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

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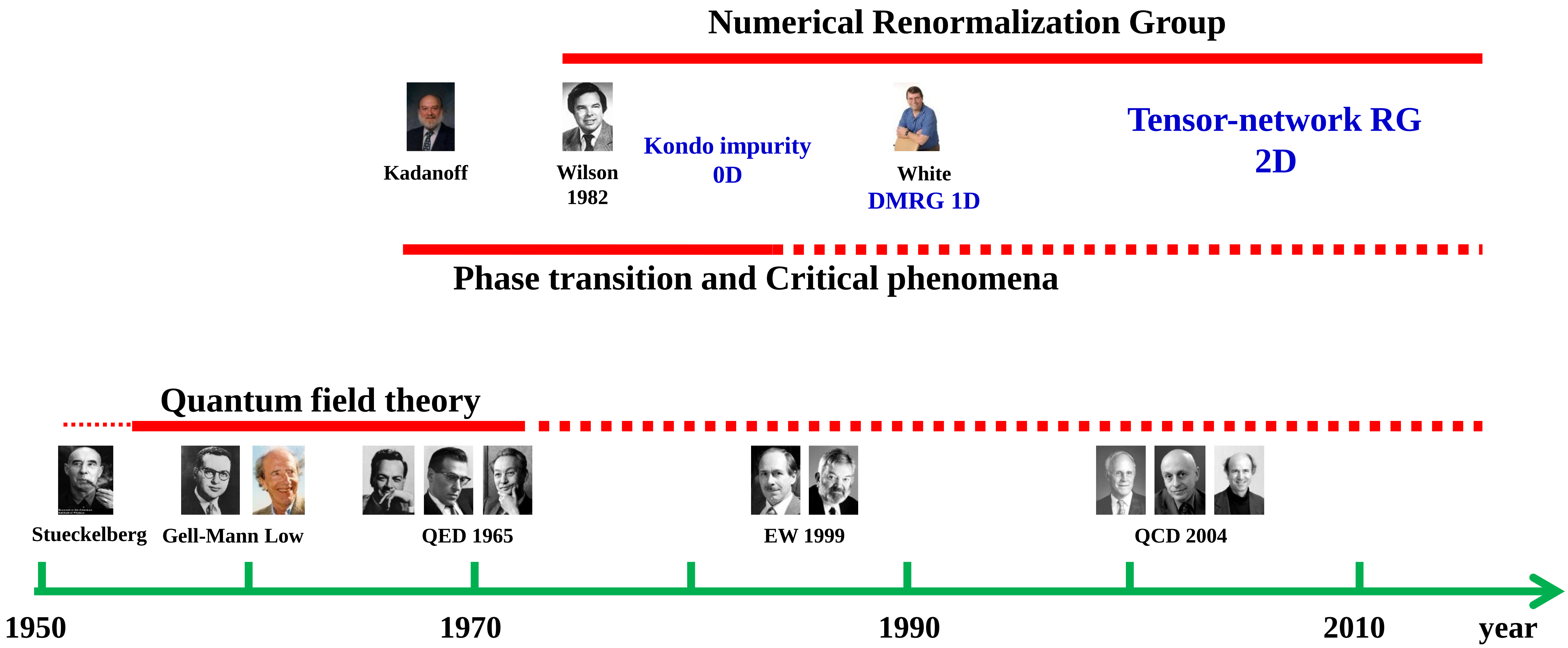
Outline

- ✓ **Brief introduction to the tensor-network renormalization group methods**

- ✓ **Critical properties of the q-state clock model**

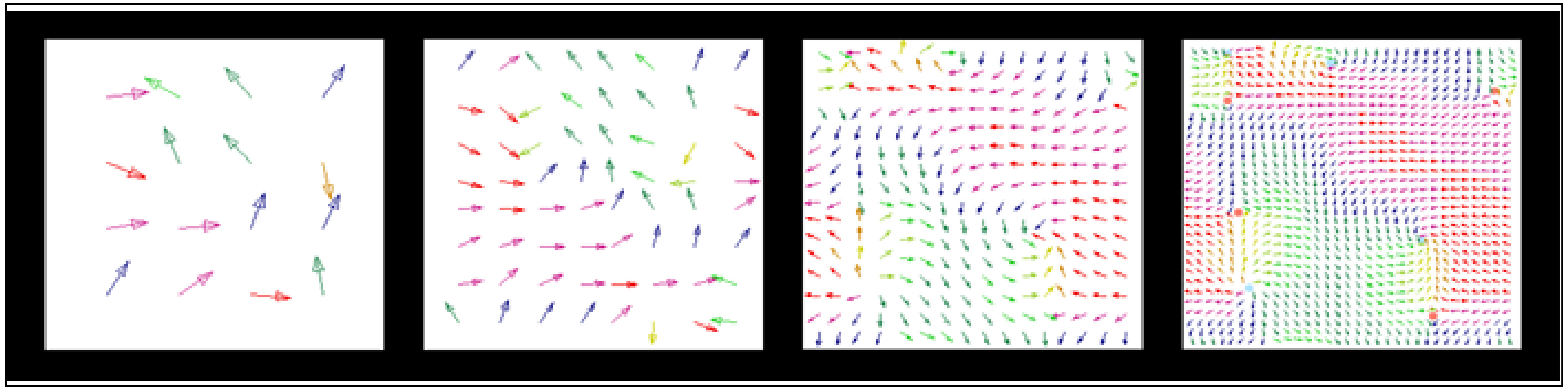
Road Map of Renormalization Group



Basic Idea of Renormalization Group

$$|\psi\rangle = \sum_{k=1}^{N_{total}} a_k\,|k\rangle \approx \sum_{k=1}^{N \ll N_{total}} a_k\,|k\rangle$$

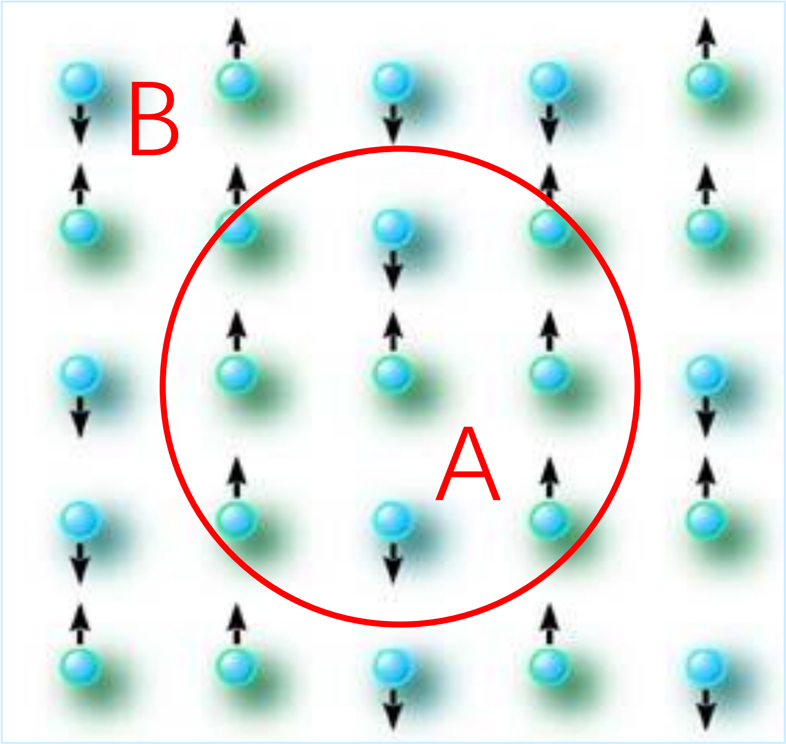
To find a small but optimized basis set to represent accurately a quantum state



Scale transformation: refine the wavefunction by local RG transformations

Is Quantum State Renormalizable?

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



L

L

$$|\psi\rangle = \sum_{k=1}^{N \ll N_{\text{total}}} a_k \, |k\rangle$$

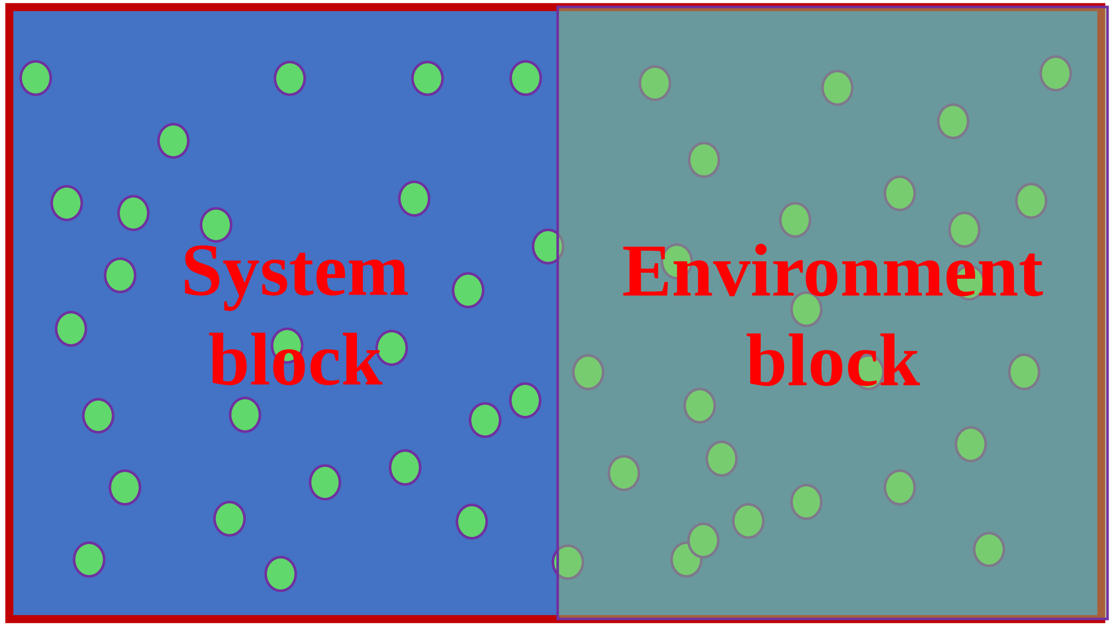
Area Law of Entanglement entropy

$$S \propto L \propto \log N$$

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

How to Determine the Optimized Basis States?

Pump-Probe



$$\rho_{sys} = Tr_{env} e^{-\beta H}$$

reduced density matrix

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

Tensor-Network State

Faithful representation of partition functions of classical/quantum models

$$Z = Tr \prod_i T_{x_i x_i' y_i y_i'}$$

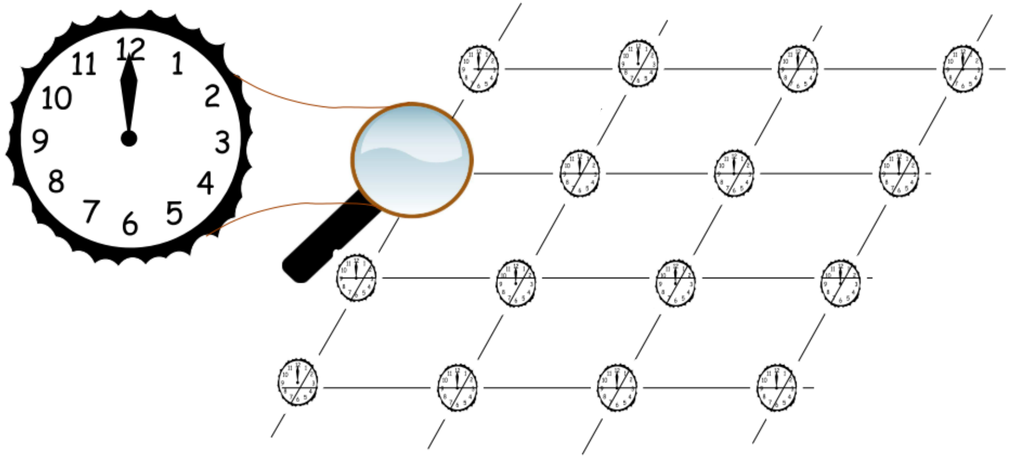
Variational wavefunctions of ground states of quantum lattice models

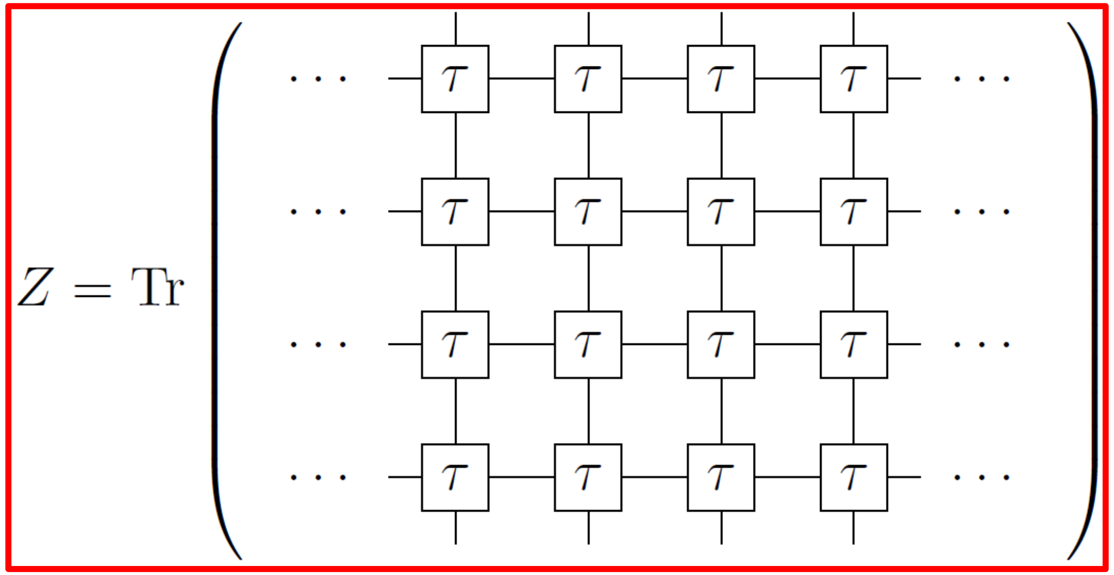
$$|\Psi\rangle = Tr \prod T_{x_i x_i' y_i y_i'}[m_i]|m_i\rangle$$

