Phases of the three-state Potts model in three spatial dimensions

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Abstract

The three-state Potts model is numerically investigated on three-dimensional simple cubic lattices of up to $128^3$ volume, concentrating on the neighborhood of the first-order phase transition separating the ordered and disordered phases. In both phases clusters of like spins are observed with irregular boundaries. In the ordered phase the two different non-favored spins are found to attract each other with a long but finite range. As a result, the neighborhoods of the non-favored spins are interpreted as domains of the disordered phase. This explains why the first-order phase transitions associated with the global $Z_3$ symmetry, including the SU(3) pure-gauge one, are so weak.
Finite-temperature systems with global $Z_3$ symmetry in three spatial dimensions have in common a weak first-order phase transition separating ordered and disordered phases. Lattice numerical calculations of the $SU(3)$ pure-gauge quantum chromodynamics (QCD) at finite temperature [1] revealed that a first-order phase transition separates a low-temperature color-confining phase and a high-temperature non-confining phase. The confining phase is disordered with the Polyakov line order parameter taking zero expectation value. The non-confining phase is ordered and the Polyakov line takes a finite expectation value falling on one of the three $Z_3$ axes in the complex plane.

The transition is considered weak because the latent heat is small and the Polyakov line correlation length grows. Numerical simulations of the three-state Potts model [2] showed there is a first-order phase transition separating a low-temperature ordered phase and a high-temperature disordered one. This transition is weak in the sense the latent heat is small. However, it is not yet understood why these phase transitions are so weak. This letter reports the author’s investigation of this problem.

We consider the simplest form of the three-state Potts model on three-dimensional simple cubic lattices. At each site, $x$, of the lattice, a spin, $\sigma_x$, is defined. It takes one of the three possible states in the $Z_3$ group, $\sigma_x \in \{0, 1, 2\}$. The thermodynamics of the system is described by the partition function,

$$Z = \exp(-H/T) = \exp(J \sum_{\langle xy \rangle} \delta(\sigma_x, \sigma_y)),$$

where the sum runs the nearest-neighbor pairs $\langle xy \rangle$ and Kronecker’s symbol is defined as $\delta(\sigma_x, \sigma_y) = 1$ if $\sigma_x = \sigma_y$ and 0 otherwise. The model is invariant under global $Z_3$ transformations. Here we consider only the “ferromagnetic” couplings, $J > 0$. The effective interactions among the Polyakov lines in the finite-temperature pure-gauge QCD are of this type [3].

Earlier numerical simulations showed that a weak first-order phase transition that separates a low-temperature ordered phase and a high-temperature disordered phase at $J \simeq 0.5505$. The phase transition is considered weak because the dimensionless internal energy density, $e \equiv \langle \delta(\sigma_x, \sigma_y) \rangle$, shows only a small gap at the phase transition, from about 0.58 to 0.53, compared with the maximum possible gap from 1 to 1/3. See Fig. 1 for distribution of this quantity. These results were, however, obtained on relatively small volumes such as $32^3$. The two broad peaks marked as “32” in Fig. 1 shows the distribution from such a small-volume simulation reproduced by the author. Although the two-peak structure is clear enough for establishing the first-order nature of this phase transition, the significant overlapping of the broad tails in the middle reflects the fact that flip-flop transitions between the two phases occur too frequently and it is hard to tell in which of the two phases the system resides at a given instant. Because of this difficulty, the natures of the individual phases could not be studied, nor the reason why the phase transition is so weak.

To avoid this difficulty one has to simulate the system on larger volumes. The author wrote a heatbath simulation code for the model that runs on an experimental parallel computer, AP1000, built by Fujitsu Laboratory [4]. On the largest existing configuration of the computer with $16 \times 32 = 512$ microcomputer “cells,” the code performs one million heatbath updates of a $128^3$ volume in about 32 hours. Typically a couple of million heatbath updates are made at four values of
the coupling, $J = 0.55025, 0.5505, 0.55075$, and $0.551$. At each of these coupling values, two independent simulations were made; one starting from a completely ordered configuration and the other starting from a completely disordered one.

At the highest temperature, $J = 0.55025$, the ordered-start simulation quickly converged to the disordered phase within 100K heatbath updates, while the disordered-start simulation remained in the disordered phase indefinitely through the duration of the simulation for more than one million updates. In contrast, at the lowest temperature, $J = 0.551$, the disordered-start simulation quickly converged to the ordered phase while the ordered-start one remained in the ordered phase indefinitely. Coexistence of the two phases is observed at both of the intermediate temperatures, $J = 0.5505$ and $0.55075$: The ordered-start simulations remained in the ordered phase and the disordered-start ones remained in the disordered phase through their durations of more than two million heatbath updates. The corresponding distribution of the internal energy density is shown in Fig. 2, marked as “128.” The two peaks are now completely separated, and there is no doubt about in which of the phases the system resides: We are now able to investigate the natures of the individual phases.

