The three-dimensional, three-state Potts Model in an External Field

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ABSTRACT

We analyze the critical behaviour of the 3-d, 3-state Potts model in the presence of an external ordering field. From a finite size scaling analysis on lattices of size up to $70^3$ we determine the critical endpoint of the line of first order phase transitions as $(\beta_c, h_c) = (0.54938(2), 0.000775(10))$. We determine the relevant temperature like and symmetry breaking directions at this second order critical point and explicitly verify that it is in the universality class of the 3-d Ising model.

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1 Introduction

The temperature driven first order phase transition of the three-dimensional, three-state Potts model has been analyzed in great detail in the absence of a symmetry breaking external field[1, 2]. This transition remains first order in the presence of a non-vanishing external field and for a critical field strength, $h_c$, it ends in a second order critical point. Although it is expected that this critical point belongs to the universality class of the 3-d Ising model, the universal behaviour in its vicinity has not been analyzed in detail so far. A first estimate for the location of the critical endpoint is given in [3].

Our interest in properties of the 3-d, 3-state Potts model in the vicinity of the second order critical point is motivated by its importance for the analysis of lines of first order transitions in lattice gauge field models. The universal behaviour in the vicinity of the second order endpoint of the line of first order transitions has recently been investigated in the U(1)-Higgs [4] and SU(2)-Higgs [5] models. Lines of first order transitions with critical endpoints do, however, also occur in QCD with light as well as heavy quarks. In the heavy quark mass limit of finite temperature QCD a line of first order phase transitions (deconfinement transition) occurs which is closely related to the phase transition in the 3-d, 3-state Potts model in an external field [6, 7]. Like in the Potts model the deconfinement transition is first order in the limit of infinitely heavy quarks and ends in a second order transition at some finite value of the quark mass. This critical point is expected to belong to the universality class of the 3-d Ising model [8]. Another line of first order transitions occurs in the case of QCD with three light quark flavours (chiral symmetry restoration). This line also ends in a second order endpoint at some critical value of the quark mass. In order to analyze the critical behaviour at these endpoints it will be important to disentangle the relevant energy- and ordering field like directions and identify the Ising-like observables at the critical points. We will address this problem here first in the simpler case of the Potts model and will explore methods used for the analysis of the liquid-gas phase transition [9] as well as lattice gauge models [4, 5].

In this letter we present an accurate determination of the critical couplings at the endpoint of the line of first order phase transitions in the 3-d, 3-state Potts model with an external ordering field. Moreover, we will determine the relevant energy-like and ordering field like directions at this endpoint as well as the related operators from which critical exponents and other universal constants (Binder cumulants) can be extracted. In the next section we fix our notation for the Potts model and introduce the new couplings and operators which control the critical behaviour at the endpoint. In section 3 we present our numerical results for the location of the critical endpoint. A more detailed discussion of the universal properties at this endpoint is given in Section 4. Finally we present our conclusions in Section 5.
2 The Model and Simulation Parameters

The three-state Potts model is described in terms of spin variables $\sigma_i \in \{1, 2, 3\}$, which are located at sites $i$ of a cubic lattice of size $V = L^3$. The Hamiltonian of the model is given by,

$$H = -\beta E - hM,$$

(2.1)

where $E$ and $M$ denote the energy and magnetization,

$$E = \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) \quad , \quad M = \sum_i \delta(\sigma_i, \sigma_g).$$

(2.2)

Here the first sum runs over all nearest neighbour pairs of sites $i$ and $j$. A non-vanishing field $h > 0$ favours magnetization in the direction of the ghost spin $\sigma_g$. On a finite lattice of size $L^3$ the partition function of the model is then given by

$$Z(\beta, h, L) = \sum_{\{\sigma_i\}} e^{-H}.$$

(2.3)

For vanishing external field the model is known to have a first order phase transition for $\beta_c(h = 0) = 0.550565(10)$ [2]. In the presence of a non-vanishing external field $h$ this first order transition weakens and ends in a second order critical endpoint, which is expected to belong to the universality class of the 3-d Ising model. A first estimate of the critical endpoint $(\beta_c, h_c)$ has been given in Ref. [3]. We will give here a more precise determination of $(\beta_c, h_c)$ and analyze the universal critical behaviour at this point.

