Coupling exponents of three-state Potts model on two dimensional square lattice

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The key idea behind studying critical behavior of physical systems with phase transition is determining their critical exponents respective to the coupling parameters, both numerically and theoretically. In a numerical aspect, methods like Finite Size Scaling and Monte Carlo Renormalization Group is utilized to characterize those universal parameters while we can also apply Real-Space Renormalization Group and Conformal Field Theory to directly calculate the exponents. Here we explicitly derive a critical exponent for the three-state Potts Model in two dimensional square lattice, and compare the numerical and theoretical results with the known value. We concluded that both Finite Size Scaling and Real-Space Renormalization Group shows an accurate results within a reasonable margin.

Keywords: Renormalization Group, 3-state Potts model, Critical Exponents, Universality Class

I. 3-STATE 2D POTTS MODEL

As a generalization of the Ising model, the Potts model named after Renfrey Potts, is a physical system of interacting spins on a crystalline lattice which shows phase transition with ferromagnetic phase. It can be generalized into several other important models in statistical physics, with examples being, but not limited to, the XY model, the Heisenberg Model, and the N-vector model.

The Potts model consists of discrete spins that are placed on a lattice. In this study, we will only consider two-dimensional square Euclidean lattice with continuous boundary condition.

The classical Hamiltonian for this model can be written by a combination of coupling parameters and spins.

$$\mathcal{H} = -\mathcal{K}\sum_{\langle i,j\rangle}\delta(s_i, s_j) - h\sum_i \delta(s_i, s_{ghost}) \tag{1}$$

While s_i is a spin respective to the location i on lattice with value from 0 to $q-1$ for q-state Potts model. $\mathcal{K}$ and h represents the coupling parameters in association with the spin and external field, respectively. In this paper, we will assume s_{ghost}; a spin interacting with an external field, to be 0 without losing generality.

As a result, the partition function and bulk free energy density for such system is given as

$$\mathcal{Z} = \sum_{\{s_i\}}\exp\left[\mathcal{K}\sum_{\langle i,j\rangle}\delta(s_i, s_j) + h\sum_i \delta(s_i, 0)\right] \tag{2}$$

$$f_{bulk} = f := -\lim_{V\to\infty}\left[\frac{\ln \mathcal{Z}}{V}\right] \tag{3}$$

It is known that the q-state Potts model on 2D square lattice has a critical fixed point on the following basis.

$$(\mathcal{K}_c, h_c) = (1/T_c, h_c) = (\ln[1+\sqrt{q}], 0) \tag{4}$$

Eq. (4) can be easily proven based on a duality relation between two coupling parameter $\mathcal{K}$ and $\mathcal{K}^*$ on 2D square lattice: $\mathcal{K} = \mathcal{K}^* = \mathcal{K}_c$ is satisfied on a critical fixed point

$$e^{-\mathcal{K}^*} = \frac{e^{\mathcal{K}}-1}{e^{\mathcal{K}}+q-1} \tag{5}$$

Note that the standard ferromagnetic Potts model in 2d shows continuous phase transition for $1 \leq q \leq 4$ and first-order phase transition for $q > 4$. In this research, we will only consider cases where q is 3.

Following the definition of Hamiltonian in Eq. (1), we determine the order parameter m to be

$$m = \frac{q\rho - 1}{q-1}, \text{ where } \rho = \frac{1}{V}\sum_i \delta(s_i, 0) \tag{6}$$

and correlation function $G(i,j)$ and correlation length $\xi(T)$ of the system to be

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$$G(i,j) = \left\langle \frac{q\delta(s_i,s_j)-1}{q-1} \right\rangle - \left\langle \frac{q\delta(s_i,0)-1}{q-1} \right\rangle \left\langle \frac{q\delta(s_j,0)-1}{q-1} \right\rangle \propto \frac{1}{|i-j|^{d-2+\eta}} \exp\left[-\frac{|i-j|}{\xi(T)}\right] \tag{7}$$

It is straight forward to prove that correlation function is 0 for both completely ordered and dis-ordered phases.

