Q-state Potts model with power-law decaying interactions: along the tricritical line

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By relying on a recently proposed multicanonical algorithm adapted to long-ranged models, we shed new light on the critical behavior of the long-ranged q-state Potts model. We refine the controversial phase diagram by an order of magnitude, over a large range of q values, by applying finite-size scaling arguments to spinodal curves. We further offer convincing evidence that the phase transition on the line of inverse-square interactions is not of the first-order, by virtue of a very unusual, previously unnoticed finite-size effect. Finally, we obtain estimates of critical couplings near the mean-field region which clearly reinforce Tsallis conjecture.

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Since the work of Kihara et al. [1] in the early 1950's, the Potts model with short-ranged (SR) interactions has been the object of extensive study. A prominent feature of this model is the dependence of the nature of the transition, either of the first- or second-order type, on both the number of states of the model and the dimensionality (see [2] for a review). Although its long-ranged (LR) counterpart exhibits much richer thermodynamical behavior as a result of the nonlocality of interactions, only very recently has it received increasing interest. This feature may be accounted for by the difficulty to implement standard analytical methods, e.g. renormalization-group (RG) approaches, and by the higher cost of numerical methods in terms of computer resources, as opposed to the SR case.

In this paper, we consider a q-state Potts model defined by the following Hamiltonian:

$$H = -\sum_{i<j} \frac{1}{|i-j|^{1+\sigma}} \delta_{s_i, s_j}$$

where the σ parameter allows to set the interaction range, the spin variable s_i can take on integer values between 1 and q, and the sum runs over all the spins of the lattice. The mean-field (MF) regime corresponds to $\sigma \to -1$, where all interactions have equal strength.

This model is known from rigorous proof to undergo a phase transition when $\sigma \leq 1.0$ ([3]), the nature of which is still, for given q and σ, a matter of intense debate. For σ above a so-called tricritical value $\sigma_c(q)$, the transition has been shown to change from a first- to a second-order one, yet numerical estimates of $\sigma_c(q)$ reported by previous works are fairly imprecise, and show strikingly high discrepancies [4, 5, 6, 7, 8]. A further unsettled issue is whether $\sigma_c(q)$ crosses the line $\sigma = 1.0$ corresponding to inverse square interactions, and if in the affirmative, at which value of q this crossing occurs (see Fig. 1). Cardy has shown, using a real-space RG analysis, that the line $\sigma = 1.0$ is the locus of Kosterlitz-Thouless (KT) transitions, whatever the number of states [9], an assertion that is convincingly supported, at least for $q = 2$ and $q = 3$, by Monte-Carlo (MC) simulations [10]. Conversely, it was claimed in [7] that the transition becomes discontinuous above $q = 8$, and the finite value of the correlation length in this latter case is obviously incompatible with the KT transition found by Cardy.

The present article addresses both of these issues by resorting to MC simulations based on a recently proposed, enhanced version of the multicanonical algorithm streamlined for LR models [11, 12]. This class of algorithms has been widely proven to efficiently overcome supercritical slowing-down in the case of first-order transitions. Our approach relies on the finite-size scaling (FSS) properties of spinodal curves, and allows us to considerably improve the precision of the phase diagram. A similar FSS analysis further demonstrates that, although the transition may appear discontinuous at finite lattice size for $\sigma = 1.0$, the thermodynamical limit clearly corresponds to a continuous transition. Finally, we show that our numerical estimates of critical couplings are in striking agreement with Tsallis conjecture [13], according to which the inverse critical coupling scales as σ whenever $\sigma \to 0^+$, *i.e.* when the system approaches the non-extensive thermodynamic region.

Our multicanonical method resorts to two key-principles: i) an iterative scheme allows to compute an estimate of the density of state $n(E)$ from successive histograms of the energy; ii) the usual Boltzmann weight $e^{-E/kT}$ is being replaced by a multicanonical weight $w(E) \propto 1/n(E)$, whereby a flat energy distribution spanning an increasingly large energy range is sampled. This in turn allows the dynamics to easily cross free-energy barriers, as witnessed in the case of discontinuous transitions. The iteration process stops whenever the histogram has become sufficiently flat over the range of interest, a long production run is carried out, then thermodynamical averages shall be computed using a reweighting procedure. For instance, the partial partition func-

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tion $Z(\beta, m)$ at inverse temperature β is estimated from a trace restricted to samples having a given magnetization m, $Z(\beta, m) = \sum_i \exp(-\beta E_i)/w(E_i)\delta_{m,m_i}$, from where on we readily derive the partial free-energy $F(\beta, m) = -\log Z(\beta, m)/\beta$.