The two-point correlation function, $C_{ij}(r)$, is defined as the probability to find a pair of spin $i$ and $j$ separated by the distance $r$. They are calculated once in every 100K heatbath updates, and are proven free of auto-correlation at least in the relevant range of $r \leq 8$.

In the disordered phase the correlations are expected to decay exponentially in Yukawa form

$$C_{ij}(r) \sim \alpha_{ij} \frac{\exp(-m_{ij}r)}{r} + p_i p_j,$$

as the distance $r$ increases toward infinity. The constant term $p_i p_j$ is given by the product of probabilities, $p_i$ and $p_j$, to find a site with spin $i$ and $j$ respectively. In the disordered phase they should all approach $1/3$ as the system size increases, because the $Z_3$ symmetry is preserved. For the same reason, there are only two different sets of correlations: the diagonal ones, $C_{00} = C_{11} = C_{22}$, and the off-diagonal ones, $C_{01} = C_{02} = C_{12}$. Moreover, because of the conservation of probability,

$$C_{i0}(r) + C_{i1}(r) + C_{i2}(r) = 1, \quad (1)$$

for any $i$, all the correlation mass must agree with each other and the amplitudes obey a simple relation $\alpha_{00} = \alpha_{11} = \alpha_{22} = -2\alpha_{01} = -2\alpha_{02} = -2\alpha_{12}$. We numerically confirmed that all the correlations are fitted well by the Yukawa form, as can be seen in Fig. 2 where the correlations are shown with the constant terms subtracted. Within statistical errors, the fitting parameters (see Table 1) satisfy the above requirements. The positive diagonal amplitudes, $\alpha_{ii} > 0$, shows the like spins attract each other, in accordance with the ferromagnetic interaction. The corresponding correlation mass of $m_{ii} \simeq 0.15$ suggests there exist clusters of like spins of

| $(ij)$     | $m$    | $\alpha$ |
|-----------|--------|---------|
| (00), (11), (22) | 0.15(1) | 0.071(3) |
| (01), (02), (12) | 0.16(1) | -0.037(1) |

Figure 2: Correlations in the disordered phase at $J = 0.5505$. The constant terms $p_i p_j$ are subtracted. The curves are obtained by the least-$\chi^2$ fittings to the Yukawa form summarized in Table 1.
the size of several lattice spacings. Indeed in the spin distributions one sees many such clusters. It is interesting to note that these clusters are neither smooth nor convex in shape, but are complex and concave.

In the ordered phase there is one favored spin which we label as 0, and two non-favored ones which we label as 1 and 2. No analytic result is known about the behavior of the correlations. The current numerical results show the Yukawa form fits them well also in this case. See Fig. 3 and 4, where the constant terms are subtracted again. The fitting parameters are given in Table 2. The positive amplitudes of the diagonal correlations, \( \alpha_{ii} > 0 \), are in accordance with the ferromagnetic interaction. Smaller correlation mass for the favored spin, 0, compared with those of non-favored spins, 1 and 2, may not be statistically significant, but nonetheless is consistent with the fact that the favored spin dominates the volume in the ordered phase. At this coupling, \( J = 0.5505 \), about 60% of the volume is covered by the favored spin, while the remaining is evenly split between the two non-favored ones. On the other hand the negative amplitudes of the correlations between the favored spin and either of the two non-favored spins, \( \alpha_{01} < 0 \) and \( \alpha_{02} < 0 \), means the favored spin repel the non-favored spins. These suggest that there form clusters of like spins, which are indeed observed in the spin distributions. Again the clusters have irregular boundaries.

