The q-state "Clock" Model Monte Carlo Results and Comparison with TRG

Leon Hostetler with Alexei Bazavov (MSU) and Ryo Sakai (UI)

Michigan State University

July 6, 2020



Outline

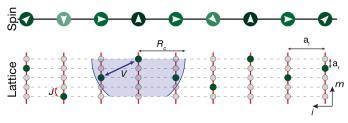
- Introduction
- 2 2-state Clock Model: Ising model
 - Energy density
 - Spin correlations
- 3-state Clock Model
 - Energy density
- Summary and Future Work

Motivation

- Lattice gauge theories are fundamental to our understanding of nature
- Unfortunately, Monte Carlo approaches are mostly limited to equilibrium physics at zero chemical potential
- Quantum computation/simulation offers the possibility of real-time and finite-density calculations:
 - ▶ Digital
 - Analog
- Challenges include: Infinite dimensional Hilbert spaces, fermions
- Ultimate goal: Quantum simulation of QCD

Example: Abelian Higgs --- Optical Lattice

- Go from Lagrangian to Hamiltonian formalism by taking the time continuum limit
- ② Truncate the "spin" states to some value s
- Simulate it on an optical lattice
 - ▶ 2 species of atoms in a Bose-Hubbard setup (1403.5238)
 - ▶ 2-leg "ladder" setup with 2s atoms per rung (1503.08354)
 - ► asymmetric ladder setup with single atom per rung (1803.11166)
- Tensor renormalization group (TRG) methods can be used to study the effect of truncations



Motivation

- Alternatively, we can start with models that already have "truncations". E.g. we look at clock models which have a small number of states
- Map such a system with finite states to an optical lattice
- Along the way, we need to validate with numerical methods like MCMC (well understood but computationally intensive) and TRG (fast even at large volumes but needs more development and validation)
- Once we can quantum simulate these simple spin models, we move on to more complicated models
- I am working on the Monte Carlo side and Ryo Sakai is working on the TRG side

q-state clock model

• For the q-state clock model¹, the Hamiltonian is

$$H = -\sum_{\langle i,j\rangle} \cos(\theta_i - \theta_j)$$

Spins reside on lattice sites with values

$$\theta_i = \frac{2\pi k}{q}, \qquad k = 0, 1, \dots q - 1$$

- ullet The model has a discrete \mathbb{Z}_q symmetry
- For q = 2, it is equivalent to the Ising model
- For q = 3, it is equivalent to the *standard* 3-state Potts model²
- ullet For $q \to \infty$, it becomes the continuous XY model

10,10,15,15,15,

6/19

¹Also called the "planar Potts model", the "vector Potts model", or the " \mathbb{Z}_q model".

²Commonly referred to as the "Potts model" or sometimes as the

[&]quot;Ashkin-Teller-Potts model".

Overview

- 1 Introduction
- 2 2-state Clock Model: Ising model
 - Energy density
 - Spin correlations
- 3-state Clock Model
 - Energy density
- 4 Summary and Future Work

2-state Clock Model: aka Ising model

• The "action" for a lattice configuration is

$$S = \sum_{\langle i,j \rangle} \delta_{q_i,q_j}.$$

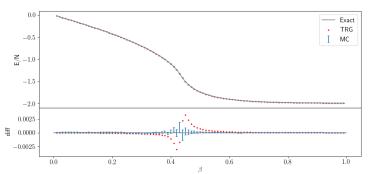
• The energy, for a lattice in *d* dimensions with *N* sites and no external magnetic field is,

$$E = -2S + dN$$
.