We have conducted MC simulations for numerous q and σ values, using lattice sizes between $L = 50$ and $L = 400$, and statistics of roughly 5.10^4 independent samples per production run. We first focus on the location of the tricritical line $\sigma_c(q)$. Due to the cluster size divergence as $\sigma \to \sigma_c(q)$, traditional estimators, e.g. latent heats or Binder cumulants [14], become impracticable. We rather resort to the observation that spinodal points, which define the limit of metastability, merge when approaching the tricritical point. We thus compute the partial free-energy $F(\beta, m)$ over a large range of temperature and magnetization: metastable states, if any, are then obtained from the condition that $dF/dm = d^2F/dm^2 = 0$. This yields two finite-size metastability temperatures, namely $T_1(L)$ and $T_2(L)$, which — mimicking the FSS theory of first-order transitions proposed in [15] — we assume to scale as a power-law of the lattice size L, e.g. $T_1(L) = T_1 + a/L^b$, where T_1 is the infinite-size temperature. As illustrated in Fig. 2 for $q = 3$, both spinodal points merge around $\sigma = 0.7$. In order to reach a higher precision, we found it convenient to fit ratios T_1/T_c and T_2/T_c to a polynomial. Here, T_c denotes the infinite-size transition temperature, and is determined by first computing finite-size transition temperatures $T_c(L)$ from both the location of peaks of the specific heat and the crossing-point of Binder cumulants of the energy [14], then fitting these temperatures to a power-law of the same form as that used for metastability temperatures, and eventually averaging over both values. The tricritical value may then be determined from the intersection of each polynomial with the horizontal line at ordinate unity (see inset in Fig. 2). As the T_2/T_c ratio turns out to produce far more precise estimates, a feature which is accounted for by the strongly asymmetric shape of $F(\beta, m)$ with respect to m, we in effect discard the estimate obtained from T_1/T_c. This yields $\sigma_c(3) = 0.72(1)$, a value which is perfectly consistent with the lower bound of 0.7 obtained in [8], and lies slightly above the interval of $(0.6, 0.7)$ reported in [4]. The same approach yields $\sigma_c(5) = 0.88(2)$, which is in agreement with $\sigma_c(5) > 0.8$ in [5], $\sigma_c(7) = 0.94(2)$, which is at least consistent with the qualitative phase diagram sketched in [7], and finally $\sigma_c(9) = 0.965(20)$. This latter estimate comes in strong contrast with the result reported in [7], whereby the transition at $\sigma = 1.0$ becomes discontinuous above $q = 8$ (see Fig. 1). In order to scrutinize this latter issue, we now turn to a detailed study of the FSS behavior of spinodal points at $\sigma = 1.0$. We concentrated our computation efforts on $q = 8$ and $q = 9$, *i.e.* at and just above the change of regime reported in [7]. As illustrated in Fig. 3, $T_2(L) \to T_1(L)$ as $L \to \infty$ for both $q = 8$ and $q = 9$, within error bars, and this accounts for the continuous nature of the transition in the thermodynamic limit. At finite size, however, the transition appears as a first-order one, with metastability temperatures being noticeably distinct already below $L = 400$. This fairly unusual FSS behavior, which has been so far unnoticed, markedly contradicts the traditional picture of first-order transitions in SR models, whereby the finite cluster size imposes that continuous transitions may be observed only as long as the lattice size is smaller than the (fixed) correlation length. We feel strongly that this behavior may be accounted for by the truncation of the LR potential at finite size: in our view, this results in the whole array of spins being more rigidly tied at small lattice sizes than at higher ones, thus artificially bringing the model closer to the MF regime and possibly favoring

