

Moving from continuous to discrete symmetry in the 2D XY model

James C. Osborn ANL **Collaborators** Nouman Butt (UIUC) Xiao-Yong Jin (ANL) Zain Saleem (ANL) Based on arXiv:2205.03548

INT workshop Tensor Networks in Many Body and Quantum Field Theory April 2023

Outline

- Examine effects of discretization and perturbations phase structure of 2d classical XY model
- Compare discretizations of XY model using HOTRG
 - Angular discretization (Z_N clock model)
 - U(1) character expansion
- Structure of TN formulations
 - Role of core and interaction tensors
- Perturbed XY model
 - Interpolates between XY and Z_N models
 - Study effect of small perturbation on phase structure
 - How large is the effect of small perturbation?



XY model discretizations

2d XY model

$$H = -\sum_{\langle xy \rangle} \cos(\theta_x - \theta_y) - h \sum_x \cos(\theta_x)$$

- Angular discretization (N states) $\rightarrow Z_N$ clock model

$$\theta_x \in \left\{ \frac{2\pi k}{N}; k = 0 \dots N - 1 \right\}$$

U(1) character expansion discretization (D = 2S+1 states)

$$e^{\beta \cos(\theta_x - \theta_y)} \approx \sum_{k=-S}^{S} I_k(\beta) e^{ik(\theta_x - \theta_y)}$$



Tensor network simulations

HOTRG method

(Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, T. Xiang 2012)

- D (N for Z_N model) = initial number of states
- D_{cut} = maximum states (after SVD)
- Observables
 - Specific heat

$$C_V = -T\partial_T^2 F$$

$$F = -\left(\ln Z\right) / (\beta V)$$

- Second derivative from 7-point polynomial fit
- Magnetization using impurity tensor method

$$\langle m \rangle = \frac{1}{V} \langle \sum_{x} \cos(\theta_{x}) \rangle$$



Specific heat of discretized XY model D_{cut} = 40



U(1) character expansion

- Peak converges well for $D \ge 5$
- Low temperature converges well for D ≥ 15
- Specific heat peak doesn't match phase transition (T_c), but similar



 Z_N clock discretization

- One peak for $N \le 4$
- Two peaks for $N \ge 5$
- Upper peak converges well for $N \ge 7$
- Larger difference from XY at low T for same number of states (D=N) Argonne

Magnetization of discretized XY model $D_{cut} = 40$ h = 10⁻⁴



Ordered phase appears in Z_N model, but not XY



Finding phase transitions

- Specific heat, magnetic susceptibility not reliable indicators of lower phase transition in Z_N (N≥5) model
- Cross derivative (Y. Chen, K. Ji, Z. Y. Xie, J. F. Yu 2020)

$$\frac{\partial^2 F}{\partial h \partial T} = -\frac{\partial \langle m \rangle}{\partial T}$$

- Seems to be good indicator of phase transitions
- Obtained from fit of magnetization to polynomial in T



Cross derivative of discretized XY model D_{cut} = 40 h = 10⁻⁴



• Gives clear peaks at phase transitions



Tensor network components Spin models

Typically start with interaction and local terms

$$H = \sum_{\langle xy \rangle} H_I(\theta_x, \theta_y) + \sum_x H_L(\theta_x)$$

Expand interaction in some basis

$$e^{-\beta H_I(\theta_x,\theta_y)} \approx \sum_{a,b} M_{ab} f_a(\theta_x) g_b(\theta_y)$$

Gives a core tensor of (for 2d)

$$C_{abcd} = \int d\theta e^{-\beta H_L(\theta)} f_a(\theta) g_b(\theta) f_c(\theta) g_d(\theta)$$



Tensor network components

XY model tensor components (U(1) character basis)

$$M_{ab} = \delta_{ab} I_a(\beta)$$

$$C_{abcd} = I_{a-b+c-d}(\beta h) \xrightarrow{h \to 0} \delta_{a-b+c-d}$$

Clock model tensor components (Z_N character basis)

$$M_{ab} = \delta_{ab} \sum_{k} I_{a+kN}(\beta)$$

$$C_{abcd} = \sum_{k} I_{a-b+c-d+kN}(\beta h) \xrightarrow{h \to 0} \sum_{k} \delta_{a-b+c-d+kN}(\beta h)$$

Can mix core and interaction tensors from different models



Specific heat for mixed XY/Z_N models D_{cut} = 40

1.75 XY,D=5 XY,D=5 periodic core XY core,Z5 interaction 1.50 2 peaks appear with **Z**5 periodic core 1.25 $(Z_5 \text{ and } XY + \text{periodic core})$ 1.00 Only one peak apparent à with XY core 0.75 0.50 Phase structure determined by symmetry 0.25 of core tensor (Y. Meurice 2019) 0.00 0.50 0.75 1.25 0.25 1.00 1.50 1.75 2.00 т



Discretization as a choice of basis

- Core, interaction decomposition not unique
- For example, can move local term into interaction

 $H_{I}'(\theta_{x},\theta_{y}) = H_{I}(\theta_{x},\theta_{y}) + \frac{1}{2d} \left[H_{L}(\theta_{x}) + H_{L}(\theta_{y}) \right] \qquad e^{-\beta H_{I}'(\theta_{x},\theta_{y})} \approx \sum_{a,b} M_{ab}'f_{a}(\theta_{x})g_{b}(\theta_{y})$