Example: Tensor-network representation of the Clock Model

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

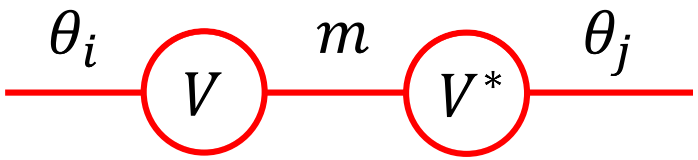
$$\theta_i = \frac{2\pi n}{q} (n = 0, \ldots, q-1)$$





q-state clock model = discretized XY-model

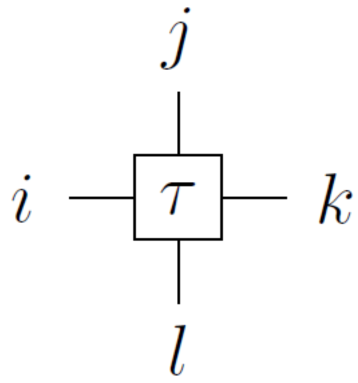
Example: Tensor-network representation of the Clock Model

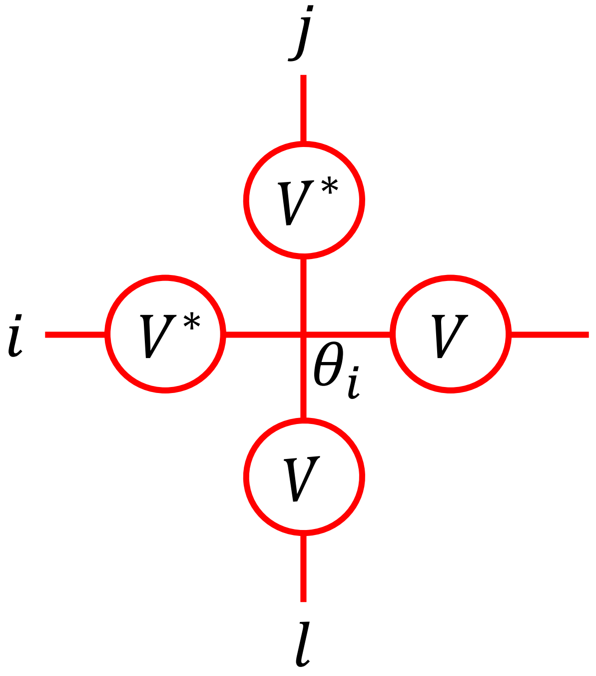
$e^{\beta\cos(\theta_i-\theta_j)} =$ 

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

Fourier transformation

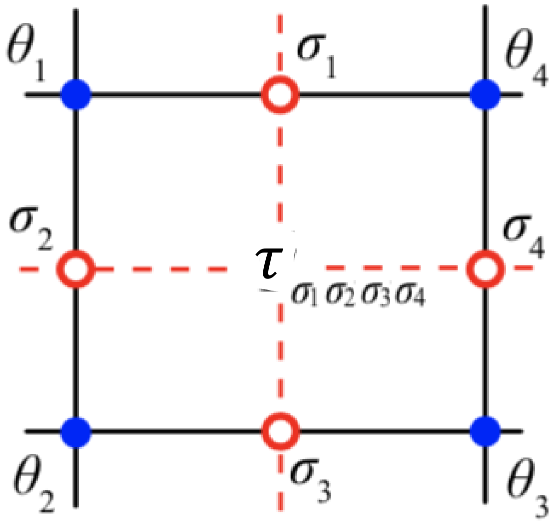
$$I_m = \sum_{n=1}^{q} e^{-im\theta_n} e^{\beta\cos\theta_n}$$

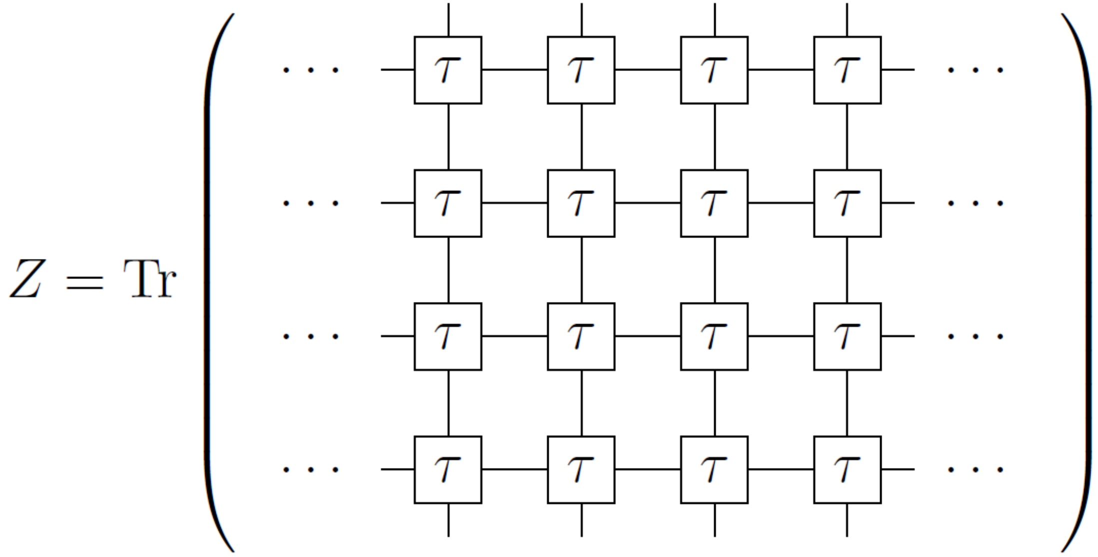
$\tau_{ijkl} =$ 

$=$ 

$\propto \sqrt{I_i I_j I_k I_l}\;\delta_{\mathrm{mod}(i+j-k-l,q)}$

Tensor-network representation in the dual lattice





$$\sigma_1 = \theta_1 - \theta_4$$
$$\sigma_2 = \theta_2 - \theta_1$$
$$\sigma_3 = \theta_3 - \theta_2$$
$$\sigma_4 = \theta_4 - \theta_3$$

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

$$\lambda_m = e^{\beta \cos \theta_m}$$

Tensor-network Methods for Quantum 1D/Classical 2D Systems

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)**

Tensor-network Methods for Quantum 1D/Classical 2D Systems

Thoroughly developed, most accurate quantum many-body computational methods

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**

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**

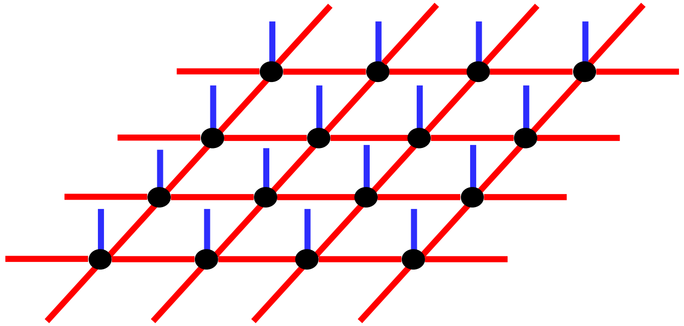
Tensor-network Methods for Quantum 2D/Classical 3D Systems

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**

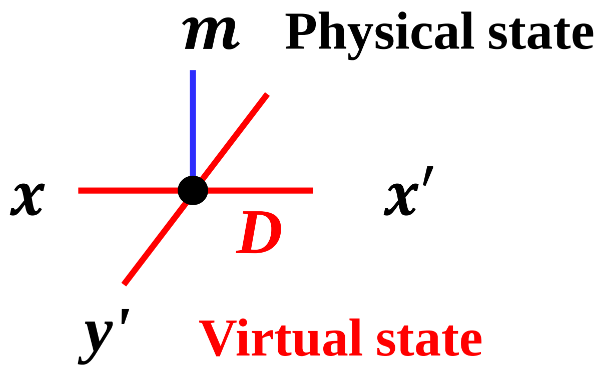
Projected Entangled Pair State (PEPS)

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



Verstraete & Cirac, cond-mat/0407066

$$T_{xx'yy'}[m] =$$



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

Determination of PEPS/PESS Wave Function

- **Simple update** — Jiang, Weng, Xiang, PRL 101, 090603 (2008)

  Fast and can access large D tensors

- **Full update** — Jordan et al PRL 101, 250602 (2008)

  more accurate than simply update

  cost high

- **Variational minimization with automatic differentiation**

  Liao, Liu, Wang, Xiang, PRX **9**, 031041 (2019)

  most accurate and reliable method

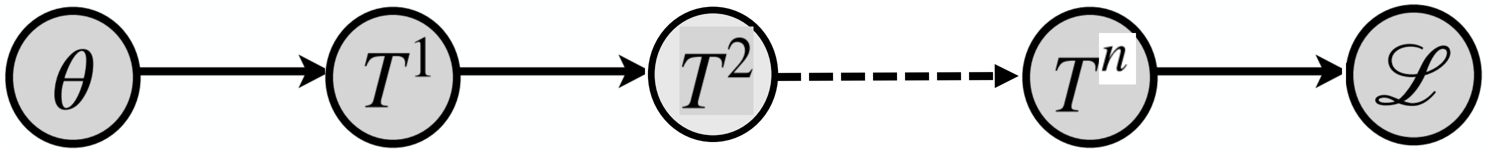
  cost high

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

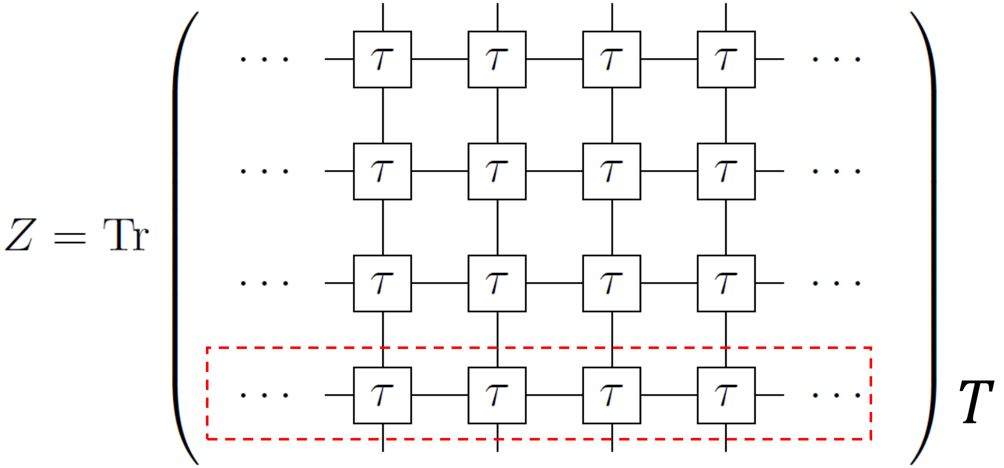
Computation Graph

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



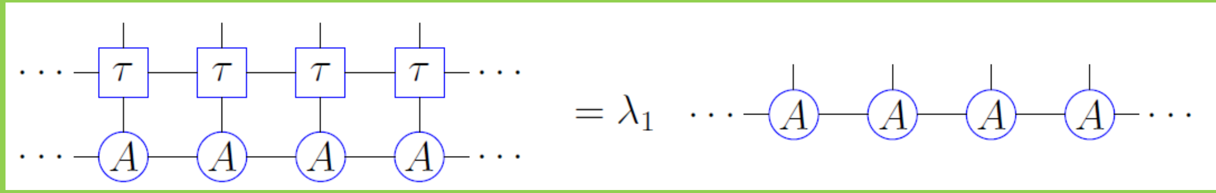
Chain rule of differentiation

TMRG: Fixed Point MPS Method

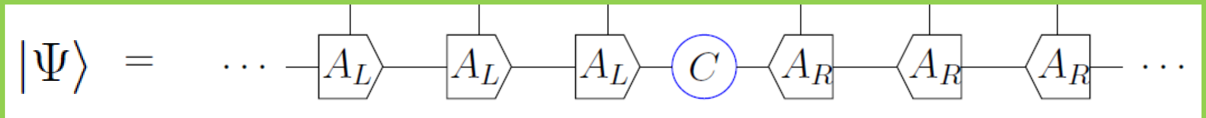


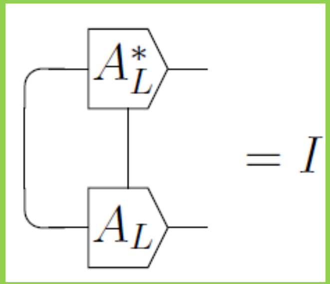
$$= \mathrm{Tr}\, T^N \underset{N \to \infty}{=} \left(\frac{\langle\Psi|T|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right)^N$$

