

Entanglement Scaling and Criticality with Tensor Networks  
at Bernoulli Center,

EPFL

#epflcampus

Nov 28—Dec 2, 2022

Finite-Size “Level Spectroscopy” Approach  
with Tensor Network Renormalization

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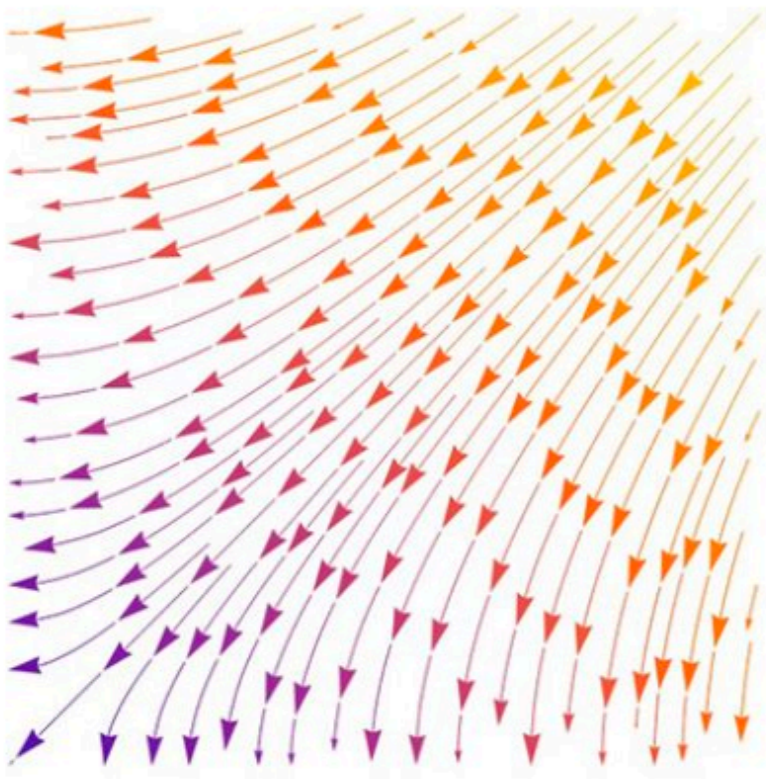
## Tensor Networks:

very powerful numerical/conceptual tool to study quantum many-body systems & stat mech

## Finite “bond dimension”:

TN can describe limited **entanglement**/correlation length  
how to study **critical phenomena**?

- change the topology of the Tensor Networks  
(MERA, etc.)
- **finite-size scaling,**  
**in particular of Transfer Matrix spectra**  
**using Tensor Networks**



Atsushi Ueda

**EDITORS' SUGGESTION**

## Resolving the Berezinskii-Kosterlitz-Thouless transition in the two-dimensional XY model with tensor-network-based level spectroscopy

The discovery of the Berezinskii-Kosterlitz-Thouless transition some fifty years ago was a subject of the 2016 Nobel Prize in Physics. However, quantitative study of the transition in the two-dimensional XY spin model still suffers from significant finite-size effects. The authors implement the level-spectroscopy method, originally developed for quantum systems. They utilize the modern tensor-network renormalization scheme. This allows for an extremely accurate determination of the critical point as well as for a visualization of the celebrated Kosterlitz renormalization-group flow.

Atsushi Ueda and Masaki Oshikawa

[Phys. Rev. B \*\*104\*\*, 165132 \(2021\)](#)

**+ Phys. Rev. E **106**, 014104 (2022)**

**+ in preparation**

# The Nobel Prize in Physics 2016

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David J. Thouless

Prize share: 1/2



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F. Duncan M. Haldane

Prize share: 1/4



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J. Michael Kosterlitz

Prize share: 1/4

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The Nobel Prize in Physics 2016 was awarded with one half to David J. Thouless, and the other half to F. Duncan M. Haldane and J. Michael Kosterlitz "for theoretical discoveries of topological phase transitions and topological phases of matter."

