Berezinskii-Kosterlitz-Thouless Criticality in the q-state Clock Model

Tao Xiang
txiang@iphy.ac.cn
Institute of Physics
Chinese Academy of Sciences
✓ Brief introduction to the tensor-network renormalization group methods

✓ Critical properties of the q-state clock model
Road Map of Renormalization Group

Numerical Renormalization Group

- Kadanoff
- Wilson 1982
- Kondo impurity 0D
- White DMRG 1D
- Tensor-network RG 2D

Phase transition and Critical phenomena

Quantum field theory

- Stueckelberg
- Gell-Mann Low
- QED 1965
- EW 1999
- QCD 2004
Basic Idea of Renormalization Group

To find a small but optimized basis set to represent accurately a quantum state

\[ |\psi\rangle = \sum_{k=1}^{N_{\text{total}}} a_k |k \rangle \approx \sum_{k=1}^{N \ll N_{\text{total}}} a_k |k \rangle \]

Scale transformation: refine the wavefunction by local RG transformations
Is Quantum State Renormalizable?

$N_{\text{total}} = 2^{L^2}$

Area Law of Entanglement entropy

$S \propto L \propto \log N$

$N \sim 2^L \ll 2^{L^2} = N_{\text{total}}$

$|\psi\rangle = \sum_{k=1}^{N \ll N_{\text{total}}} a_k |k\rangle$
How to Determine the Optimized Basis States?

Use a sub-system as a pump to probe the other part of the system

Importance is measured by the entanglement or reduced density matrix

\[
\rho_{\text{sys}} = Tr_{\text{env}} e^{-\beta H}
\]

reduced density matrix
Faithful representation of partition functions of classical/quantum models

\[ Z = Tr \prod_i T_{x_i x'_i y_i y'_i} \]

Variational wavefunctions of ground states of quantum lattice models

\[ |\Psi\rangle = Tr \prod_i T_{x_i x'_i y_i y'_i}[m_i]|m_i\rangle \]
Example: Tensor-network representation of the Clock Model

\[ H = - \sum_{(i,j)} \cos(\theta_i - \theta_j) \]

\[ \theta_i = \frac{2\pi n}{q} \quad (n = 0, \ldots, q - 1) \]

q-state clock model = discretized XY-model
Example: Tensor-network representation of the Clock Model

\[ e^\beta \cos(\theta_i - \theta_j) = \theta_i \ V \ m \ V^* \ \theta_j \]

\[ V_{\theta,m} = \sqrt{I_m} e^{im\theta} / q \]

\[ I_m = \sum_{n=1}^{q} e^{-im\theta_n} e^\beta \cos \theta_n \]

\[ \tau_{ijkl} = \begin{cases} i \ V \ k \ V^* \ j \ V \ l \ V^* \ & \text{if } k \mod (i+j-k-l+q) = 0 \\ i \ V \ l \ V^* \ j \ V \ k \ V^* \ & \text{otherwise} \end{cases} \]

\[ k \propto \sqrt{I_i I_j I_k I_l} \ \delta_{\mod(i+j-k-l,q)} \]
Tensor-network representation in the dual lattice

\[ \tau_{ijkl} = \sqrt{\lambda_i \lambda_j \lambda_k \lambda_l} \delta_{\text{mod}(i+j-k-l,q)} \]

\[ \lambda_m = e^{\beta \cos \theta_m} \]
Thoroughly developed, most accurate quantum many-body computational methods

1. Ground state
   ✓ **Density-matrix renormalization group** (DMRG, White 1992)
   ✓ **Simple update, time evolving block decimation** (TEBD, Vidal 2004)
   ✓ **Variational minimization of MPS** (FBC, PBC)

2. Thermodynamics
   ✓ **Transfer-matrix renormalization group** (TMRG, Nishino coworkers/classical 2D 1995, Xiang coworkers/quantum 1D 1996)
   ✓ **Corner transfer matrix renormalization** (Nishino et al 1996)
   ✓ **Coarse-graining tensor renormalization** (TRG, SRG, HOTRG, HOSRG, TNR, loop-TNR)
   ✓ **Ancilla purification approach** (Verstraete et al 2004)
3. Dynamic correlation functions
   ✓ Lanczos DMRG
   ✓ Lanczos MPS
   ✓ Chebyshev MPS
   ✓ Correction vector method

4. Time-dependent problem
   ✓ Pace-keeping DMRG
   ✓ TEBD
   ✓ Adaptive time-dependent DMRG
   ✓ Folded transfer matrix method

5. Excitation spectra
   ✓ MPS ansatz of single-mode approximation

Thoroughly developed, most accurate quantum many-body computational methods
Evolution of Coarse-Graining Tensor-Network Renormalization