At $(\beta_c, h_c)$ the original operators for the energy and magnetization, $E$ and $M$, loose their meaning as operators being conjugate to the temperature-like and symmetry breaking couplings. One rather has to determine the new relevant directions at the critical endpoint, which take over the role of temperature-like and symmetry breaking directions and allow the determination of the two relevant critical exponents at the second order endpoint. This also fixes the new order parameter and energy-like observables as mixed operators in terms of the original variables $E$ and $M$. Following the discussion of the corresponding problem for the liquid-gas transition [9] we introduce new operators

$$\tilde{M} = M + sE \quad , \quad \tilde{E} = E + rM,$$

(2.4)
as superpositions of the original variables $E$ and $M$. The Hamiltonian of the Potts model can then be rewritten in terms of these new operators,

$$H = -\tau \tilde{E} - \xi \tilde{M},$$

where the new couplings are given by

$$\xi = \frac{1}{1 - rs}(h - r\beta), \quad \tau = \frac{1}{1 - rs}(\beta - sh).$$

We note that the general ansatz given by Eqs. 2.4 to 2.6 does allow for the possibility that the new couplings $\tau$ and $\xi$ do not define orthogonal directions in the space of the original couplings $\beta$ and $h$, i.e. they need not result from a rotation of the couplings $\beta$ and $h$.

In the presence of a non-vanishing external field the line of first order phase transitions, $\beta_c(h)$, singles out a direction which corresponds to the low temperature, symmetry broken part of a temperature-driven transition. The new temperature-like direction $\tau$ thus is identified with $\beta_c(h)$. In the vicinity of the critical endpoint the slope of this line determines the mixing parameter $r$,

$$r^{-1} = \left(\frac{d\beta_c(h)}{dh}\right)_{h=h_c}.$$  

The second mixing parameter, $s$, is determined by demanding that the energy-like fluctuations and those of the ordering field are uncorrelated,

$$\langle \delta \tilde{M} \cdot \delta \tilde{E} \rangle \equiv 0,$$

with $\delta \tilde{X} = \tilde{X} - \langle \tilde{X} \rangle$ for $X = M$ and $E$. This insures that the expectation value of the new ordering field operator, $\langle \tilde{M} \rangle$, fulfills a basic property of an order parameter, i.e. for $\xi = \xi_c$ it stays $\tau$-independent in the symmetric phase. Eqs. 2.7 and 2.8 give two independent conditions which are sufficient to determine the mixing parameters $r$ and $s$.

All our simulations have been performed on lattices of size $L^3$ with $L = 40, 50, 60$ and 70. We use periodic boundary conditions and perform simulations with a cluster algorithm described in Ref. [10]. Independent of the lattice size we call a new configuration the spin configuration obtained after 1000 cluster updates. Typically we have for each value of the external field $h$ performed simulations at 3 to 4 $\beta$-values in the vicinity of the critical point. For each pair of couplings $(\beta, h)$ we generated about 10000 configurations which then have been used in a Ferrenberg-Swendsen
Reweighting analysis [11] to calculate observables at intermediate parameter values. Autocorrelation times have been estimated by monitoring the time evolution of the energy $E$. Close to the pseudo-critical points they vary between 7 and 25 configurations on the smallest and largest lattices, respectively. All errors quoted below have been obtained from a jackknife analysis.

3 Determination of the critical endpoint

The basic observables for the determination of the pseudo-critical couplings on finite lattices are susceptibilities constructed from the Hamiltonian $H$, and the magnetization $M$,

$$c_L = \frac{1}{L^3} \left( \langle H^2 \rangle - \langle H \rangle^2 \right) \quad ,$$

$$\chi_L = \frac{1}{L^3} \left( \langle M^2 \rangle - \langle M \rangle^2 \right) \quad .$$

(3.1)

(3.2)

The location of the maxima in these observables define pseudo-critical couplings, $\beta_{c,L}(h)$, which may differ for different observables. We generally find that the locations of $c_{L,max}$ and $\chi_{L,max}$ differ by about one standard deviation of the statistical errors on $\beta_{c,L}(h)$ for our smaller lattices and agree within errors for the largest lattice, $L = 70$. The maxima have been obtained from a combined Ferrenberg-Swendsen analysis which takes into account all data sets at fixed values of $h$ at $\beta$-values in the vicinity of the pseudo-critical points. In Tab. 1 we quote results for $\beta_{c,L}(h)$ obtained from $\chi_{L,max}$ for couplings, $h$, in the vicinity of the critical endpoint.

