Critical exponents of the 3D antiferromagnetic three-state Potts model using the Coherent-Anomaly Method

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June 26, 2018

Abstract

The antiferromagnetic three-state Potts model on the simple-cubic lattice is studied using the coherent-anomaly method (CAM). The CAM analysis provides the estimates for the critical exponents which indicate the XY universality class, namely $\alpha = -0.011, \beta = 0.351, \gamma = 1.309$ and $\delta = 4.73$. This observation corroborates the results of the recent Monte Carlo simulations, and disagrees with the proposal of a new universality class.

Key words: Potts model, critical exponents, coherent-anomaly method, series expansion

Running title: AF-Potts model critical exponents using CAM

1 Introduction

The three-dimensional antiferromagnetic three-state Potts model has been investigated intensively during the last decade. However, our understanding of its low-temperature properties is still far from complete. There are several controversial results suggesting different universality classes of its phase transition as well as different types of the low-temperature ordering. In the present article, we concentrate on the critical properties.

The existence of the finite-temperature second-order phase transition from the disordered to the low-temperature phase is generally accepted, but there has been a discussion about its universality class. Let us review the previous results in brief.

Banavar et al. conjectured that the model under investigation belongs to the universality class of the three-dimensional XY ($O(2)$) model. Ono observed a Kosterlitz-Thouless phase with a vanishing order parameter in his Monte Carlo study, but that was probably a consequence of the short simulation time. While the first Monte Carlo estimates of the critical exponents by Wang et al. lay somewhere between the Ising

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and the XY universality classes, improved measurements \[4\] were in good agreement with the later. On the other hand, using the Monte Carlo twist method, Ueno et al. \[5\] obtained the critical exponents which indicate a new universality class. They also found some evidence of a new type of the low-temperature phase. Later, Okabe \[6\] estimated the exponents $\beta$ and $\nu$ by Monte Carlo renormalization group approach, and obtained results which were again in favor of the XY class. Recently, Gottlob and Hasenbusch \[7, 8\] obtained high-precision Monte Carlo estimates of $\gamma$ and $\nu$ in a very good agreement with the estimates for the XY model. They also measured various critical amplitudes, again in full agreement with the XY universality class. Estimates for critical indices are listed in Table 1 together with the corresponding values calculated for the $O(2)$-model \[9, 10\]. It seems that arguments for the XY universality class predominate. On the other hand, Ueno et al. \[11\] later argued that the low-temperature phase is an incompletely ordered phase, and that its nature is not compatible with the XY picture. In order to help to clear up this controversy, we present our results based on the coherent-anomaly method.

We use the same technique which was applied recently to the three-dimensional Ising model and provided accurate critical exponents. The present treatment is nothing but an obvious generalization of the method described in detail in the Ref. \[12\]. Therefore, we only briefly sketch its main points in the next section. In Section 3., we present the results of our analysis. Concluding remarks are given in Section 4.

2 Mean-field solutions based on a series expansion

The coherent-anomaly method \[13, 14, 15\] is a general approach for investigation of critical phenomena (see Ref. \[16\] for a recent review). It is based on the analysis of a suitable set of mean-field type approximations for the given system. Here, we use the variational series-expansion approach \[17, 18, 19\] to generate the series of approximate solutions.

Let us consider the simple-cubic Potts model described by the Hamiltonian

$$H = \sum_{<i,j>} \delta(s_i, s_j) - \sum_{i \in a} \sum_{s=1}^{3} H^a_s \delta(s, s_i) - \sum_{i \in b} \sum_{s=1}^{3} H^b_s \delta(s, s_i)$$

with spin variables $s_i$ taking on three different values, say $\{1, 2, 3\}$. The first summation in $H$ runs over all nearest-neighbor pairs of the cubic lattice, while the second and the third summations correspond to the interaction with external fields. We distinguish between the $a$- and $b$-sublattices in order to be able to take into account the antiferromagnetic order appearing below the critical point. The notation $h^{a,b}_s = \beta H^{a,b}_s$ is used below for the dimensionless external fields.

