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# Correlation length of 2D Potts models: numerical vs exact results

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We report Monte Carlo simulations of 2D $q$-state Potts models with $q = 10, 15$, and 20 in the disordered phase and compare numerical results for the correlation length $\xi_d$ at the first-order transition point $\beta_t$ with an analytic formula. To measure the exponential decay of the correlation function over several decades with the desired accuracy we made extensively use of cluster-update techniques and improved estimators. As a byproduct we also obtain the energy moments in the disordered phase in very good agreement with a recent large $q$ expansion at $\beta_t$.

## 1. INTRODUCTION

The two-dimensional $q$-state Potts model defined by the partition function

$$Z = \sum_{\{s_i\}} e^{-\beta E}; E = -\sum_{\langle ij \rangle} \delta_{s_i s_j}; s_i = 1, \ldots, q, \quad (1)$$

is one of the rare statistical systems for which non-trivial exact results are available [1]. On square lattices it exhibits at $\beta_t = \ln(1+\sqrt{q})$ a 2nd (1st) order phase transition for $q \leq 4$ ($q \geq 5$). For $q \geq 5$, also the energies $e_o$ and $e_d$ of the ordered and disordered phase at $\beta_t$ as well as the difference $\Delta c = c_d - c_o$ of the corresponding specific heats are known exactly.

Recently the 7-state model has served as a testing ground for numerical techniques to extract the interface tension $\sigma_{od}$ between the coexisting phases at $\beta_t$ [2–4]. Depending on the employed technique, the numerical predictions for $\sigma_{od}$ differed by a factor of eight. Only shortly after these numerical investigations a formula for the correlation length $\xi_d(\beta_t)$ in the disordered phase [5] could be converted into an explicit expression for the interface tension, $\sigma_{od} = 1/2\xi_d$ [6], which clearly supported the histogram technique [7] used in Ref.[4] and initiated many more refined simulation studies of the interface tension $\sigma_{od}$ [8]. Besides duality arguments the derivation involves the (weak) assumption of complete wetting which can only be proven in the limit of large $q$.

Here we focus on the correlation length and present direct numerical tests of the formula for $\xi_d(\beta_t)$ [9]. As a byproduct we also compare various energy moments with recently derived large $q$ expansions [10].

## 2. SIMULATION

Using the single-cluster (SC) update algorithm [11] we ran simulations for $q = 10, 15$ and 20 on lattices of size $V = L \times L$ with $L = 150, 60$ and 40 ($\approx 14\xi_d$) and periodic boundary conditions. The lattice sizes proved to be large enough to suppress tunneling events such that, starting from a completely random configuration, the system remained a sufficiently long time in the disordered phase. The choice of update algorithm is based on measurements of the integrated autocorrelation time $\tau$ of the spatial correlation function. As is illustrated for $q = 20$ in Fig.1, at large distances the SC update decorrelates (in real time) much faster than the heat-bath algorithm.

After many SC steps we performed one multiple-cluster [12] update to facilitate the most efficient use of the "improved estimator" for measurements of the correlation function

$$G(i,j) \equiv \langle \delta_{s_i s_j} - \frac{1}{q} \rangle = \frac{q-1}{q} \langle \Theta(i,j) \rangle, \quad (2)$$

where $\Theta(i,j) = 1$, if $i$ and $j$ belong to the same cluster, and $\Theta = 0$ otherwise. In the analysis we focussed on the $k_y = 0$ projection $g$ of $G$ in order to avoid power-like prefactors in the large-distance behavior.

All error bars are estimated by means of the jack-knife technique.