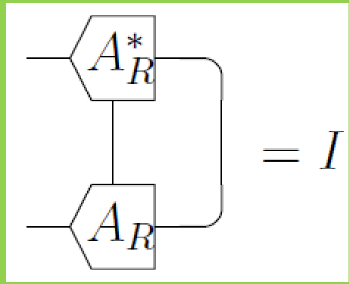
Fixed point MPS equation:



Fixed gauge by left and right canonicalization



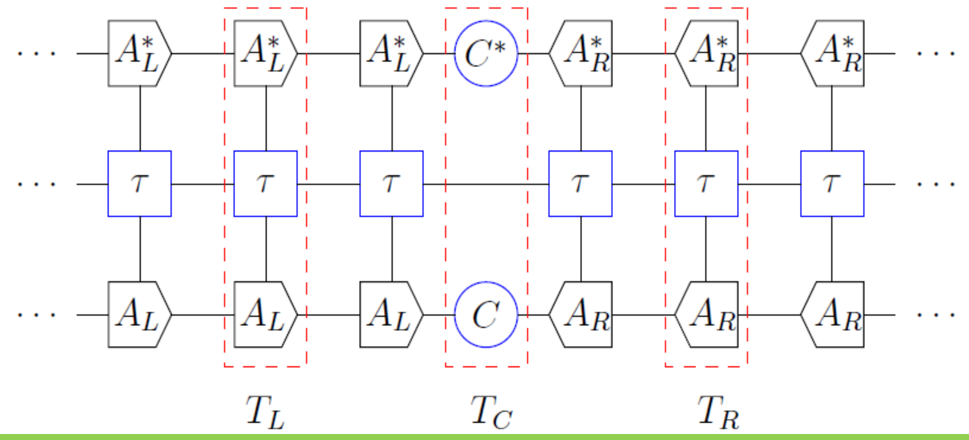




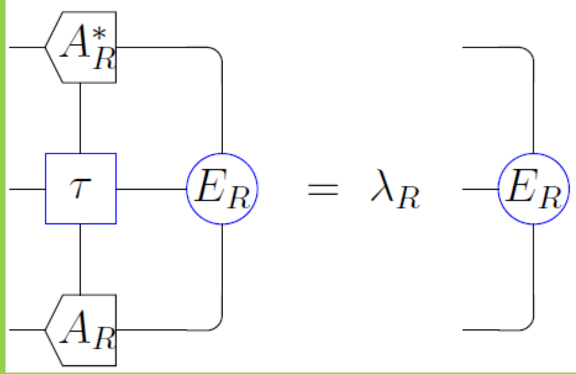
TMRG: Fixed Point MPS Method

$$\langle \Psi | T | \Psi \rangle = \mathrm{Tr}\left(T_{A_L}^{N_L} T_C T_{A_R}^{N_R}\right)$$

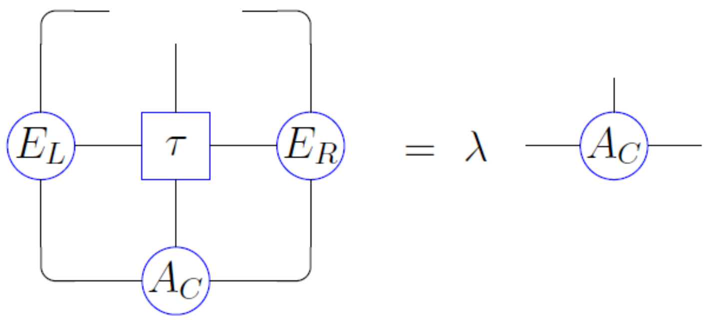
$$=$$



To determine the local tensor, one needs to solve the following equations:



$$A_C[\sigma] = A_L[\sigma]C = C\,A_R[\sigma]$$



Outline

- ✓ Brief introduction to tensor-network renormalization group methods

- ✓ **Critical properties of the q-state clock model**

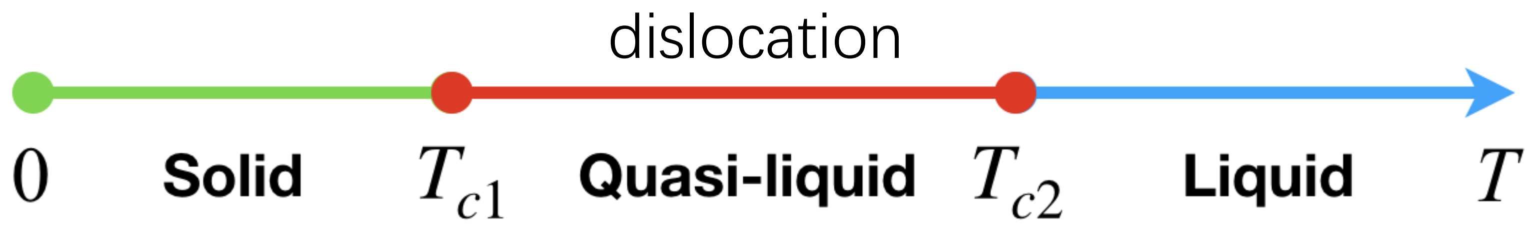
q-state Clock Model

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

$$\theta_i = \frac{2\pi n}{q} (n = 0, \dots, q-1)$$

Understanding the nature of topological phase transition without symmetry breaking

2D melting:



I. Halperin and D. R. Nelson, PRL. 41, 121 (1978); Phys. Rev. 8 19, 2457 (1979).

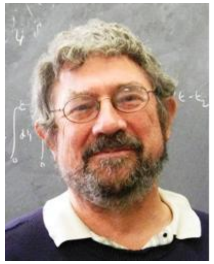
Berezinskii-Kosterlitz-Thouless Transition

XY-model

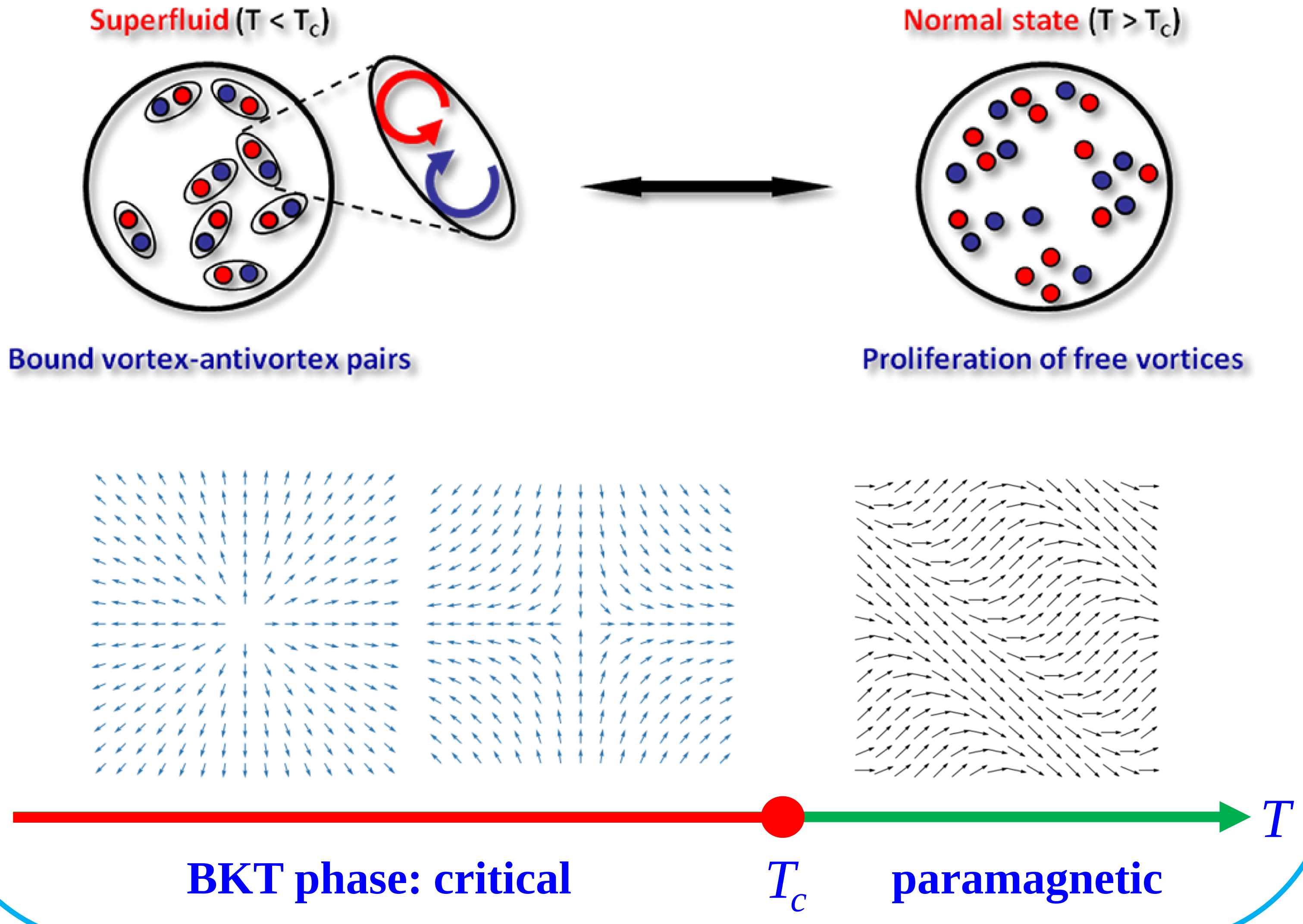
$$H = -\sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$

Berezinkii

Thouless



Kosterlitz



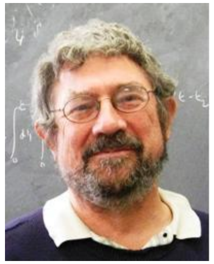
Effective Low Energy Theory

XY-model

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

Berezinkii

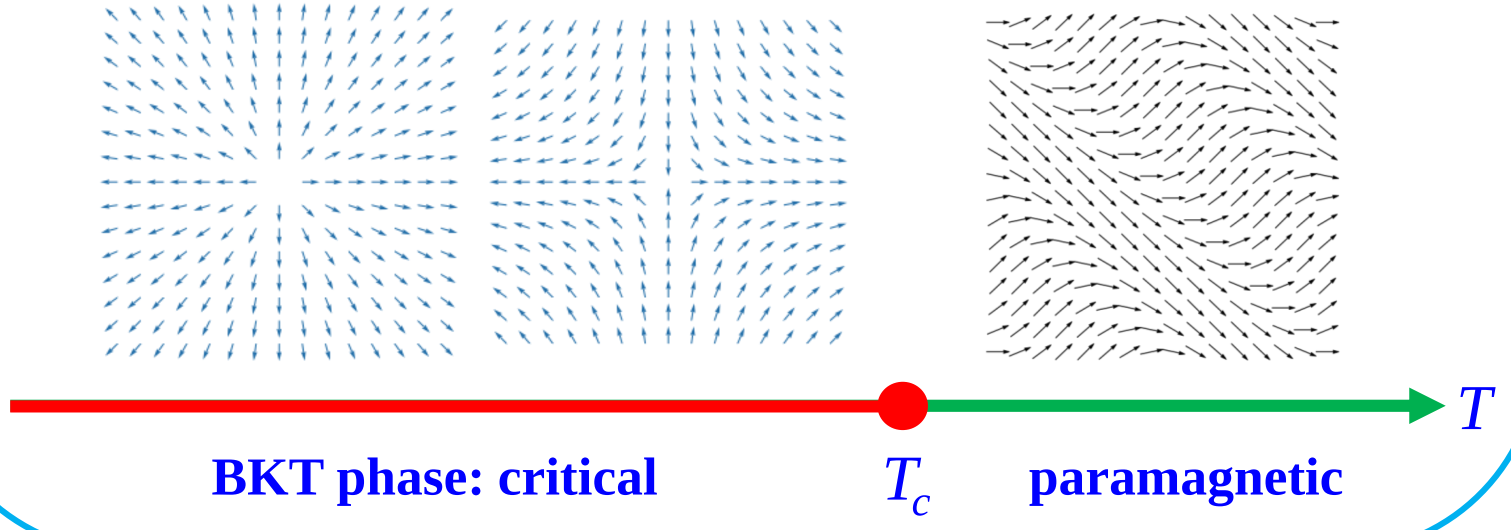
Thouless



Kosterlitz

Sine-Gordon Model:

