Symmetry Breaking and Clock Model Interpolation in 2D Classical O(2) Spin Systems

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August 4, 2023

Outline

1. Motivation
2. Introduction
3. The Extended-O(2) Model
   - The $h_q \to \infty$ limit
   - Phase Diagram
4. Phase Diagram at Finite-h_q
5. Summary & Outlook

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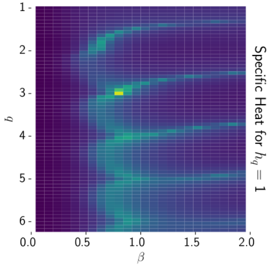
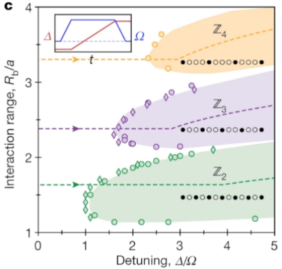
Motivation

1. Field digitization in quantum simulation
   1. Can approximate U(1) by $\mathbb{Z}_q$
   2. Need to optimize the approximation
   3. It is useful to have a continuous family of models that interpolate among the different q
2. Playground for tensor methods
3. Early results suggested a phase diagram similar to that found in Rydberg atom chains (Bernien et. al. Nature 551, 579-584 (2017), Keesling et. al. Nature 568, 207 (2019))





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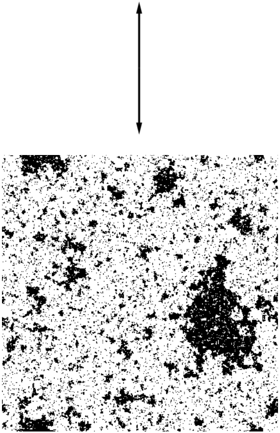
Introduction

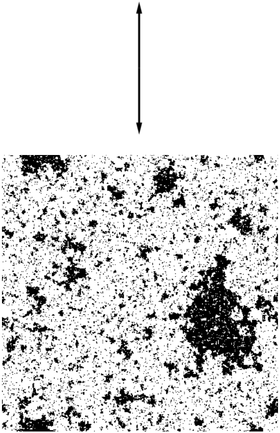
$$S = -J \sum_{x,\mu} \vec{S}_x \cdot \vec{S}_{x+\hat{\mu}} = -J \sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x)$$



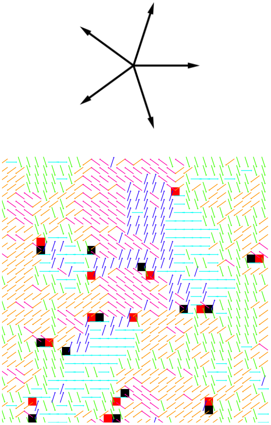
(a) Ising Model

Introduction

$$S = -J \sum_{x,\mu} \vec{S}_x \cdot \vec{S}_{x+\hat{\mu}} = -J \sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x)$$



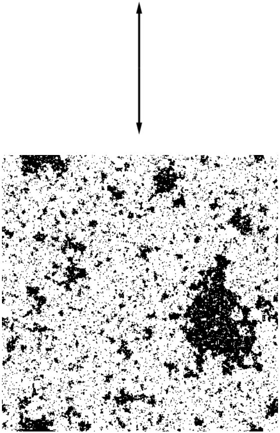
(a) Ising Model



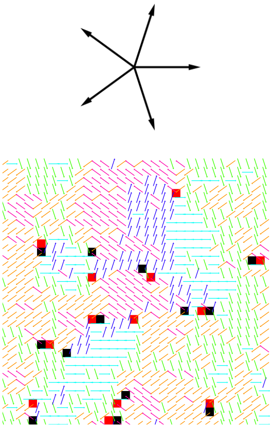
(b) Clock Models

Introduction

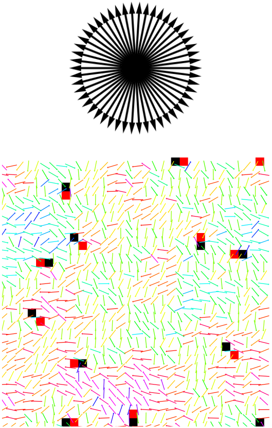
$$S = -J \sum_{x,\mu} \vec{S}_x \cdot \vec{S}_{x+\hat{\mu}} = -J \sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x)$$



(a) Ising Model



(b) Clock Models



(c) XY Model

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- The $h_q \to \infty$ limit
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4 Phase Diagram at Finite-h_q

5 Summary & Outlook

The Extended-O(2) Model

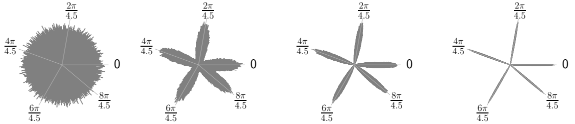
- We consider an extended-O(2) model in 2D with action

$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$

- When $h_q = 0$, this is the classic XY model, with a BKT transition
- When $h_q \to \infty$, the continuous angle φ is forced into the discrete values

$$\varphi_0 \le \varphi_{x,k} = \frac{2\pi k}{q} < \varphi_0 + 2\pi$$

  - For $q \in \mathbb{Z}$, this is the ordinary q-state clock model with $\mathbb{Z}_q$ symmetry
  - For $q \notin \mathbb{Z}$, this defines an interpolation of the clock model for noninteger q