# “Topological Phase Transitions”

Prototype: Berezinskii-Kosterlitz-Thouless Transition  
which is also closely related to “Haldane Gap”

Canonical model for the BKT transition:  
2D classical XY model

$$H_{XY} = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$

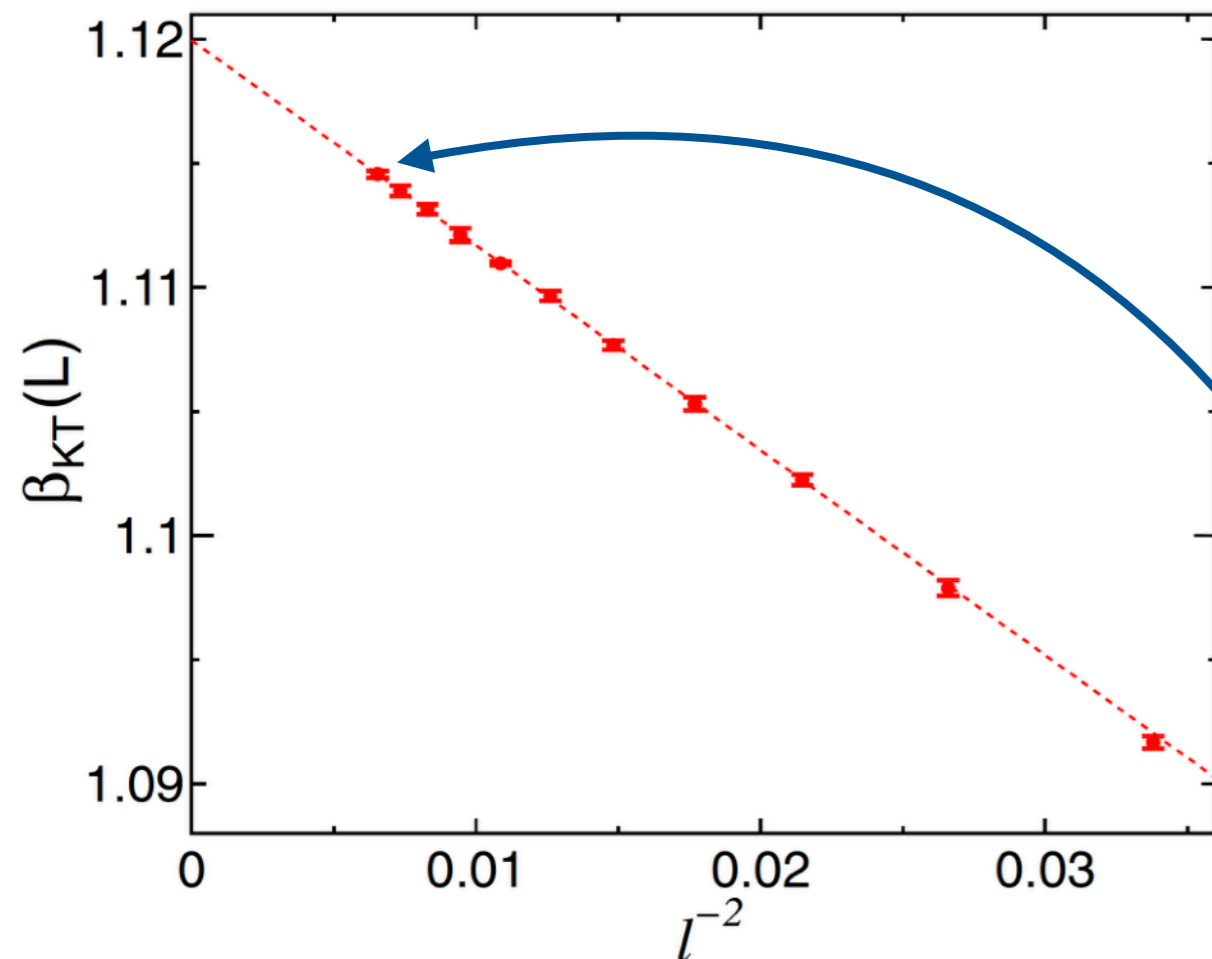
Classical stat mech: no negative sign problem, etc.  
Easily studied with Monte Carlo, right?