II. CRITICAL EXPONENTS AND SCALING RELATIONS

The basic approach to quantitatively analyzing the system in statistical physics is to follow the variation of physical quantities as we increase the length scale. Such approach is known as coarse graining and rescaling, which allows us to systematically take into account fluctuations near the critical point by tracing out short-range fluctuations and shift our attention to longer-length behavior of the system.

The basis of coarse graining and rescaling analysis is the rule that the partition function is invariant.

$$\mathcal{Z}(\mathcal{H}) = \sum_{s'}\sum_{s} e^{-\mathcal{H}} = \sum_{s'} e^{-\mathcal{H}'} = \mathcal{Z}'(\mathcal{H}') \tag{8}$$

$$\text{where } e^{-\mathcal{H}'} = \sum_{s} e^{-\mathcal{H}} \leftrightarrow \mathcal{H}' = -\ln\left[\sum_{s} e^{-\mathcal{H}}\right] \tag{9}$$

Combining Eqs. (3) and (8), the bulk free energy density of the system changes as we rescale the system with scale factor $b > 1$.

$$f(\mathcal{K}) = b^{-d} f(\mathcal{K}') \tag{10}$$

Eq. (10) is known as the fundamental relation in thermodynamics and statistical physics. For $\mathcal{K}$ consisting of nearest-neighbor coupling and external magnetic field, we arrive at

$$f(t,h) = b^{-d} f(b^{y_t}t, b^{y_h}h), \text{ where } t = \frac{T-T_c}{T_c} \tag{11}$$

Where y_t and y_h are the thermal and magnetic coupling exponents, respectively. It is worth noting that Eq. (11) leads to several important scaling relations in critical phenomena.

The degree of singularity of physical quantities near the critical point is described by the critical exponents defined below, note that each exponents represents the asymptotic behavior of each physical quantities as the system reaches criticality.

$$\lim_{t\to 0} C_v \propto |t|^{-\alpha}, \text{ where } C_v := -T\left.\frac{\partial^2 f(t,h)}{\partial t^2}\right|_{h=0} \text{ is a Specific Heat} \tag{12}$$

$$\lim_{t\to 0-} M(h=0) \propto (-t)^{\beta}, \text{ where } M := -\frac{\partial f(t,h)}{\partial h} \text{ is a Order Parameter} \tag{13}$$

$$\lim_{t\to 0} X_T \propto |t|^{-\gamma}, \text{ where } X_T := -\left.\frac{\partial^2 f(t,h)}{\partial h^2}\right|_{h=0} \text{ is a Susceptibility} \tag{14}$$

$$\lim_{h\to 0} M(t=0) \propto |h|^{1/\delta} \tag{15}$$

$$\lim_{t\to 0} \xi(t) \propto |t|^{-\nu} \tag{16}$$

$$\lim_{t\to 0} G(i,j) \propto \frac{1}{|i-j|^{d-2+\eta}}, \text{ where } d \text{ and } \eta \text{ is a dimension and an anomalous dimension, respectively} \tag{17}$$

Combining Eq. (11) with Eqs. (12) to (15), we can determine the critical exponents α, β, γ, and δ as follows:

$$-\alpha y_t + 2y_t - d = 0 \to \alpha = 2 - d/y_t \tag{18}$$

$$\beta y_t + y_h - d = 0 \to \beta = (d - y_h)/y_t \tag{19}$$

$$-\gamma y_t + 2y_h - d = 0 \to \gamma = (2y_h - d)/y_t \tag{20}$$

$$y_h/\delta + y_h - d = 0 \to \delta = y_h/(d - y_h) \tag{21}$$

One can also derive the relations for ν and η by applying fluctuation-dissipation theorem and a trivial scaling relation for correlation length $\xi(t) = b\xi(tb^{y_t})$, please refer to Appendix A for further details regarding the relationship between the correlation function and susceptibility.

$$-\nu y_t + (2y_h - d)/(2-\eta) = 0 \to \nu = 1/y_t \tag{22}$$

$$(2y_h - d)/(2-\eta) = 1 \to \eta = d - 2y_h + 2 \tag{23}$$

III. NUMERICAL METHOD 1: FINITE SIZE SCALING

A. Monte Carlo Simulation and Heat-Bath Method

Monte Carlo simulations are realized as the numerical implementation of stochastic dynamics represented by the master equation, which describes how the set of probabilities evolves with time.

