Symmetry Breaking in an Extended-O(2) Model

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QuLAT Collaboration

Outline

Outline

Motivation

- Ultimately, we want to do quantum simulation of lattice QCD
- First, we must be able to do this with simpler Abelian models
- Given the limited number of qubits available, it is important to optimize the discretization procedure
- One can make a $\mathbb{Z}_q$ approximation of a continuous $U(1)$ symmetry
- To optimize such a $\mathbb{Z}_q$ approximation, it is useful to build a continuous family of models that interpolate among the various possibilities
- This brings us to our extended-$O(2)$ model

Outline

The Extended-O(2) Model

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

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

- When $\gamma = 0$, this is the classic XY model, with a BKT transition
- When $\gamma > 0$, the second term breaks periodicity and we must choose $\varphi \in [\varphi_0, \varphi_0 + 2\pi)$ for some choice φ_0
- When $\gamma \to \infty$, the continuous angle φ is forced into the discrete values

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

  - 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
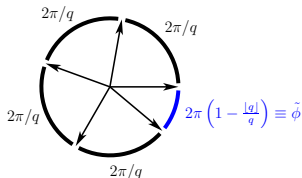
Previous Work: The $\gamma \to \infty$ limit

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

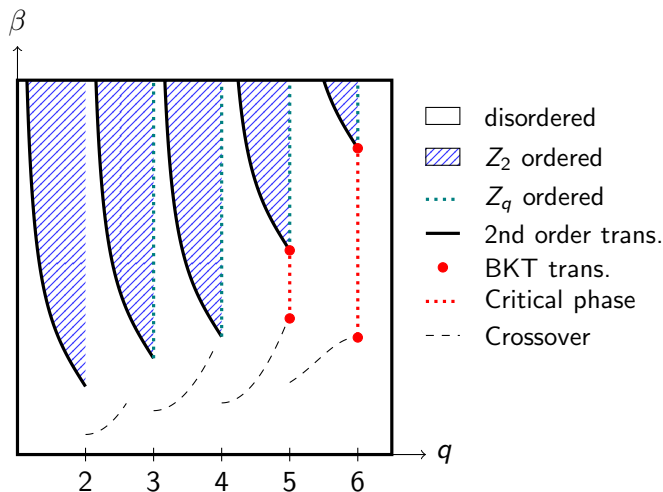$$S_{\text{ext-}q} = -\beta \sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x)$$

- 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":

Previous Work: The $\gamma \to \infty$ limit[1]

- ☐ disordered
- ▨ Z_2 ordered
- ⋯ Z_q ordered
- — 2nd order trans.
- ● BKT trans.
- ⋯ Critical phase
- – – Crossover

[1]PRD 104 (5), 054505

Previous Work: The $\gamma \to 0$ limit for $q \in \mathbb{Z}$

- Previous work on this model by others includes work by Jose, Kadanoff, Kirkpatrick, and Nelson in 1977 (PRB 16 3)
  - They considered the same model but with integer q and $\gamma \to 0$ as a symmetry-breaking perturbation to the O(2) model
  - They study it using two schemes—Migdal approximation and a generalized Villain model and spin-wave expansion
  - Key finding is that any $\gamma > 0$ perturbation will force the system away from O(2) behavior if β is sufficiently large
- Previous work on this model by others includes work by N. Butt, X.-Y. Jin, J. C. Osborn, and Z. H. Saleem in 2022 (arXiv:2205.03548)
  - They considered the same model also with integer q and $\gamma \to 0$ as a symmetry-breaking perturbation to the O(2) model
  - They study it using a tensor formulation
  - A key finding is that even a small perturbation results in an additional phase transition which has a non-zero critical temperature even in the limit $\gamma \to 0$

Phase Diagram

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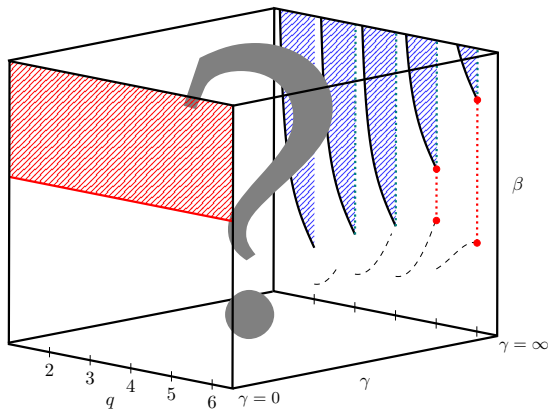
Algorithm Developments