# Large-Scale Monte Carlo Simulation of Two-Dimensional Classical XY Model Using Multiple GPUs

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(Received August 27, 2012; accepted September 24, 2012; published online October 12, 2012)



finite-size scaling of  $T_c$

$$l = \ln bL$$

largest system:

$$L=65536$$

calculation using 256GPUs

# Sine-Gordon Field Theory for BKT

$$\mathcal{L} = \frac{1}{2\pi K} (\partial_\mu \phi)^2 - y_\kappa (\partial_\mu \phi)^2 + y_V V$$

$\theta$  angle of the XY spin  $\longleftrightarrow$   $\phi$   
dual (mutually non-local)  $\phi \sim \phi + \pi$   
 $\theta \sim \theta + 2\pi$

$$V = \cos 2\phi = \frac{1}{2} (e^{2i\phi} + e^{-2i\phi})$$

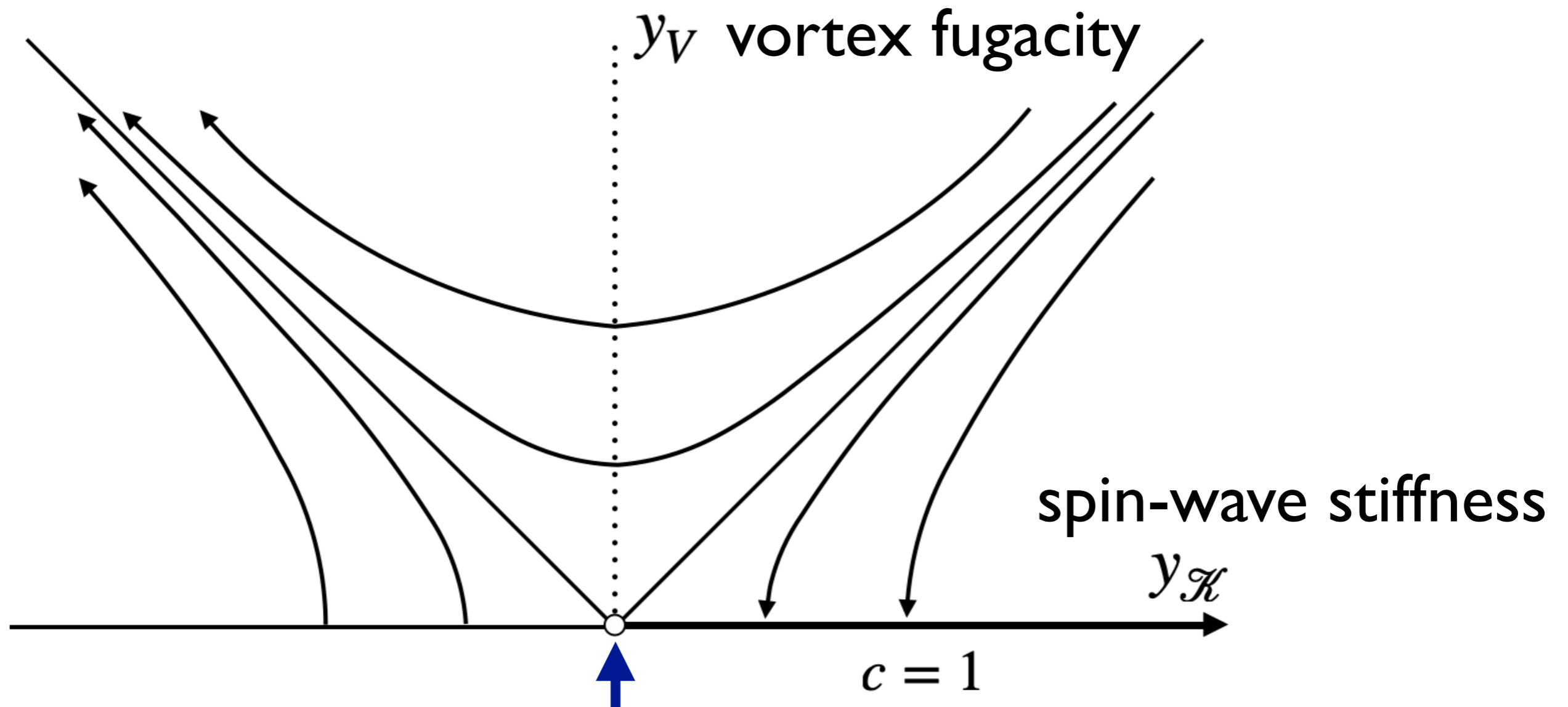
scaling dimension  $2/K$   
marginal at  $K=2$

Single vortex **creation** / **annihilation** operator

$y_V$  vortex fugacity

$y_\kappa$  renormalization of Luttinger parameter  $K$

# Kosterlitz RG Flow



Luttinger parameter  $K=2$  (vortex operator marginal)

BKT transition:  $y_V = y_K = g$

$$\frac{dg}{dl} = -g^2$$

$$g \sim \frac{1}{l} \sim \frac{1}{\ln L}$$

slow decay



log-corrections



# BKT Transition in $S=1/2$ XXZ Chain

$$\mathcal{H} = \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z)$$

Single vortex creation/annihilation operator

$$\cos 2\phi \sim (-1)^j \vec{S}_j \cdot \vec{S}_{j+1}$$

$$\sin 2\phi \sim (-1)^j S_j^z$$

Forbidden in Hamiltonian by the translation symmetry!