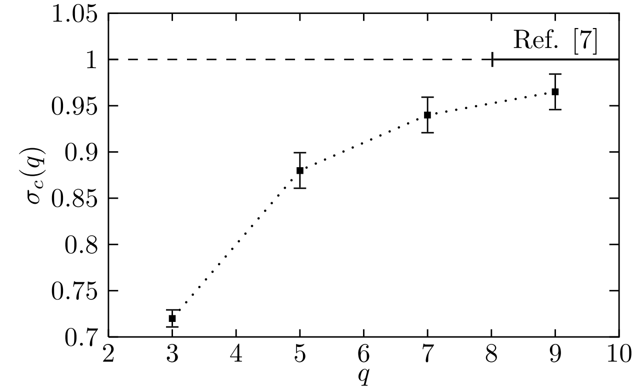

FIG. 1: Filled squares sketch our own estimate of the tricritical line $\sigma_c(q)$ above which the transition changes from a first-order to a second-order one (dotted lines are guides to the eyes). The horizontal dashed line at $\sigma = 1.0$ corresponds to inverse square interactions; according to Cardy [9], it is the locus of KT transitions for all q's, while it was claimed in [7] that $\sigma_c(q)$ crosses this line at $q = 8$ and that first-order transitions set in for $q \geq 8$ (rightmost solid line).

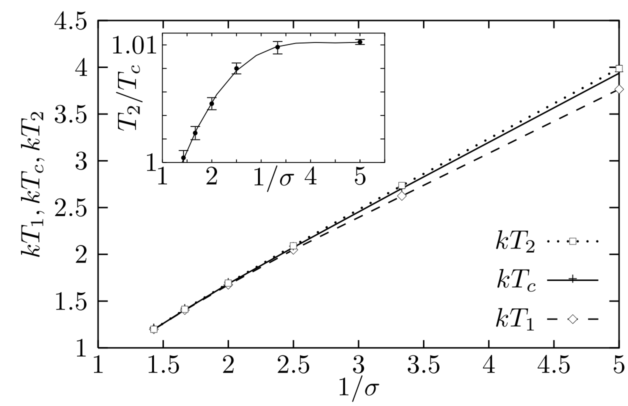

FIG. 2: Spinodal curve for $q = 3$. Metastability temperatures T_1 and T_2, as well as the transition temperature T_c, were obtained by a fit of finite-size estimates to a power-law of the lattice size. The inset shows a plot of the third-order polynomial fitted to the ratio T_2/T_c. Lines are guides to the eyes.

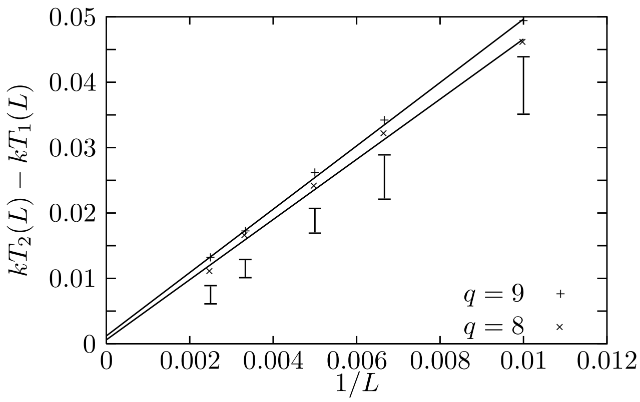

FIG. 3: Metastability temperature differences $T_2(L) - T_1(L)$ on the line $\sigma = 1.0$ for $q = 8$ and $q = 9$, compared with the corresponding linear fits (solid lines). For the sake of clarity, the size of the error for each lattice size is shown as a bar; the error shown corresponds to the largest of both errors computed for $q = 8$ and $q = 9$.

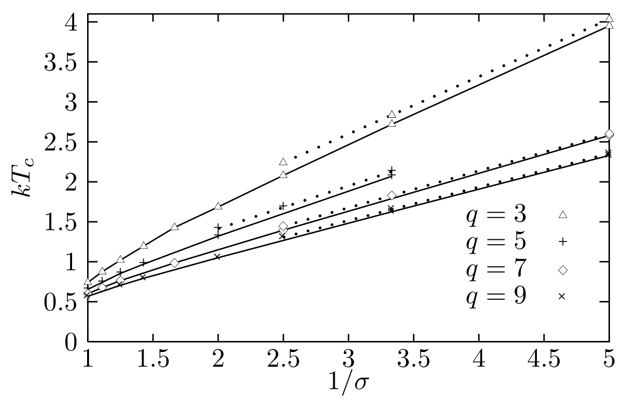

FIG. 4: Critical couplings for $q = 3, 5, 7, 9$, from top to bottom (solid lines). MF predictions are shown for comparison (dotted lines).

the onset of a first-order transition. The latter feature should be especially apparent at higher q since, according to our estimates of $\sigma_c(q)$, we expect $\sigma_c(q) \to 1.0$ whenever $q \to \infty$ (see Fig. 1), hence the artificial shift towards the MF regime makes the system wade across the thin second-order region far more easily. This interpretation is in effect supported by a comparison of our results at $q = 8$ and $q = 9$ as illustrated in Fig. 3, and has been confirmed by our simulations at $q = 3$, where the transition appears continuous at all sizes.