The partition function can be rewritten as follows:

$$Z = \sum_{\{s_i\}} \exp(-\beta H) = \sum_{\{s_{abc}\}} \Pi_{(xyz)} w(s_{xyz}, s_{x+1yz}, s_{x+y+1z}, s_{xy+z}, s_{xy+1z}, s_{x+1y}, s_{x+y+1z+1}, s_{x+1y+1z+1}, s_{xy+1z+1})$$

where the product runs only over the triples $(xyz)$ in which all entries are either even or odd, and
\[ w(s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8) = \]
\[ \exp[-\beta(\delta(s_1, s_2) + \delta(s_2, s_3) + \delta(s_3, s_4) + \delta(s_4, s_1) + \delta(s_5, s_6) + \delta(s_6, s_7) + \delta(s_7, s_8) + \delta(s_8, s_5) + \delta(s_1, s_9) + \delta(s_2, s_6) + \delta(s_3, s_7) + \delta(s_4, s_8))] \]
\[ \times \exp[\sum_{s=1}^{3} h^a_s(\delta(s, s_1) + \delta(s, s_3) + \delta(s, s_6) + \delta(s, s_8))] \]
\[ \times \exp[\sum_{s=1}^{3} h^b_s(\delta(s, s_2) + \delta(s, s_4) + \delta(s, s_5) + \delta(s, s_7))] \] .  \hspace{1cm} (3)

The sum (2) is nothing but the partition function of a three-state vertex model defined on the bcc lattice, with the vertex weights \( w \) determined by (3). Our strategy is to make use of the gauge invariance \([20, 21]\) of the vertex models to construct a set of mean-field solutions of the model. We parameterize the gauge transformation in the following way:

\[ \tilde{w}_a(s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8) = \]
\[ \sum_{\{r\}} A_{s_1, r_1} A_{s_2, r_2} A_{s_3, r_3} B_{s_4, r_4} A_{s_5, r_5} B_{s_6, r_6} A_{s_7, r_7} B_{s_8, r_8} w(r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) \]  \hspace{1cm} (4)

\[ \tilde{w}_b(s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8) = \]
\[ \sum_{\{r\}} B_{s_1, r_1} A_{s_2, r_2} A_{s_3, r_3} B_{s_4, r_4} A_{s_5, r_5} B_{s_6, r_6} A_{s_7, r_7} B_{s_8, r_8} w(r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) \] ,  \hspace{1cm} (5)

where \( A \) and \( B \) are orthogonal matrices with their first rows parameterized as

\[ \{A_{11}, A_{12}, A_{13}\} = \sqrt{1 - x_1^2 - x_2^2} \{1, 1, 1\}/\sqrt{3} + x_1 \{0, 1, -1\}/\sqrt{2} + x_2 \{-2, 1, 1\}/\sqrt{6} \]
\[ \{B_{11}, B_{12}, B_{13}\} = \sqrt{1 - x_3^2 - x_4^2} \{1, 1, 1\}/\sqrt{3} + x_3 \{0, 1, -1\}/\sqrt{2} + x_4 \{-2, 1, 1\}/\sqrt{6} \]  \hspace{1cm} (6)

Apart from the orthogonality condition, the remaining rows are arbitrary; their parameterization does not effect the calculation. Alternatively, we use the parameterization

\[ x_1 = r_A \cos \phi_A \quad x_2 = r_A \sin \phi_A \]
\[ x_3 = r_B \cos \phi_B \quad x_4 = r_B \sin \phi_B \]  \hspace{1cm} (7)

when it is appropriate. The gauge invariance consists in the fact that the partition function does not change when one replaces the original weights \( w \) by the transformed weights \( \tilde{w}_a \) and \( \tilde{w}_b \) on the sublattices (of the bcc lattice) \( a \) and \( b \), respectively.