- In the $\gamma \to \infty$ limit, the DOF can 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 γ
- For finite γ, 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 $\gamma \to \infty$ limit
- We needed to make some algorithmic developments
  - We implemented a *biased Metropolis heatbath algorithm*[2] (BMHA) which is designed to approach heatbath acceptance rates
  - To explore large volumes, we implemented a Gaussian quadrature method (see presentation by Ryo Sakai on this)

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

Outline

1. Motivation

2. The Extended-O(2) Model
   - Previous Work
   - Phase Diagram

3. **Monte Carlo Exploration**
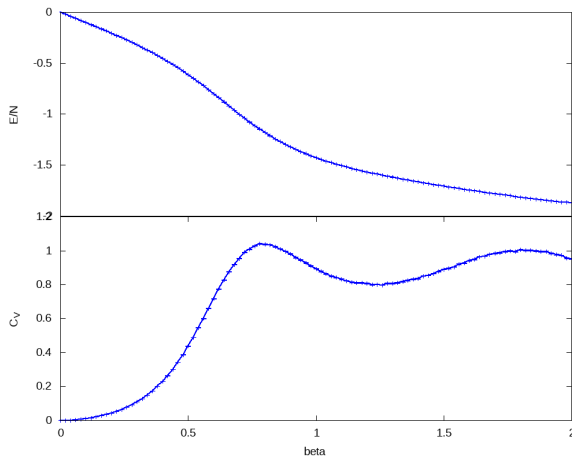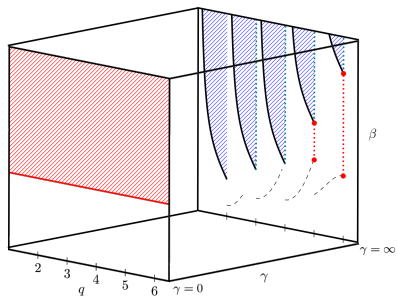
4. Summary & Outlook

Monte Carlo Exploration

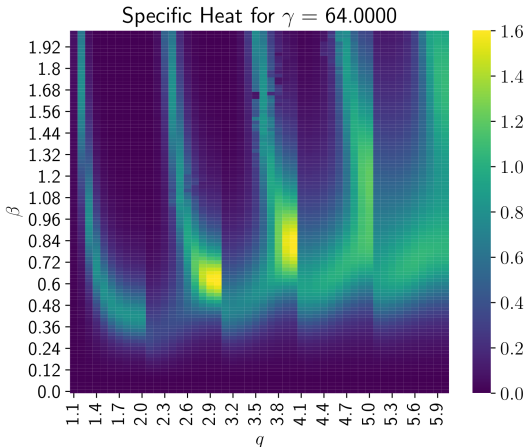Figure: Example on 4×4 lattice with $q = 5.9$, $\gamma = 4$, and $\beta \in [0, 2]$.
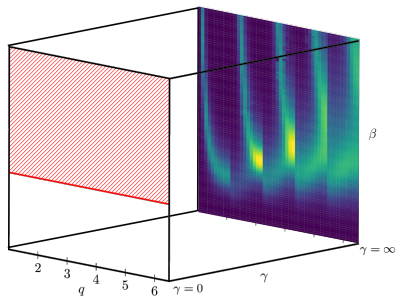
Monte Carlo Exploration

$$S_{\text{ext-}O(2)} = -\beta \sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - \gamma \sum_x \cos(q\varphi_x)$$
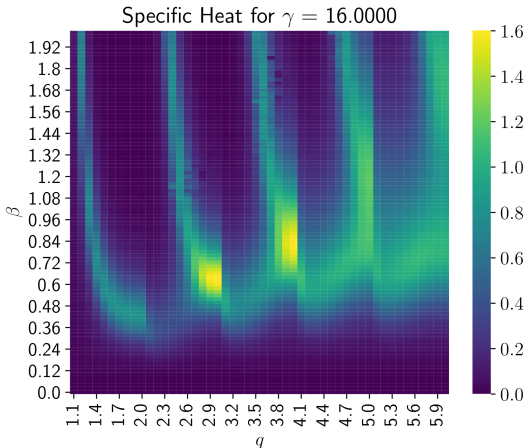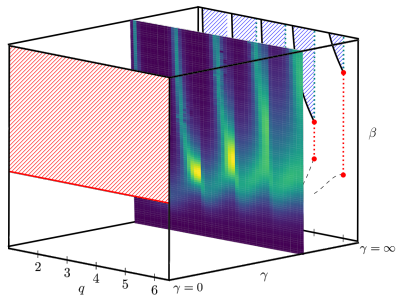
Monte Carlo Exploration: $\gamma = 64$