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



Scaling Dimension Δ

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

$\Delta < 2$ relevant

$\Delta = 2$ marginal

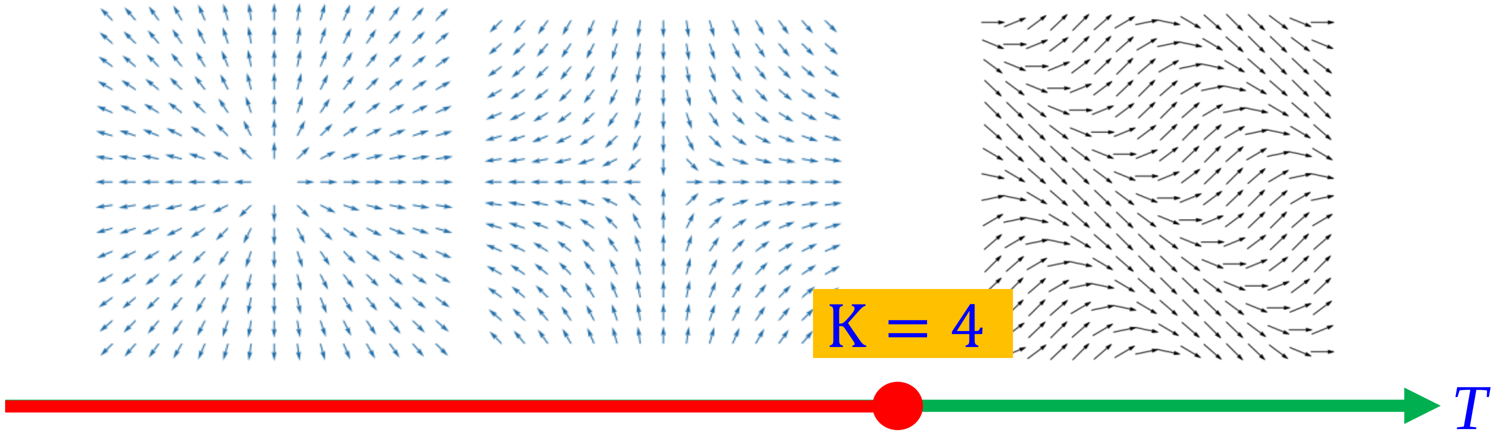
$\Delta > 2$ irrelevant

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**



BKT phase: critical T_c **paramagnetic**

Central Charge c

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

$\Delta < 2$ relevant

$\Delta = 2$ marginal

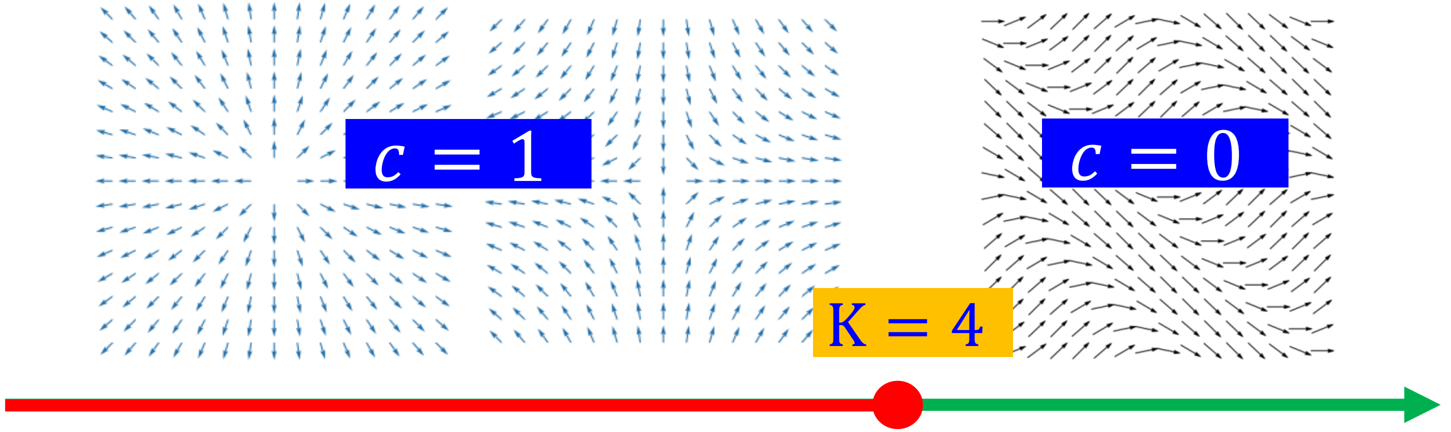
$\Delta > 2$ irrelevant

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



BKT phase: critical T_c **paramagnetic**

q-state Clock Model: Large q Limit

$$S = \underbrace{\underbrace{\frac{1}{2\pi K}\int d^2r(\nabla\varphi)^2 + \frac{g_1}{2\pi}\int d^2r\cos(\sqrt{2}\,\varphi)}_{\text{XY Model}} + \frac{g_2}{2\pi}\int d^2r\cos(q\sqrt{2}\,\theta)}_{\text{Clock Model}}$$

$\boldsymbol{\theta}$ is dual to $\boldsymbol{\varphi}$: $\partial_x\varphi = -\partial_y(K\theta)$ $\partial_y\varphi = \partial_x(K\theta)$

P. B. Wiegmann, J. Phys. C 11, 1583(1978)

q-state Clock Model: Large q Limit

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

Scaling dimension

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

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

$\Delta < 2$ relevant

$\Delta = 2$ marginal

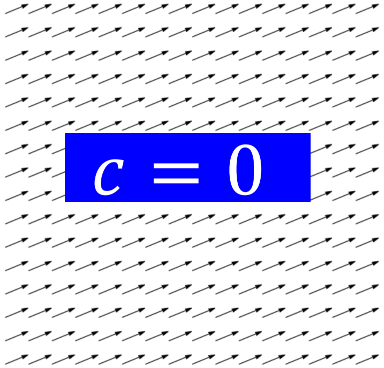
$\Delta > 2$ irrelevant

q-state Clock Model: Large q Limit

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

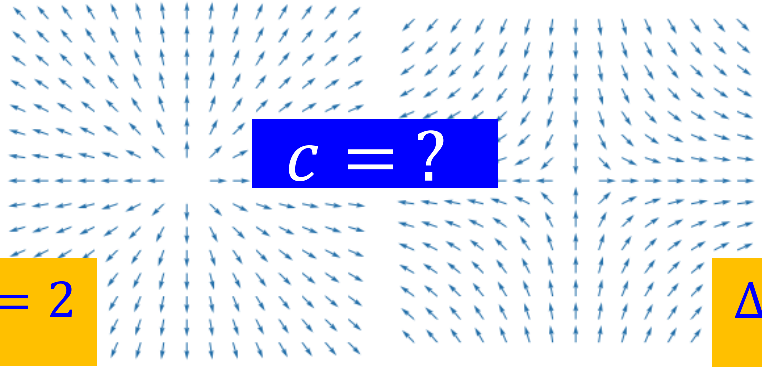
$\Delta_{\cos(\sqrt{2}\varphi)} > 2$

$\Delta_{\cos(q\sqrt{2}\theta)} < 2$



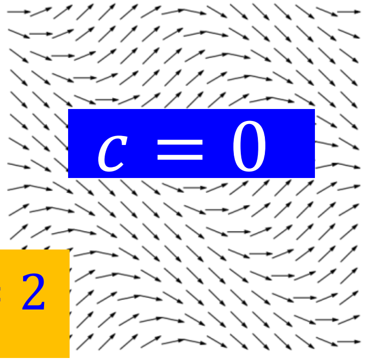
$\Delta_{\cos(\sqrt{2}\varphi)} > 2$

$\Delta_{\cos(q\sqrt{2}\theta)} > 2$



$\Delta_{\cos(\sqrt{2}\varphi)} < 2$

$\Delta_{\cos(q\sqrt{2}\theta)} > 2$



$\Delta_{\cos(q\sqrt{2}\theta)} = 2$

$\Delta_{\cos(\sqrt{2}\varphi)} = 2$

T

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

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

When K = q, $g_1 = g_2$, the model is invariant under dual transformation

$$\varphi \leftrightarrow q\theta$$

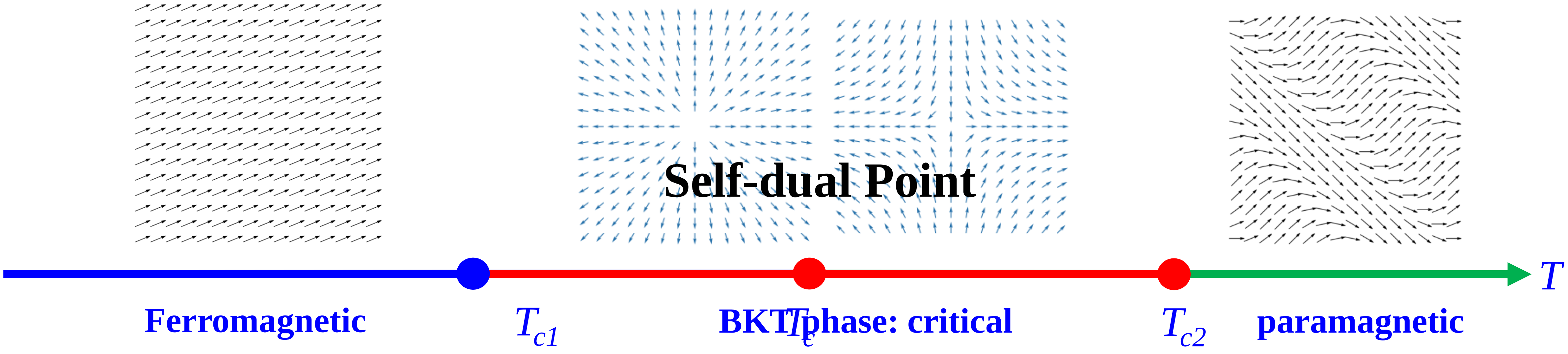
At the self-dual point

$$\Delta_{\cos(\sqrt{2}\varphi)} = \Delta_{cos(q\sqrt{2}\theta)} = \frac{q}{2} \to K_{sd} = q$$

The self-dual point is a critical point for $q \leq 4$
The self-dual point is not a critical point when $q > 4$

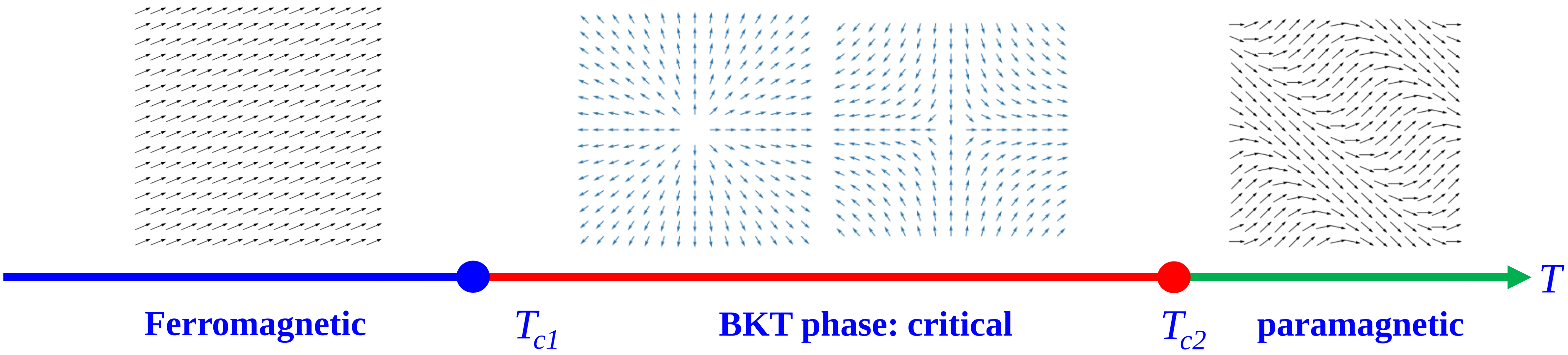
q-state Clock Model: Small q Limit

q	T_c	c	
2	$2\ln^{-1}(1+\sqrt{2})$	1/2	Ising, Majorana fermion
3	$(3/2)\ln^{-1}(1+\sqrt{3})$	4/5	Z_3 Parafermion
4	$\ln^{-1}(1+\sqrt{2})$	1	Two copies of Ising



q-state Clock Model: Intermediate q (≥ 5)

1. Is the intermediate phase still a BKT phase?
2. Can the critical temperatures and conformal parameters (c and K) be accurately determined?



