Ordered vs disordered: Correlation lengths of 2D Potts models at $\beta_t$

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We performed Monte Carlo simulations of two-dimensional $q$-state Potts models with $q = 10$, 15, and 20 and measured the spin-spin correlation function at the first-order transition point $\beta_t$ in the disordered and ordered phase. Our results for the correlation length $\xi_d(\beta_t)$ in the disordered phase are compatible with an analytic formula. Estimates of the correlation length $\xi_o(\beta_t)$ in the ordered phase yield strong numerical evidence that $R \equiv \xi_o(\beta_t)/\xi_d(\beta_t) = 1$.

1. INTRODUCTION

Correlation lengths or inverse masses are among the most important quantities to characterize the properties of a statistical system. Unfortunately there are only very few models for which the correlation length $\xi$ is exactly known and can thus serve as a testing ground for the employed numerical techniques. The best known example is the two-dimensional (2D) Ising model where $\xi$ is exactly known at all temperatures. But the situation is already much more involved for 2D $q$-state Potts models with a partition function

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

where $i = (i_x,i_y)$ denote the lattice sites of a square lattice of size $V = L_x \times L_y$, $\langle ij \rangle$ are nearest-neighbor pairs, and $\delta_{s_i,s_j}$ is the Kronecker delta symbol. Here only the correlation length $\xi_d(\beta_t)$ in the disordered phase could be derived analytically [1], where $\beta_t = \ln(1+\sqrt{q})$ is the first-order transition point of this model for $q \geq 5$. For the correlation length $\xi_o(\beta_t)$ in the ordered phase no analytical results are available. One goal of the present investigations was to test the conjecture that $R \equiv \xi_o(\beta_t)/\xi_d(\beta_t) = 1/2$, which was suggested quite heuristically by previous Monte Carlo (MC) studies [2].

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2. SIMULATION

We studied the Potts model (1) in both the disordered and ordered phase and measured correlation functions at $\beta_t$ for $q = 10$, 15 and 20 on lattices of size $V = L \times L$ and $V = 2L \times L$ with $L = 150, 60$ and $40$ ($\approx 14 \xi_d$). To take advantage of translational invariance we used periodic boundary conditions. We carefully checked that our lattice sizes are large enough to suppress tunneling events such that, starting from a completely random or ordered configuration, the system remained a sufficiently long time in the disordered or ordered phase to perform statistically meaningful measurements. Analyses of autocorrelation times suggested to use in the disordered phase the single-cluster and in the ordered phase the heat-bath update algorithm. All error bars are estimated by means of the jack-knife technique.

To determine the correlation length $\xi$ we considered the $k_y = 2\pi n/L_y$ momentum projections,

$$ g^{(n)}(i_x,j_x) = 1/L_y \sum_{i_y,j_y} G(i,j) e^{ik_y(i_y-j_y)}, \quad (2) $$

of the spin-spin correlation function and its improved cluster estimator

$$ G(i,j) \equiv \langle \delta_{x,y} - 1 \rangle = \frac{q-1}{q} \langle \Theta(i,j) \rangle, \quad (3) $$

where $\Theta(i,j) = 1$, if $i$ and $j$ belong to the same Swendsen-Wang cluster, and $\Theta = 0$ otherwise. The projection removes the power-like prefactor...
in the large-distance behaviour of $G$ and thus allows fits of $g^{(n)}(x) \equiv g^{(n)}(\xi, 0)$ to the Ansatz
\begin{equation}
\xi^{(n)} = \xi / \sqrt{1 + (2 \pi n / L_y)^2} \approx (1 + (n / L_y)^2). (5)
\end{equation}
In the ordered phase (4) can only be used for $n \neq 0$.

3. RESULTS

3.1. Disordered phase

A preliminary report of a first set of simulations in the disordered phase on $L \times L$ lattices was already given in Ref [3]. In the meantime we have further increased the statistics and added another set of simulations on asymmetric $2L \times L$ lattices [4]. For both lattice geometries the first three energy moments are found in very good agreement with the exact result for the average energy and with dual transformed large $q$ expansions [4,5].

In the disordered phase we concentrated on the $k_y = 0$ projection of the correlation function (3). In a first step we fixed $\xi(0) = \xi_d$ at its theoretical value (see Table 1) and optimized only the remaining three parameters in (4). For $q = 10$ the resulting fits to the $L \times L$ and $2L \times L$ data are shown in Fig. 1 as dotted and solid lines, respectively. While the lines are excellent interpolations of the data over a wide range up to $x \approx (5 \ldots 6) \xi_d$, we also see a clear tendency of the fits to lie systematically above the data for very large $x$. In unconstrained fits to the Ansatz (4) this is reflected by a systematic trend to underestimate $\xi_d$. By restricting the fit interval to larger $x$ values the estimates for $\xi_d$ increase, but then also the statistical errors grow rapidly [4]. Table 1 shows our results for $\xi_d(\beta)$ using the fit range $[x_{\min}, L/2]$ with $x_{\min} \approx 2 \xi_d$. We further estimate $c \approx 1.5 - 2$, independent of $q$, which stabilizes to $c = 1.5(1)$ if $\xi_d$ is held fixed at its theoretical value.