(a) $h_q = 0$ (b) $h_q = 1$ (c) $h_q = 4$ (d) $h_q = 64$

The $h_q \to \infty$ limit[1]

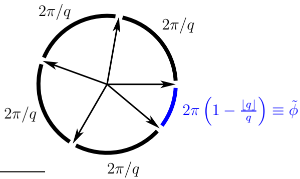
- In the limit $h_q \to \infty$, we can replace the action with

$$S_{\text{ext-}q} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x)$$

- We directly restrict the previously continuous angles to the discrete values

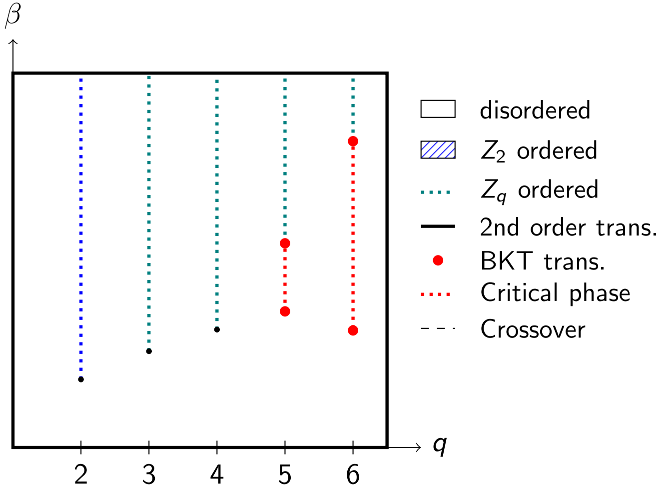
$$\varphi_0 \leq \varphi_{x,k} = \frac{2\pi k}{q} < \varphi_0 + 2\pi$$

- We choose $\varphi_0 = 0$, i.e. $\varphi \in [0, 2\pi)$, but we also investigate $\varphi_0 = -\pi$
- For $q \notin \mathbb{Z}$, divergence from ordinary clock model behavior is driven by the introduction of a "small angle":



[1] PRD 104 (5), 054505 and PoS(LATTICE2021)353

The $h_q \to \infty$ limit[2]



[2] PRD 104 (5), 054505 and PoS(LATTICE2021)353

TRG results at large volume[3]

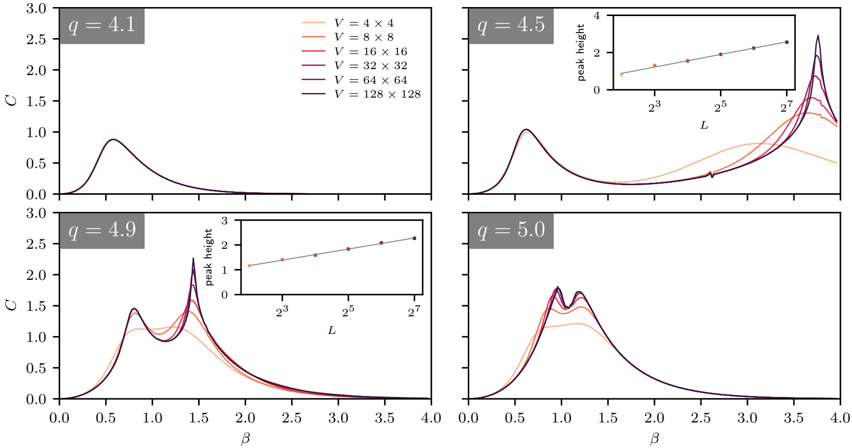
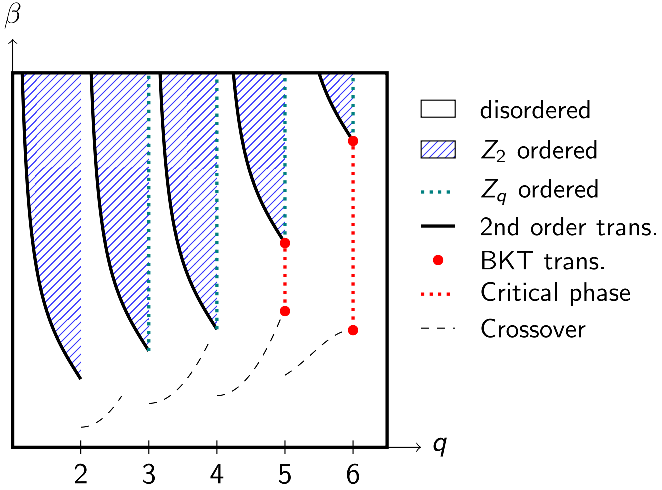


Figure: Specific heat results for the extended-q clock model from TRG obtained by Ryo for $q = 4.1$, 4.5, 4.9, and 5.0 at volumes from $2^2 \times 2^2$ up to $2^7 \times 2^7$.