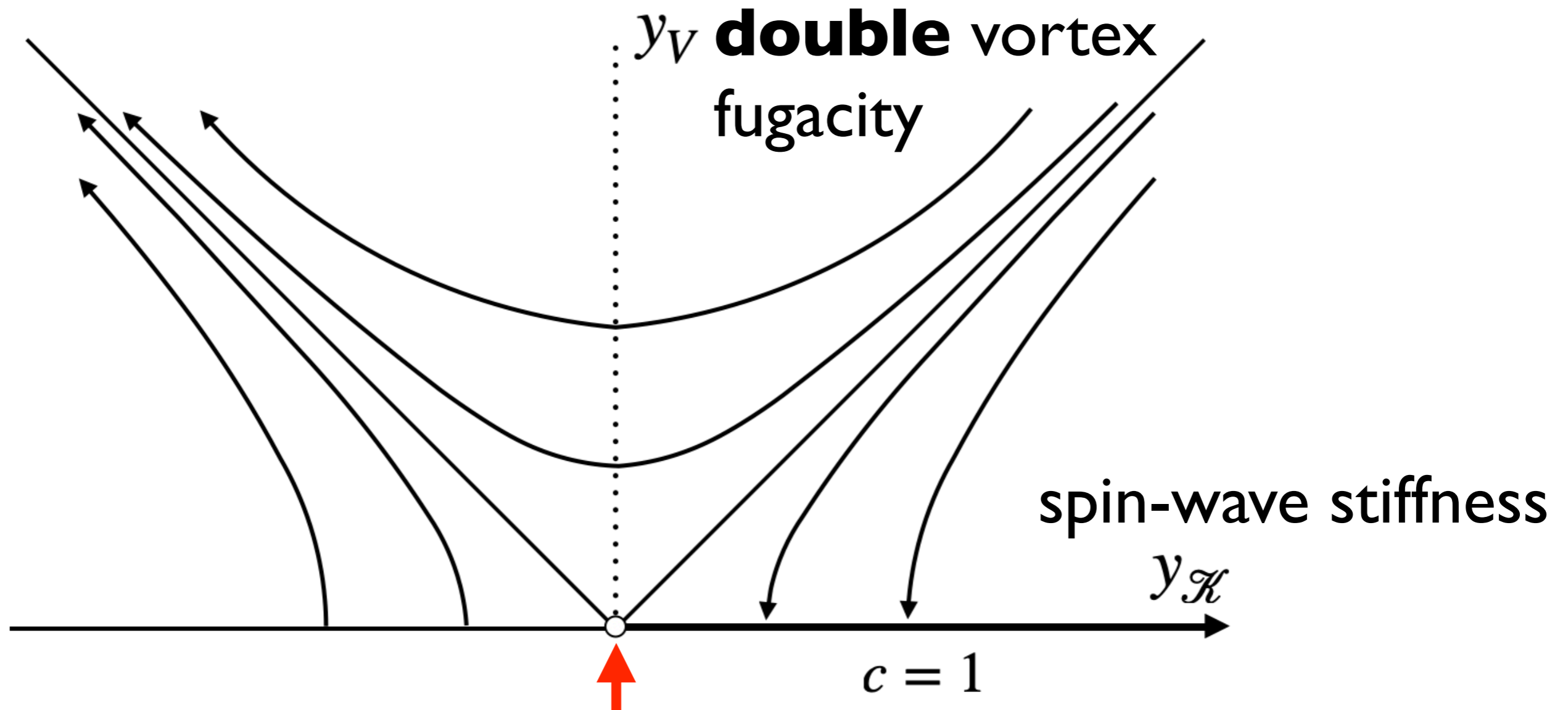
(**Haldane 1980** → “Haldane conjecture”

related to Lieb-Schultz-Mattis theorem etc.)