Critical Phase is Difficult to Study

- Marginal operators lead to strong finite size effect with logarithmic corrections

Spin-spin correlation function

$$\sim r^{1/4} \ln^{1/8} r$$

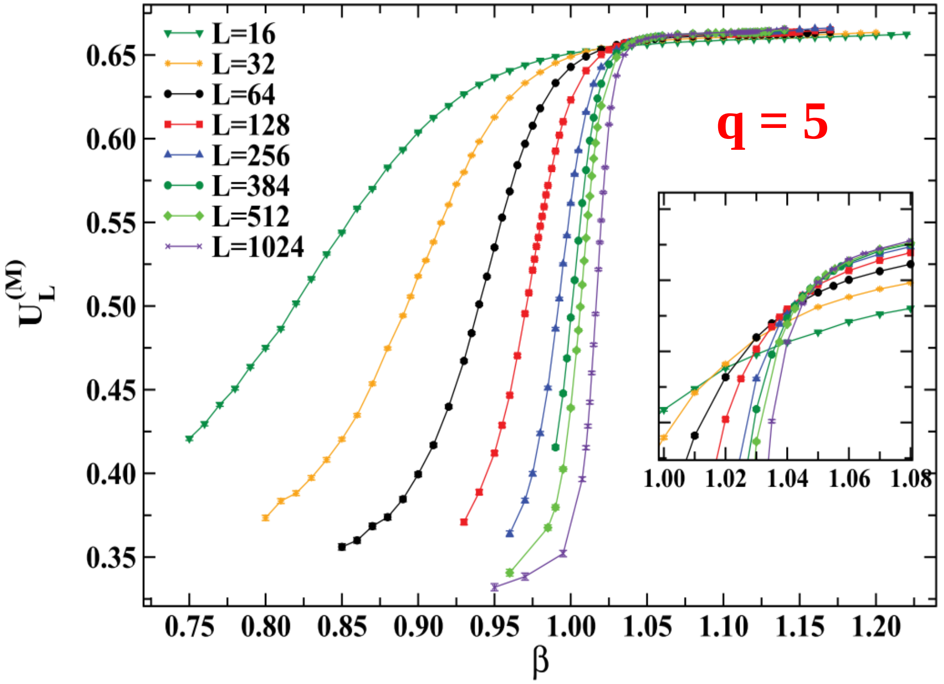
J M Kosterlitz, J. Phys. C 7, 1046 (1974)

- Correlation length diverges exponentially

$$\xi \sim \mathrm{e}^{a|T-T_{BKT}|^{-1/2}} \qquad T > T_{BKT}$$

Monte Carlo: Binder Ratio

$$U_L^{(M)} = 1 - \frac{\langle M_L^4 \rangle}{3\langle M_L^2 \rangle^2}$$



Borisenko et. al., PRE 83, 041120(2011)

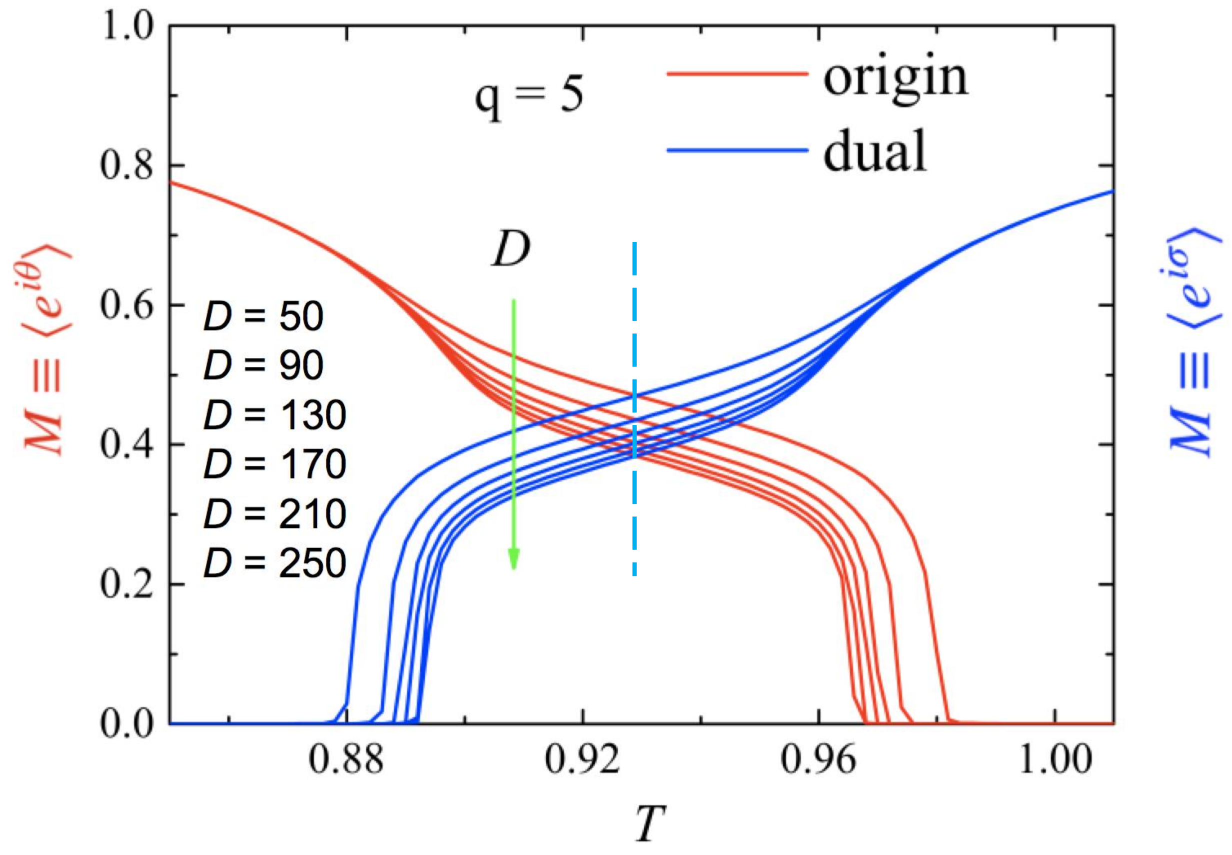
Critical Temperatures

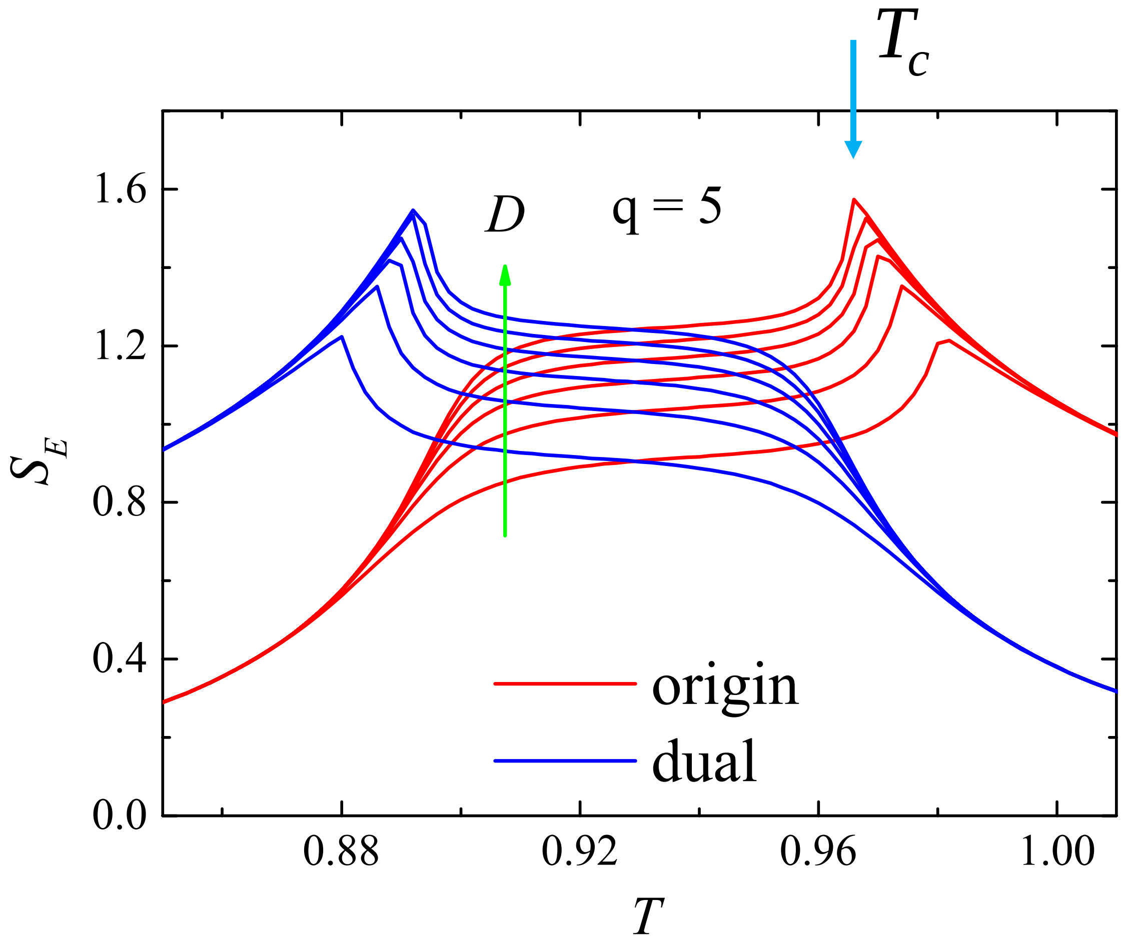
$q = 5$	T_{c1}	T_{c2}	Method
Tobochnik, et.al., PRB(1982)	0.8	1.1	MC
Borisenko, et.al., PRE(2011)	0.905(1)	0.951(1)	MC
Kumano, et.al., PRB(2013)	0.908	0.944	HTSE
Chatelain, et.al., JSM(2014)	0.914(12)	0.945(17)	DMRG
Chatterjee, et.al., PRE(2018)	0.897(1)	-	MC
Chen, et.al., CPB(2018)	0.9029(1)	0.9520(1)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