[3] PRD 104 (5), 054505 and PoS(LATTICE2021)353

The $h_q \to \infty$ limit[4]



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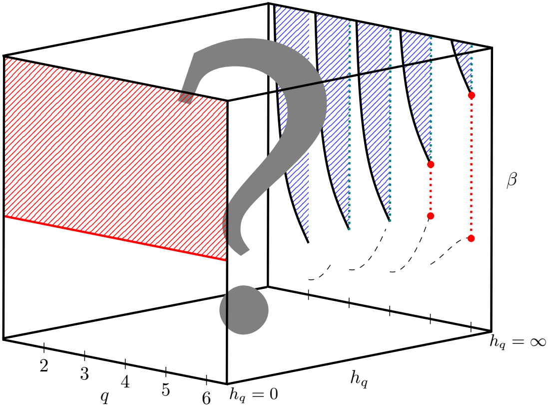
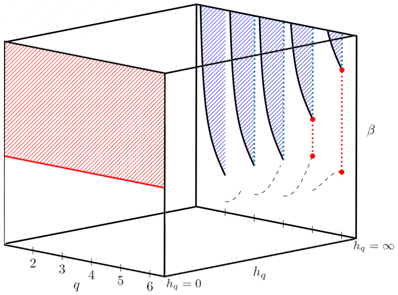
Phase Diagram

$$S = -\sum_{x,\mu} \cos\left(\varphi_{x+\hat{\mu}} - \varphi_x\right) - h_q \sum_x \cos(q\varphi_x)$$



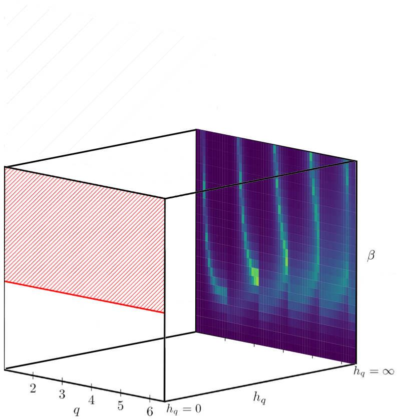
Phase Diagram at Finite-h_q

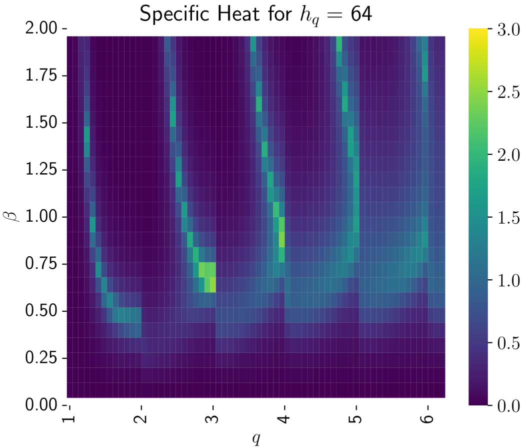
$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$



Specific Heat from TRG with $L = 1024$ and $h_q = 64$

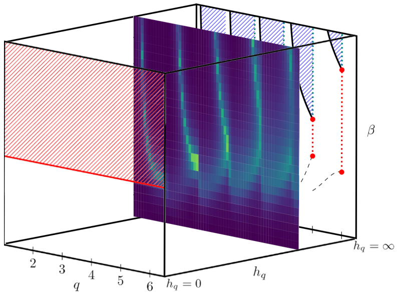
$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$

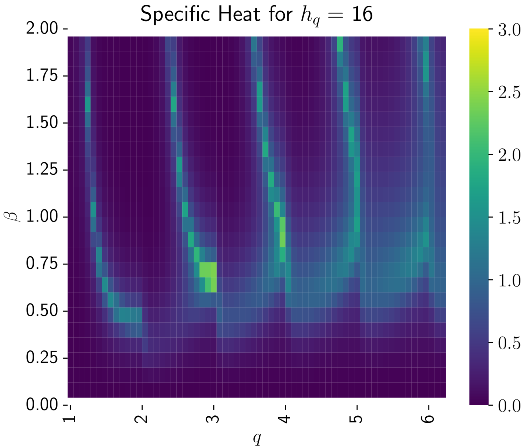




Specific Heat from TRG with $L = 1024$ and $h_q = 16$

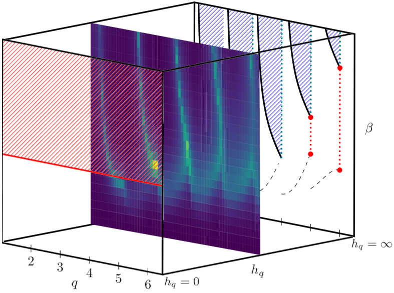
$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$