The correlation between the two different non-favored spins, \( C_{12}(r) \), is the most interesting. It starts from zero at the origin as it should be, but then overshoots the asymptotic value \( p_1p_2 \), and approaches it from above (see Fig. 4.) This means an attractive force acts between the two different non-favored spins. The attractive part alone can be fitted by the Yukawa form if we limit the range of fitting to \( r \geq 3 \) (Fig. 4.) Note that the correlation mass, \( m_{12} = 0.03 \pm 0.03 \), is much smaller than those for the other cases, the smallest of which is \( m_{00} = 0.14 \pm 0.02 \). It is not appropriate, however, to consider this as a truly long-range correlation with zero correlation mass. Again because of the conservation of probability, the correlation

Table 2: Two-point correlations in the ordered phase at \( J = 0.5505 \). Two-parameter least-\( \chi^2 \) fit to the Yukawa form for the range \( r \geq 3 \). The favored spin is 0.

| \((ij)\)  | \(m\)     | \(\alpha\) |
|----------|-----------|------------|
| (00)     | 0.14(2)   | 0.081(3)   |
| (11), (22)| 0.18(3) | 0.028(4)   |
| (01), (02)| 0.15(1) | -0.041(1)  |
| (12)     | 0.03(3)   | 0.010(1)   |
mass $m_{12}$ in the long-distance limit $r \to \infty$ must be equal to the smaller of the masses $m_{01}$ and $m_{11}$. Much smaller value of $m_{12}$ we are seeing must come from subtle balance of the two terms $C_{01}(r)$ and $C_{11}(r)$ in the range we are looking at, and has to give way to the true correlation mass at some longer range. For this reason, we will call this attractive part as the “middle-range” attraction in the remainder of this letter.

Yet it is useful to explore what would happen if we had a really long-range attraction between the two different non-favored spins: such an attraction is likely to cause instability of the ordered phase, because the repulsion against the non-favored spins from the favored ones can then be compensated by paring the two different non-favored spins attracting each other. Hence we expect that the smaller the correlation mass $m_{12}$, the weaker the phase transition. Indeed in the spin distribution of this phase one finds many clusters of the non-favored spins. And such a non-favored cluster almost always accompany clusters of the other non-favored spin in its neighborhood. It should be noted that such pairing of the clusters of the two different non-favored spins is a way to maintain the global $Z_3$ symmetry which requires the volumes occupied by the two non-favored spins must be equal.

As was mentioned earlier, these clusters of the non-favored spins appear in irregular shapes. The neighborhood of such a cluster of complex-shaped clusters of the non-favored spins can be interpreted as an island of the disordered phase in the sea of the ordered phase. This is clearly seen by looking at the local-averaged internal energy density, $c_i(r)$, which is defined in the sphere of radius $r$ with spin $i$ at its center. See Fig. 5 for its dependence on the radius. In the disordered phase, the quantity does not show any dependence and stays at its asymptotic value of $\simeq 0.53$. In the ordered phase, the one around the favored spin approaches the asymptotic value of $\simeq 0.58$ monotonously from above, while the other around the two non-favored spins starts from a value smaller than in the disordered phase and approaches the asymptotic value monotonously from below. These disordered domains increases the internal energy density of the ordered phase and explains why the latent heat is so small.

Irregular boundaries of the non-favored clusters and disordered domains in the ordered phase near the transition may be consistent with very small surface tension at the confined-deconfined phase boundaries found by a MIT-bag calculation [7] as well as by lattice QCD numerical calculations [8]. Note, however, that the irregular boundaries themselves suggests inadequacy of the sharp spherical boundaries assumed or imposed in these calculations.

The “middle-range” attractive correlation between the two different non-favored spins remains attractive down to the lowest temperature simulated, $J = 0.551$. Its range, however, decreases to $m_{12} = 0.07(3)$ at $J = 0.55075$ and $0.11(3)$ at 0.551. This way the ordered phase away from the first-order transition consolidates itself.

It would be interesting to check if the above mechanism of weakening the first-order phase transition works in the pure-gauge QCD thermodynamics. As a first step, the author generated several hundred pure-gauge configurations on a $16^3 \times 2$ lattice by the “APE6” computers in Rome, using a hybrid Monte Carlo algorithm written by the APE group [9]. From each gauge configuration a distri-
bution of Polyakov lines is calculated. Near the first-order phase transition, most of the Polyakov lines are found in the neighborhood of the three \( Z_3 \) axes with non-zero magnitude, even in the disordered phase. Each Polyakov line is projected onto the nearest of the \( Z_3 \) axes, resulting in distributions of the Potts-model spins. Correlations of the spins are then calculated, and found to behave in the same manner as their counterparts in the three-state Potts model. Most notably, the correlation between the two different non-favored spins in the ordered phase shows the same kind of “middle-range” attraction. This allows one to speculate that the deconfined phase of QCD near the phase transition is susceptible to mixture of complex-shaped “droplets” of the confined phase \[1\]. If such is indeed the case, perturbation calculations of the QCD deconfined phase would be useless near the phase transition. Hence it is important to investigate this point in more detail.

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