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LETTER TO THE EDITOR

FIRST-ORDER PHASE TRANSITION IN $1d$ POTTS MODEL WITH LONG-RANGE INTERACTIONS

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The first-order phase transition in the one-dimensional q-state Potts model with long-range interactions decaying with distance as $1/r^{1+\sigma}$, has been studied by Monte Carlo numerical simulations for $0 < \sigma \leq 1$ and integer values of $q > 2$. On the basis of the finite-size scaling analysis of interface free energy ΔF_L, specific heat and Binder's fourth order cumulant, we obtain the first-order transition which occurs for σ below a threshold value $\sigma_c(q)$.

The subject of our study is the one-dimensional ($1d$) Potts model with ferromagnetic long-range (LR) interactions decaying with distance as $1/r^{1+\sigma}$, defined by the Hamiltonian

$$H = -\sum_{i<j} \frac{J}{|i-j|^{1+\sigma}}\, \delta(s_i, s_j)\ , \tag{1}$$

where $J > 0$, s_i denotes the q-state Potts variable at site i, δ is the Kronecker symbol, and summation is taken over all pairs in the system. The phase transition at nonzero temperature, shown rigorously [1] for the Ising $(q = 2)$ case with $\sigma \leq 1$ and by renormalization group for the continuous n-component models with $\sigma < 1$ [2], exists also in model (1) for $\sigma \leq 1$ and $q > 0$ [3,4] and goes through a variety of universality classes by variation of q and σ. Model (1) has been used as a relevant model for describing a number of phenomena involving LR interactions, from spin glasses to neural networks, but may also be of interest for possible analogies [5], in some cases very direct [6], with short-range (SR) models in higher dimensions.

An important feature of Potts models with SR interactions is the onset of the first-order phase transition for q above some threshold value $q_c(d)$, which depends on dimensionality [7]. For example, in $d = 2$ [8] and $d = 4$ [9] analytical results yield q_c equal to 4 and 2, respectively, while for $d = 3$, the approximate methods give a non-integer value for q_c, slightly lower than 3 [10], so that the $3d$ 3-state Potts model has an extremely weak first-order transition, very difficult to detect [11]. Such distinct situations created by variation of d and q make this model a canonical example for the study of various aspects of temperature-driven first-order phase transitions [12].

One can expect similar behaviour to occur for the Potts model with LR interactions, although certain related quantities (e.g. the interface energy) may require different interpretation. Generally, this model has been much less explored than its SR version, due to non-locality of interactions, which makes difficult the application of standard renormalization group techniques in direct space, otherwise appropriate for discrete models. A few studies that have been done concern mostly the mean-field region and its vicinity by using an $\varepsilon-$expansion within Ginzburg-Landau continuous formalism [13], and the special case of $\sigma = 1$ [3]. We have recently proposed the finite-range scaling (FRS) approach [14] suitable for study of the Hamiltonian (1), with both σ and q arbitrary and continuous [4]. This approach is, however, inherently insensitive to discern the first-order transitions and remained inconclusive in this respect. The problem was not resolved in other recent works [15,16] on the LR Potts model either.

For this reason we present here the results based on simple numerical simulations performed with intention to examine the existence of a first-order transition in this model and get a qualitative estimate of its dependence on q and σ.

It has been recently pointed out [17], that the temperature-driven first-order transitions can be identified from finite-size scaling (FSS) analysis of maxima of the energy probability distribution

$$P_L(E) = \frac{1}{Z_L(K)} \mathcal{N}_L(E)\, \mathrm{e}^{-KE} \,, \tag{2}$$

where $K = J/k_BT$, $Z_L(K)$ is the partition function, $\mathcal{N}_L(E)$ is the number of configurations with energy E, and index L denotes the system size. Due to the coexistence of phases, at the temperature of a first-order phase transition $P_L(E)$ has two maxima, corresponding to the two wells of the free energy. The barrier separating them, which represents the interface free energy, is defined by

$$\Delta F_L = \ln \left. \frac{P_L(E_{min})}{P_L(E_{max})} \right|_{K_L} \,, \tag{3}$$

where E_{min} and E_{max} denote the energies corresponding to the minimum and one of the two maxima, respectively, the finite-size temperature K_L being adjusted so as to make the two maxima equal. For a first-order phase transition, ΔF_L should diverge for $L \to \infty$. In systems with SR interactions it scales like a surface, i.e. $\sim L^{d-1}$, while in the present case it is expected to scale rather like a volume, i.e. $\sim L$.