- Tensor renormalization group (TRG, Levin, Nave, 2007)
- Second renormalization group (SRG, Xie et al 2009)
- TRG with HOSVD (HOTRG, HOSRG Xie et al 2012)
- Tensor network renormalization (TNR, Evenbly, Vidal 2015)
- Loop TNR (Yang et al 2016)

- TNR and loop TNR are more accurate at the critical points
- HOTRG and HOSRG can be applied to 2D quantum and 3D classical models
Tensor-network Methods for Quantum 2D/Classical 3D Systems

Still under development, already applied to quantum spin/interacting electron models

1. Ground state: based on the PEPS/PESS ansatz

2. Thermodynamics: coarse-graining tensor renormalization

3. Excitations: single-mode approximation

Projected Entangled Pair State (PEPS)

\[ |\Psi\rangle = \text{Tr} \prod T_{x_i x'_i y_i y'_i} [m_i] |m_i\rangle \]

Verstraete & Cirac, cond-mat/0407066
Ground state: Problems need be solved

1. Determination of PEPS/PESS wave function

$$|\Psi\rangle = Tr \prod T_{x_i x'_i y_i y'_i} [m_i] |m_i\rangle$$

2. Evaluation of expectation values (high cost)

$$\langle \hat{O} \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$\langle \Psi | \hat{O} | \Psi \rangle$ and $\langle \Psi | \Psi \rangle$ are each a 2D tensor-network
Simple update

Fast and can access large D tensors

Jiang, Weng, Xiang, PRL 101, 090603 (2008)

Full update

more accurate than simply update

cost high


Variational minimization with **automatic differentiation**

most accurate and reliable method

cost high

Liao, Liu, Wang, Xiang, PRX 9, 031041 (2019)
Automatic Differentiation (AD)

➢ a cute technique which computes exact derivatives, whose errors are limits only floating point error
➢ a powerful tool successfully used in deep learning

\[
\frac{\partial L}{\partial \theta} = \frac{\partial L}{\partial T^n} \frac{\partial T^n}{\partial T^{n-1}} \cdots \frac{\partial T^2}{\partial T^1} \frac{\partial T^1}{\partial \theta}.
\]

Computation Graph

Chain rule of differentiation
TMRG: Fixed Point MPS Method

Fixed point MPS equation:

\[
\begin{pmatrix}
\vdots & \tau & \tau & \tau & \tau & \cdots \\
\vdots & \tau & \tau & \tau & \tau & \cdots \\
\vdots & \tau & \tau & \tau & \tau & \cdots \\
\vdots & \tau & \tau & \tau & \tau & \cdots \\
\vdots & \tau & \tau & \tau & \tau & \cdots \\
\vdots & \tau & \tau & \tau & \tau & \cdots \\
\end{pmatrix}
\]

\[ Z = \text{Tr} \left( T^N \right) N \to \infty = \left( \frac{\langle \Psi | T | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right)^N = \lambda_1 \]

Fixed gauge by left and right canonicalization

\[
|\Psi\rangle = \cdots A_L A_L A_L \bigcirc A_R A_R A_R A_R \cdots
\]

\[
A^*_L A_L = I \quad A^*_R A_R = I
\]
To determine the local tensor, one needs to solve the following equations:
✓ Brief introduction to tensor-network renormalization group methods

✓ Critical properties of the q-state clock model
q-state Clock Model

\[ H = - \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \]

\[ \theta_i = \frac{2\pi n}{q} (n = 0, \ldots, q - 1) \]

Understanding the nature of topological phase transition without symmetry breaking

2D melting:

0 \quad \text{Solid} \quad T_{c1} \quad \text{Quasi-liquid} \quad T_{c2} \quad \text{Liquid} \quad T

Berezinskii-Kosterlitz-Thouless Transition

**XY-model**

\[ H = - \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \]

Berezinskii  | Thouless  | Kosterlitz

Superfluid \( (T < T_c) \)

Bound vortex-antivortex pairs

Normal state \( (T > T_c) \)

Proliferation of free vortices

BKT phase: critical

\[ T_c \]

paramagnetic

\( T \)
Effective Low Energy Theory

**XY-model**

\[ H = -\sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \]

**Sine-Gordon Model:**

\[
S = \frac{1}{2\pi K} \int d^2r (\nabla \varphi)^2 + \frac{g_1}{2\pi} \int d^2r \cos(\sqrt{2} \varphi)
\]

Berezinskii  Thouless  Kosterlitz

BKT phase: critical  \( T_c \)  paramagnetic
Scaling Dimension $\Delta$

\[ \Delta_{\cos(\sqrt{2}\varphi)} = \frac{K}{2} \]