For spin configuration $a = \{s_1, s_2, ...s_N\}$, let us denote the state of a system using a probability that the system has a configuration a at time t, $P(a,t)$. For the ising model, the total number of possible configuration a is 2^N while for q-state Potts model, it is q^N. Suppose that the configuration changes from a to b with the transition probability $w(a \to b)\Delta t$ in a small time interval Δt. The net change of the probability for the system in configuration a should satisfy the following master equation.

$$P(a, t + \Delta t) - P(a, t) = -\sum_{b \neq a} w(a \to b)P(a, t)\Delta t + \sum_{b \neq a} w(b \to a)P(b, t)\Delta t \tag{24}$$

It is critical to choose appropriate transition probabiltiles in Monte Carlo simulations so that the equilibrium distribution is of the Gibbs-Boltzmann form $P(a,t) = e^{-H(a)}/\mathcal{Z} := P_{eq}(a)$. Suppose that an equilibrium has been achieved in the master equation Eq. (24) with $P(a,t) = P_{eq}(a)$. Then, the left-hand side vanishes and consequently

$$\sum_{b \neq a} w(a \to b)P_{eq}(a) = \sum_{b \neq a} w(b \to a)P_{eq}(b) \tag{25}$$

A sufficient condition for the above relation to hold is to equate both sides term by term,

$$w(a \to b)P_{eq}(a) = w(b \to a)P_{eq}(b) \tag{26}$$

$$\frac{w(a \to b)}{w(b \to a)} = e^{-\beta[H(b) - H(a)]} \tag{27}$$

This relation is called the detailed balance condition that the transition probability should satisfy. A common choide of the transition probability that satisfied such condition is a Heat-Bath method described below.

$$w(a \to b) = \frac{e^{-\beta H(b)}}{e^{-\beta H(a)} + e^{-\beta H(b)}} \tag{28}$$

Note that in Monte Carlo simulations one regards the calculation of the expectation value of a physical quantity O as an average over the configurations generated by the stochastic dynamics.

B. Finite Size Scaling

To extract coupling exponents from numerical data, we would have to run simulations where critical phenomena take place in macroscopic system. We can, however, carry out numerical computations only for finite-size systems. Therefore, it is not possible for our physical quantities to show authentic singular behavior since critical phenomena only happens at the thermodynamic limit, i.e. either when system size it infinite or the temperature is zero.

Since the parameter should be carefuly tuned for the system to reach the critical point, we should include the inverse of system size L^{-1} in the argument of free energy density.

$$f(t, h, L^{-1}) = b^{-d} f(b^{y_t} t, b^{y_h} h, bL^{-1}) \tag{29}$$

If we combine Eq. (29) with the definition described in Eq. (12), (13), and (14), we obtain

$$C_v(t, 0, L^{-1}) = b^{2y_t - d} \partial_t^2 f(b^{y_t} t, 0, bL^{-1}) \tag{30}$$

$$m(t, h, L^{-1}) = b^{y_h - d} \partial_h f(b^{y_t} t, b^{y_h} h, bL^{-1}) \tag{31}$$

$$X_T(t, 0, L^{-1}) = b^{2y_h - d} \partial_h^2 f(b^{y_t} t, 0, bL^{-1}) \tag{32}$$

If we insert $b = L$ and rewrite the equation,

$$L^{d-2y_t} C_v(t, L^{-1}) = \Phi_1(L^{y_t} t) \tag{33}$$

$$L^{d-y_h} m(t, L^{-1}) = \Phi_2(L^{y_t} t) \tag{34}$$

$$L^{d-y_h} m(h, L^{-1}) = \Phi_3(L^{y_h} h) \tag{35}$$

$$L^{d-2y_h} X_T(t, L^{-1}) = \Phi_4(L^{y_t} t) \tag{36}$$

Therefore, we can estimate the exact value of coupling exponents by plotting physical quantities on graph with appropriate x and y axis in respective to Eqs. (33) to (36).