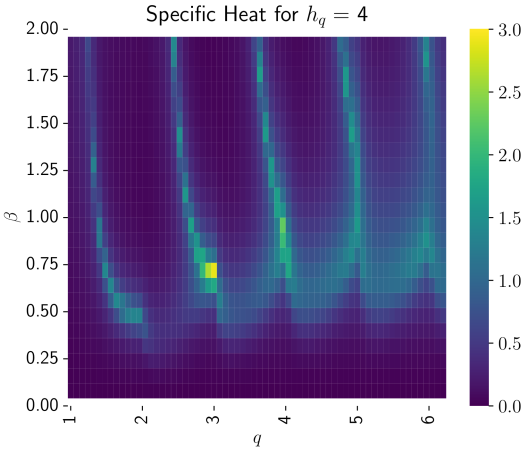




Specific Heat from TRG with $L = 1024$ and $h_q = 4$

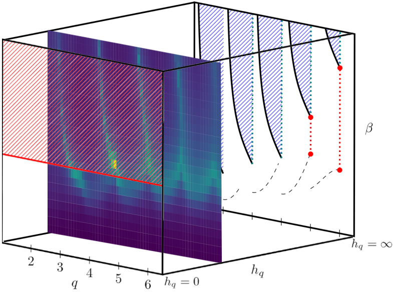
$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$

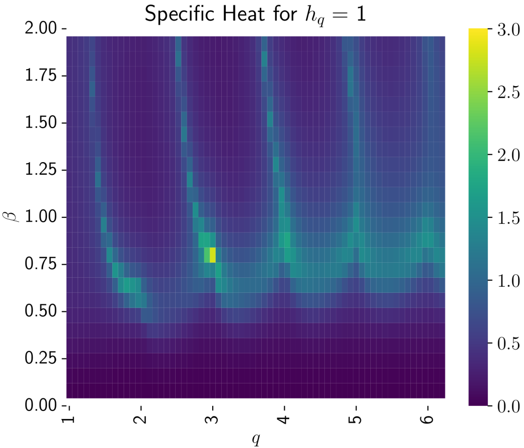




Specific Heat from TRG with $L = 1024$ and $h_q = 1$

$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$





Specific Heat from TRG with $L = 1024$ and $h_q = 1$

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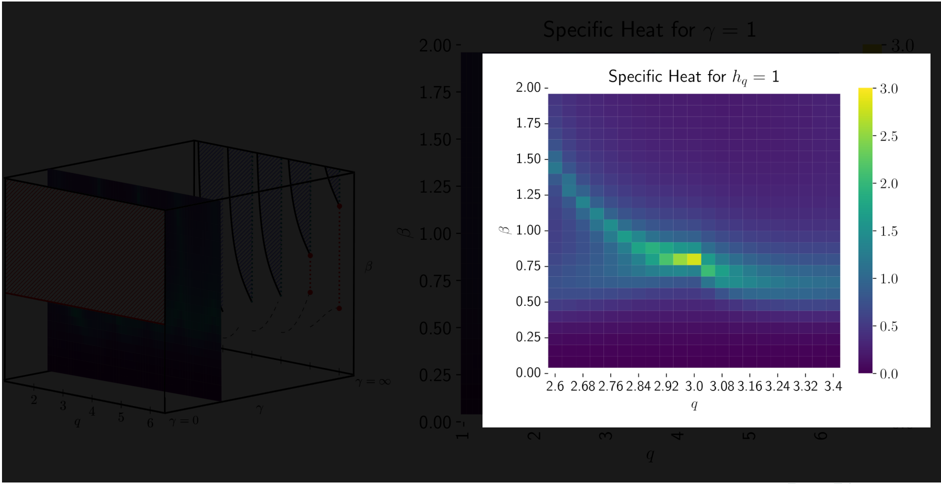
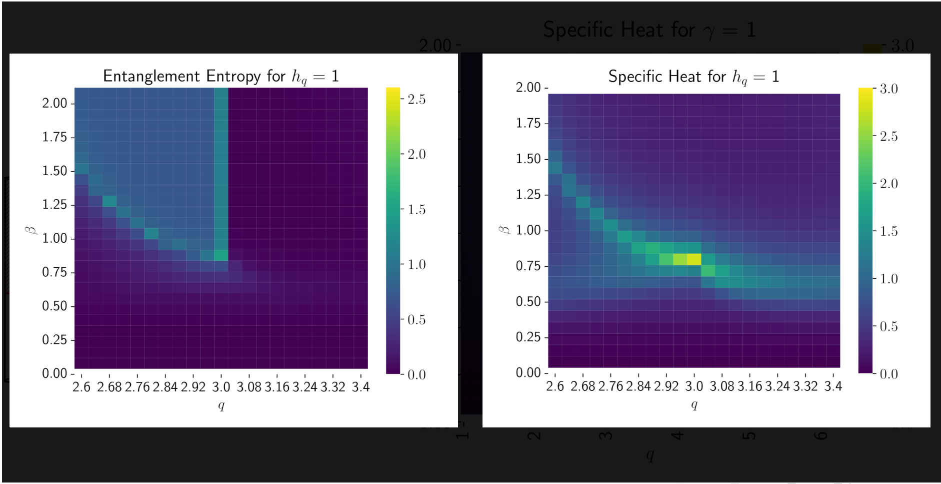


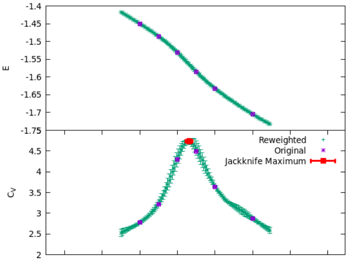
Specific Heat from TRG with $L = 1024$ and $h_q = 1$