$$S_{\text{ext-}O(2)} = -\beta \sum_{x,\mu} \cos(\varphi_{x+\hat{\mu}} - \varphi_x) - \gamma \sum_x \cos(q\varphi_x)$$
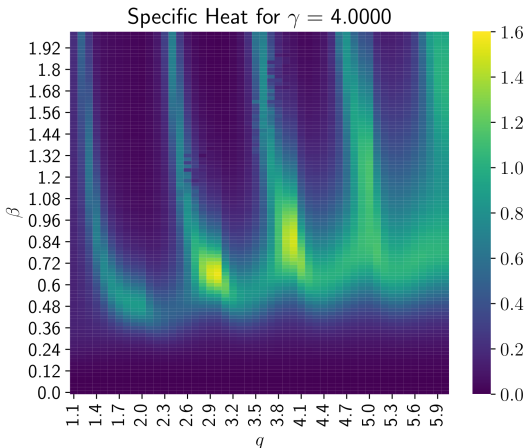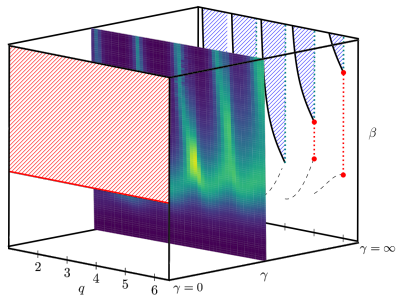
Monte Carlo Exploration: $\gamma = 16$

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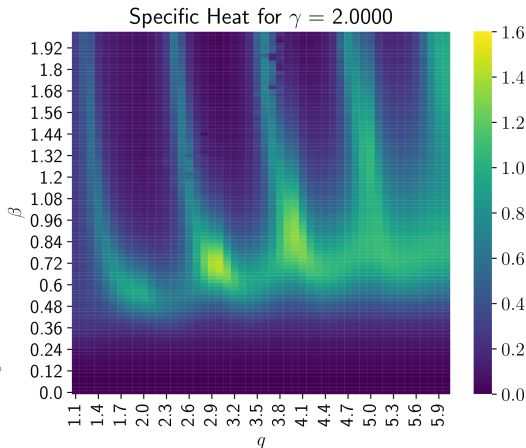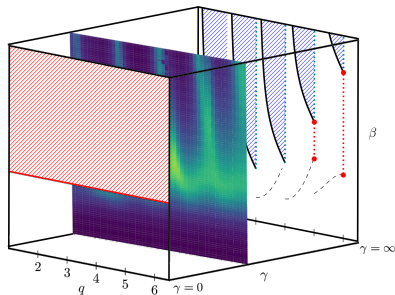

Specific Heat for $\gamma = 16.0000$

Monte Carlo Exploration: $\gamma = 4$

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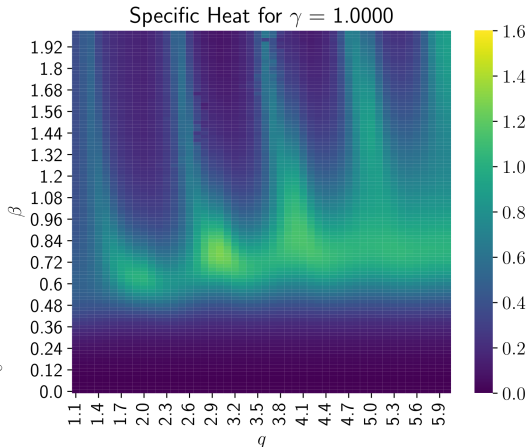

Specific Heat for $\gamma = 4.0000$

Monte Carlo Exploration: $\gamma = 2$

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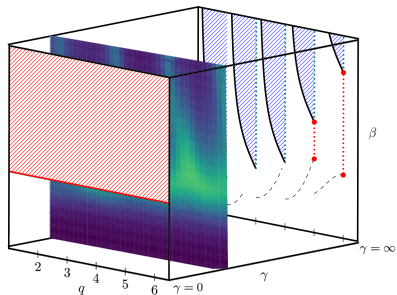