A first indication for the location of the critical region is obtained from an analysis of the volume dependence of the peak heights in the susceptibilities. In the region of first order phase transitions ($h < h_c$) $\chi_{L,max}$ is expected to increase proportional to the volume, while for $h > h_c$ the peak heights will approach a finite value in the infinite volume limit. Results for $\chi_{L,max}$ obtained on different size lattices are shown in Fig. 1. From this figure as well as from a similar analysis of $c_{L,max}$ it is clear that the critical endpoint will be located in the interval $0.0005 \leq h \leq 0.001$. In this interval we find that the dependence of the pseudo-critical couplings $\beta_{c,L}(h)$ on the external field $h$ is well approximated by a leading order Taylor-expansion,

$$\beta_{c,L}(h_1) - \beta_{c,L}(h_2) = \frac{1}{r_L} (h_1 - h_2) \quad , \quad h_1, h_2 \in [0.0005, 0.001] \quad .$$

(3.3)

For our largest lattice, $L = 70$, this dependence is shown in Fig. 2. A straight line fit to these data yields, $r_{70} = -0.689(8)$. Results from other lattice sizes are
Figure 1: The maxima of $\chi_L$ (a) and $\chi_L$ in units of the volume $V = L^3$ (b) as a function of the external field $h$ on various size lattices.
<table>
<thead>
<tr>
<th>$h$</th>
<th>$L = 40$</th>
<th>$L = 50$</th>
<th>$L = 60$</th>
<th>$L = 70$</th>
</tr>
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<tr>
<td>0.00050</td>
<td>0.549800(16)</td>
<td>0.549798(10)</td>
<td>0.549792 (8)</td>
<td>0.549790 (6)</td>
</tr>
<tr>
<td>0.00055</td>
<td>0.549742(16)</td>
<td>0.549724(12)</td>
<td>0.549718 (8)</td>
<td>0.549716 (6)</td>
</tr>
<tr>
<td>0.00060</td>
<td>0.549668(18)</td>
<td>0.549652(12)</td>
<td>0.549644 (8)</td>
<td>0.549642 (6)</td>
</tr>
<tr>
<td>0.00065</td>
<td>0.549596(20)</td>
<td>0.549578(14)</td>
<td>0.549572 (8)</td>
<td>0.549568 (6)</td>
</tr>
<tr>
<td>0.00070</td>
<td>0.549524(20)</td>
<td>0.549506(14)</td>
<td>0.549498 (8)</td>
<td>0.549496 (6)</td>
</tr>
<tr>
<td>0.00075</td>
<td>0.549454(20)</td>
<td>0.549434(14)</td>
<td>0.549426 (8)</td>
<td>0.549424 (6)</td>
</tr>
<tr>
<td>0.00080</td>
<td>0.549382(22)</td>
<td>0.549362(16)</td>
<td>0.549354(10)</td>
<td>0.549352 (6)</td>
</tr>
<tr>
<td>0.00085</td>
<td>0.549312(22)</td>
<td>0.549292(16)</td>
<td>0.549282(10)</td>
<td>0.549280 (8)</td>
</tr>
<tr>
<td>0.00090</td>
<td>0.549240(22)</td>
<td>0.549220(18)</td>
<td>0.549212(10)</td>
<td>0.549208(10)</td>
</tr>
<tr>
<td>0.00095</td>
<td>0.549170(24)</td>
<td>0.549150(18)</td>
<td>0.549140(10)</td>
<td>0.549136(10)</td>
</tr>
</tbody>
</table>

Table 1: Pseudo-critical couplings determined from the location of the peak in $\chi_L$ on different size lattices at various values of the external field $h$.

<table>
<thead>
<tr>
<th>$L$</th>
<th>40</th>
<th>50</th>
<th>60</th>
<th>70</th>
<th>$\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_L$</td>
<td>-0.706(21)</td>
<td>-0.694(15)</td>
<td>-0.690 (9)</td>
<td>-0.689 (8)</td>
<td>-0.685(10)</td>
</tr>
<tr>
<td>$s_L$</td>
<td>0.696 (1)</td>
<td>0.696 (1)</td>
<td>0.694 (1)</td>
<td>0.690 (3)</td>
<td>0.690(2)</td>
</tr>
</tbody>
</table>

Table 2: Slope parameter, $r_L$, determined from the dependence of the pseudo-critical couplings on the external field $h$ (Eq. 2.7) and the second mixing parameter $s_L$ determined from Eq. 2.8 for different lattice sizes.

summarized in Tab. 2. The slope parameter $r_L$ is slightly volume dependent which, of course, reflects the volume dependence of the pseudo-critical couplings. We thus have extrapolated $r_L$ to the infinite volume limit using the ansatz $r_L = r_\infty + c/L^3$. This yields $r_\infty = -0.685(10)$ and fixes the mixing parameter $r$ defined in Eq. 2.4.