$\Delta < 2$ relevant

$\Delta = 2$ marginal

$\Delta > 2$ irrelevant

**Sine-Gordon Model:**

\[ S = \frac{1}{2\pi K} \int d^2r (\nabla \varphi)^2 + \frac{g_1}{2\pi} \int d^2r \cos(\sqrt{2} \varphi) \]

$K > 4$ free boson

$K < 4$ non-critical

$K = 4$

BKT phase: critical

$T_c$

paramagnetic
Central Charge $c$

$$\Delta \cos(\sqrt{2}\varphi) = \frac{K}{2}$$

\[ \begin{align*} 
\Delta < 2 \quad & \text{relevant} \\
\Delta = 2 \quad & \text{marginal} \\
\Delta > 2 \quad & \text{irrelevant}
\end{align*} \]

Sine-Gordon Model:

$$S = \frac{1}{2\pi K} \int d^2 r (\nabla \varphi)^2 + \frac{g_1}{2\pi} \int d^2 r \cos(\sqrt{2} \varphi)$$

- $K > 4$ free boson
- $K < 4$ non-critical

$\Delta = 2$

$\Delta < 2$ relevant

$\Delta = 2$ marginal

$\Delta > 2$ irrelevant

$\Delta = \frac{2}{K}$

$K = 4$

BKT phase: critical

$T_c$

paramagnetic
q-state Clock Model: Large q Limit

\[ S = \frac{1}{2\pi K} \int d^2r (\nabla \varphi)^2 + \frac{g_1}{2\pi} \int d^2r \cos(\sqrt{2} \varphi) + \frac{g_2}{2\pi} \int d^2r \cos(q\sqrt{2} \theta) \]

\( \theta \) is dual to \( \varphi \):

\[ \partial_x \varphi = -\partial_y (K\theta) \quad \partial_y \varphi = \partial_x (K\theta) \]

q-state Clock Model: Large $q$ Limit

$$S = \frac{1}{2\pi K} \int d^2 r (\nabla \phi)^2 + \frac{g_1}{2\pi} \int d^2 r \cos(\sqrt{2} \phi) + \frac{g_2}{2\pi} \int d^2 r \cos(q\sqrt{2} \theta)$$

Scaling dimension

$$\Delta_{\cos(\sqrt{2}\phi)} = \frac{K}{2}$$
$$\Delta_{\cos(q\sqrt{2}\theta)} = \frac{q^2}{2K}$$

$\Delta < 2$ relevant
$\Delta = 2$ marginal
$\Delta > 2$ irrelevant
q-state Clock Model: Large \( q \) Limit

\[
S = \frac{1}{2\pi K} \int d^2r (\nabla \varphi)^2 + \frac{g_1}{2\pi} \int d^2r \cos(\sqrt{2} \varphi) + \frac{g_2}{2\pi} \int d^2r \cos(q\sqrt{2} \theta)
\]

\[
\Delta \cos(\sqrt{2} \varphi) > 2 \\
\Delta \cos(q\sqrt{2} \theta) < 2
\]

\[
\Delta \cos(\sqrt{2} \varphi) > 2 \\
\Delta \cos(q\sqrt{2} \theta) > 2
\]

\[
\Delta \cos(\sqrt{2} \varphi) < 2 \\
\Delta \cos(q\sqrt{2} \theta) > 2
\]

\[
c = 0
\]

\[
c = ?
\]

\[
c = 0
\]

\[
\Delta \cos(q\sqrt{2} \theta) = 2
\]

\[
\Delta \cos(\sqrt{2} \varphi) = 2
\]

Ferromagnetic \( T_{c1} \) BKT phase: critical \( T_{c2} \) paramagnetic

J. V. Jose, et al, PRB 16,1217(1977)
q-state Clock Model: Self-dual Point

\[
S = \frac{1}{2\pi K} \int d^2r (\nabla \varphi)^2 + \frac{g_1}{2\pi} \int d^2r \cos(\sqrt{2} \varphi) + \frac{g_2}{2\pi} \int d^2r \cos(q\sqrt{2} \theta)
\]

When \( K = q, \ g_1 = g_2 \), the model is invariant under dual transformation

\[
\varphi \leftrightarrow q\theta
\]

At the self-dual point

\[
\Delta \cos(\sqrt{2} \varphi) = \Delta \cos(q\sqrt{2} \theta) = \frac{q}{2} \rightarrow K_{sd} = q
\]

The self-dual point is a critical point for \( q \leq 4 \)