- Energy density, or energy per site is E/N
- Here, we focus on d = 2

Energy density: Numerical results



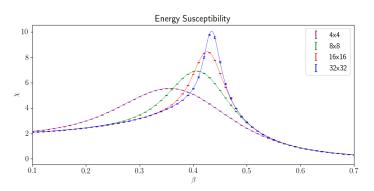


- ullet For MC results, 100K equilibrating HB sweeps followed by 1K×1K sweeps. Error bars are calculated from binned data
- TRG results do not have error bars yet
- "Exact" results are from numerical differentiation of the partition function

● Bottom plot gives the deviation from the exact result () () ()

Leon Hostetler (MSU) Clock Model July 6, 2020 9/19

Energy susceptibility



Plotted is the energy susceptibility

$$-\frac{1}{N}\frac{dE}{d\beta} = \frac{1}{N}\Big(\langle E^2 \rangle - \langle E \rangle^2\Big)$$

LHS can be calculated "exactly" from the partition function and gives the solid curves. RHS can be estimated by MC sampling and gives the points with error bars.

Leon Hostetler (MSU) Clock Model July 6, 2020 10 / 19

Spin-spin Correlation Functions from MC

Schematically,

$$G(r) = \langle \sigma_{0,0} \sigma_{0,r} \rangle ,$$

where $\sigma_{i,j}$ is the spin at Cartesian coordinate (i,j). Some authors subtract the magnetization $\langle \sigma_{0,0} \rangle^2$

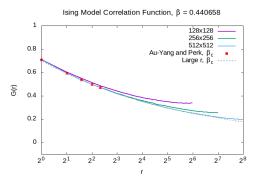
- Can use translation invariance to maximize statistics
- We consider only correlations in the vertical and horizontal directions (no diagonals). Then for the 2d Ising model,

$$G(r) = \frac{1}{4N} \sum_{i} \sum_{j} \left[\sigma_{i,j} \sigma_{i-r,j} + \sigma_{i,j} \sigma_{i+r,j} + \sigma_{i,j} \sigma_{i,j-r} + \sigma_{i,j} \sigma_{i,j+r} \right],$$

where N is the number of sites in the lattice.

◆ロト ◆母 ト ◆ き ト ◆ き ト き 目 を り へ ○ ○

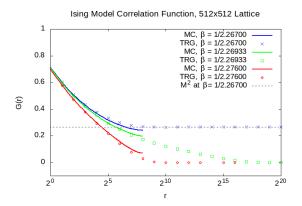
MC Validation near T_c



- At $T = T_c$ and small r, G(r) can be calculated exactly via Toeplitz determinants. See Au-Yang and Perk (1984)
- At $T=T_c$, and large r, we know from Wu (1966) that $G(r)\simeq 0.70338/r^{1/4}$
- Note: $\beta_c = \frac{1}{2} \ln(1 + \sqrt{2}) \approx 0.4406867935$
- No error bars yet!



Comparison with TRG Results



- In the ordered phase, we expect the asymptotic value of the correlation function to be the spontaneous magnetization squared. The dashed line gives the exact infinite volume M^2 at the value of β corresponding to the blue curve and blue points
- Neither MC nor TRG results have error bars yet

Overview

- 1 Introduction
- 2 2-state Clock Model: Ising model
 - Energy density
 - Spin correlations
- 3-state Clock Model
 - Energy density
- 4 Summary and Future Work

3-state Clock Model

- The 3-state clock model is equivalent to the standard 3-state Potts model. One only needs to make a substitution in the factor out front $2 \rightarrow 3/2$
- Energy function is

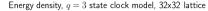
$$E = -rac{3}{2}\sum_{\langle i,j
angle}\delta_{q_iq_j} + rac{1}{2}dN$$

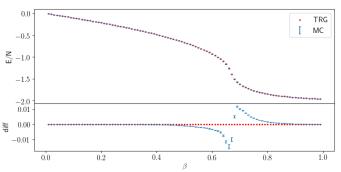
Site variables are

$$q_i \in \{0,1,2\}$$



Energy density





- MC results from 10K equilibrating HB sweeps followed by 1K histograms of 1K sweeps each
- Bottom plot gives difference between MC and TRG results
- Note, no error bars on the TRG results yet