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Table 1
Comparison of numerical and analytical results for energy moments in the disordered phase.

| | $q=10$ | $q=15$ | $q=20$ |
|---|---|---|---|
| $e_d$(MC) | −0.96823(10) | −0.75065(9) | −0.62659(6) |
| $e_d$(exact) | −0.968203... | −0.750492... | −0.626529... |
| $C_d$(MC) | 18.41(13) | 8.701(37) | 6.153(16) |
| $C_d$(large $q$) | 18.51(4) | 8.661(5) | 6.133(3) |
| $\mu_d^{(3)}$(MC) | −2066(81) | −175(5) | −55.8(9) |
| $\mu_d^{(3)}$(large $q$) | $\approx -1780$ | $\approx -175$ | $\approx -56$ |

## 3. RESULTS

To convince ourselves that the system was always in the disordered phase, we monitored the time series of the energy and measured the first three moments of the energy distribution, $e_d \equiv \langle E\rangle/V$, $C_d = \beta_t^2\mu_d^{(2)} \equiv \beta_t^2(\langle E^2\rangle - \langle E\rangle^2)/V$, and $\mu_d^{(3)} = \langle(E-\langle E\rangle)^3\rangle/V$. By using duality they can be related to the corresponding moments in the ordered phase ($C_d = C_o + \beta_t^2(e_d - e_o)/\sqrt{q}$, $\mu_d^{(3)} = -\mu_o^{(3)} + 2(1-q)/q^{3/2} + 3(e_d - e_o)/q + 6C_o/\beta_t^2\sqrt{q}$), which have recently been computed by means of large $q$ expansions [10]. For a comparison with our numerical results see Table 1.

Our data for the projected correlation functions $g(x)$ for $q = 10, 15$, and 20 is shown in the semi-log plots of Fig.1. The quite pronounced curvature for relatively small $x$ indicates that the simplest Ansatz taking into account just the lowest excitation (largest correlation length) can only be justified for very large $x$. We have therefore considered the more general Ansatz

$$g(x) = a\,\mathrm{ch}\Big(\frac{L/2-x}{\xi_d}\Big) + b\,\mathrm{ch}\Big(c\frac{L/2-x}{\xi_d}\Big), \qquad (3)$$

with four parameters $a, b, c$, and $\xi_d$. Since nonlinear four-parameter fits are notoriously difficult to control, we first fixed $\xi_d$ at its theoretical value ($\xi_d = 10.559519...$, 4.180954..., and 2.695502... for $q = 10, 15$, and 20, respectively), and optimized only the remaining three parameters. The resulting fits are shown in Fig.1 as solid lines. We see that over a wide range the lines are excellent fits to the data, but noteworthy is also the tendency of the data to be systematically lower at large distances. This suggests that fits to the Ansatz (3) with $\xi_d$ as a *free* parameter should somewhat underestimate the value of $\xi_d$.

In fact, from four-parameter fits over the same $x$ range we obtain values of $\xi_d = 9.2(8), 3.6(2)$ and 2.2(1) for $q = 10, 15$ and 20, respectively, which are about $15-20\%$ lower than the analytical values. Restricting the fit interval to larger $x$ values, we observe a tendency to higher values, but also the errors increase rapidly. The problem is that at the distances we have studied so far ($x_{\max} = L/2 \approx 7\xi_d$) even higher excitations cannot be neglected. Due to convexity properties it is then natural that $\xi_d$ is underestimated by using the truncated Ansatz (3).

As a check we put $q = 2$ in our programs, and thus simulated the Ising model in the disordered phase at $\beta = 0.71 \approx 0.80\beta_c$. Here the exactly known correlation length, $\xi_d = 2.7289\ldots$, is comparable to that of the $q = 20$ model at $\beta_t$. Our data points for $g(x)$ on a $40 \times 40$ lattice look perfectly straight in a semi-log plot. Consequently, a much simpler fit of the form (3) with $b \equiv 0$ was sufficient. As a result we obtained $\xi_d = 2.726(3)$, in very good agreement with the theoretical value.

In both situations we also tried so-called correlated fits which, in general, seemed to be a little more stable. The resulting values for $\xi_d$, however, did not change significantly.