Following the usual procedure of the variational series-expansion method, we generate a formal series expansion for the transformed vertex model described by the weights \( \tilde{w}_a \) and \( \tilde{w}_b \) without fixing the gauge parameters \( \{x_i\} \). There are totally \( 2 \times 3^8 \) kinds of the vertex weights for a general three-state model with two nonequivalent sublattices. For the purpose of the series expansion, we classify them into \( 2 \times 495 \) classes \( \{\omega_{a,b}^{i,j}\}_{i=0}^{494} \) induced by the lattice symmetry. We fix the notation such that \( \omega_{a,b}^0 = \tilde{w}_{a,b}(1, 1, 1, 1, 1, 1, 1, 1) \). Then, we calculate the formal series expansion for the free energy in powers of \( \omega_i^a/\omega_0^a \) and \( \omega_i^b/\omega_0^b \). (See Refs. \([12, 22]\) for technical details.) Thus, our expansion for the logarithm of the partition function has the form

\[ F_L = \frac{1}{2} \log(\omega_0^a/\omega_0^b) + \sum_{n=2}^{L} f_n(\{\omega_i^{a,b}/\omega_0^{a,b}\}) \] ,  \hspace{1cm} (8)
where \( \{f_n\} \) are homogeneous polynomials of order \( n \), and \( L \) denotes the maximal order included in the expansion. Because of the large number of variables \( \omega \), this is a huge formula containing thousands of terms and we cannot present it here. The calculation of the series is the limiting factor in the variational series-expansion approach. In this case we were able to generate the series only up to the order \( L = 6 \). Nevertheless, within the present formulation, the approximation \( \mathcal{F}_6 \) includes quite large excitation encompassing up to 40 original spins. (Note that the graph-counting here is rather different from that of the usual series expansions).

Having calculated the formal expansion for the free energy, we can return to the original model described by the weights \( \tilde{w}_a \) and \( \tilde{w}_b \). Thus, \( \mathcal{F}_L \) becomes a function of the temperature, external fields and of the gauge parameters \( \{x_i\} \). Within the variational series-expansion method, the gauge parameters are fixed by the stationarity conditions

\[
\frac{\partial \mathcal{F}_L}{\partial x_i} = 0 \quad (i = 1, 2, 3 \text{ and } 4).
\]

Let us describe the structure of the solutions to (9). In the high-temperature phase and in zero external fields, there exists only a single solution, namely \( x_i = 1 \) (i.e. \( r_A = r_B = 0 \)). New solutions characterized by finite \( r_A \) and \( r_B \) appear at the critical point. However, our mean-field solutions \( \mathcal{F}_L \) exhibit a nearly perfect rotational symmetry in a broad region around the critical point. This means that we have always \( r_A = r_B = r \) and \( \phi_A = \phi_B + \pi = \phi \), and, moreover, \( \mathcal{F}_L(r, \phi) \) does not depend on the angle \( \phi \). Perturbations of this rotational symmetry are at least of the order \( r^6 \), and are therefore completely irrelevant to the CAM analysis. This property can be shown explicitly in the lowest-order approximation.

The symmetric properties of our solutions reflect the restoration of the rotational symmetry of the model at its critical point, and are in agreement with what was observed in Ref. [7]. In fact, without this property, it would be impossible to extract any reliable estimates for critical exponents using the CAM.

### 3 CAM analysis

The coherent-anomaly method is based on the scaling of the so-called mean-field critical coefficients [13, 14, 15]. Similarly as in Ref. [18], we expand the approximant \( \mathcal{F}_L \) in the vicinity of its critical point in order to calculate the coefficients. The only difference from the calculation in Ref. [18] is that we have four gauge parameters to take into account. We are interested mainly in the magnetizations and the susceptibilities

\[
m_i^\alpha = \frac{\partial \mathcal{F}}{\partial h_i^\alpha}, \quad \chi_{ij}^{\alpha \beta} = \frac{\partial m_i^\alpha}{\partial H_j^\beta}.
\]