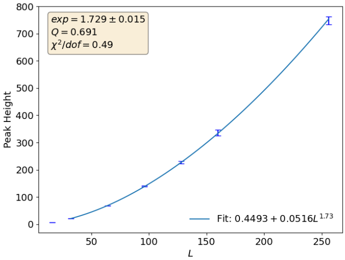
$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$



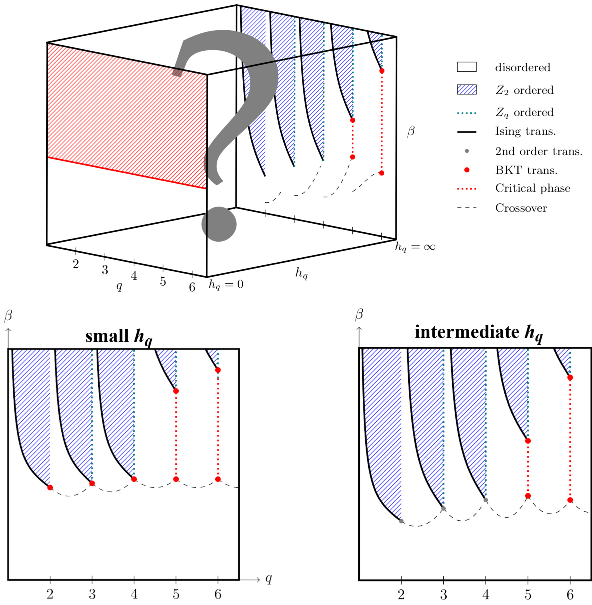
Finishing Up: Reweighting and Finite Size Scaling

$$\left.\frac{dU_M}{d\beta}\right|_{max} = U_0 + U_1 L^{1/\nu}$$
$$C_V|_{max} = C_0 + C_1 L^{\alpha/\nu}$$
$$\langle M\rangle|_{infl} = M_0 + M_1 L^{-\beta/\nu}$$
$$\chi_M|_{max} = \chi_0 + \chi_1 L^{\gamma/\nu}$$
$$F(\vec{q})|_{max} = F_0 + F_1 L^{2-\eta}.$$





Phase Diagram



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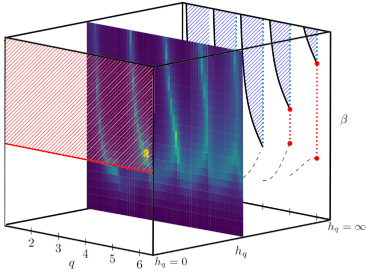
Summary & Outlook

1. We looked at an extended O(2) model with parameters β, h_q, and q

$$S = -\sum_{x,\mu} \cos\left(\varphi_{x+\hat{\mu}} - \varphi_x\right)$$



2. Rich phase diagram with crossovers, second-order phase transitions of various universality classes and BKT transitions

Thank you!

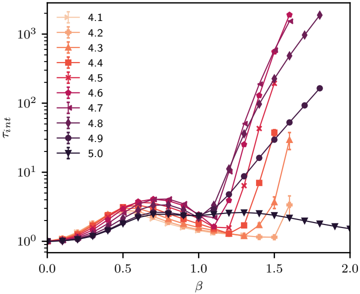
Additional Slides:

Previous Work on the Extended-$O(2)$ Model

- José, Kadanoff, Kirkpatrick, and Nelson, Phys. Rev. B 16, 1217 (1977).
- Landau, Journal of Magnetism and Magnetic Materials 31-34, 1115 (1983)
- Hu and Ying, Physica A: Statistical Mechanics and its Applications 140, 585 (1987)
- Bramwell, Holdsworth, and Rothman, Modern Physics Letters B 11, 139 (1997)
- Calabrese and Celi, Phys. Rev. B 66, 184410 (2002)
- Rastelli, Regina, and Tassi, Phys. Rev. B 69, 174407 (2004)
- Rastelli, Regina, and Tassi, Phys. Rev. B 70, 174447 (2004)
- Taroni, Bramwell, and Holdsworth, Journal of Physics: Condensed Matter 20, 275233 (2008)
- Nguyen and Ngo, Advances in Natural Sciences: Nanoscience and Nanotechnology 8, 015013 (2017)
- Chlebicki and Jakubczyk, Phys. Rev. E 100, 052106 (2019)
- Butt, Jin, Osborn, and Saleem, (2022), arXiv:2205.03548

TRG for Extended-q-state Clock Model

- In the Monte Carlo approach, we use a Markov chain importance-sampling algorithm to generate equilibrium configurations
  - Monte Carlo has difficulty sampling this model appropriately at $\beta > 1$ for $q \notin \mathbb{Z}$
  - Integrated autocorrelation time explodes, and we have to perform billions of heatbath sweeps already on a 4×4 lattice
  - Studying this model on larger lattices with Monte Carlo is challenging



- Tensor renormalization group (TRG) approach can be used instead
  - We validate TRG against Monte Carlo in the regime accessible to Monte Carlo
  - Then we use TRG to explore lattice sizes and β-values beyond the reach of Monte Carlo