## 4. CONCLUSIONS

Our data for the projected correlation function $g(x)$ in the disordered phase at $\beta_t$ is compatible with the asymptotic decay predicted by the analytical value for $\xi_d(\beta_t)$. By performing four-parameter fits, however, we systematically underestimate $\xi_d$. We attribute this to higher mass excitations which cannot be neglected at the dis-

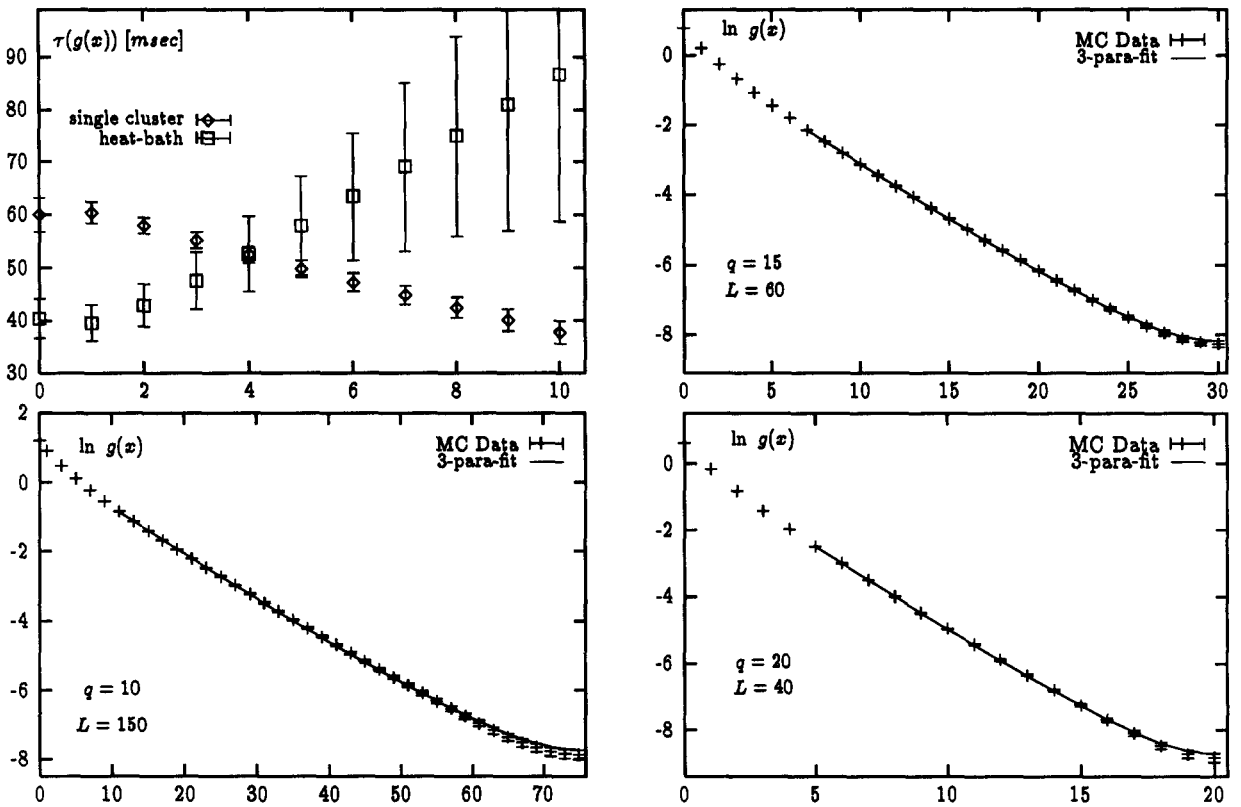


Figure 1. Autocorrelation times for $q = 20$, and semi-log plots of the correlation functions $g(x)$ vs distance $x$ for $q = 10, 15$, and 20. The solid lines are fits to the Ansatz (3) with $\xi_d$ fixed at its theoretical value.

tances investigated so far. Since including further correction terms in the fits is a hopeless enterprise, we are currently performing additional simulations on elongated $2L \times L$ lattices, which should allow a study of correlations over larger distances in reasonable computer time.

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