Naturally, these quantities are not independent. Actually, there is only one independent susceptibility because we have \( \chi_{ii}^{\alpha \alpha} = -\chi_{kl}^{\alpha \alpha} / 2 \) (\( k \neq l \)) and \( \chi_{kl}^{\alpha \beta} = -\chi_{kl}^{\alpha \beta} \). In the same way, we have effectively only one critical coefficient for the magnetizations because of the rotational symmetry mentioned above. Therefore, we omit the indices \( i \) and \( j \) corresponding to the three Potts states as well as the sublattice indices \( \alpha \) and \( \beta \).

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After some straightforward calculations, we obtain the following expressions for the mean-field critical coefficients of the specific heat $\bar{c}_L$, the magnetization $\bar{m}_L$, the susceptibility $\bar{\chi}_L$ and the critical magnetization $\bar{m}_L^c$:

\[
\bar{c}_L = \beta_L^* \beta^* (\partial_{rrr} \mathcal{F})^2 / \partial_{rrrr} \mathcal{F}, \\
\bar{m}_L = \partial_{hr} \mathcal{F}(-6 \beta_L^* \partial_{rr} \mathcal{F} / \partial_{rrrr} \mathcal{F})^{1/2}, \\
\bar{\chi}_L = \partial_{hr} \mathcal{F} \partial_{hx} \mathcal{F} / \partial_{rr} \mathcal{F}
\]

and

\[
\bar{m}_L^c = \partial_{hr} \mathcal{F}(-6 \beta_L^* \partial_{hx} \mathcal{F} / \partial_{rrrr} \mathcal{F})^{1/3}.
\]

Here, the symbol $\partial_x$ means the derivative with respect to the gauge parameter $x_1$ or $x_2$, $\partial_h$ stands for the derivative with respect to the external field, and $\partial_r$ is the derivative with respect to the radius gauge parameter. All the derivatives in (11-14) are to be calculated at the critical point $\beta = \beta_L^*$, $x_i = 1$ ($r = r_A = r_B = 0$). Taking different gauge parameters $x$'s and external fields $h$ results in equivalent sets of mean-field critical coefficients. Namely, the critical coefficients can be rescaled so that they may be equal to unity in the lowest order approximation $L = 0$. This does not affect the subsequent analysis, and it turns out that one is left with only one set of coefficients for each quantity. This is a consequence of the model symmetry.

Now, we can estimate the true critical exponents of the model from the CAM scaling formulas as \[12\]

\[
\bar{c}_L \sim \left( \frac{t^*_L}{t^*} \right)^{\alpha/2} \left( \frac{|t^* - t^*_L|}{t^*} \right)^{-\alpha} = (|\Delta_L|)^{-\alpha}, \\
\bar{m}_L \sim \left( \frac{t^*_L}{t^*} \right)^{(1/2 - \beta)/2} \left( \frac{|t^* - t^*_L|}{t^*} \right)^{\beta - 1/2} = (|\Delta_L|)^{\beta - 1/2}, \\
\bar{\chi}_L \sim \left( \frac{t^*_L}{t^*} \right)^{(\gamma - 1)/2} \left( \frac{|t^* - t^*_L|}{t^*} \right)^{1 - \gamma} = (|\Delta_L|)^{1 - \gamma}
\]

and

\[
\bar{m}_L^c \sim \left( \frac{t^*_L}{t^*} \right)^{\psi/2} \left( \frac{|t^* - t^*_L|}{t^*} \right)^{-\psi} = (|\Delta_L|)^{-\psi}, \quad \psi = \gamma(\delta - 3) / 3(\delta - 1)
\]

where $\Delta_L = (t^*/t^*_L)^{1/2} - (t^*_L/t^*)^{1/2}$ with $t$ standing for the temperature or for the inverse temperature; $t^*$ is the exact critical value while $t^*_L$ is its $L$th order approximation.