The calculations were performed on chains of size $100 \leq L \leq 400$ with periodic boundary conditions. We used the simple Metropolis single-spin-flip algorithm with $1 \times 10^6 - 3 \times 10^6$ Monte Carlo (MC) sweeps per spin. The number of necessary runs for the precise localization of each of the size-dependent critical temperatures K_L has been reduced by applying the Ferrenberg and Swendsen [18] histogram method.

We considered integer values of $q \geq 2$ in the interval $0 < \sigma \leq 1$. While for $q = 2$ (Ising case), the simulations at T_c show only a single maximum in $P_L(E)$ in the entire range of σ, for higher values of q, the two peaks emerge for σ sufficiently low. They become more pronounced with increasing q or decreasing σ. For illustration, in Fig. 1 are shown the maxima corresponding to different values of σ, taken from three typical sets of simulations with the fixed values $q = 3$ and $L = 400$.

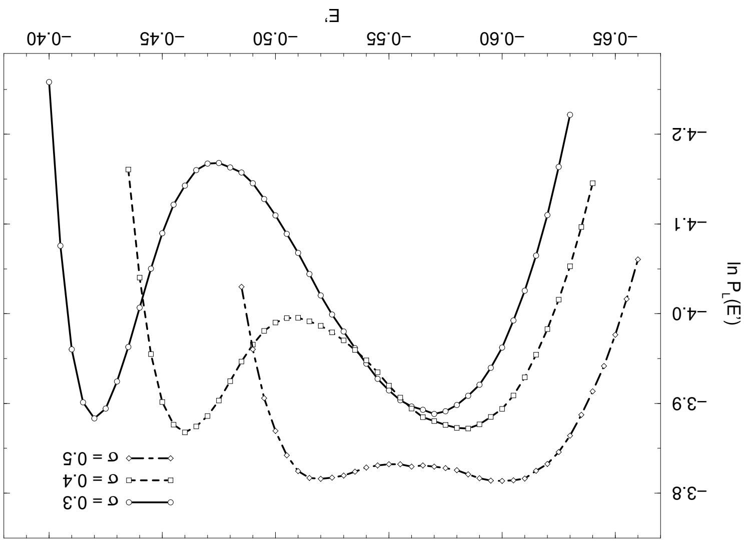

Fig. 1. Maxima of $\ln P_L(E')$ for $q = 3, L = 400$ and $\sigma = 0.3, 0.4$ and 0.5, taken at respective values of K_L. $E' = E/|E_0(\sigma)|$, where $E_0(\sigma)$ stand for the zero-temperature energies.

We report here the systematic results for two chosen values, $q = 3$ and $q = 5$, in the whole interval $0 < \sigma \leq 1$ taken with increment 0.1.

Figures 2a and b summarize the results for the free energy barrier plotted as a function of chain size L for $q = 3$ and $q = 5$, respectively. The corresponding critical temperatures extrapolated to $L \to \infty$, given in Table 1, are found to be in good agreement with our earlier FRS results [4], as well as with other known approximate results [16].

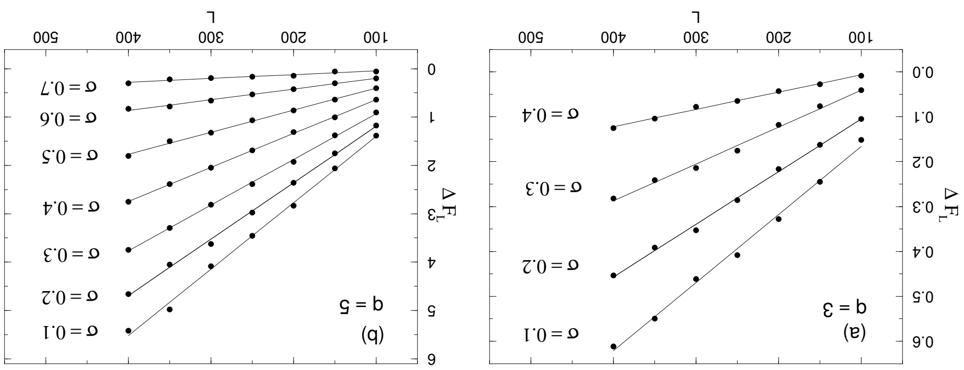

Fig. 2. MC *results of the free energy barrier* ΔF_L *for sizes* $L = 100$ *to* 400 *for: (a)* $q = 3, \sigma = 0.1$ *to* 0.4, *(b)* $q = 5, \sigma = 0.1$ *to* 0.7. *Notice that the slope is by an order of magnitude larger in the case (b). The size of the numerical error bars is comparable to or smaller than the size of the points.*