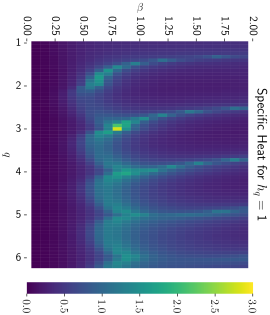
Algorithm Developments Needed for Extended-$O(2)$ Model

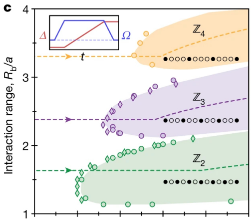
- In the $h_q \to \infty$ limit, the DOF could be treated as discrete
  - Which means we could use an MCMC *heatbath* algorithm
  - We could use a TRG method for large volumes
- The model is more difficult to study at finite h_q
- For finite h_q, the DOF are continuous
  - MCMC heatbath is not an option, so we're left with the Metropolis, which suffers from low acceptance rates and leads to large autocorrelations in this model
  - Furthermore, our TRG method was only designed for the $h_q \to \infty$ limit
- We needed to make some algorithmic developments
  - We implemented a *biased Metropolis heatbath algorithm*[5] (BMHA) which is designed to approach heatbath acceptance rates
  - To explore large volumes, Ryo Sakai implemented a Gaussian quadrature method

[5] A. Bazavov and B. A. Berg, PRD 71, 114506 (2005)

Connections to Quantum Simulation

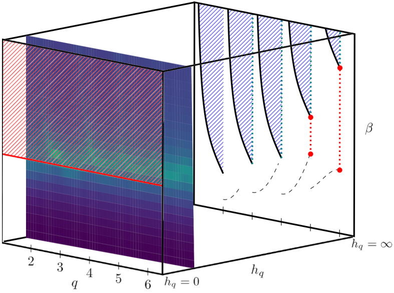
1. Field digitization in quantum simulation
    1. Can approximate U(1) by $\mathbb{Z}_q$
    2. Need to optimize the approximation
    3. It is useful to have a continuous family of models that interpolate among the different q
2. The extended-O(2) model shows interesting behavior already on very small lattices making it a good test case for analog simulation
3. Quantum simulation of similar models with a continuously tunable parameter have been done with Rydberg atoms (Bernien et. al. Nature 551, 579-584 (2017), Keesling et. al. Nature 568, 207 (2019))
    - The resulting phase diagram (right) shows similarities to the phase diagram of the extended-O(2) model at finite h_q.

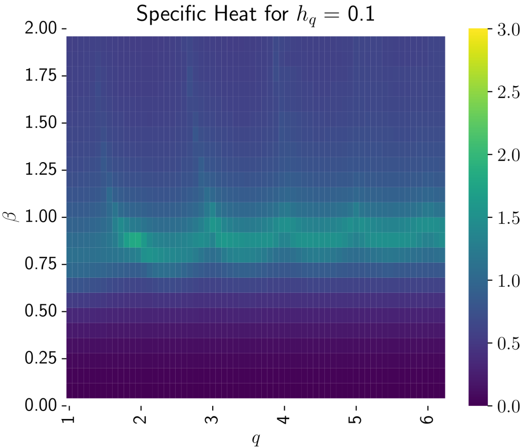




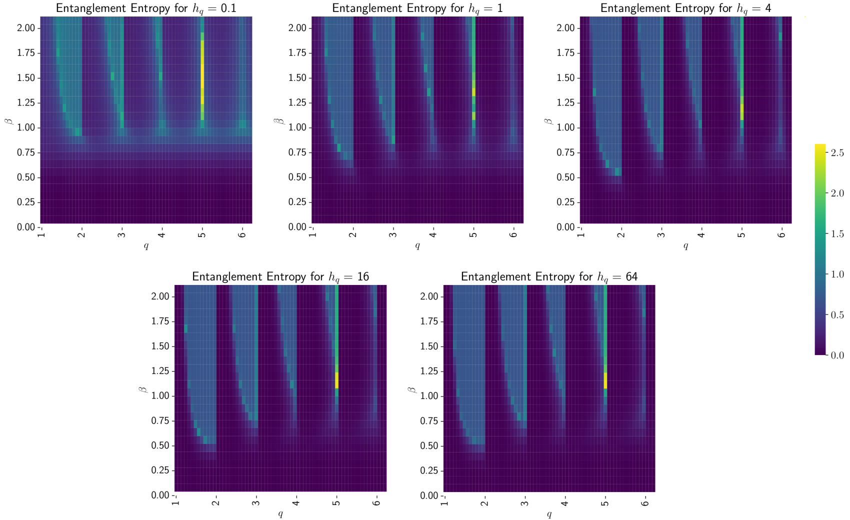
Specific Heat from TRG with $L = 1024$ and $h_q = 0.1$

$$S_{\text{ext-}O(2)} = -\sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - h_q \sum_x \cos(q\varphi_x)$$