Critical Temperatures

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

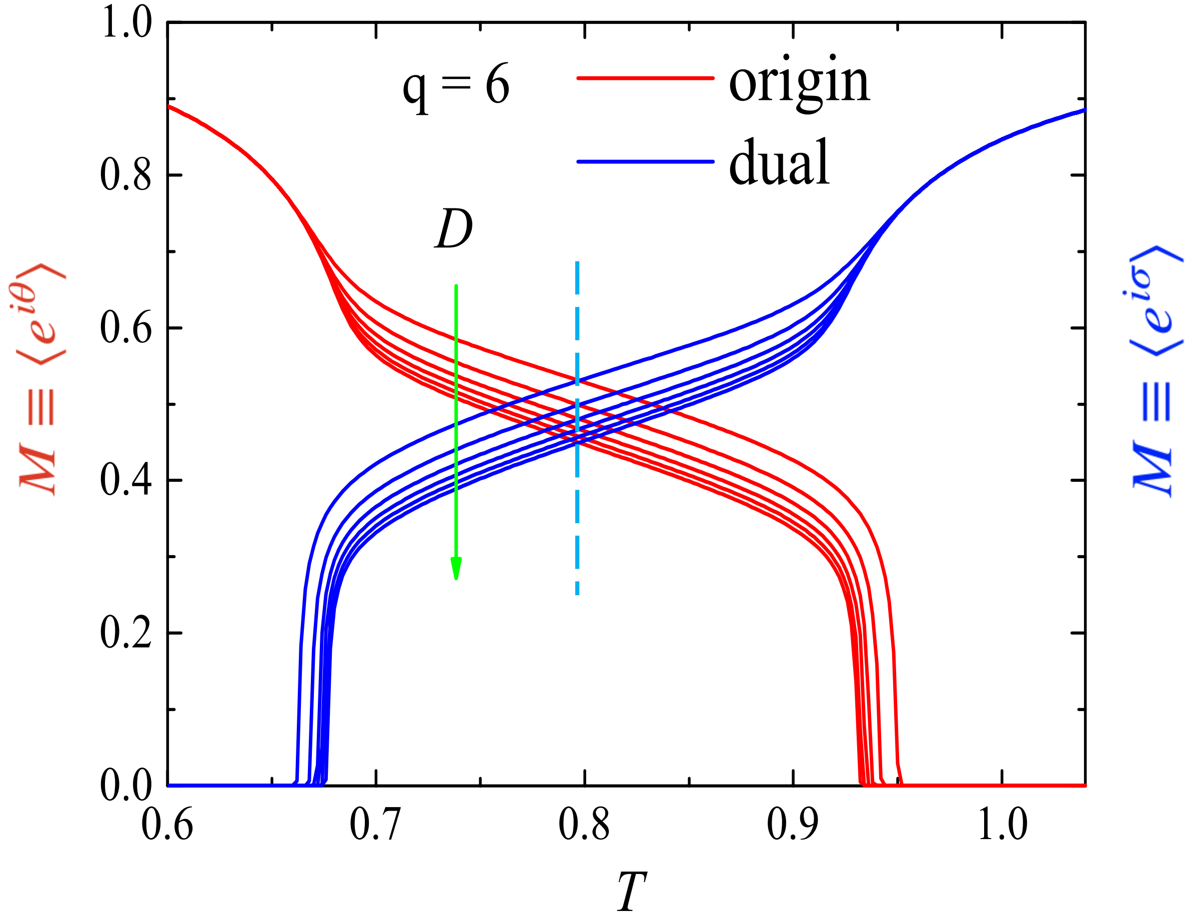
Magnetization and Entanglement Entropy

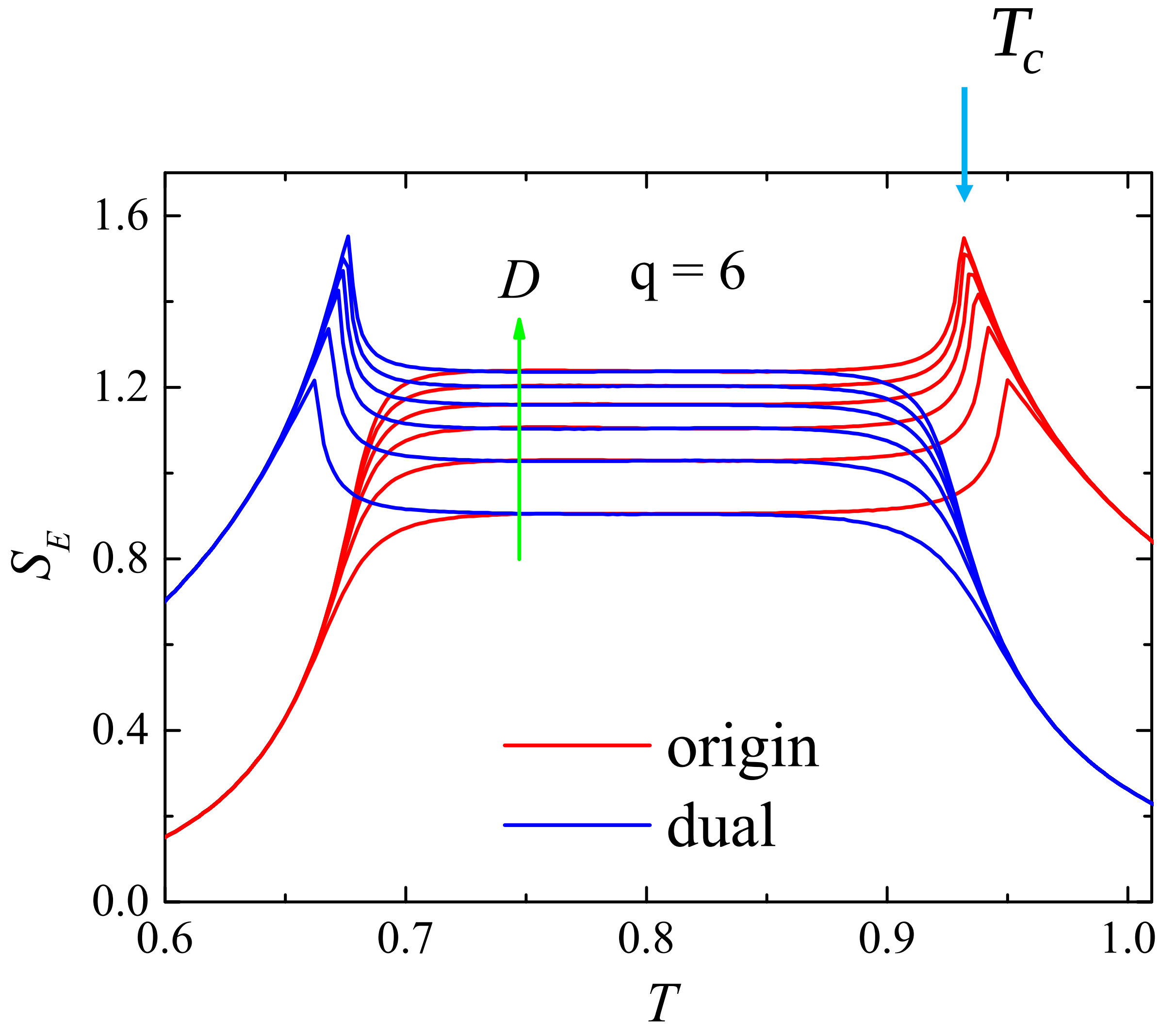




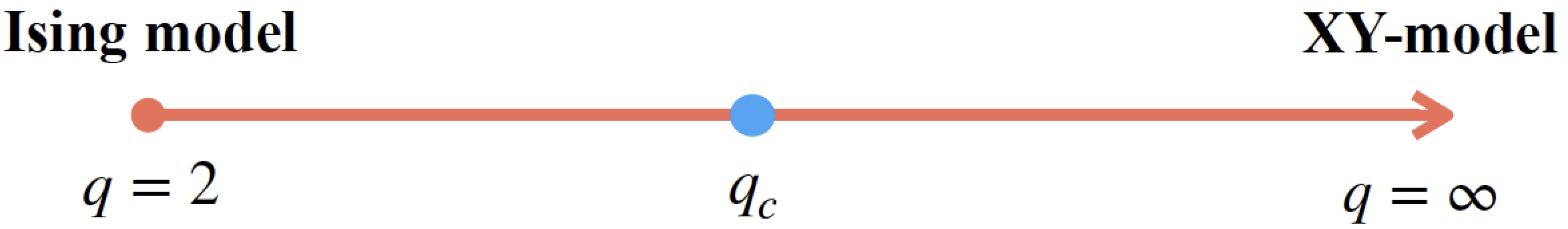
Peak positions determine the critical temperatures

Magnetization and Entanglement Entropy





What is the critical q for the BKT transition?



Field theory: $q_c = 5$

J. V. Jose, et.al., PRB 16,1217(1977).
S. Elitzur, et.al., PRD 19,3698(1979).

Monte Carlo: $q_c = 8$

C. M. Lapilli, *et.al.*, PRL 96, 140603 (2006)

Monte Carlo: $q_c = 7$

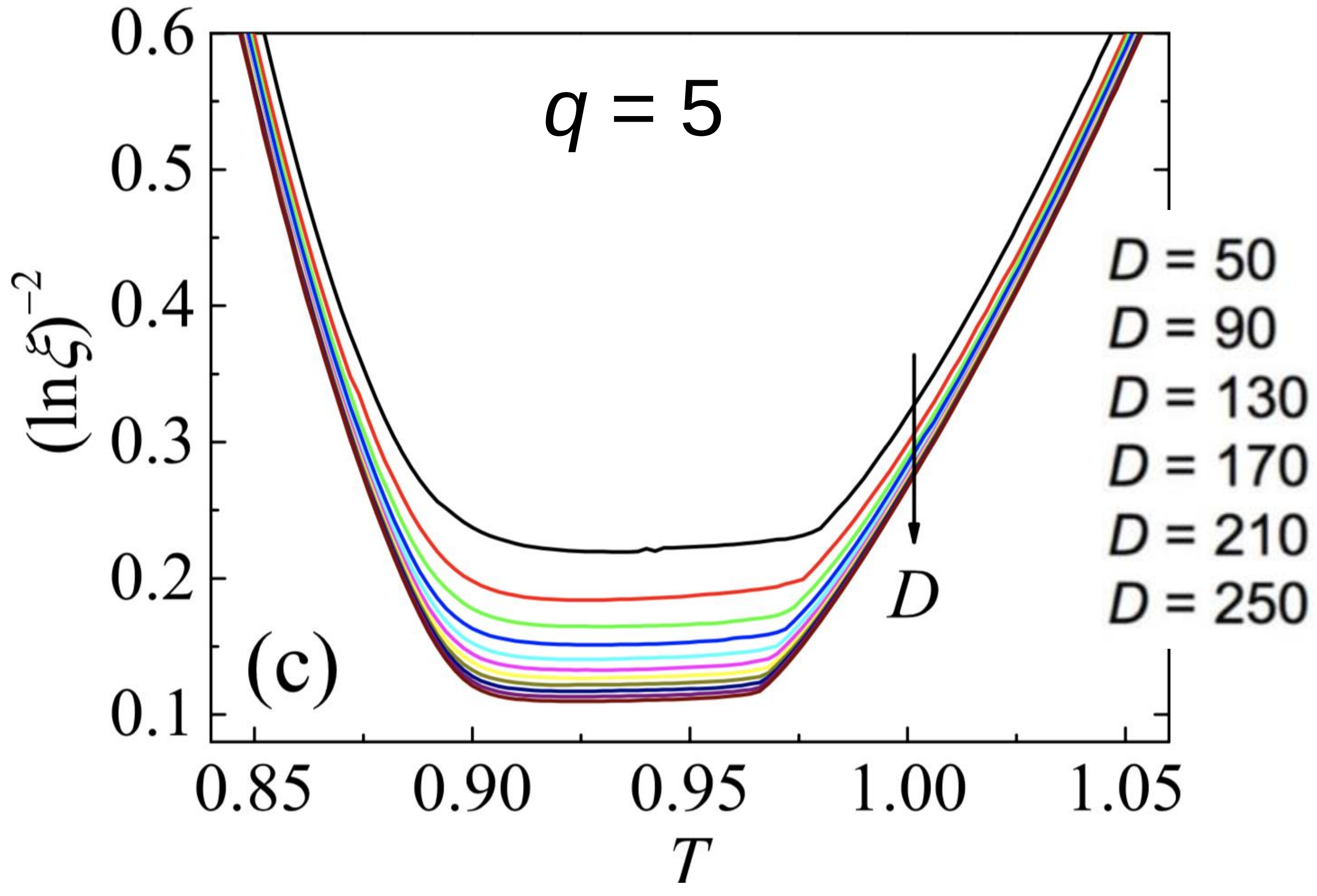
C. Hwang, PRE. 80.042103(2009)

Monte Carlo: $q_c = 6$

S. Baek, *et.al.*, PRE.88.012125(2013)

BKT signature: Exponentially Diverging Correlation Length

$$\xi \sim e^{a|T-T_c|^{-1/2}} \quad \rightarrow \quad (T - Tc) \sim \ln^{-2}\xi$$

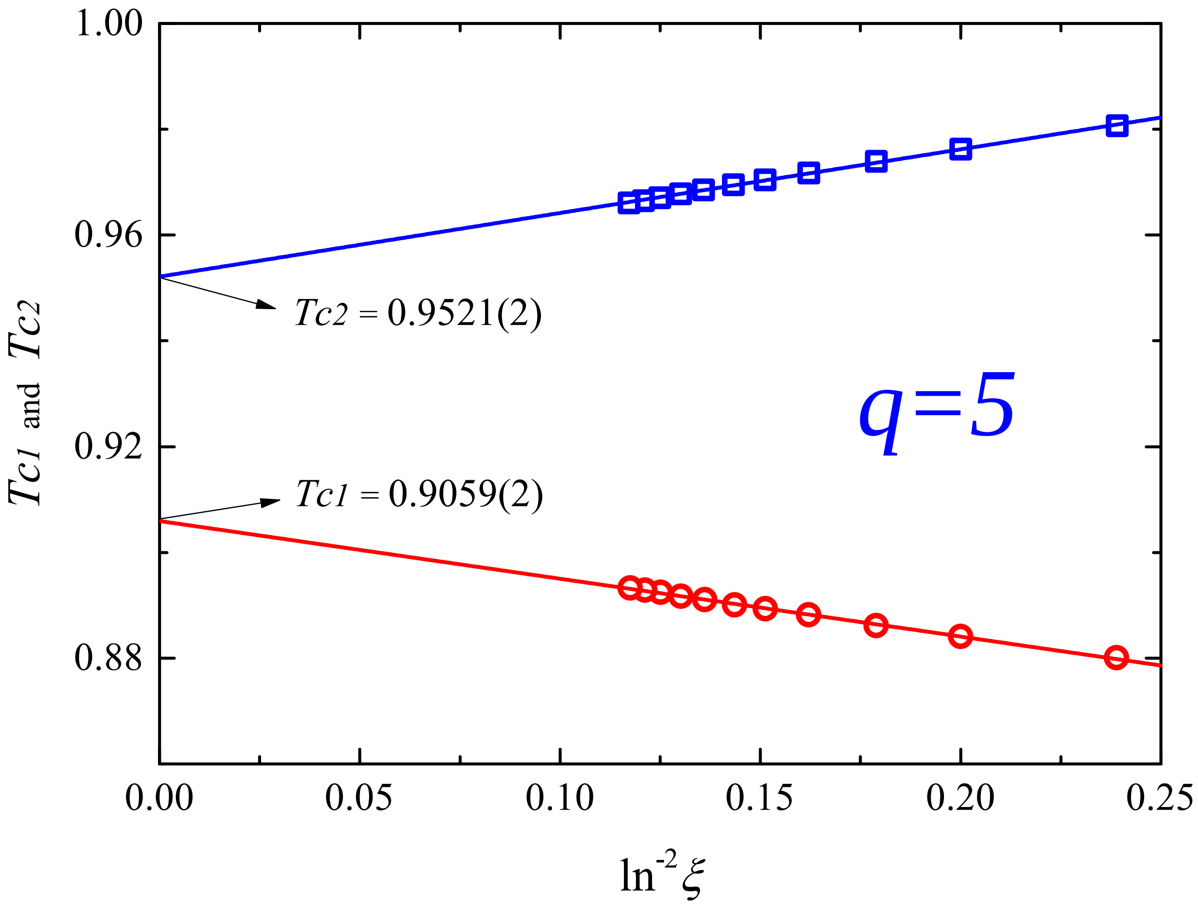


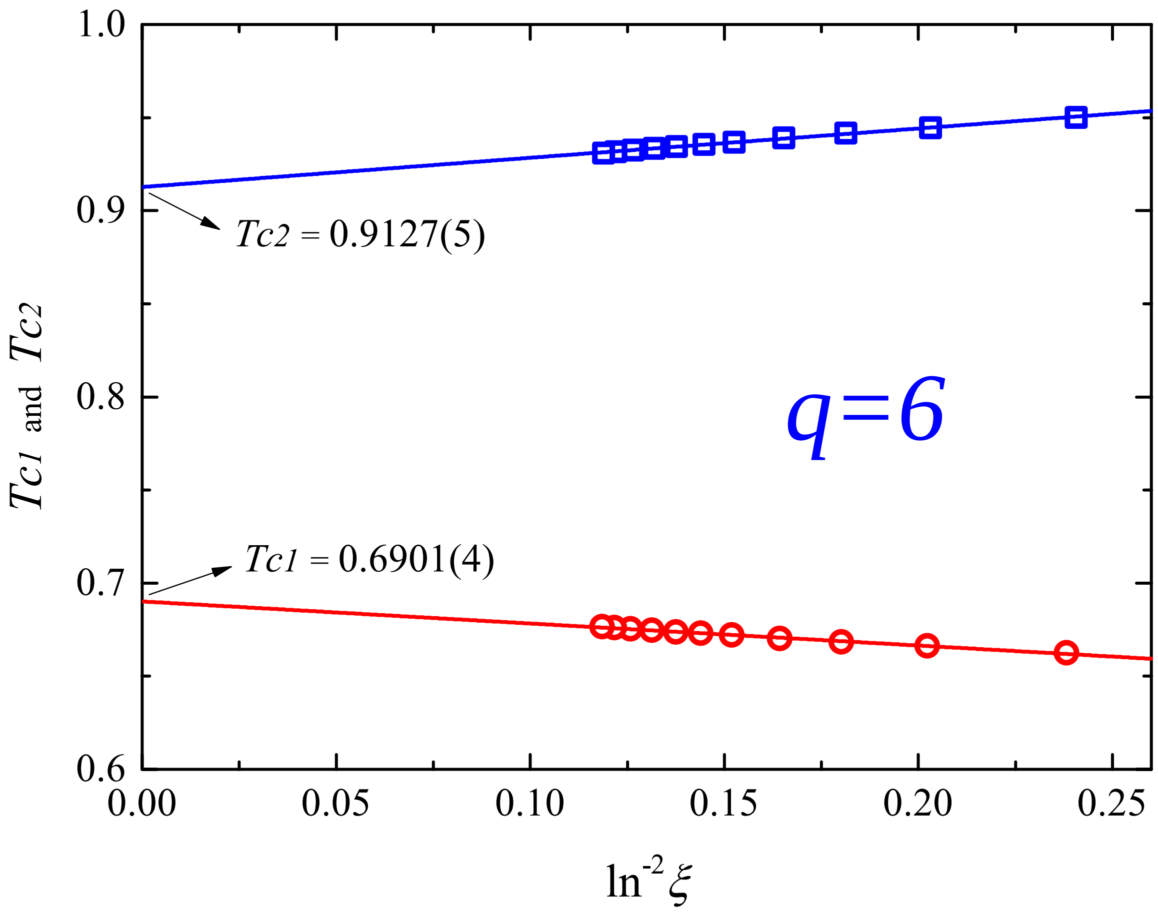
Exponential divergence of the correlation length suggests that the critical transition is BKT like and