The result of the numerical computation is displayed from Fig. 1 to 8, each containing a corresponding physical quantities introduced in Section II. In general, the critical exponents that forms the universality class of 3-state 2D Potts Model coincides with the numerical data generated by Monte Carlo simulations, refer to Table I in Appendix C for the full list of critical exponents.

IV. THEORETICAL METHOD 1: REAL-SPACE RENORMALIZATION GROUP

V. NUMERICAL METHOD 2: MONTE CARLO RENORMALIZATION GROUP

TBA

VI. THEORETICAL METHOD 2: CONFORMAL FIELD THEORY

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VII. CONCLUSIONS

Conclusion.

ACKNOWLEDGMENTS

The code that generates data for Finite Size Scaling in Section III in this paper is available at .

Appendix A: Fluctuation-dissipation theorem

Fluctuation-dissipation theorem

Appendix B: Real-Space Renormalization Group for Ising Model on two dimensional square lattice

Real-space Renormalization Group for Ising Model on two dimensional square lattice

Appendix C: Universality Class

Universality Class

TABLE I. A table with numerous columns that still fits into a single column. Here, several entries share the same footnote. Inspect the LaTeX input for this table to see exactly how it is done.

Class	d	α	β	γ	δ	ν	η
Ising	2	0	1/8	7/4	15	1	1/4
Ising	3	0.11	0.33	1.24	4.79	0.63	0.04
3-state Potts	2	1/3	1/9	13/9	14	5/6	4/15
4-state Potts	2	2/3	1/12	7/6	15	2/3	1/4
XY	3	-0.02	0.35	1.32	4.78	0.67	0.04
Heisenberg	3	-0.12	0.37	1.40	4.78	0.71	0.04
Mean Field		0	1/2	1	3	1/2	0

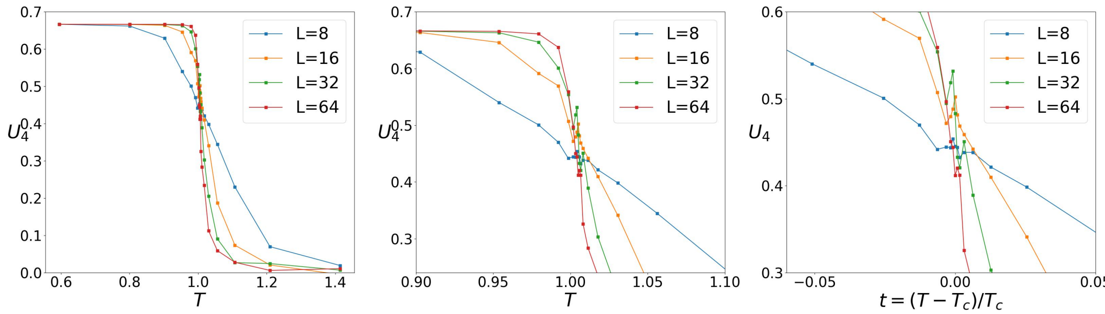

FIG. 1. Binder Cumulant U_4 of the system at Size = 8, 16, 32, and 64. The T_c where the cumulant intersect is 1.005.

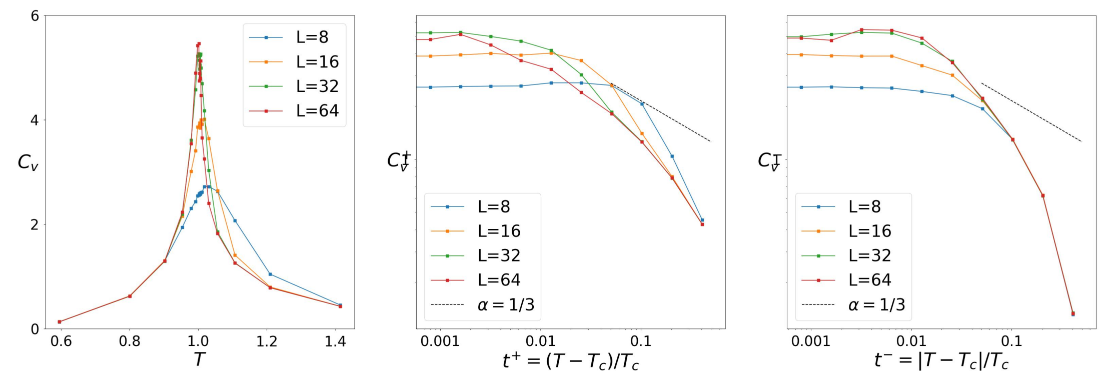

FIG. 2. Specific Heat C_v of the system at Size = 8, 16, 32, and 64. $\alpha = 1/3$