Core tensor then determined only by basis

$$e^{-\beta H'_{I}(\theta_{x},\theta_{y})} \approx \sum_{a,b} M'_{ab} f_{a}(\theta_{x}) g_{b}(\theta_{y})$$
$$C'_{abcd} = \int d\theta f_{a}(\theta) g_{b}(\theta) f_{c}(\theta) g_{d}(\theta)$$

- Z_N clock model as approximation to interaction term using a rectangular step function basis, each over distinct angular range of $2\pi/N$, zero elsewhere
 - Evaluating interaction at center of each interval reproduces clock model
- Could choose other sets of basis functions, expansion approximations
- Evaluating error in discrete approximation to interaction term may help determine which basis is best (does this consider symmetries?)
 - RMS error for Z_N basis is larger than U(1) character basis
- Could use this to optimize basis for given model



Moving between XY and Z_N models

- Previously looked at Z_N for increasing N
- Instead consider fixed N
 - interpolate between periodic, non-periodic core tensor

$$C_{abcd} = \sum_{k} \alpha_{k}(h_{N})I_{a-b+c-d+kN}(\beta h)$$

Perturbed XY model (Jose, Kadanoff, Kirkpatrick, Nelson 1977)

$$H = -\sum_{\langle xy \rangle} \cos(\theta_x - \theta_y) - h \sum_x \cos(\theta_x) - h_N \sum_x \cos(N\theta_x)$$
$$\alpha_k(h_N) \propto \frac{I_k(\beta h_N)}{I_0(\beta h_N)} = \begin{cases} \delta_k : h_N = 0 \ (XY) \\ 1 : h_N \to \infty (ZN) \end{cases}$$

Interested in behavior of lower phase transition for small h_N



Perturbed model N=5

D_{cut} = 40 h = 1e-5





Perturbed XY model RG analysis

 RG analysis using Villain approximation in JKKN paper

$$1 - \cos(\theta_x - \theta_y) \approx (\theta_x - \theta_y)^2/2$$

- For fixed h_N > 0, found
 - 2 critical temperatures for N > 4
 - At N=4 collapse to single T_c
- Value of $T_2(h_N \rightarrow 0)$ not clear from RG analysis
- Interested if non-zero, and how large
- If large, infinitesimal perturbation has large effect on phase diagram



(Jose, Kadanoff, Kirkpatrick, Nelson 1977)



Determining peaks of cross derivative

- Calculated <m> with spacing Δ T = 0.004
- Fit 11 consecutive points to 4th order polynomial
 - Plots of cross derivative from derivative of polynomial at center of interval
 - Peak location from zero of 2nd derivative of polynomial
- Consider only peak fits where peak is well within interval
- Peak temperature and height averaged over fit intervals



Cross derivative peak example $h_5 = 0.2$ h = 2e-7

- D_{cut}=81 not enough
- Peak temperature consistent for D_{cut}=91, 101
- D_{cut}=91 seems sufficient for T_c
- Peak height still moving lower a bit
- Lowest $h_5 = 0.2$, simulations became unstable around h=1e-7 for $h_5 < 0.2$





Cross derivative peak fits

$h_5 = 0.2 h = 1e-7$

- ~4 points fell well within fit interval
- Peak determined from average, error from variance
- Error is systematic error of fit
- For peak height additional error from D_{cut}





Lower peak temperature h₅ = 0.2

- D_{cut} = 81 not accurate enough at small h
- D_{cut} = 91 and 101 agree within errors
- Used D_{cut} = 91 for most of remaining results





Lower peak height h₅ = 0.2





Lower peak temperature versus h





Lower critical temperature versus h₅

- Error bars too large for power-law fit
- Trending down at lower h₅
- Still far from 0, but unable to do ⊢[~] reliable extrapolation with this approach





Peak temperature versus h₅

- First fit to h₅ at fixed h
- power-law in h₅

 $T_{peak}(h_5) - T_{peak}(0) \propto h_5^{\alpha}$

23

• Then extrapolate $T_{peak}(h_5 \rightarrow 0)$ to h = 0



Extrapolated peak temperature versus h

- Power-law fit extrapolates to $T_{peak}(h_5 \rightarrow 0) = 0.44(3)$
- About half the temperature of XY T_c ~ 0.89
- Small perturbation seems to have large effect on phase diagram





Peak height

- Need to check that system is critical (peak height diverges) as h→0
- Fit peak heights to power-law

height $\propto h^{-\gamma}$

• Check if gamma is nonzero as $h_5 \rightarrow 0$





Peak height scaling





Summary

- XY truncation using U(1) character expansion has less effect on low energy behavior than angular discretization
- Expansion basis for TN construction determines core tensor symmetries, which in turn has large effect on phase structure
- Choosing basis that preserves symmetries
 - Does that also minimize error in truncated interaction expansion?
- Studied location of lower-T phase transition in perturbed XY model as function of h₅
 - consistent with non-zero $T_c~~(\sim 0.5~T_{XY})$ as $h_5 \rightarrow 0$
- Small symmetry-breaking perturbations can have large effect on phase structure

