Study of Ising model and three state Pott's model cumulants in 2D lattice

Swati Saha*

(In collaboration with Prof. Rajiv V. Gavai[#] and Prof. Bedangadas Mohanty*)



- * National Institute of Science Education and Research, HBNI, India
- # Indian Institute of Science Education and Research, Bhopal, India



*** WORK IN PROGRESS

Outline:

- → Motivation
- Ising and Pott's model
- Observables
- Analysis details
- → Results
- → Summary and outlook

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We want to understand the ordering of susceptibility χ using simple models having phase-transition at (i) high temperature (ii) low temperature and its (iii) volume dependence



Overview of models



Ising model

For a d-dimensional lattice, each lattice site having spin σ_k = {+1,-1}, energy of the lattice configuration

$$\mathcal{H} = -\mathcal{J} \sum_{\langle i,j
angle} \sigma_i \sigma_j$$

Stephen G. Brush, Rev. Mod. Phys. 39, 883

Order-parameter *m* where *N* is the number of lattice site in a lattice configuration

$$m = \frac{\sum_{i=1}^{N} \sigma_i}{N}$$

-> Critical temperature T_c of Ising model in d = 2 lattice $T_C = \frac{2}{\ln(1 + \sqrt{2})} = 2.269 \text{ J/}k_B$

Lars Onsager, Phys. Rev. 65, 117

q=3 state Pott's model

• For a d-dimensional lattice, each lattice site having spin $\sigma_k = \{0,1,2\}$, energy of the lattice configuration

$$\mathcal{H} = -\mathcal{J}\sum_{\langle i,j\rangle} \delta(\sigma_i,\sigma_j)$$

Order-parameter *m* where *N* is the number of lattice site in a lattice configuration

$$m = \frac{3 \cdot \max(N_0, N_1, N_2) - N}{2N}$$

• Critical temperature T_c of q=3 state Pott's model in d = 2 lattice $T_C = \frac{1}{\ln(1 + \sqrt{3})} = 0.995 \text{ J/}k_B$

R.B. Potts, Proc. Cambridge Philos. Soc. 48 (1952) 106

F. Y. Wu, Rev. Mod. Phys. 54, 235



Simulation in 2D lattice





Order parameter m for each lattice configuration (after reaching equilibrium) is calculated at temperature T. Cumulants of m are further calculated for different T.



Observables



Cumulants of order parameter *m* :

$$C_{1} = \langle m \rangle$$

$$C_{2} = \mu_{2}N$$

$$C_{3} = \mu_{3}N$$

$$C_{4} = (\mu_{4} - 3\mu_{2}^{2})N$$

$$C_{5} = (\mu_{5} - 10\mu_{3}\mu_{2})N$$

$$C_{6} = (\mu_{6} - 15\mu_{4}\mu_{2} - 10\mu_{3}^{2} + 30\mu_{2}^{3})N$$

$$\langle m \rangle = \frac{1}{S_{\text{tot}}} \sum_{k=1}^{S_{\text{tot}}} m_k$$
$$\mu_n = \langle (m - \langle m \rangle)^n \rangle$$

- → m_k is order parameter in the kth
 state of lattice at a temp (T)
- S_{tot} = total no of states
- N = total no of lattice sites

Model	Ising model		q = 3 state Pott's model	
Lattice size (L)	50 x 50	80 x 80	50 x 50	80 x 80
States (iteration)	2 x 10 ⁵	2 x 10⁵	2 x 10 ⁵	2 x 10 ⁵
Independent states	9000	9000	3600	3600

For each lattice, simulation performed for different T near critical temperature T_c .

(i) for Ising model: T in [2.2, 2.8] J/ $k_{\rm B}$, (ii) for q=3 state Pott's model: T in [0.9, 1.1] J/ $k_{\rm B}$



Cumulants in Ising model





- \rightarrow C₂ and higher order cumulants show non-monotonic variation with temperature.
- → FWHM decreases with lattice size (for C_2 , 37% reduction from L = 50 to L = 80). For all higher-order cumulants as well, the region of critical behaviour narrows with lattice size.



Cumulants in q=3 state Pott's model





 \rightarrow q=3 state Pott's model also shows non-monotonic variation with *T*.









- Critical exponents are in good agreement with theory. $T_{C,L}$ obtained for lattices in both models.



Ratio of cumulants in Ising model





- Cumulant ratios show a nonmonotonic variation with *T/T_{C,L}*.
- → The critical region is volume dependendent, it narrows with increase in lattice size.
- Uncertainities are statistical (computed using subsampling method)



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Ordering in Ising model





LQCD prediction

 $T_{C,L}$ = 2.312 (50x50) $T_{C,L}$ = 2.297 (80x80)

 $C_{\rm s}/C_{\rm s} < C_{\rm s}/C_{\rm s} < C_{\rm s}/C_{\rm s} < C_{\rm s}/C_{\rm s}$

- C_6/C_2 does not follow the ordering of cumulant ratios.
- → Ordering is observed from C₃/C₁ to C₅/C₁ in a narrow region close to critical temperature (T_{C,L}). For T > T_{C,L}
 C₅/C₁ < C₄/C₂ < C₃/C₁
- For $T < T_{C,L}$ inequality of the ordering is reversed, - $C_5/C_1 > C_4/C_2 > C_3/C_1$
- Temperature at which inequality is reversed varies with lattice size.