Specific Heat for $\gamma = 2.0000$

Monte Carlo Exploration: $\gamma = 1$

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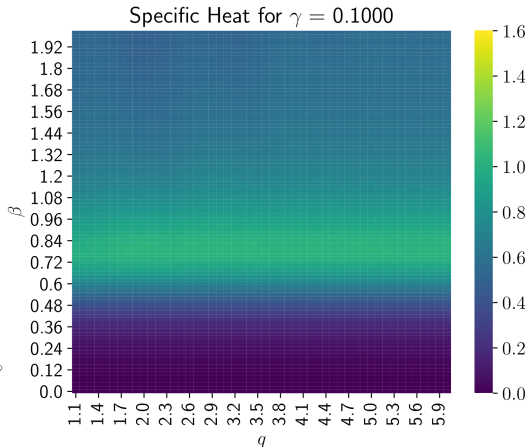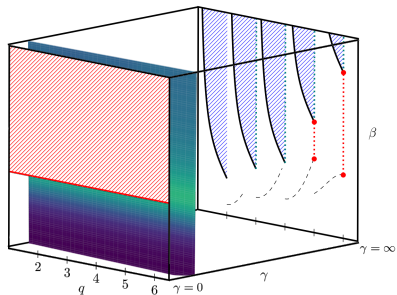

Specific Heat for $\gamma = 1.0000$

Monte Carlo Exploration: $\gamma = 0.1$

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

Specific Heat for $\gamma = 0.1000$

Outline

1. **Motivation**

2. **The Extended-O(2) Model**
   - **Previous Work**
   - **Phase Diagram**

3. **Monte Carlo Exploration**

4. **Summary & Outlook**

Summary & Outlook

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

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

2. Previously, we established the $\gamma = \infty$ slice of the 3D phase diagram
   - When $q \in \mathbb{Z}$, we recover the classic q-state clock model which has a single second-order phase transition for $q = 2, 3, 4$ and two BKT transitions for $q \geq 5$
   - When $q \notin \mathbb{Z}$, we get a crossover and a second-order phase transition

3. We are currently exploring the finite γ region of the phase diagram
   - Finite size scaling
   - Ryo Sakai is studying the model on large lattices using tensor methods

4. This model may be a good candidate for analog quantum simulation as a small step toward the ultimate goal of simulating QCD on a quantum computer

5. Perhaps on Rydberg arrays. See (Keesling et. al. Nature **568**, 207 (2019))

Thank you!

Additional Slides:

Angle Histograms

In the Extended-O(2) model, each spin variable can be represented by an angle $\varphi \in [0, 2\pi)$. Histograms of this angle over many configurations and over all sites in a configuration can help to illustrate what is happening when q and γ are varied.
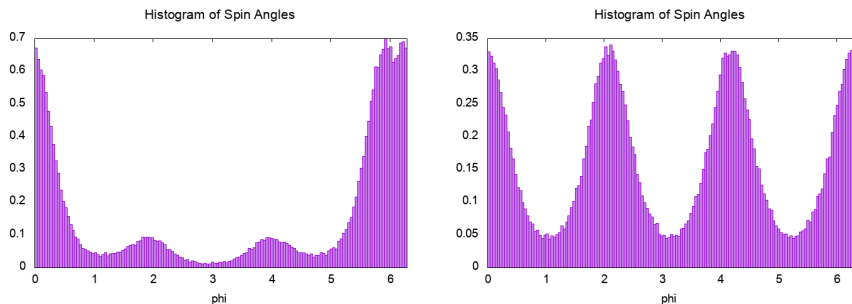

Figure: (LEFT) An example angles histogram for the case $q = 3.2$, $\gamma = 1.0$, and $\beta = 0.8$. (RIGHT) An example angles histogram for the case $q = 3.0$, $\gamma = 1.0$, and $\beta = 0.8$.
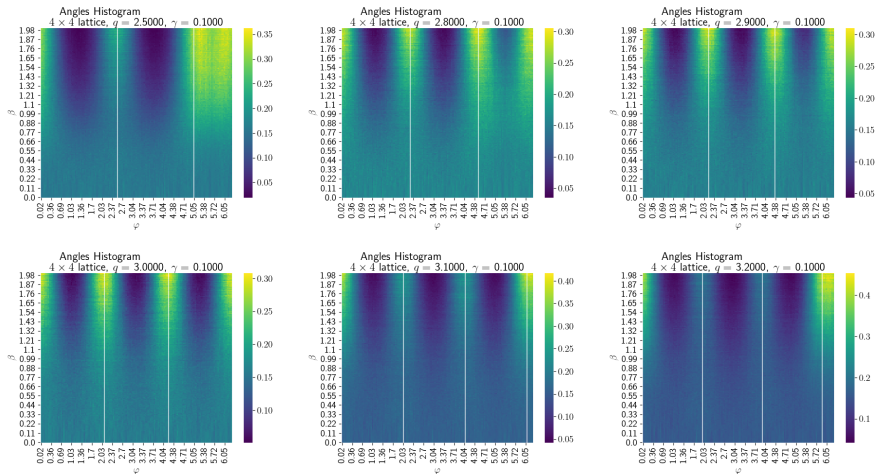
Angle Histograms at $\gamma = 0.1$