The mixing parameter $r_L$ determined above may be used in connection with Eq. 2.8 to determine the second mixing parameter $s_L$. We have done so and within statistical errors we found $s_L = -r_L$, i.e. the couplings $(\tau, \xi)$ can be obtained from a rotation in the space of the original couplings $(\beta, h)$. An alternative approach thus is to assume $s_L = -r_L$ and use Eq. 2.8 to determine $s_L$. In this way we also can make use of the information on diagonal correlations $\langle (\delta X)^2 \rangle$, $X = E$, $M$ and determine $s_L$ from a diagonalization of the fluctuation matrix [4, 5]. The results obtained in this way for $s_L$ on different size lattices are also given in Tab. 2. We note that within errors this approach is consistent with the determination of $r_L$ from the slope of the critical line. The statistical errors are, however, significantly smaller.
Figure 2: The dependence of the critical coupling on the external field on a $70^3$ lattice in the vicinity of the second order endpoint whose location is indicated by an asterisk.

This shows that the transformation of variables, $(\beta, h) \rightarrow (\tau, \xi)$ defined in Eq. 2.6 indeed is a rotation. In the following we will use for the mixing parameters $r = -s$ with $s = 0.690$.

Having fixed the mixing parameters we can perform an analysis of the critical behaviour in the vicinity of the critical endpoint using standard techniques to study temperature driven second order phase transitions in the absence of an external symmetry breaking field. In particular, we can use Binder cumulants to locate the critical endpoint,

$$B_{3,L} = \frac{\langle (\delta \tilde{M})^3 \rangle}{\langle (\delta \tilde{M})^2 \rangle^{3/2}}, \quad B_{4,L} = \frac{\langle (\delta \tilde{M})^4 \rangle}{\langle (\delta \tilde{M})^2 \rangle^2}.$$  \hspace{1cm} (3.4)

For given values of $h$ and $L$ we find that the cumulant $B_{3,L}(\beta, h)$ vanishes and $B_{4,L}(\beta, h)$ acquires a minimum at values of the coupling $\beta$ which agree with each other within statistical errors. This, in turn, defines a pseudo-critical coupling, which again agrees within errors with the pseudo-critical couplings given in Tab. 1. The minima of the second Binder cumulant, $B_{4,L}$, calculated on different size lattices should have a unique crossing point when plotted, for instance, versus the external field $h$. This is indeed the case, as can be seen in Fig. 3. The crossing point yields the critical field $h_c$ at the second order endpoint.
From the crossing points of the Binder cumulants we find for the critical endpoint

$$\beta_c = 0.54938(2) \quad , \quad h_c = 0.000775(10)$$ \hspace{1cm} (3.5)

or equivalently in terms of the rotated couplings,

$$\left( \tau_c, \xi_c \right) = (0.37182(2), 0.25733(2))$$ \hspace{1cm} (3.6)

At this point the Binder cumulant takes on the value $B_4 = 1.609(4)(10)$, where the first error only takes into account the fluctuation of $B_{4,L}$ on the different size lattices at $(\beta_c, h_c)$ and the second error estimates the uncertainties arising from the errors on the location of the endpoint. Our result agrees within errors with the value found for the three dimensional Ising model, $B_4 = 1.604(1)$ [12].

### 4 Universality class of the endpoint

The value of the Binder cumulant $B_4$ determined at the critical endpoint strongly suggests that the critical endpoint belongs to the universality class of the 3-d Ising model. Rather impressive support for Ising-like behaviour at the critical endpoint, which at the same time also demonstrates the importance of the correct choice of
energy- and ordering field like variables, is given by the contour plots obtained from the joined probability distributions (two-dimensional histograms) of the operators $(E, M)$ and $(\tilde{E}, \tilde{M})$, respectively. These are shown in Fig. 4 for the $70^3$ lattice at $(\beta_c, h_c)$. Although the contour plot for $(\tilde{E}, \tilde{M})$ is still slightly asymmetric, a comparison with the corresponding contour plot of the 3-d Ising model [5] clearly shows the same characteristic fingerprint. We have checked that this asymmetry is well within the uncertainties of our determinations of $(\beta_c, h_c)$ as well as the mixing parameters $r$ and $s$.