∢ロト ∢団ト ∢ミト ∢ミト 亳川三 幻久♡

Leon Hostetler (MSU) Clock Model July 6, 2020 16 / 19

Overview

- 1 Introduction
- 2 2-state Clock Model: Ising model
 - Energy density
 - Spin correlations
- 3-state Clock Model
 - Energy density
- 4 Summary and Future Work

Summary and Future Work

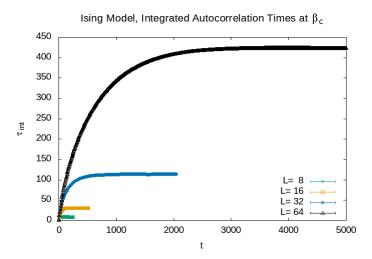
- The ultimate goal is to simulate LGTs on optical lattices
- We start by looking at the simpler clock model and develop the numerical tools needed
- With 2-state clock model (i.e. Ising model), we validate MC and TRG against exact results
- We have started looking at the 3-state clock model—TRG results will be validated by MC
- Next: Study phase transition of n-state clock models with MC, TRG, and optical lattices

References

- A. Bazavov et. al. "Gauge-invariant implementation of the Abelian Higgs model on optical lattices." Phys. Rev. D 92, 076003 (2015) arXiv:1503.08354
- B. A. Berg, Markov Chain Monte Carlo Simulations and Their Statistical Analysis, World Scientific. (2004) link
- B. A. Berg, Fortran Code, World Scientific. (2004) https://www.worldscientific.com/page/5602-stmc
- T. T. Wu, "Theory of Toeplitz Determinants and the Spin Correlations of the Two-Dimensional Ising Model. I." Phys. Rev. D. **149** 1 (1966)
- H. Au-Yang and J. H. H. Perk, "Ising correlations at the critical temperature." Phys. Lett. 104A 3 (1984)
- J. Zhang et. al. "Quantum simulation of the universal features of the Polyakov loop." Phys. Rev. Lett. 121, 223201 (2018) arXiv:1803.11166
- H. Zou et. al. "Progress towards quantum simulating the classical O(2) model." Phys. Rev. A 90, 063603 (2014) arXiv:1403.5238

EXTRA SLIDES

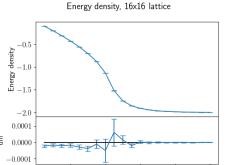
Ising τ_{int}



Asymptotic plateau gives the integrated autocorrelation time at β_c .

 Leon Hostetler (MSU)
 Clock Model
 July 6, 2020
 2 / 11

Energy density: Numerical results

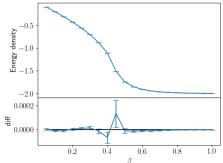


0.4

0.6

02

Energy density, 32x32 lattice



• 500K equilibrating HB sweeps followed by $10K \times 10K$ ($10K \times 4K$) sweeps for 16x16 (32x32) lattice. Error bars are calculated from "binned" data

1.0

- \bullet Integrated autocorrelation time is ~ 30 for 16x16 and ~ 110 for 32x32
- Bottom plots give difference from exact results

0.8

Leon Hostetler (MSU) Clock Model July 6, 2020 3 / 11

Ising Energy density: Statistics and error

For each simulation:

- **1** 10K HB sweeps are followed by $n \times m$ sweeps:
 - \bullet The data is separated into n histograms
 - **②** Each histogram contains data for *m* sweeps. The histogram is updated at each spin flip.
- ② The mean action is calculated for each histogram. Now we have a vector S containing n action means
- ullet From these action means, the final action mean \overline{S} is calculated and the error bar is calculated from the unbiased variance of the action means

$$\hat{S} = \overline{S} \pm \frac{\sigma}{\sqrt{n}}, \qquad \sigma^2 = \frac{1}{n-1} \sum_{i} \left(S_i - \overline{S} \right)^2$$

The energy is proportional to the action plus a shift

Summary: Error bars are calculated from binned data, but no jackknifing is performed.