Figure: Heatmaps of the angle histograms for several q. Brighter colors correspond to higher peaks in the angle histogram. The vertical white lines were added to indicate the preferred angles (i.e. $2\pi k/q$ for $k = 0, 1, \ldots, \lfloor q \rfloor$) for that value of q.

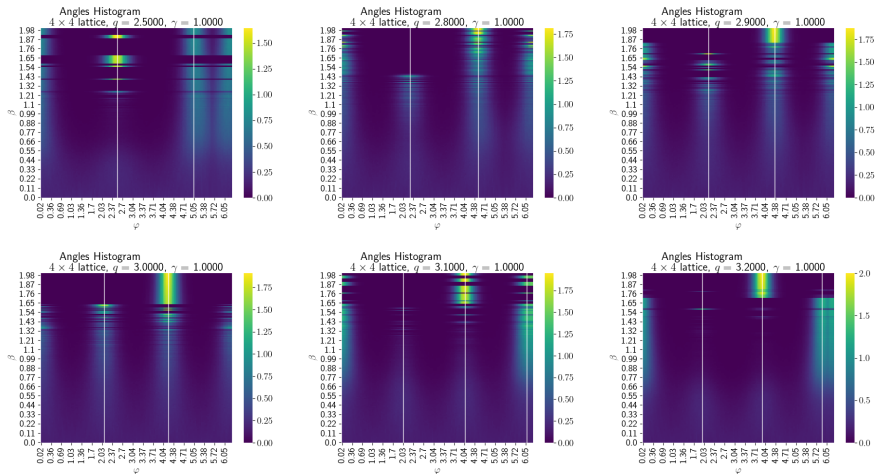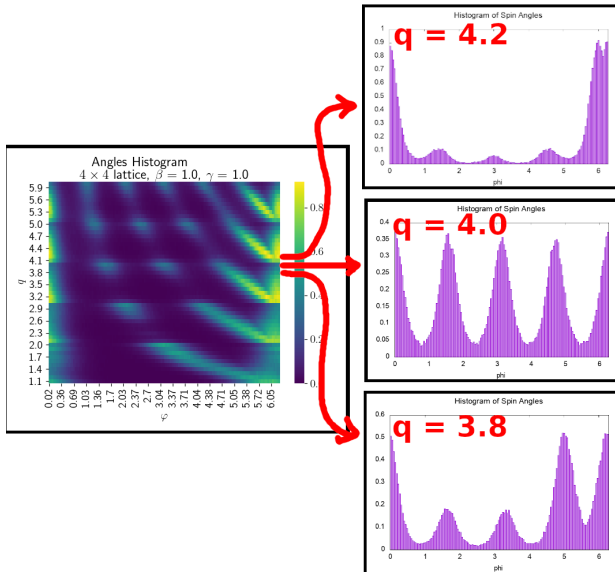# Angle Histograms at $\gamma = 1$

Figure: Heatmaps of the angle histograms for several q with $\gamma = 1$ and $\beta \in [0, 2]$. At large β, artifacts develop due to freezing/insufficient statistics, thus, one should ignore the upper parts i.e. $\beta \gtrsim 1.2$ of these heatmaps.
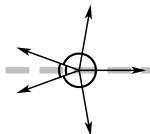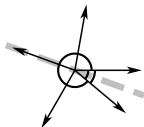
Angle Histograms along a line of Constant β

Choice of φ_0

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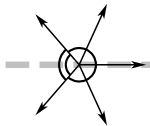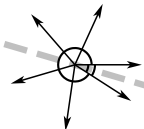- We choose $\varphi_0 = 0$, i.e. $\varphi \in [0, 2\pi)$, but we also investigate $\varphi_0 = -\pi$