The leading (most relevant) perturbation is thus  
double vortex creation/annihilation op.  $\cos 4\phi$

# BTK Transition in $S=1/2$ XXZ Chain

$$\mathcal{L} = \frac{1}{2\pi K} (\partial_\mu \phi)^2 - y_{\mathcal{K}} (\partial_\mu \phi)^2 + y_V V \quad V = \cos 4\phi$$



Luttinger parameter  $K=1/2$   
(**double** vortex operator marginal)

# BKT Transition in $S=1/2$ XXZ Chain

$$\mathcal{H} = \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z)$$

BKT transition at  $\Delta=1$  (SU(2) symmetric point)

IR fixed point at the BKT transition:

Free boson (Tomonaga-Luttinger Liquid) at  $K=1/2$

equivalent to Level 1 SU(2) Wess-Zumino-Witten

Effective theory in the vicinity of the BKT transition

$$\mathcal{L} = \mathcal{L}_{k=1}^{\text{WZW}} + g \mathbb{J}^L \cdot \mathbb{J}^R + t \left( -\frac{1}{2} J_+^L J_+^R - \frac{1}{2} J_-^L J_+^R + J_z^L J_z^R \right)$$

$$y_V = g + t, y_\kappa = g - t$$

BKT transition  $\Leftrightarrow t=0 \Leftrightarrow$  SU(2) symmetry

# Level Spectroscopy

Determination of the critical point from the finite-size spectrum [Okamoto-Nomura 1994, ...]

“Double vortex” BKT transition at  $K=1/2$  can be identified by  $SU(2)$  symmetry of the finite-size spectrum!

State-operator correspondence and Finite-Size Scaling in CFT [Cardy 1984, 1986]

$$E_n - E_0 = \frac{2\pi}{L} \left( x_n + \sum_m c_{nnm} y_m L^{2-x_m} + \dots \right)$$

BKT transition  $\Leftrightarrow$

Energy levels form  $SU(2)$  singlet, triplet, ...

# 1D $S=1/2$ XXZ vs 2D Classical XY

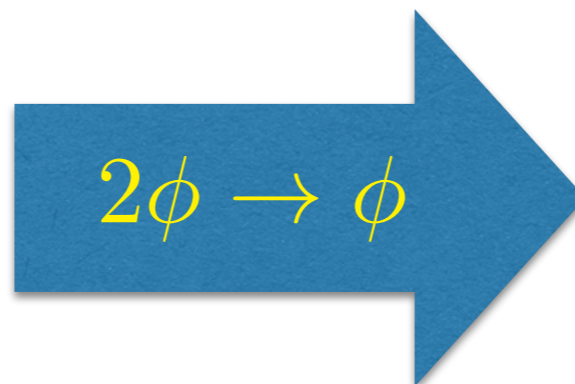
$$\mathcal{L} = \frac{1}{2\pi K} (\partial_\mu \phi)^2 - y_K (\partial_\mu \phi)^2 + y_V V$$

## $S=1/2$ XXZ

$K=1/2$  (SU(2)<sub>1</sub> WZW)

$$V \sim \cos 4\phi$$

double vortex op.



## Classical XY

$$K=2 \quad \phi \sim \phi + \pi$$

$$V \sim \cos 2\phi$$

single vortex op.

$$\cos 2\theta, \sin 2\theta, \sin \phi$$

half-vortex op.

(eigenstate under antiperiodic b.c.)

SU(2) triplet (degenerate at BKT)

$$n^x \sim \cos \theta, \quad n^y \sim \sin \theta, \quad n^z \sim \sin 2\phi$$

**Nomura-Kitazawa 1998**

# Level Spectroscopy for 2D Stat Mech

Level spectroscopy has been developed for quantum 1D,  
but why not for 2D stat mech models (such as XY)??