In order to extract accurate estimates of critical exponents, it is necessary to know the critical temperature with a high accuracy. We have used the value $\beta^* = 0.81563$ obtained from the high-precision Monte Carlo simulation by Gottlob and Hasenbusch \[8\], and fitted the critical exponents to the above coherent-anomaly scaling formulas. We would like to stress that within the CAM approach the resulting exponents always fulfill the scaling relations $\alpha + 2\beta + \gamma = 2$ and $\gamma = \beta(\delta - 1)$.

We excluded the approximants for $L = 0, 2$ and $3$ from our analysis as usual, because their critical behavior is the same. Actually, they represent the same approximation which has a Bethe-like character; it does not take into account properly even the shortest cycle of the lattice. This is why the critical coefficients for $0 \leq L \leq 3$ do not follow the CAM scaling very well for the type of the expansion used here. On the other hand, even the
approximation with \( L = 4 \) takes account of quite large loops, and reflects the structure of the lattice much better.

Therefore, we have fitted the critical exponents to the data obtained only from the approximations with \( L = 4, 5 \) and 6. The values thus obtained are shown in the bottom of Table 2, and the corresponding CAM plots are presented in Fig. 1. Unfortunately, unlike in the Ising case, we are not able to estimate the error of our results, because we have effectively only three data points. However, the same method works extremely well for the Ising model, which is in fact a special case of the present system. This is why we believe that our estimates would be essentially unchanged also for higher-order approximations. Now, let us compare our results to the previously calculated exponents shown in Table 1. Our estimates of \( \gamma \) are in a very good agreement with the the values of the XY universality class. The values for \( \alpha \) and \( \beta \) are also consistent with the XY universality class, though the differences between various fits indicate a relatively larger error.

4 Conclusion

We have calculated the estimates of critical exponents \( \alpha, \beta, \gamma \) and \( \delta \) of the three-dimensional antiferromagnetic Potts model. Our calculation is based on the variational-expansion approach combined with the coherent-anomaly method. The most difficult part of the computation in the present investigation was the generation of the series expansion. We have calculated the necessary series up to the order \( L = 6 \). This relatively short series provides only three points for the subsequent CAM analysis, and therefore, we cannot estimate the error bars for our estimates. The extension of the series seems to be rather infeasible even for the order \( L = 7 \). Hence, the present method may not be competitive with the Monte Carlo simulation for the model under investigation. However, all the recent estimates of critical exponents calculated directly for the Potts model come from Monte Carlo studies. In the present situation in which similar results by different methods are not available, it is important to obtain at least some results independently of the Monte Carlo studies, in order to confirm the universality class. The agreement of our estimates with the XY universality class is fairly good and the discrepancy between our results and the values proposed by Ueno is large. We thereby conclude that our estimates corroborate the XY universality class, and are clearly against the new universality class as proposed by Ueno [5].

Finally, let us make a brief remark concerning the low-temperature phase. As described above, our mean-field solutions exhibit approximate rotational symmetry in the order-parameter space. From the point of view of the mean-field critical behavior, we can regard them as perfectly symmetric, because the deviations from the symmetry do not affect the calculation of the mean-field critical coefficients. However, it is the asymmetry which determines the direction of the sublattice-symmetry breaking. Unfortunately, the deviations from the perfect symmetry are so small that the differences between the free energies corresponding to different solutions under the stationarity conditions (3) are practically negligible compared to the expected accuracy of our approximations. This is why we cannot determine the type of the low-temperature ordering from the present calculations. It is possible that this peculiar behavior of our approximations reflects the nature of the low-temperature phase, namely that the order parameter of the model be-
comes effectively continuous. This would be in line with the restoration of the rotational symmetry observed by Gottlob and Hasenbusch [7]. It would also elucidate the origin of the XY critical indices. Clearly, the interesting properties of the low-temperature phase deserve further investigation.