The self-dual point is not a critical point when \( q > 4 \)
### q-state Clock Model: Small q Limit

<table>
<thead>
<tr>
<th>q</th>
<th>$T_c$</th>
<th>c</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$2 \ln^{-1}(1 + \sqrt{2})$</td>
<td>1/2</td>
<td>Ising, Majorana fermion</td>
</tr>
<tr>
<td>3</td>
<td>$(3/2) \ln^{-1}(1 + \sqrt{3})$</td>
<td>4/5</td>
<td>$Z_3$ Parafermion</td>
</tr>
<tr>
<td>4</td>
<td>$\ln^{-1}(1 + \sqrt{2})$</td>
<td>1</td>
<td>Two copies of Ising</td>
</tr>
</tbody>
</table>

#### Phase Diagram
- **Ferromagnetic**
- **Self-dual Point**
- **BKT/phase: critical**
- **paramagnetic**
q-state Clock Model: Intermediate $q \geq 5$

1. Is the intermediate phase still a BKT phase?
2. Can the critical temperatures and conformal parameters $(c$ and $K)$ be accurately determined?
Marginal operators lead to strong finite size effect with logarithmic corrections.

Spin-spin correlation function

\[ \sim r^{1/4} \ln^{1/8} r \]


Correlation length diverges exponentially

\[ \xi \sim e^{a|T-T_{BKT}|^{-1/2}} \quad T > T_{BKT} \]

Borisenko et. al., PRE 83, 041120(2011)
### Critical Temperatures

<table>
<thead>
<tr>
<th>$q = 5$</th>
<th>$T_{c1}$</th>
<th>$T_{c2}$</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tobochnik, et.al., PRB(1982)</td>
<td>0.8</td>
<td>1.1</td>
<td>MC</td>
</tr>
<tr>
<td>Borisenko, et.al., PRE(2011)</td>
<td>0.905(1)</td>
<td>0.951(1)</td>
<td>MC</td>
</tr>
<tr>
<td>Kumano, et.al., PRB(2013)</td>
<td>0.908</td>
<td>0.944</td>
<td>HTSE</td>
</tr>
<tr>
<td>Chatelain, et.al., JSM(2014)</td>
<td>0.914(12)</td>
<td>0.945(17)</td>
<td>DMRG</td>
</tr>
<tr>
<td>Chatterjee, et.al., PRE(2018)</td>
<td>0.897(1)</td>
<td>-</td>
<td>MC</td>
</tr>
<tr>
<td>Chen, et.al., CPB(2018)</td>
<td>0.9029(1)</td>
<td>0.9520(1)</td>
<td>HOTRG</td>
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<td>Surungan, et.al., arXiv(2019)</td>
<td>0.911(5)</td>
<td>0.940(5)</td>
<td>MC</td>
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</tbody>
</table>
## Critical Temperatures

<table>
<thead>
<tr>
<th>$q = 6$</th>
<th>$T_{c1}$</th>
<th>$T_{c2}$</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tobochnik, et.al., PRB(1982)</td>
<td>0.6</td>
<td>1.3</td>
<td>MC</td>
</tr>
<tr>
<td>Challa, et.al., PRB(1986)</td>
<td>0.68(2)</td>
<td>0.92(1)</td>
<td>MC</td>
</tr>
<tr>
<td>Yamagata, et.al., JPA(1991)</td>
<td>0.68</td>
<td>0.90</td>
<td>MC</td>
</tr>
<tr>
<td>Tomita, et.al., PRB(2002)</td>
<td>0.7014(11)</td>
<td>0.9008(6)</td>
<td>MC</td>
</tr>
<tr>
<td>Hwang, et.al., PRE(2009)</td>
<td>0.632(2)</td>
<td>0.997(2)</td>
<td>MC</td>
</tr>
<tr>
<td>Brito, et.al., PRE(2010)</td>
<td>0.68(1)</td>
<td>0.90(1)</td>
<td>MC</td>
</tr>
<tr>
<td>Baek, et.al., PRE(2013)</td>
<td>-</td>
<td>0.9020(5)</td>
<td>MC</td>
</tr>
<tr>
<td>Kumano, et.al., PRB(2013)</td>
<td>0.700(4)</td>
<td>0.904(5)</td>
<td>HTSE</td>
</tr>
<tr>
<td>Krcmar, et.al., arXiv(2016)</td>
<td>0.70</td>
<td>0.88</td>
<td>CTMRG</td>
</tr>
<tr>
<td>Chen, et.al., CPL(2017)</td>
<td>0.6658(5)</td>
<td>0.8804(2)</td>
<td>HOTRG</td>
</tr>
<tr>
<td>Chatterjee, et.al., PRE(2018)</td>
<td>0.681(1)</td>
<td>-</td>
<td>MC</td>
</tr>
<tr>
<td>Surungan, et.al., arXiv(2019)</td>
<td>0.701(5)</td>
<td>0.898(5)</td>
<td>MC</td>
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<tr>
<td>Seongpyo, et.al., arXiv(2019)</td>
<td>0.693</td>
<td>0.904</td>
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</table>
Magnetization and Entanglement Entropy