3.2. Ordered phase

Also in the ordered phase we first checked that the average energy agrees with the exact result, and compared the higher moments with the large $q$ expansions of Ref [5]. For the specific heat see Table 2. Furthermore we looked at the magnetization $m = (q \langle \text{max} \{n_i\} \rangle / V - 1) / (q - 1)$ and its cluster estimator $m' = \langle |C|_{\text{max}} / V \rangle$, where $n_i$ denotes the number of spins of “orientation” $i = 1, \ldots, q$ and $|C|_{\text{max}}$ is the size of the largest (spanning) cluster. Also here we find very good agreement with the exact answer [6] (for $q = 10$ and $2L \times L$, e.g., $m = m' = 0.857113(49)$, $m_{\text{ex}} = 0.857106 \ldots$).

To determine $\xi_d$ we followed Gupta and Irbäck [2] and studied the $k_y = 2 \pi / L_y$ projection $g^{(1)}(x)$ of $G$. Since this removes constant background

\begin{table}[h]
\centering
\caption{Correlation length $\xi_d(\beta)$ in the disordered phase.}
\begin{tabular}{lccc}
\hline
$q$ & $q = 10$ & $q = 15$ & $q = 20$ \\
\hline
$L \times L$ & 9.0(5) & 3.70(16) & 2.24(6) \\
$(2L \times L)_x$ & 10.2(9) & 3.59(10) & 2.23(5) \\
$(2L \times L)_y$ & 9.3(7) & 3.62(16) & 2.33(7) \\
exact & 10.5595... & 4.1809... & 2.6955... \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Specific heat at $\beta_0$ in the ordered phase.}
\begin{tabular}{lccc}
\hline
$q$ & $q = 10$ & $q = 15$ & $q = 20$ \\
\hline
$L \times L$ & 17.95(13) & 8.016(21) & 5.351(15) \\
$(2L \times L)$ & 17.81(10) & 8.004(19) & 5.3612(55) \\
large $q$ & 18.1(1) & 8.00(3) & 5.362(5) \\
\hline
\end{tabular}
\end{table}
terms, \( g^{(1)}(x) \) can be fitted with the Ansatz (4) also in the ordered phase. For \( q = 10 \) the qualitative behaviour of \( g^{(1)} \) is illustrated in the semi-log plot of Fig. 2. The comparison with \( g^{(0)} \) of the disordered phase suggests that the two correlation functions are governed by the same asymptotic decay law, i.e., that \( \xi_o(\beta_t) = \xi_d(\beta_t) \). In fact, the dotted line interpolating the \( g^{(1)} \) data is a constrained fit to (4) assuming that \( \xi_o = \xi_d = 10.5595 \ldots \). To make this statement even more convincing we have plotted in Fig. 3 the ratio \( R_{\text{eff}} = \xi_{\text{eff}} / \xi_d^{\text{eff}} \), where \( \xi_{\text{eff}} = 1 / \ln[g(x)/g(x+1)] \) is the usual effective correlation length (with the correction (5) for \( \xi_o \) already taken into account). The corresponding plots for \( q = 15 \) and \( q = 20 \) look similar.

4. DISCUSSION

The numerical results for \( \xi_d(\beta_t) \) confirm the analytical expression to about 10 – 20%. The systematic underestimate is presumably caused by higher excitations which are neglected in the fits. Using a non-zero momentum projection in the ordered phase we believe that \( \xi_o(\beta_t) \) is of about the same accuracy. By comparing the two correlation length at \( \beta_t \) we obtain strong numerical evidence that \( \xi_o = \xi_d \). At first sight this is in striking disagreement with a very recent exact proof [7] of the earlier conjecture \( \xi_o = \xi_d / 2 \) for a certain definition of the ordered correlation length, \( \xi_o,1 \). For another definition, \( \xi_o,2 \), however, only the relation \( \xi_o,2 \geq \xi_o,1 \) could be established, which would be consistent with our results if we identify the numerically determined \( \xi_o \) with \( \xi_o,2 \). We are currently investigating this problem in more detail [8] by using precisely the definitions of Ref.[7] which are based on geometrical properties of Potts model clusters such as, e.g., their diameter.

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