^- \sim \beta J \delta (V + c S)$ and appears with a density, $-\ln \rho_- \sim V + c S$. Note that there is a difference in the sign of the surface term comparing with the high-temperature case. The limiting size of clusters, $l_- (\delta)$, can be estimated as above and the free energy of the optimal set can be written in an analogous form with eq. (4):

$$-\beta N f_- \simeq 1 + N \beta J z + N \sum_{l \geq l_- (\delta)} (\Delta f_\alpha^-(l) - \Delta f_\alpha(l)) \rho_-(l),$$

and it is dominated by the contribution with $l = l_- (\delta)$. The asymmetry in the densities in the two phases, $\rho_+$ and $\rho_-$, leads to a shift in the critical temperature, $\ln(T_c (\delta) - T_c (0)) \sim -\delta^{-3}$, and similarly to a reduction of the latent heat and the jump of the magnetization at the transition point:

$$\ln (1 - \Delta c / T_c) \sim \ln (1 - \Delta m) \sim \frac{1}{\delta^3}.$$

Thus the phase transition stays first order and as the disorder is switched on there is an essential singularity in the thermodynamical quantities as a function of $\delta^{-3}$.

For finite values of disorder the optimal set (and thus the free energy and the magnetization) is exactly calculated by a combinatorial optimization algorithm [15], which works in strongly polynomial time. In the numerical calculations we studied periodic systems of cubic shape with a linear size $L = 16, 24, 32$ and in some cases $L = 40$. For the largest size the computation of the optimal set for a single sample typically took from 5 to 20 hour CPU time in a 2.8GHz processor. (Since the breaking-up length [16] at $\delta = 0.40$ is $L_br \approx 40$ we restricted ourselves to $0.40 \leq \delta \leq 1$.) The number of realizations were several thousands, for the largest size several hundreds.

We start to show in fig. 1 the numerically calculated phase diagram as a function of the strength of disorder. Here the phase boundary between the ordered and disordered phases is obtained from the condition that the largest cluster in the optimal set starts to percolate and the finite-size results are then extrapolated, see the inset of fig. 1. The transition points obtained by this method agree, within the error of the calculation, with those calculated from
the position of the maxima of the specific heat. Before analyzing the properties of the phase transition we mention that the structure of the optimal set in the ordered phase can be of two different types. For weak disorder, \( \delta < \delta_{pr} \), or for low temperature, \( T < T_{pr} \), in the optimal set the isolated sites form finite clusters, otherwise the isolated sites are percolating. In the dilute model with \( \delta = 1 \) and \( J_1 = 2J \) the percolation temperature is at \( T_{pr}(1) = J_1 \). Indeed the optimal set for \( T < J_1 \) contains all the strong bonds, whereas from this optimal set for \( T > J_1 \) the dangling bonds are removed. Since the dangling bonds represent a finite fraction of the bonds the non-occupied sites become percolating.

For \( \delta < 1 \) the skeleton of dangling bonds of \( J_1 \) couplings are decorated by weak \( J_2 \) couplings, and by removing one strong dangling bond one has also to remove four weak decorated ones, which is possible in the temperature range:

\[
T_c > T > T_{pr}(\delta) = J(5 - 3\delta) .
\]

The numerical results indicate that at \( T_{pr}(\delta) \) in a finite fraction of samples there is a giant cluster of isolated sites which spans the finite cube.

The temperature dependence of the magnetization for different values of the disorder is illustrated in fig. 2 in a finite system of \( L = 16 \). For \( \delta < \delta_c \) in the first-order transition regime the magnetization has a finite jump, \( \Delta m > 0 \). \( \Delta m(L) \) is estimated from the relation: \( \Delta m(L) \approx 2m[T_c(L)] \), and the extrapolated values are shown in the inset of fig. 2 for different values of \( \delta \). From this we estimate the position of the tricritical disorder \( \delta_c = 0.65(2) \). It is interesting to observe that this value, within the relatively large error coincides with the
limiting value of disorder, $\delta_{pr} = 0.658(1)$, where the percolation of isolated sites in the ordered phase starts. Physically it is very intuitive that percolation of isolated sites is the prerequisite of a continuous transition in the system. Indeed the correlation length in the ordered phase, which is measured by the linear size of the largest finite (i.e. not the giant) ordered cluster can be divergent, if it is embedded in an infinite cluster of isolated sites. Therefore we tend to conjecture that $\delta_c = \delta_{pr}$.

In the second-order transition regime we have made the most detailed calculations at $\delta = 7/8$, but universality is checked at other values of the disorder at $\delta = 0.75$, 0.80, 0.925 and 1. The fractal dimension, $d_f$, of the percolating connected cluster is estimated in such a way that fixing a reference point we measured the average number of points, $s(r, L, T)$, within a shell around the reference point of unit width and radius, $r$. Close to the transition point: $t = (T - T_c)/T_c \ll 1$ it is expected to scale as:

$$s(r, L, t) = L^{d_f - 1} \tilde{s}(r/L, t L^{1/\nu}) .$$

Since the exact value of the critical temperature is not known we can not fix the second argument of the scaling function as $\tilde{s}(\rho, \tau = 0)$. Instead we set $T = T_{sp}(L)$, which is the temperature, where the connected cluster spans the cube of the given size and we average over disorder. Evidently with this choice the second argument of the scaling function, $\tau$, is asymptotically constant and the scaling function depends only on one parameter: $\tilde{s} = \tilde{s}(r/L)$. Our scaling picture is verified in fig. 3 in which the scaling plot of the mass in the shell is shown. From the optimal scaling collapse [17] we obtained for the fractal dimension, $d_f = 2.40(2)$.

The correlation length critical exponent, $\nu$, is calculated from the scaling behavior of the
magnetization: \( m(t, L) = L^x \tilde{m}(tL^{1/\nu}) \). From an optimal scaling collapse [17] as shown in the inset of fig. 3 we have obtained \( \nu = 0.73(1) \). Note that \( \nu \) satisfies the rigorous bound for disordered systems [18]: \( \nu \geq 2/d \). Due to strong cross-over effects we could not determine the tricritical exponents with sufficient accuracy. However, the tricritical correlation length exponent, \( \nu_{tr} \), is related [6] to the exponents of the random-field Ising model as: \( \nu_{tr} = \nu_{RF}/(2 - \alpha_{RF} - \beta_{RF}) \). Using numerical estimates [19] we obtain \( \nu_{tr} \approx 0.69 \).

In Table I we have collected the presently known numerical results about the critical exponents of random \( q \)-state Potts models in 3d, including also the Ising model (\( q = 2 \)) and percolation, which formally corresponds to \( q = 1 \). The \( q \)-dependence of the exponents, in particular that of \( \beta/\nu \) is non-monotonic.

In our model thermal fluctuations play a negligible role and the physical properties are solely determined by disorder effects, which is characteristic at a so called infinite disorder fixed point [20]. In the two-dimensional problem an isomorphism is conjectured [7] with the phase transition in the strongly anisotropic random transverse-field Ising model in 1d. However, our numerical results indicate that this type of relation does not seem to work in

| \( q \)  | \( \nu \)  | \( \beta/\nu \) |
|---------|-----------|----------------|
| perc. 21 | 0.877     | 0.477          |
| \( q = 2 \) [22] | 0.684(5) | 0.518(2)       |
| \( q = 3 \) [10] | 0.690(5) | 0.539(2)       |
| \( q = 4 \) [11] | 0.747(10) | 0.732(20)     |
| \( q \to \infty \) | 0.73(1)  | 0.60(2)        |
higher dimensions.

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