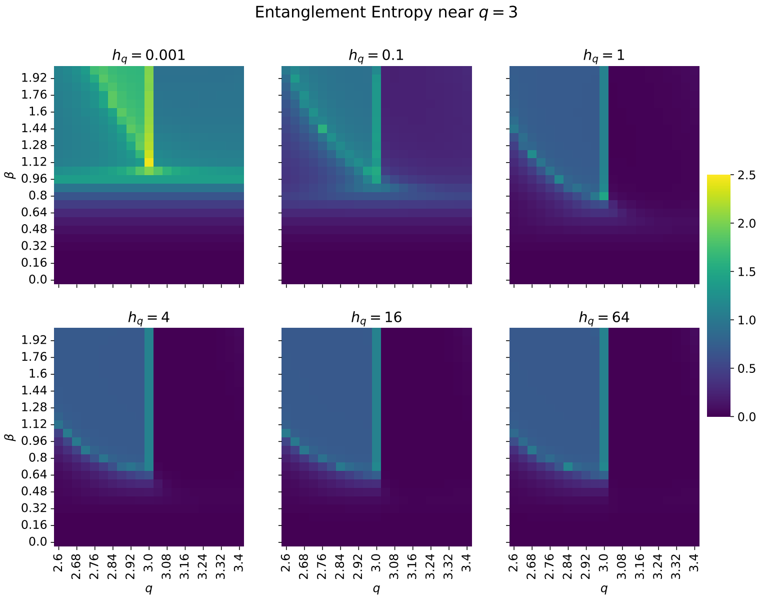




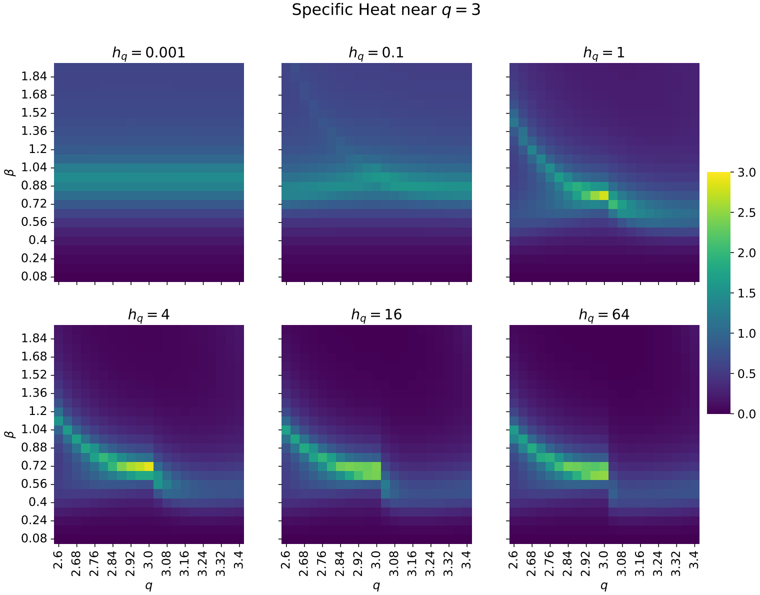
Entanglement Entropy from TRG with $L = 1024$



Entanglement Entropy from TRG with $L = 1024$

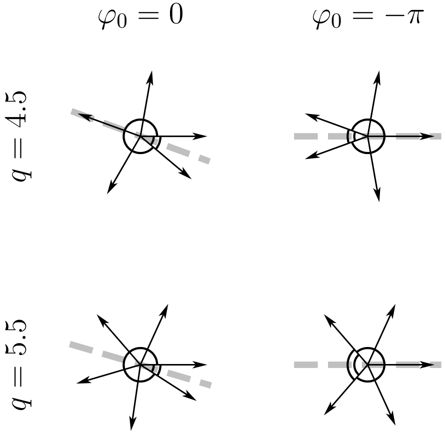


Specific Heat from TRG with $L = 1024$

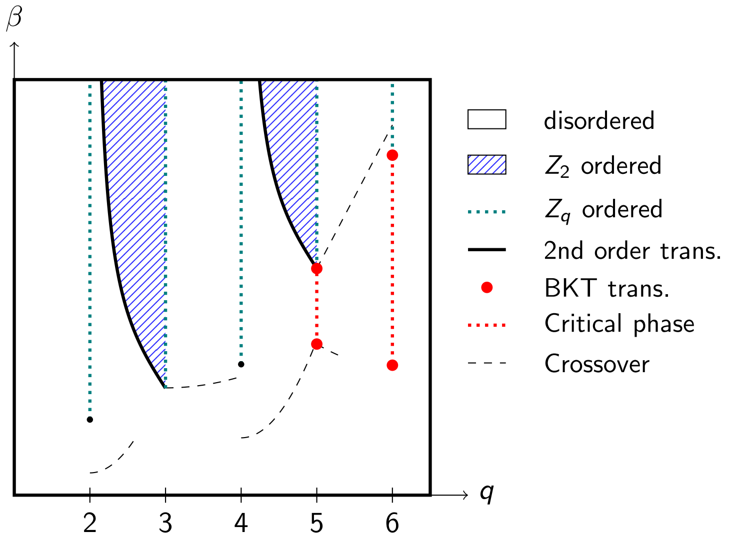


Choice of φ_0

- Choice of φ_0 can change the DOF in the model
- We choose $\varphi_0 = 0$, i.e. $\varphi \in [0, 2\pi)$, but we also investigate $\varphi_0 = -\pi$