TABLE 1. Inverse critical temperatures (K_e^{MC}) *obtained by extrapolation of* K_L *compared to* FRS *extrapolated values* (K_e^{FRS}) [4].

σ	K_e^{MC}	K_e^{FRS}	K_e^{MC}	K_e^{FRS}
	$q = 3$		$q = 5$	
0.1	0.190	0.136	0.262	0.28
0.2	0.279	0.270	0.333	0.45
0.3	0.380	0.386	0.492	0.576
0.4	0.489	0.494	0.637	0.690
0.5			0.771	0.803
0.6			0.901	0.920
0.7			1.019	1.046

For both considered values of q, there is a wide range of σ, where ΔF_L increases with size, indicating the first-order transition. As expected for the LR interactions, ΔF_L is proportional to the volume rather than surface and depends linearly on L. The slope is larger by an order of magnitude for $q = 5$ in comparison to $q = 3$, showing that the first-order character becomes stronger with increasing q, like for the SR interactions. In both cases the slope decreases with increasing σ to the point where ΔF_L becomes of the order of numerical error. Beyond this value, at least for the sizes considered here, the $P_L(E)$ exhibits a single maximum indicating the onset of the second-order phase transition. In present calculation, taken with a rough increment of 0.1 in σ, this change is observed around $\sigma = 0.5$ and $\sigma = 0.8$ for $q = 3$ and $q = 5$, respectively. These values should be taken with caution and only as a lower limit for the threshold value σ_c between the first- and the second-order transition. Namely, the present model allows the continuous approach to the threshold value σ_c, whereby the first-order transition becomes arbitrarily weak and very difficult to detect, comparable to the situation with the $3d$ 3-state Potts model with SR interactions. The above results, however, strongly suggest that σ_c is considerably larger for $q = 5$ than for $q = 3$, and that dependence $\sigma_c(q)$ should be expected, analogous to the threshold dependence $d_c(q)$ in the SR model.

Two other energy-related quantities are more conventionally [19] used for determination of the first-order transition in context of FSS analysis of MC simulation results: specific heat and Binder's fourth order cumulant [20], which both can be derived from $P_L(E)$, and expressed in terms of higher energy momenta $\langle E^n\rangle_L = \sum_E E^n P_L(E)$. The specific heat is given by

$$C_L = \frac{K^2}{L^d}\left(\langle E^2\rangle_L - \langle E\rangle_L^2 \right) . \tag{4}$$

According to the FSS theory, for second-order transitions its maximum scales as $C_L^{max} \sim L^{\alpha/\nu}$, where α and ν are the critical exponents of the specific heat and the correlation length, respectively. When the transition is of the first order, it scales as a volume, i.e. $C_L^{max} \sim L^d$. Instead of the Binder fourth cumulant $V_L^{(4)} = 1 - U_L^{(4)}/3$, we consider here the ratio

$$U_L^{(4)} = \frac{< E^4 >_L}{< E^2 >_L^2} . \tag{5}$$

For the first-order transitions, $\lim_{L\to\infty} U_L^{(4)} = 1$ when $T \neq T_c$, while at $T = T_c$ $\lim_{L\to\infty} U_L^{(4)} = const > 1$. For the second-order transitions it always tends to one.

We present the behaviour of those two quantities on two examples: $q = 5$, $\sigma = 0.2$ and $q = 3$, $\sigma = 0.8$, representative of the first- and second-order regimes, respectively.

In Figs. 3a and b, one can observe two kinds of behaviour of C_L^{max} in the two cases: linear and power law. The fit to the form $C_L^{max} \sim L^x$ in the latter case gives the value $x = 0.24$ for $q = 3, \sigma = 0.8$. The bare extrapolation error bars for x are estimated to be of order of 10%. The hyper-scaling relation with the substitution of FRS result [4] $\nu = 1.74$ gives $\alpha/\nu = 0.15$. The difference can be attributed to the general difficulty in extracting the critical exponents from the specific heat, and to the fact that the calculated exponent is small, and additional correction terms due to finite-size gain importance.