Finally, we shortly consider the agreement of our critical couplings estimates with MF predictions. According to MF theory, the transition temperature is given by $kT_c = \zeta(1+\sigma)\frac{q-2}{(q-1)\,\log(q-1)}$, where $\zeta(1+\sigma)$ is the Riemann zeta function [2]. T_c is thus expected to scale as $1/\sigma$ when $\sigma \to 0^+$ (see also [13]). Our results are plotted in Fig. 4 for $q = 3, 5, 7, 9$ and $0.2 \le \sigma < 1.0$, together with MF predictions. The agreement with MF results at low σ is exceptionally good, thus lending strong support to Tsallis conjecture [13]. It is also markedly better than most previous studies [4, 5, 16], with e.g. the ratio between T_c and the corresponding MF prediction amounting to $98.7\%, 95.9\%, 93.3\%$ for $q = 3$, $\sigma = 0.2, 0.3, 0.4$, and $97.4\%, 93.5\%$ for $q = 5$, $\sigma = 0.3, 0.5$, whereas two previous MC studies [4, 5] led to $91.7\%, 95.2\%, 92.9\%, 95.6\%, 91.8\%$ respectively. It is important to mention, however, that a cluster mean-field approach yielded estimates very similar to ours [17].

To sum up, we have obtained a refinement of the phase diagram of the LR Potts model by an order of magnitude, with numerical estimates of $\sigma_c(q)$ supporting a two-digit precision. Near the MF region, the observed scaling behavior of transition temperatures as $1/\sigma$ lends clear support to Tsallis conjecture. Finally, our detailed FSS analysis along the line $\sigma = 1.0$ shows that the observation of discontinuous transitions at finite size may be viewed as an artefact due to the truncation of the LR potential. We therefore strongly expect $\sigma_c(q)$ to approach the line of square interactions in the high-q limit, and the transition to be continuous along the whole line $\sigma = 1.0$, in agreement with Cardy's conjecture. Whether this transition is characterized by exponentially diverging rather than power-law correlation lengths, is still an open question however, and we think this would deserve extensive studies at higher lattice sizes.

[1] T. Kihara, Y. Midzuno, T. Shizume, *J. Phys. Soc. Jpn.*, **9**, 681 (1954).
[2] F.Y.Wu, *Rev. Mod. Phys.*, **54**, 235 (1982).
[3] B.Simon, A.Sokal, *J. Stat. Phys.*, **25**, 679 (1981).
[4] Z. Glumac, K. Uzelac, *Phys. Rev. E*, **58**, 4372 (1998).
[5] K. Uzelac, Z. Glumac, *Fizika B*, **6**, 133 (1997).
[6] Z. Glumac, K. Uzelac, *Physica A*, **271**, 147 (1999).
[7] E. Bayong, H.T. Diep, V. Dotsenko, *Phys. Rev. Letter*, **83**, 14 (1999).
[8] M. Krech, E. Luijten, *Phys. Rev. E*, **61**, 2058 (2000).
[9] J.L. Cardy, *J. Phys. A*, **14**, 1407 (1981).
[10] E.Luijten, H.Messingfeld, *Phys. Rev. Lett.*, **86**, 5305 (2001).
[11] B.A.Berg, T.Neuhaus, *Phys. Rev. Lett.*, **68**, 9 (1992).
[12] S. Reynal, H.T. Diep, *Reexamination of the long-ranged Potts model: a multicanonical approach*, unpublished.
[13] C. Tsallis, *Fractals*, **3**, 541 (1995).
[14] K.Binder, *Z. Phys. B*, **43**, 119 (1981); K.Binder, *Phys. Rev. Lett.*, **47**, 693 (1981).
[15] M.S.S. Challa, D.P.Landau, K.Binder, *Phys. Rev. B*, **34**, 1841 (1986).
[16] Z. Glumac, K. Uzelac, *J. Phys. A*, **26**, 5267 (1993).
[17] J.L.Monroe, *J. Phys. A*, **32**, 7803 (1999).