Further support for the Ising universality class of the critical endpoint comes from a more conventional finite size scaling analysis performed for the newly defined mixed operators $\tilde{M}, \tilde{E}$ and the related susceptibilities. In particular we have considered the order parameter

$$\tilde{m}(\tau, \xi) = \frac{1}{L^3} \left( \tilde{M}(\tau, \xi) - \langle \tilde{M}(\tau_c, \xi_c) \rangle \right)$$

and the susceptibility

$$\tilde{\chi}_L = L^3 \left( \langle \tilde{m}^2 \rangle - \langle |\tilde{m}| \rangle^2 \right).$$

These observables indeed show the usual finite size behaviour in the vicinity of the critical point. For fixed $\xi \equiv \xi_c$ the susceptibility $\tilde{\chi}_L$ reaches a maximum at a pseudo-critical coupling $\tau_{pc}$. Critical exponents can then be determined from the scaling of the order parameter, $\langle |\tilde{m}| \rangle \sim L^{-\beta/\nu}$, the peak height of the susceptibility, $\tilde{\chi}_{L,max} \sim L^{-\gamma/\nu}$, and the pseudo-critical couplings, $(\tau_{pc} - \tau_c) \sim L^{-1/\nu}$. In our analysis of the critical behaviour we have first fixed the critical point $(\tau_c, \xi_c)$ and determined critical exponents from two-parameter fits. Errors have then be determined by also varying $(\tau_c, \xi_c)$ within the errors given in Eq. 3.6. In Tab. 3 we summarize the results of this analysis and compare the calculated exponents with known values for the 3-d Ising model. As can be seen the agreement is quite satisfactory although in our analysis the lattices have not yet been large enough to reach an accuracy similar to that obtained for the 3-d Ising model [2, 12].

Most sensitive to the correct choice of the new, mixed observables are the new energy-like observable, $\langle \tilde{e} \rangle = \langle \tilde{E}/L^3 \rangle$, and the corresponding susceptibility, $c_e \sim (\partial \tilde{e}/\partial \tau)_\xi$. Their critical behaviour is controlled by the thermal critical exponent $(y_t)$ which fixes the critical exponent $\alpha$. In particular, the energy density calculated at $(\tau_c, \xi_c)$ is expected to scale like $\langle \tilde{e} \rangle = c_0 + c_1 L^{-(1-\alpha)/\nu}$ at $(\tau_c, \xi_c)$. It is obvious from Eq. 2.4 that this scaling behaviour can hold only if in the mixed observable $\tilde{e}$ the leading singular behaviour of $E/L^3$ and $M/L^3$, which in general is proportional to $L^{-\beta/\nu}$, gets canceled. For the 3-d Ising model the exponent $\alpha$ is small ($\alpha = 0.11$).
Figure 4: Correlations between the original fields $E$ and $M$ (left) and the new energy-like and ordering field like operators $\tilde{E}$ and $\tilde{M}$. Shown are contour plots obtained from joint histograms for these observables on a $70^3$ lattice at $(\beta_c, h_c)$. The histograms have been obtained from a Ferrenberg-Swendsen reweighting in $\beta$ and $h$. Actually shown are the normalized observables which have vanishing expectation value and a variance that is equal to unity, $(X - \langle X \rangle)/\langle (X - \langle X \rangle)^2 \rangle^{1/2}$. 
Table 3: Critical exponents determined from a finite size scaling analysis in the vicinity of the critical endpoint of the Potts model. The last column is based on the exponents for the 3-d Ising model given in [12].

As a consequence the dominant singular behaviour in $\tilde{e}$ is expected to behave like $\sim L^{-1.41}$ rather than $\sim L^{-0.52}$ as would be the case for $E/L^3$ and $M/L^3$ separately. As can be seen from Tab. 3 this is supported by our analysis of the finite size scaling behaviour of the energy-like observable $\langle \tilde{e} \rangle$, although in this case the critical exponent shows the largest deviation from the corresponding value of the 3-d Ising model.

5 Conclusions

We have determined the critical endpoint of the 3-d, 3-state Potts model in the presence of an external ordering field and have analyzed the critical behaviour in the vicinity of this second order phase transition. New energy-like and ordering field like couplings and observables have been obtained through a rotation of the original couplings and fields. At the critical endpoint of the line of first order phase transitions the joined probability distribution of these new observables shows a correlation pattern which is characteristic for the 3-d Ising model. A finite size scaling analysis performed with the newly defined rotated observables further supports that the critical endpoint belongs to the universality class of the 3-d Ising model.

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References