Ordering in q=3 state Pott's model





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- → Lattice QCD predicted an ordering of baryon susceptibility χ_B ratios which STAR experiment seems to have observed. QCD critical point in T-µ plane is expected to be Ising class with µ playing the role of magnetic field. Hence, we tried to study the ordering using cumulants of order parameter in spin models.
- → Our study shows that the ordering of cumulant ratios is followed from C_3/C_1 to C_5/C_1 only above critical temperature. Below that, inequality of the ordering is reversed. Temperature at which inequality is reversed seems to be volume dependent.
- A more realistic simulation would be q=3 state Pott's model in 3-dimensional lattice with magnetic field *B*, where *B* will correspond to chemical potential μ_B. This is a work in progress.











Simulation performed using Wolf-Cluster algorithm

Phys. Rev. Lett. 62, 361

- (1) Select a random spin configuration of 2d-lattice
- (2) Using random number generator, select a lattice site i randomly
- (3) Get the nearest neighbour of ith lattice site, i.e j. For each neighbour j, if spins of i and j are parallel, and the bond is not considered before, then j is added to the cluster with probability $1-\exp(-2\beta J)$
- (4) After all i's neighbours, j have been considered, we repeat the same process from step 2 for the j sites that are added to the cluster.
- (5) The process is repeated until the cluster grows as much as possible.
- (6) The spins of the cluster is inverted.







Errors are estimated using sub-sampling method

- → Total available statistics is divided into smaller groups. Each group is a sub-sample. N = 25 samples are created in our case.
- C_n is calculated for each sub-sample.
- Statistical error on C_n is given by

$$\sigma_{C_{\rm n}} = \sqrt{\frac{\sum_{i=1}^{N} (C_{{\rm n},i} - C_{\rm n})^2}{N(N-1)}}$$

where $C_{n,i}$ is the value of C_n calculated for the ith sub-sample





→ Time auto-correlation function is defined by \$\varphi(t)\$ where \$M(0)\$ and \$M(t)\$ are the order parameters a t²=0 and t²=t time

$$\phi(t) = \frac{\langle M(0)M(t) \rangle - \langle M \rangle^2}{\langle M^2 \rangle - \langle M \rangle^2}$$

→ In discrete case, if we have *n* number of states produced at different mc-times, *M_s* and *M_{s+i}* are the magnetization per spin of states at *s* and *s+i*th mc time, the function can be written as

$$\phi_i = \frac{\frac{1}{n-i} \sum_{s=1}^{n-i} M_s M_{s+i} - \langle M \rangle^2}{\langle M^2 \rangle - \langle M \rangle^2}$$

• The auto-correlation time can be extracted using the relation $\phi(t) = exp\left(-\frac{t}{t_r}\right)$







Characteristic feature of a second-order phase transition is the divergence of the correlation length at a critical temperature $T_c = T_c(\infty)$

$$\xi(T) = \xi_0 + |1 - T/T_C|^{\nu} + \dots$$

This leads to the singularities of the specific heat, magnetization ($T < T_c$), susceptibility parameterized by the critical exponents (2D Ising model: $\nu = 1$, $\alpha = 0$, $\gamma = 7/4$, $\beta = 1/8$

$$C(T) = C' + C_0 |1 - T/T_C|^{-\alpha} + \dots \qquad m(T) = m_0 |1 - T/T_C|^{\beta} + \dots$$
$$\xi(T) = \xi_0 |1 - T/T_C|^{-\gamma} + \dots$$

In any numerical simulation the system size is finite, and hence near T_c the role of ξ is taken over by the linear system size L

$$|1 - T/T_C(\infty)| \propto \xi(T)^{-1/\nu} \to |1 - T/T_C(\infty)| \propto L^{-1/\nu}$$

As a critical temperature of the finite lattice T_c (L) we take the location of the specific-heat peak (or susceptibility). This leads to

$$T_{C,L} - T_{C,\infty} \propto L^{\frac{-1}{\nu}}$$



Ordering in Ising model



→ $L = 50 - T/T_{C,L} \le 1.008$, inequality reversed ($T/T_{C,L} \ge 1.012$, inequality maintained); the boundary line is between (1.008, 1.012), ~ $T = 1.01T_{C,L}$

→ $L = 80 - T/T_{C,L} \le 1.001$, inequality reversed $(T/T_{C,L} \ge 1.006)$, inequality maintained); the boundary line is between (1.001, 1.006), ~ $T = 1.003T_{C,L}$



→ L = 50 -----> $T/T_{C,L} \le 1.002$, inequality reversed ($T/T_{C,L} \ge 1.007$ inequality maintained); the boundary line is between (1.002, 1.007), ~ $T = 1.005 T_{C,L}$

→ $L = 80 = T/T_{C,L} \le 1.00$, inequality reversed $(T/T_{C,L} \ge 1.005)$, inequality maintained); the boundary line is between (1.0, 1.005), $\sim T = 1.003 T_{C,L}$