The convergence of the maxima of $U_L^{(4)}$ with size is presented in Figs. 3c and d. The points for the Ising model with $\sigma = 0.5$ are added as a reference for the second-order transition behaviour. Within the limits of accuracy, the case $q = 3, \sigma = 0.8$ shows a clear convergence towards 1. The points for $q = 5, \sigma = 0.2$ converge towards a much larger value, which is approximately 2.4 when we take into account larger values of L and use the linear extrapolation.

Thus, the two quantities confirm earlier conclusions based upon the behaviour of ΔF_L. However, at the present stage, we could not extract from these quantities any better precision in the determination of $\sigma_c(q)$, so we do not reproduce any systematic study of them.

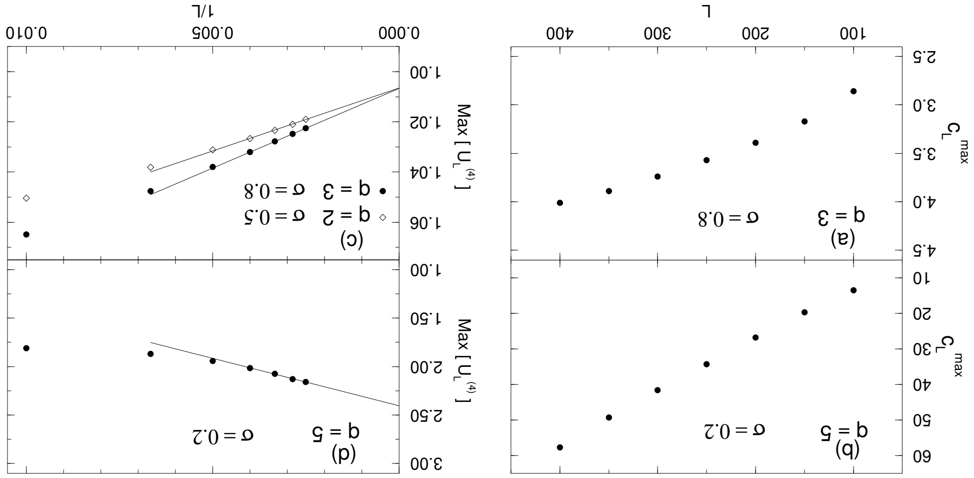

Fig. 3. M*C data for sizes* $L = 100$ *to* 400*: specific heat maxima are plotted for (a)* $q = 3, \sigma = 0.8$*, (b)* $q = 5, \sigma = 0.2$*; ratio* $U_L^{(4)}$ *maxima are plotted in function of inverse size for: (c)* $q = 3, \sigma = 0.8$*, (d)* $q = 5, \sigma = 0.2$ *(full circles). The diamonds correspond to* $q = 2, \sigma = 0.5$ *taken as a reference. Lines show the linear extrapolations. Notice the common scale on* x*-axis, but different scales on* y*-axis. The size of the numerical error bars is smaller than the size of the points.*

In summary, by simple numerical calculations, in combination with FSS arguments, we have shown that the $1d$ LR Potts model for integer $q > 2$ exhibits the first-order phase transition for σ below some threshold value σ_c generally depending on q. The first-order character becomes weaker with the increase of σ, which represents a continuous parameter leading from the first- to the second-order phase transition regime. More intensive numerical approach [21] is needed in the future in order to determine the threshold value $\sigma_c(q)$.

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FAZNI PRIJELAZ PRVOGA REDA U 1*d* POTTSOVOM MODELU S DUGODOSEŽNIM MEĐUDJELOVANJEM

U jednodimenzijskom Pottsovom modelu q–stanja s dugodosežnim međudjelovanjima koja opadaju s udaljenošću kao $1/r^{1+\sigma}$, Monte Carlo simulacijama je promatran fazni prijelaz prvog reda za $0 < \sigma \leq 1$ i cjelobrojne vrijednosti $q > 2$. Na temelju *scaling* analize slobodne energije međuplohe, specifične topline i Binderovog kumulanta četvrtog reda, dobivamo prijelaz prvoga reda za σ manji od granične vrijednosti $\sigma_c(q)$.