$q_c = 5$

Two Critical Temperatures

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

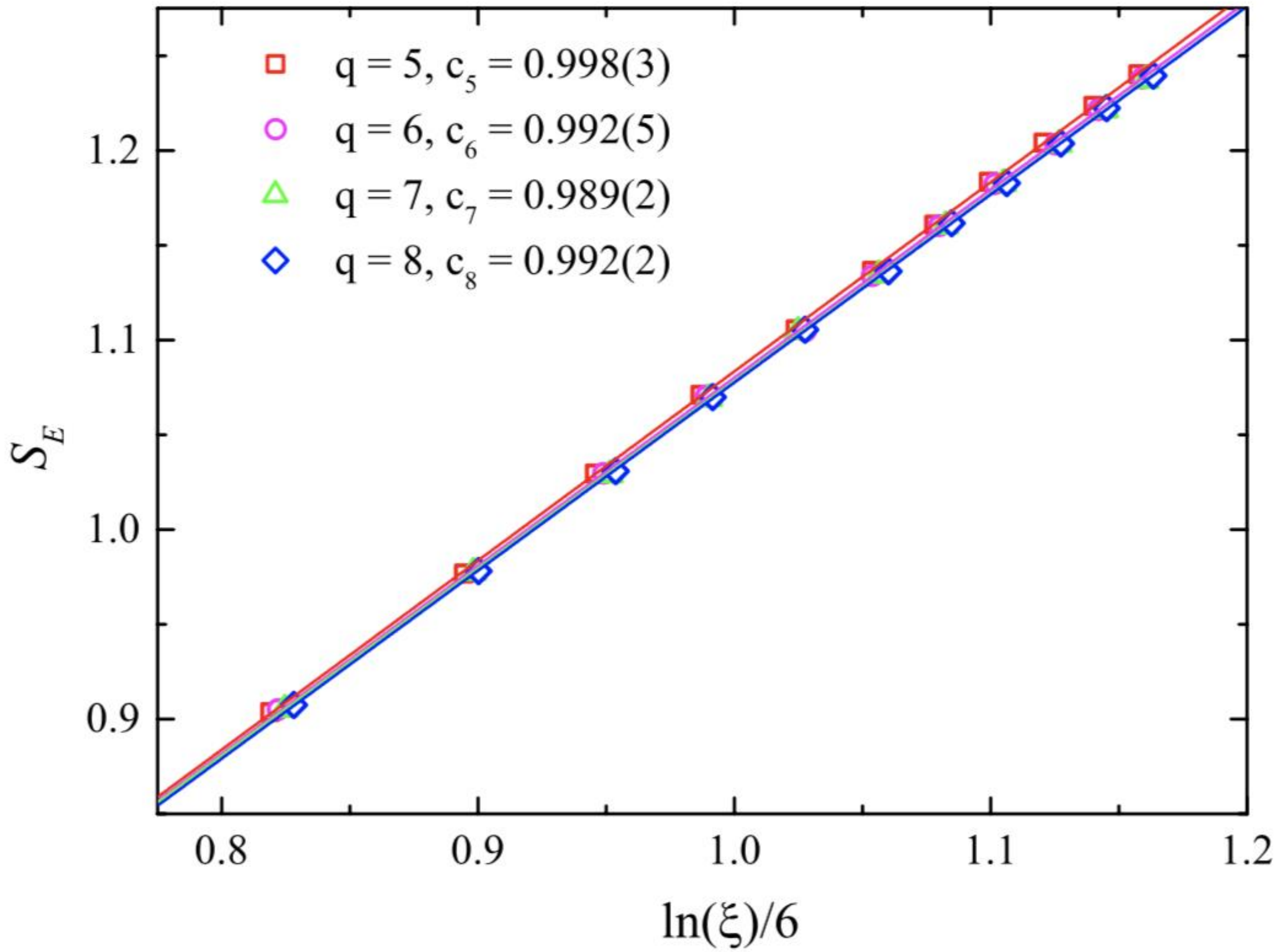




Critical Temperatures

$q = 5$	T_{c1}	T_{c2}	Method
Tobochnik, et.al., PRB(1982)	0.8	1.1	MC
Borisenko, et.al., PRE(2011)	0.905(1)	0.951(1)	MC
Kumano, et.al., PRB(2013)	0.908	0.944	HTSE
Chatelain, et.al., JSM(2014)	0.914(12)	0.945(17)	DMRG
Chatterjee, et.al., PRE(2018)	0.897(1)	-	MC
Chen, et.al., CPB(2018)	0.9029(1)	0.9520(1)	HOTRG
Surungan, et.al., arXiv(2019)	0.911(5)	0.940(5)	MC
Seongpyo, et.al., arXiv(2019)	0.908	0.945	HOTRG
Current work	0.9059 (2)	0.9521(2)	TMRG

Central Charge c ~ 1



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

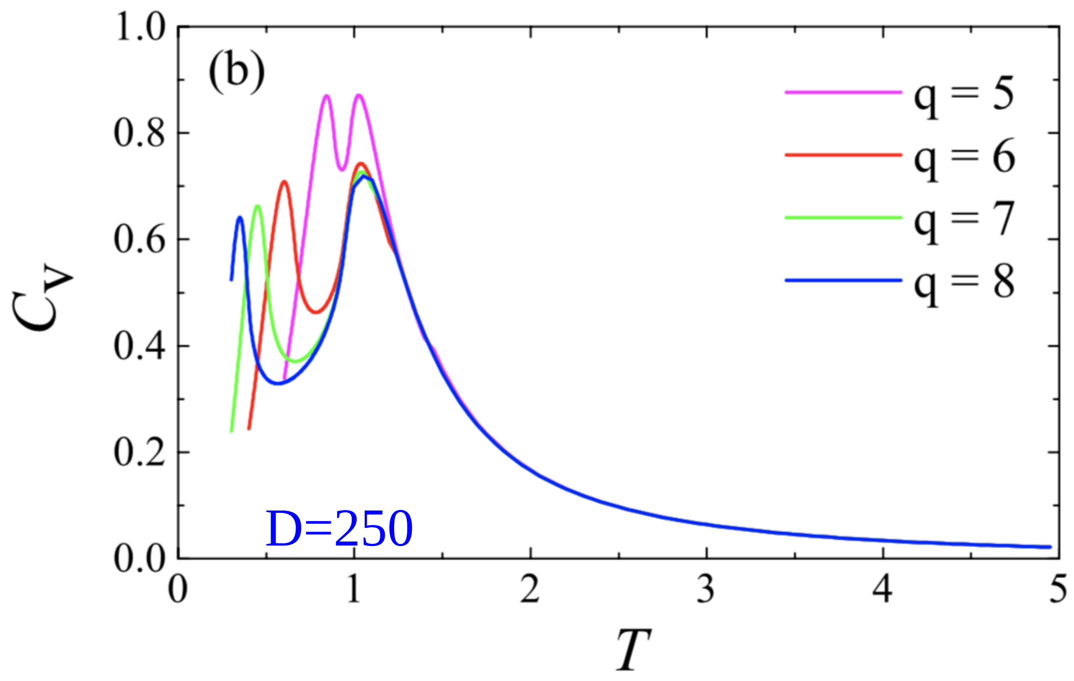
Calabrese & Cardy, J Stat Mech (2004)

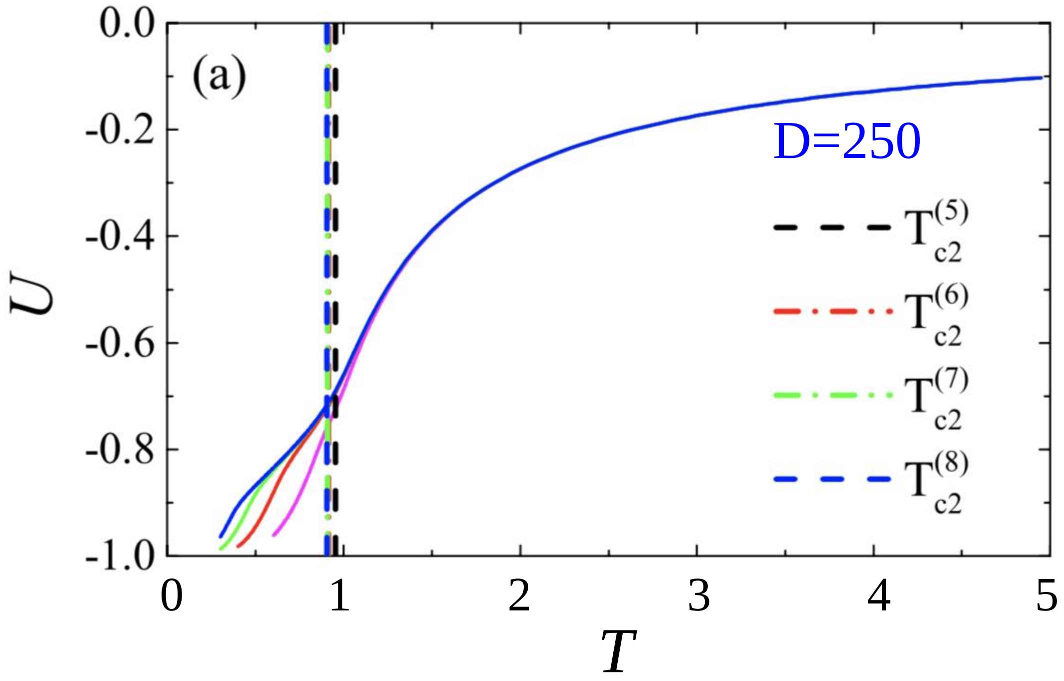
q = 5	T = 0.928
q = 6	T = 0.794
q = 7	T = 0.693
q = 8	T = 0.614

Inside the critical phase

High-temperature Behaviors

Thermodynamic observables are q-independent





irrelevant

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

C. M. Lapilli, *et.al.*, PRL 96, 140603 (2006)

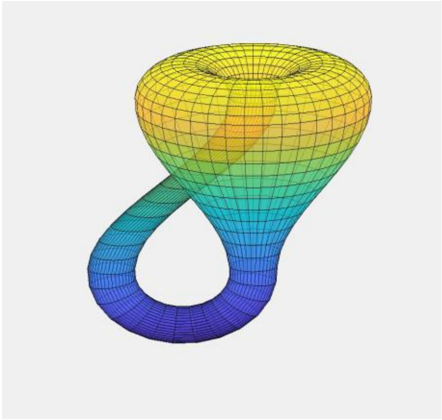
Determination of Luttinger Parameter K

- 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

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



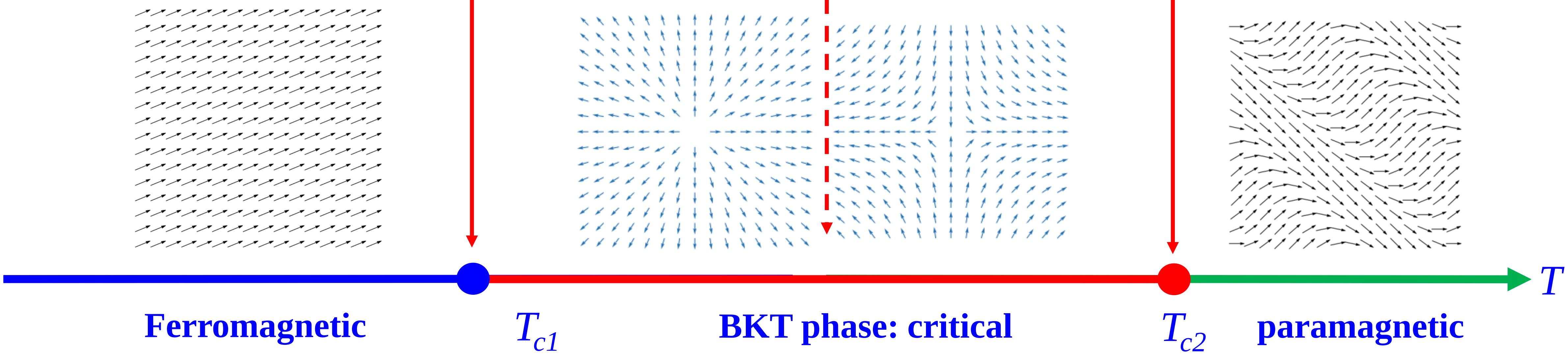
H.H. Tu, PRL 119, 261603 (2017)
W. Tang, *et.al.*, PRB 99, 115105 (2019)