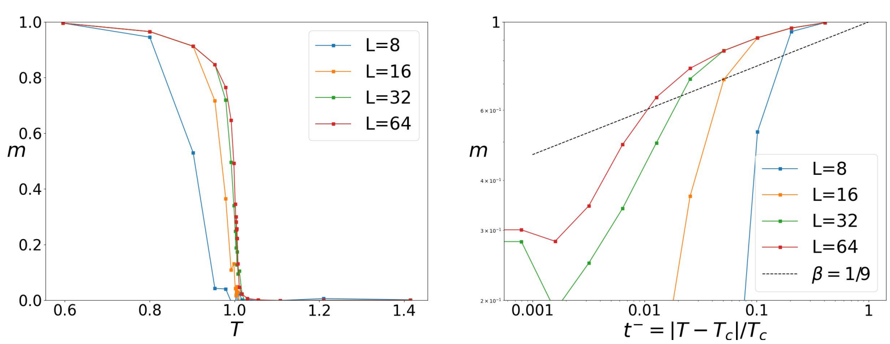

FIG. 3. Order Parameter m of the system with no external field at Size = 8, 16, 32, and 64. $\beta = 1/9$

TABLE II. A table with numerous columns that still fits into a single column. Here, several entries share the same footnote. Inspect the LaTeX input for this table to see exactly how it is done.

Class	d	y_t	y_h
Ising	2	1	15/8
Ising	3	1.59	2.48
3-state Potts	2	6/5	28/15
4-state Potts	2	3/2	15/8
XY	3	1.49	2.48
Heisenberg	3	1.41	2.48

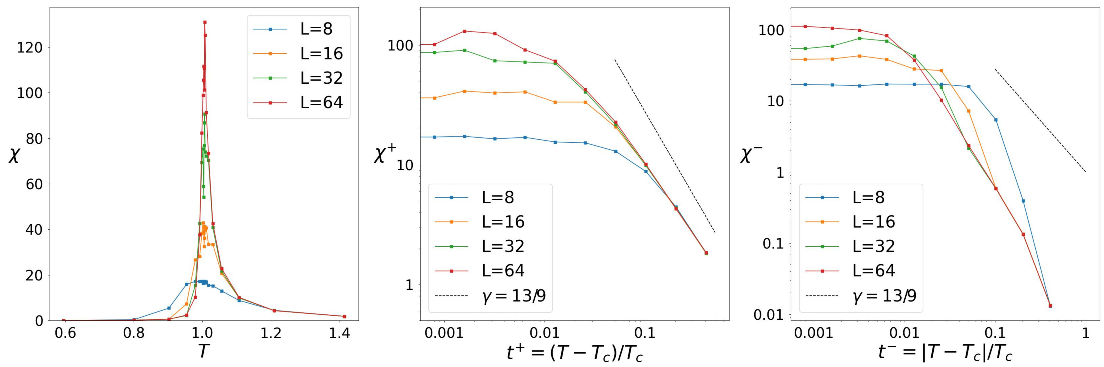

FIG. 4. Susceptibility X_T of the system at Size = 8, 16, 32, and 64. $\gamma = 13/9$

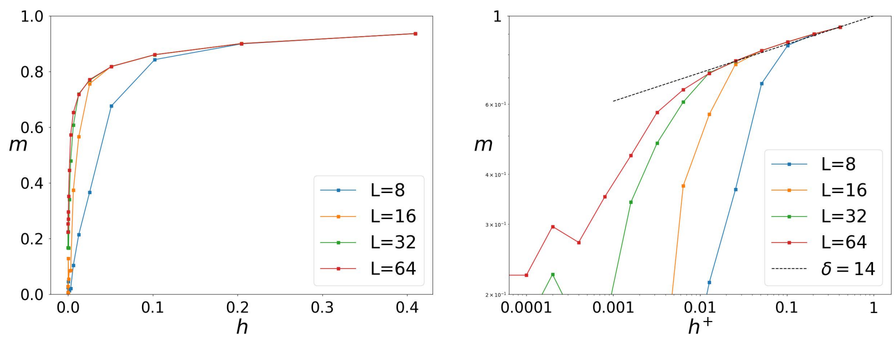

FIG. 5. Order Parameter m of the system at $t = 0$ at Size = 8, 16, 32, and 64. $\delta = 14$