Acknowledgment

One of us (M.K.) would like to express his gratitude to the Nishina Memorial Foundation for granting him a scholarship.
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| Author     | year | Ref. | α      | β       | γ      | ν      |
|-----------|------|------|--------|---------|--------|--------|
| Wang      | 1989 | [3]  | 1.27(5)| 0.63(4) |        |        |
| Wang      | 1990 | [4]  | 1.31(3)| 0.66(3) |        |        |
| Ueno      | 1989 | [5]  | 0.15   | 0.34(2) | 1.10(2)| 0.58(1)|
| Okabe     | 1992 | [6]  | 0.33(2)| 0.66(2) |        |        |
| Gottlob   | 1994 | [7]  | 1.310(9)|   | 0.664(4)|
| Gottlob   | 1994 | [8]  | 0.663(4)|   |        |        |
| LeGuillou | 1980 | [9]  | −0.007(6)| 0.345(2)| 1.3160(25)| 0.669(2)|
| LeGuillou | 1985 | [10] | 0.3485(35)| 1.315(7)|        | 0.671(5)|

Table 1. Recent estimates for critical exponents of the antiferromagnetic three-state Potts model in three dimensions. We have also included the exponents calculated for the 3D XY model for comparison. The values in Refs. [3] and [4] are the standard RG estimates and the results from the $\epsilon$-expansion, respectively.
Table 2. Critical temperatures and critical mean-field coefficients as calculated for various approximation orders $L$. The critical exponents were fitted to the data from approximations with $L > 3$ and the resulting estimates are shown in the bottom row of the table. The numbers in the first column correspond to the approximations used.

| $L$ | $T^*_L$ | $\bar{c}_L$ | $\bar{m}_L$ | $\bar{\chi}_L$ | $\bar{m}_L$ |
|-----|---------|-------------|-------------|----------------|-------------|
| 0-3 | 1.3943  | 1.0         | 1.0         | 1.0            | 1.0         |
| 4   | 1.3014  | 1.09957     | 1.15608     | 1.21551        | 1.17556     |
| 5   | 1.2998  | 1.11207     | 1.16766     | 1.22603        | 1.18680     |
| 6   | 1.2735  | 1.09982     | 1.23997     | 1.39797        | 1.29054     |
| data used | $\alpha$ | $\beta$ | $\gamma$ | $\delta$ |
| 5,6:       | −0.025 | 0.359 | 1.306 | 4.63 |
| 4,6:       | 0.001 | 0.344 | 1.311 | 4.81 |
| 4,5,6:     | −0.011 | 0.351 | 1.309 | 4.73 |
Figure caption

**Fig. 1.** CAM scaling of the critical mean-field coefficients $\bar{Q}_L$ for the specific heat, $\bar{c}_L$ (◇), magnetization, $\bar{m}_L$ (+), susceptibility, $\bar{\chi}_L$ (□) and for the critical magnetization, $\bar{m}_c^L$ (×). The distance from the true critical point is measured in $\Delta_L = (\beta*/\beta_L)^{1/2} - (\beta_L/\beta*)^{1/2}$. Critical coefficients were rescaled so that $\bar{Q}_0=1$ (see the text).
\[ \log(Q_L) \_ \_ -0.1 \_ 0.0 \_ 0.1 \_ 0.2 \_ 0.3 \_ 0.4 \_ 0.5 \_ 0.6 \_ 0.7 \_ 0.8 \_ 0.9 \_ 1.0 \_ 1.1 \_ 1.2 \_ 1.3 \_ 1.4 \_ 1.5 \_ 1.6 \_ 1.7 \_ 1.8 \_ 1.9 \_ 2.0 \]

\[ \log(\Delta_L) \]

The graph shows a plot of \( \log(Q_L) \) against \( \log(\Delta_L) \). Several lines are displayed, each representing different data points. The x-axis represents \( \log(\Delta_L) \) with values ranging from -3.2 to -2.0, while the y-axis represents \( \log(Q_L) \) with values ranging from -0.1 to 0.4.