Prediction of Conformal Field Theory ($q \to \infty$)

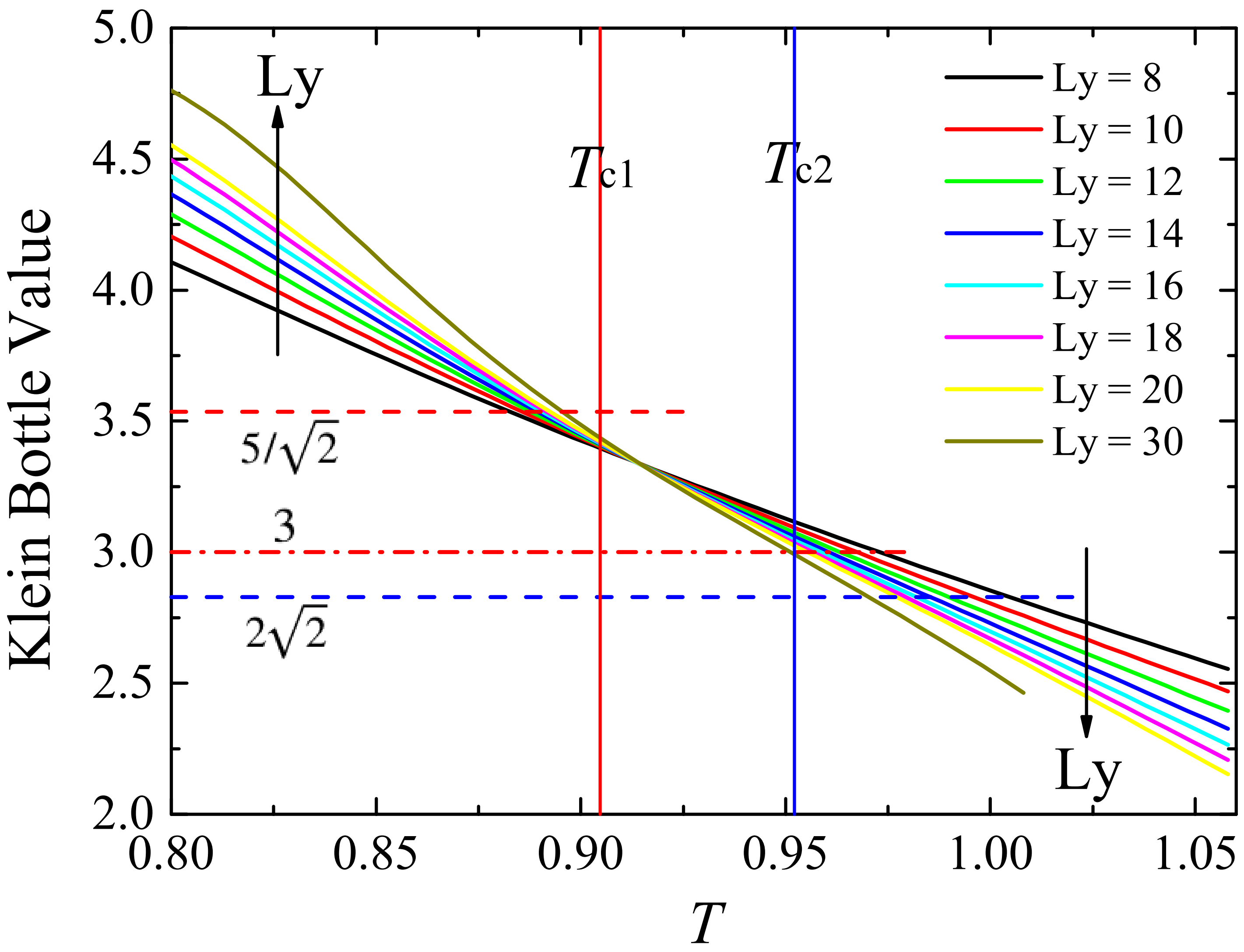
$$R(T_{\text{self dual}}) = \sqrt{2q}$$

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

$$R(T_{c2}) = 2\sqrt{2}$$



Luttinger Parameter (q=5)

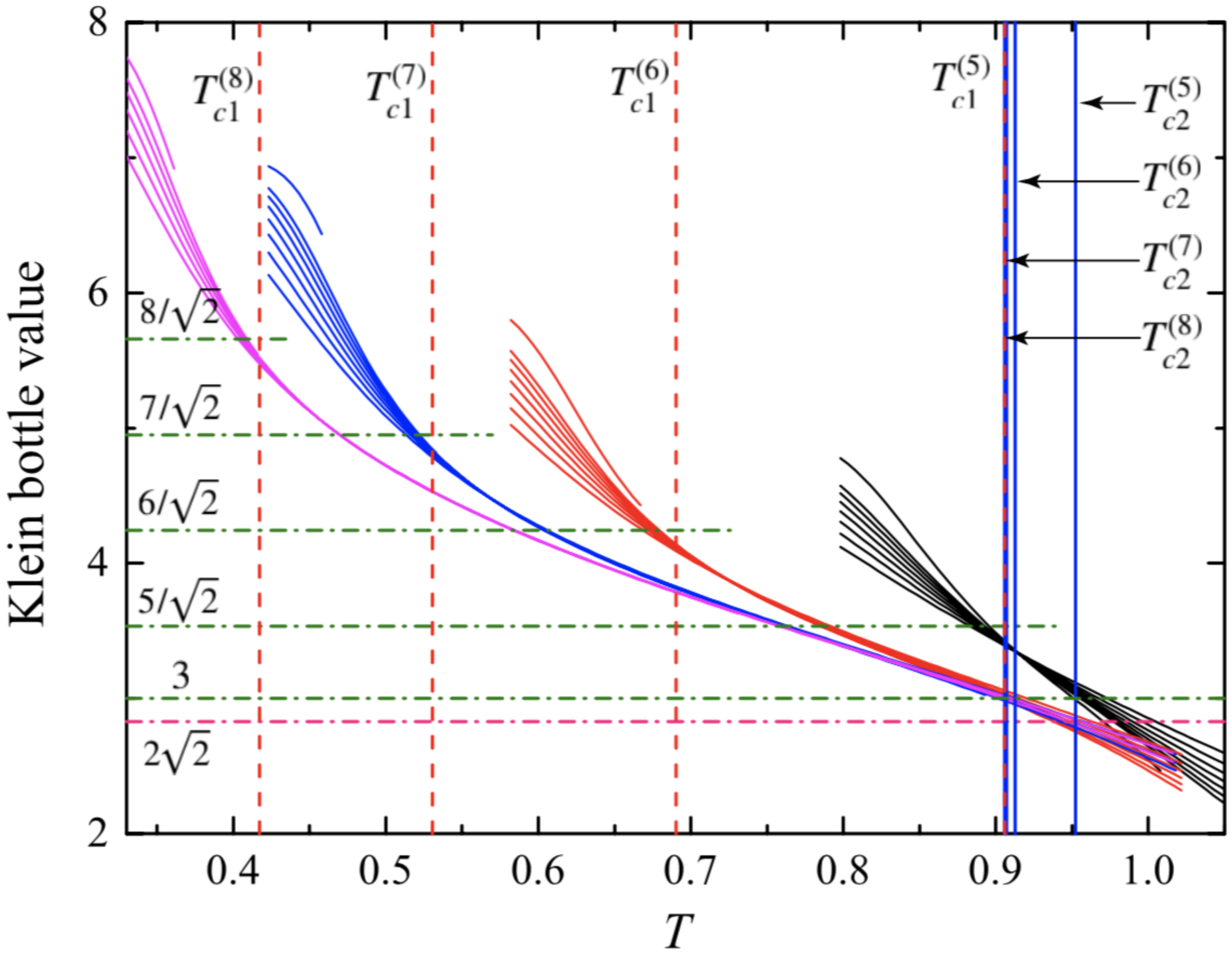


$$R(T_{c2}) = 2\sqrt{2}$$

$$R(T_{c1}) = \frac{5}{\sqrt{2}}$$

Discrepancy are mainly caused by the marginal terms

Luttinger Parameter

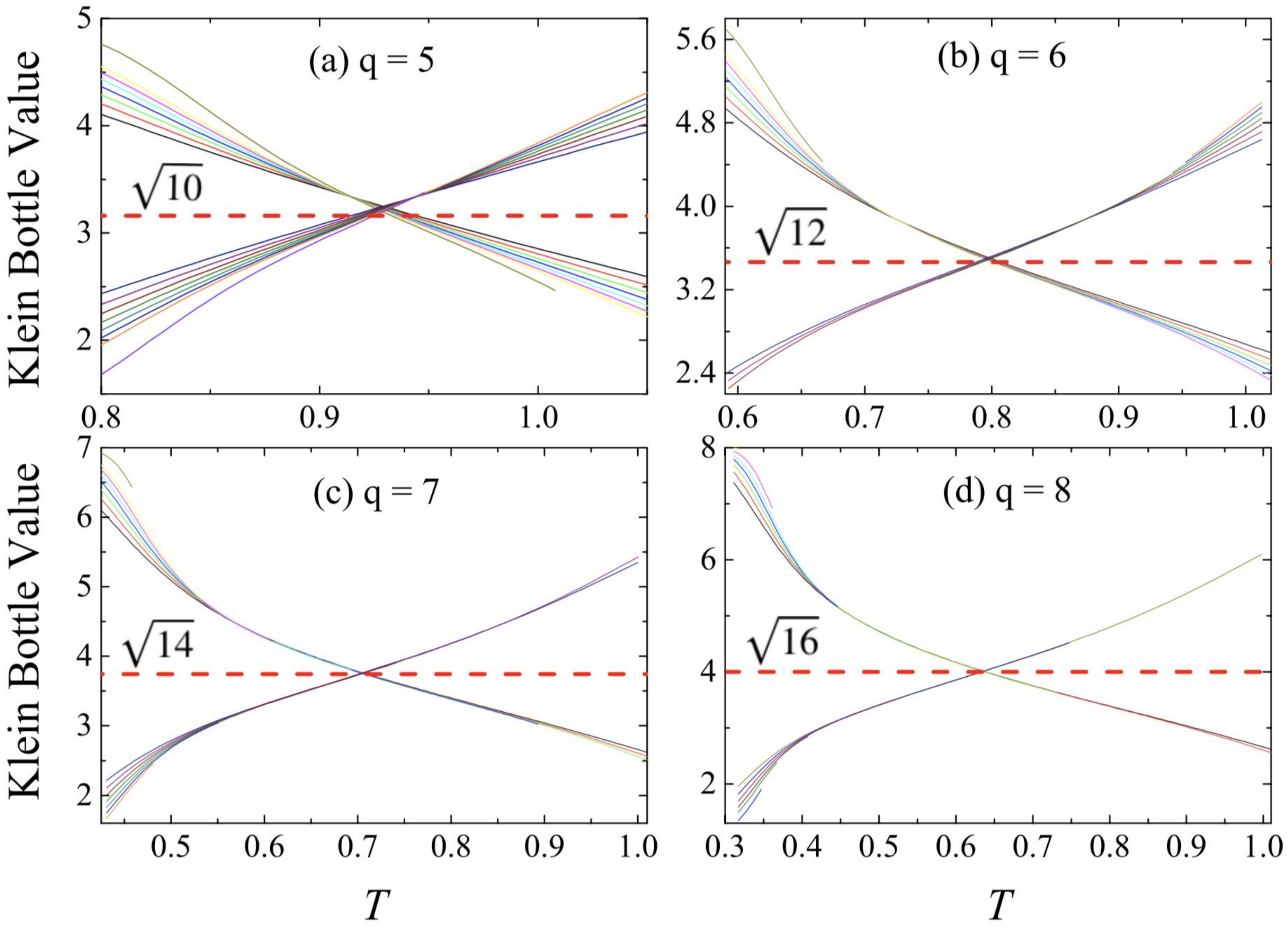


$$R(T_{c2}) = 2\sqrt{2}$$

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

Discrepancy are mainly caused by the marginal terms

Luttinger Parameter at the Self-dual Point



$$R(T_{\mathrm{self\,dual}}) = \sqrt{2q}$$

Discrepancy becomes smaller and smaller with increasing q

Summary

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

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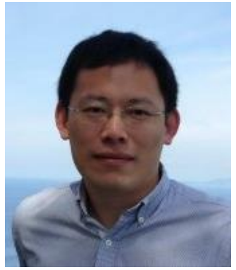

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