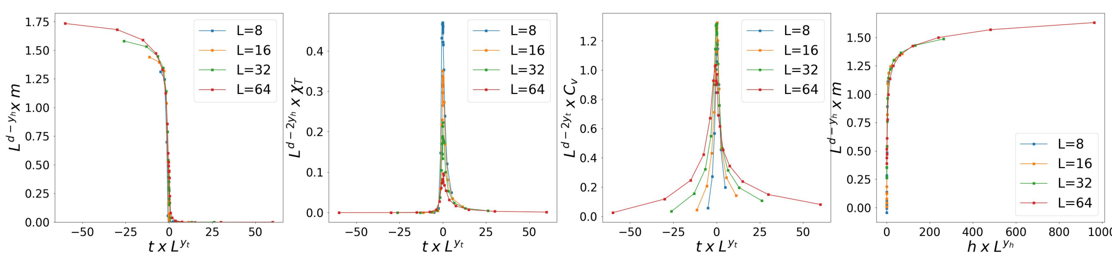

FIG. 6. Finite Size Scaling of the system at Size = 8, 16, 32, and 64. $y_t = 6/5$ and $y_h = 28/15$

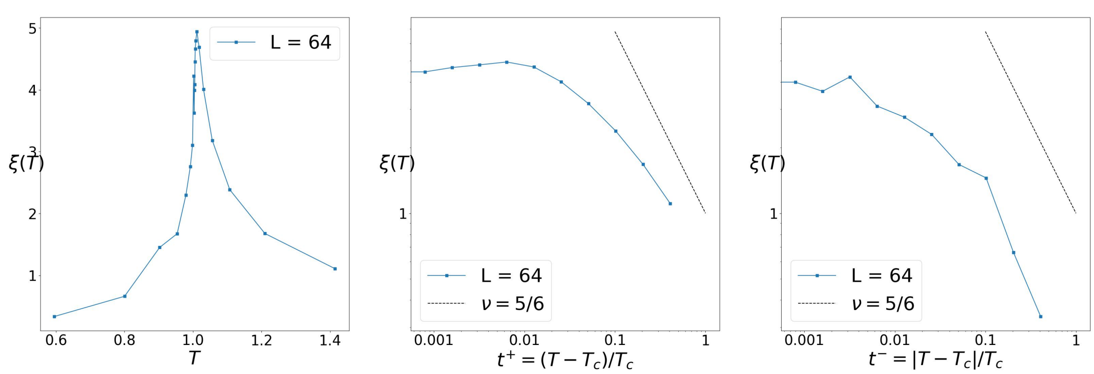

FIG. 7. Correlation Length ξ of the system at Size = 64. $\nu = 5/6$

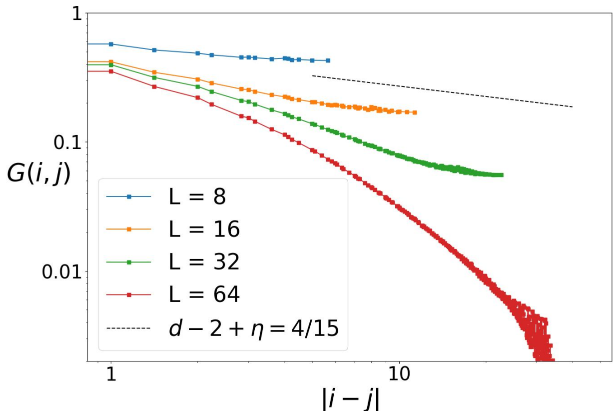

FIG. 8. Correlation Function $G(i, j)$ of the system at critical fixed point at Size = 8, 16, 32, and 64. $\eta = 4/15$ since $d = 2$