Magnetization

• To match Ising convention, where the spins are $\{-1,1\}$ instead of $\{0,1\}$, we calculate the magnetization on the lattice as

$$M = \left| \langle \delta_{q_i,0} \rangle - \langle \delta_{q_i,1} \rangle \right|$$

instead of the usual $M = |\langle spin \rangle|$.

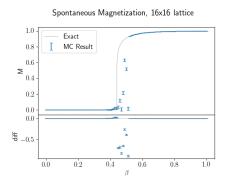
• Exact spontaneous magnetization (infinite volume) for 2d Ising model with isotropic interaction $J_h=J_\nu=1$ is

$$M(\beta) = \left[1 - \frac{1}{\sinh^4(2\beta)}\right]^{1/8}$$

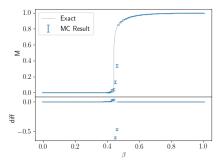
This formula was presented by Onsager (1948) and proved by Yang (1952).

◆ロト ◆昼 ト ◆ き ト ◆ き ト を り へ ○

Spontaneous Magnetization



Spontaneous Magnetization, 32x32 lattice



- 10K equilibrating HB sweeps followed by 1K histograms of 1K sweeps each
- Bottom plots give difference between MC results and exact results in infinite volume
- There is a finite size effect—critical point shifts left toward infinite volume result as lattice volume is increased

MC Validation at T_c

At $T = T_c$, we can calculate G(r) exactly for the 2d Ising model on a lattice via an inefficient procedure involving Toeplitz determinants. The first several values given in Au-Yang and Perk (1984) [5]:

$$G(0) = 1$$

$$G(1) = \frac{1}{\sqrt{2}}$$

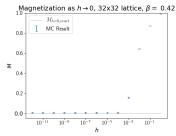
$$G(2) = 1 - \frac{4}{\pi^2}$$

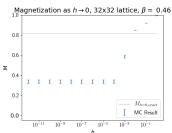
$$G(3) = 2\sqrt{2}\left(1 - \frac{8}{\pi^2}\right)$$

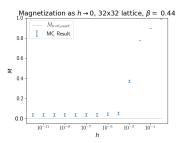
$$G(4) = 16\left(1 - \frac{112}{9\pi^2} + \frac{256}{9\pi^4}\right)$$

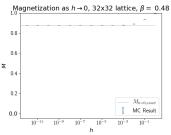
$$G(5) = 128\sqrt{2}\left(1 - \frac{88}{9\pi^2}\right)\left(1 - \frac{64}{9\pi^2}\right).$$

Magnetization as $h \rightarrow 0$

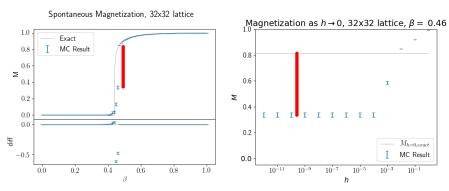






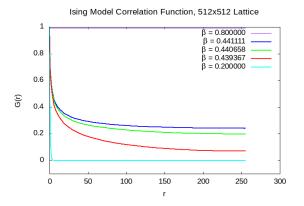


Magnetization



The discrepancy is due to a finite size shift of the critical point.

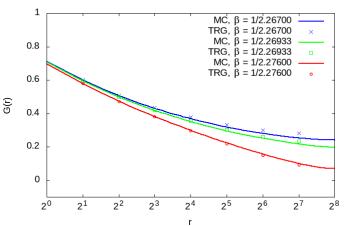
Results for 512x512 Lattice



- 500K equilibrating heatbath (HB) sweeps followed by 128 measurements each separated by 10K HB sweeps
- Measured at all integers $r \in [0, 512]$, plot shows up to r = 256
- No error bars yet.

Comparison with TRG Results

Ising Model Correlation Function, 512x512 Lattice



- Both MC and TRG results are from the same size lattice
- No error bars yet

11 / 11