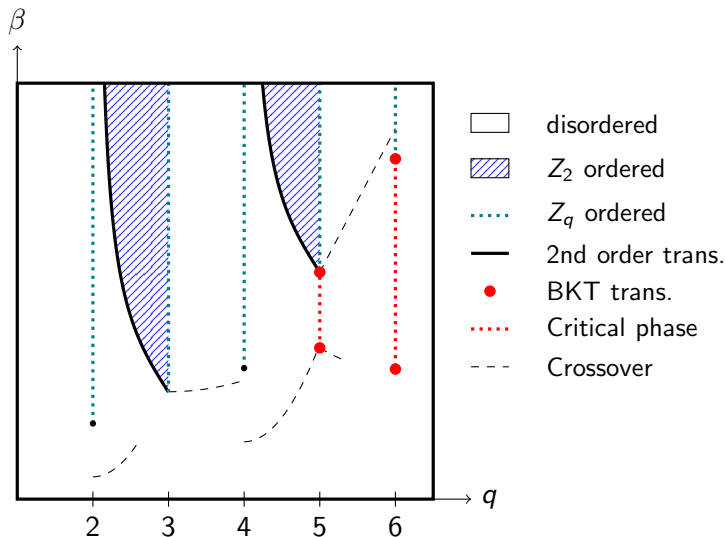$$\varphi_0 = 0 \qquad\qquad \varphi_0 = -\pi$$

$q = 4.5$

$q = 5.5$

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

Placement of β

- One can define the model as

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

  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

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

  with Boltzmann factor $e^{-\beta S}$, where β is the inverse temperature

- The two definitions are related by $\gamma' = \gamma/\beta$
- We have used both definitions, however, the Monte Carlo results shown in these slides are from the definition with β factored out front
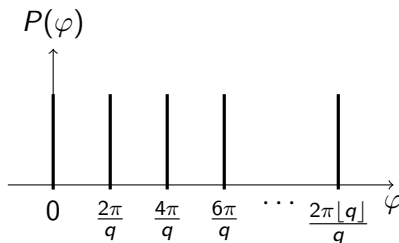
The Need to Shift the Angles: A Subtlety

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

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

- 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"

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

The Need to Shift the Angles: A Subtlety

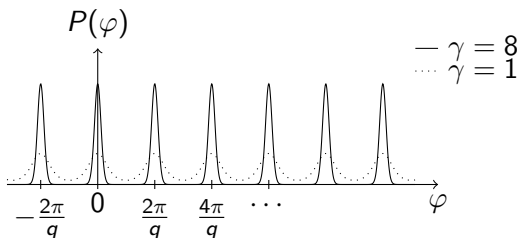- In the Extended-O(2) model, we have the energy function

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

- 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

$$P_{q,\varphi_0}^{extO2}(\varphi) \sim e^{\gamma \cos(q\varphi)}$$
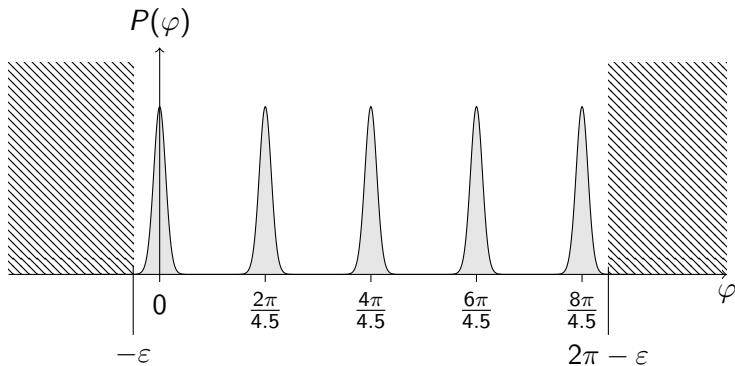
The Need to Shift the Angles: A Subtlety

Figure: To recover the Dirac comb of the clock model distribution in the $\gamma \to \infty$ 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 $\gamma \to \infty$ limit, it should be sufficient to choose ε such that

$$P_{q,\varphi_0}^{extO2}(\varphi) \xrightarrow[\gamma \to \infty]{} P_{q,\varphi_0}^{clock}(\varphi)$$

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 $P_{q,\varphi_0}^{extO2}(\varphi)$ are centered in the domain $[-\varepsilon, 2\pi - \varepsilon)$