Peak positions determine the critical temperatures

$T_c$
Magnetization and Entanglement Entropy

\[ M \equiv \langle e^{i\theta} \rangle \]

\[ S_E \]

- \( q = 6 \)
- \( \text{origin} \)
- \( \text{dual} \)

\[ T_c \]
What is the critical $q$ for the BKT transition?

<table>
<thead>
<tr>
<th>Ising model</th>
<th>XY-model</th>
</tr>
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<tr>
<td>$q = 2$</td>
<td>$q = \infty$</td>
</tr>
<tr>
<td>$q_c$</td>
<td></td>
</tr>
</tbody>
</table>

**Field theory:** $q_c = 5$

**Monte Carlo:** $q_c = 8$

**Monte Carlo:** $q_c = 7$
- C. Hwang, PRE 80.042103 (2009)

**Monte Carlo:** $q_c = 6$
- S. Baek, et al., PRE 88.012125 (2013)
BKT signature: Exponentially Diverging Correlation Length

\[ \xi \sim e^{q|T-T_c|^{-1/2}} \rightarrow (T-T_c) \sim \ln^{-2}\xi \]

Exponential divergence of the correlation length suggests that the critical transition is BKT like and

\[ q_c = 5 \]
Two Critical Temperatures

Correlation length \( \xi(D) \sim e^{a|T-T_c(D)|^{-1/2}} \)

\( T - T_c \sim \ln^{-2} \xi \)

\( q=5 \)

\( T_{c1} = 0.9059(2) \)

\( T_{c2} = 0.9521(2) \)

\( q=6 \)

\( T_{c1} = 0.6901(4) \)

\( T_{c2} = 0.9127(5) \)
## Critical Temperatures

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</tr>
<tr>
<td><strong>Current work</strong></td>
<td><strong>0.9059 (2)</strong></td>
<td><strong>0.9521(2)</strong></td>
<td><strong>TMRG</strong></td>
</tr>
</tbody>
</table>
Central Charge $c \sim 1$

$$S_E \sim \frac{c}{6} \ln \xi$$


$q = 5 \quad T = 0.928$
$q = 6 \quad T = 0.794$
$q = 7 \quad T = 0.693$
$q = 8 \quad T = 0.614$

Inside the critical phase
Thermodynamic observables are \( q \)-independent

\[
S = \frac{1}{2\pi K} \int d^2r (\nabla \varphi)^2 + \frac{g_1}{2\pi} \int d^2r \cos(\sqrt{2} \varphi) + \frac{g_2}{2\pi} \int d^2r \cos(q \sqrt{2} \theta)
\]

Determination of Luttinger Parameter $K$

- $K$ is difficult to determine, unknown before
- Critical phase described by compactified boson CFT of radius $R = \sqrt{2K}$

$$S = \frac{1}{8\pi} \int d^2r (\nabla \theta)^2$$

$R$ is related to the ratio of partition functions on the Klein Bottle and Torus

$$R = \frac{Z^{\text{Klein}}(2L_x, \frac{L_y}{2})}{Z^{\text{Torus}}(L_x, L_y)}$$

H.H. Tu, PRL 119, 261603 (2017)
Prediction of Conformal Field Theory \((q \rightarrow \infty)\)

\[
R(T_{\text{self dual}}) = \sqrt{2q}
\]

\[
R(T_{c1}) = \frac{q}{\sqrt{2}}
\]

\[
R(T_{c2}) = 2\sqrt{2}
\]
Luttinger Parameter (q=5)

Discrepancy are mainly caused by the marginal terms

\[ R(T_{c2}) = 2\sqrt{2} \]

\[ R(T_{c1}) = \frac{5}{\sqrt{2}} \]
Discrepancy are mainly caused by the marginal terms.

\[ R(T_{c2}) = 2\sqrt{2} \]

\[ R(T_{c1}) = \frac{q}{\sqrt{2}} \]
Discrepancy becomes smaller and smaller with increasing $q$

$$R(T_{\text{self-dual}}) = \sqrt{2q}$$
We calculated the Luttinger parameter $K$ of the q-state clock model in the critical phase for the first time, and determined accurately the critical temperatures and other physical quantities.