Phase diagram for $h_q = \infty$ and $\varphi_0 = -\pi$



Placement of β

- One can define the model as

$$S = -\beta \sum_{x,\mu} \cos\left(\varphi_{x+\hat{\mu}} - \varphi_x\right) - h_q \sum_x \cos(q\varphi_x)$$

  where β is multiplying the first term like a field-theoretic coupling. Then the Boltzmann factor is e^{-S}
- Alternatively, one can factor β out front and define the model as

$$S = -\sum_{x,\mu} \cos\left(\varphi_{x+\hat{\mu}} - \varphi_x\right) - h'_q \sum_x \cos(q\varphi_x)$$

  with Boltzmann factor $e^{-\beta S}$, where β is the inverse temperature
- The two definitions are related by $h'_q = h_q/\beta$
- We have used both definitions, however, the Monte Carlo results shown in these slides are from the definition with β factored out front

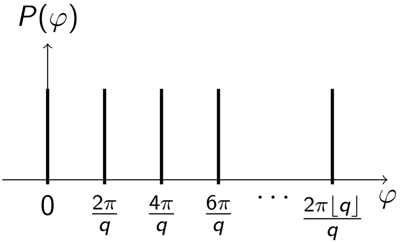
The Need to Shift the Angles: A Subtlety

- In the ordinary clock model, we have the energy function

$$S = -\sum_{\langle x,y \rangle} \cos(\varphi_x - \varphi_y)$$

- The angles $\varphi_x^{(k)}$ are selected discretely as $\varphi_0 \leq \varphi_x^{(k)} = \frac{2\pi k}{q} < \varphi_0 + 2\pi$
- When $\beta = 0$ and with $\varphi_0 = 0$, the spins are selected uniformly from a "Dirac comb"

$$P^{clock}_{q,\varphi_0=0}(\varphi) \sim \sum_{k=0}^{\lfloor q \rfloor} \delta\left(\varphi - \frac{2\pi k}{q}\right)$$



The Need to Shift the Angles: A Subtlety

- In the Extended-O(2) model, we have the energy function

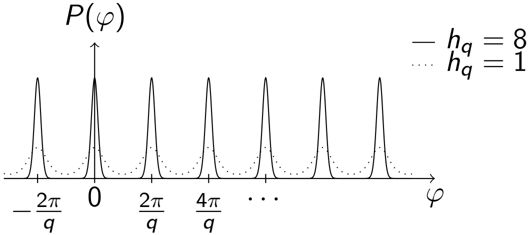
$$S = -\sum_{\langle x,y \rangle} \cos(\varphi_x - \varphi_y) - h_q \sum_x \cos(q\varphi_x)$$

- The angles φ_x are now selected continuously in

$$\varphi_0 \leq \varphi \in \mathbb{R} < \varphi_0 + 2\pi$$

- When $\beta = 0$ and with $\varphi_0 = 0$, the spins are selected from a distribution

$$P^{extO2}_{q,\varphi_0}(\varphi) \sim e^{h_q \cos(q\varphi)}$$



The Need to Shift the Angles: A Subtlety

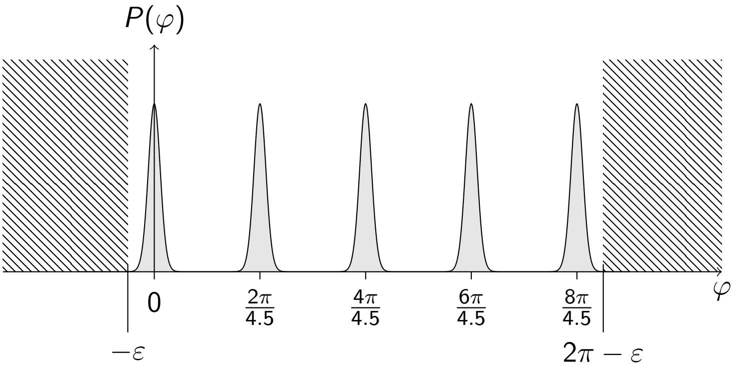


Figure: To recover the Dirac comb of the clock model distribution in the $h_q \to \infty$ limit, the angle domain must be shifted by some ε so that the histogram includes all relevant peaks.

The Need to Shift the Angles: A Subtlety

- To match the clock model in the $h_q \to \infty$ limit, it should be sufficient to choose ε such that

$$P^{extO2}_{q,\varphi_0}(\varphi) \xrightarrow[h_q \to \infty]{} P^{clock}_{q,\varphi_0}(\varphi)$$

  where for the clock model, angles are selected from $[\varphi_0, \varphi_0 + 2\pi)$, but for the Extended-O(2) model, they are selected from $[\varphi_0 - \varepsilon, \varphi_0 - \varepsilon + 2\pi)$
- In our case, we use $\varphi_0 = 0$, and choose

$$\varepsilon = \pi \left(1 - \frac{\lfloor q \rfloor}{q}\right)$$

  so that the $\lceil q \rceil$ peaks of the distribution $P^{extO2}_{q,\varphi_0}(\varphi)$ are centered in the domain $[-\varepsilon, 2\pi - \varepsilon)$