1D quantum Hamiltonian  $\Leftrightarrow$

Transfer matrix for 2D stat mech

Continuous spin: series expansion of Boltzmann weight

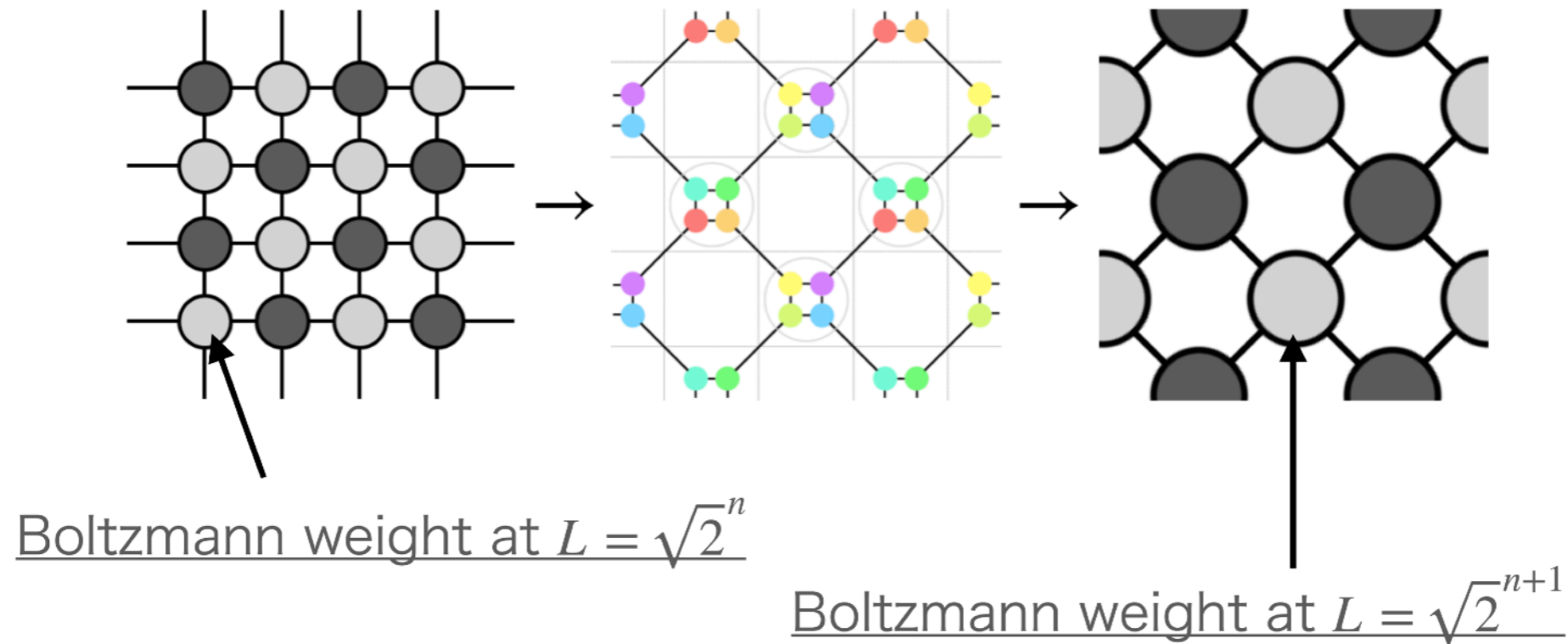
$$e^{\beta \cos(\theta_i - \theta_j)} = \sum_{n=-\infty}^{\infty} e^{in(\theta_i - \theta_j)} I_n(\beta),$$

the series may be  
truncated to  $-15 \leq n \leq 15$

Transfer matrix still “too large” to be diagonalized  
 $\Rightarrow$  we utilize Tensor Network Renormalization

(We used Loop-TNR)

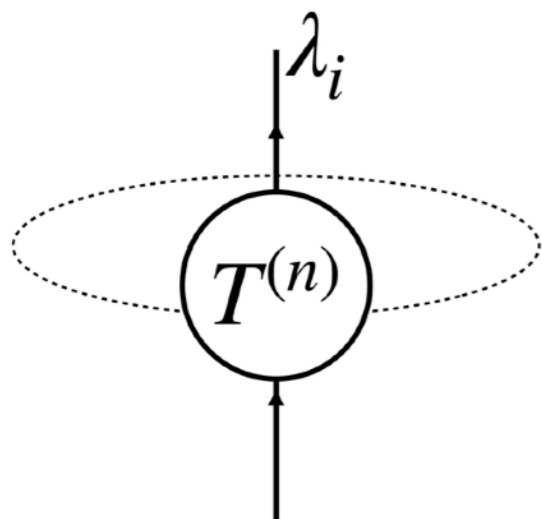
# TNR Construction of Transfer Matrix



after  $n$  steps, a single tensor represents  
a square block of linear size  $L = \sqrt{2}^n$

contract horizontal indices

$\Rightarrow$  transfer matrix in vertical direction

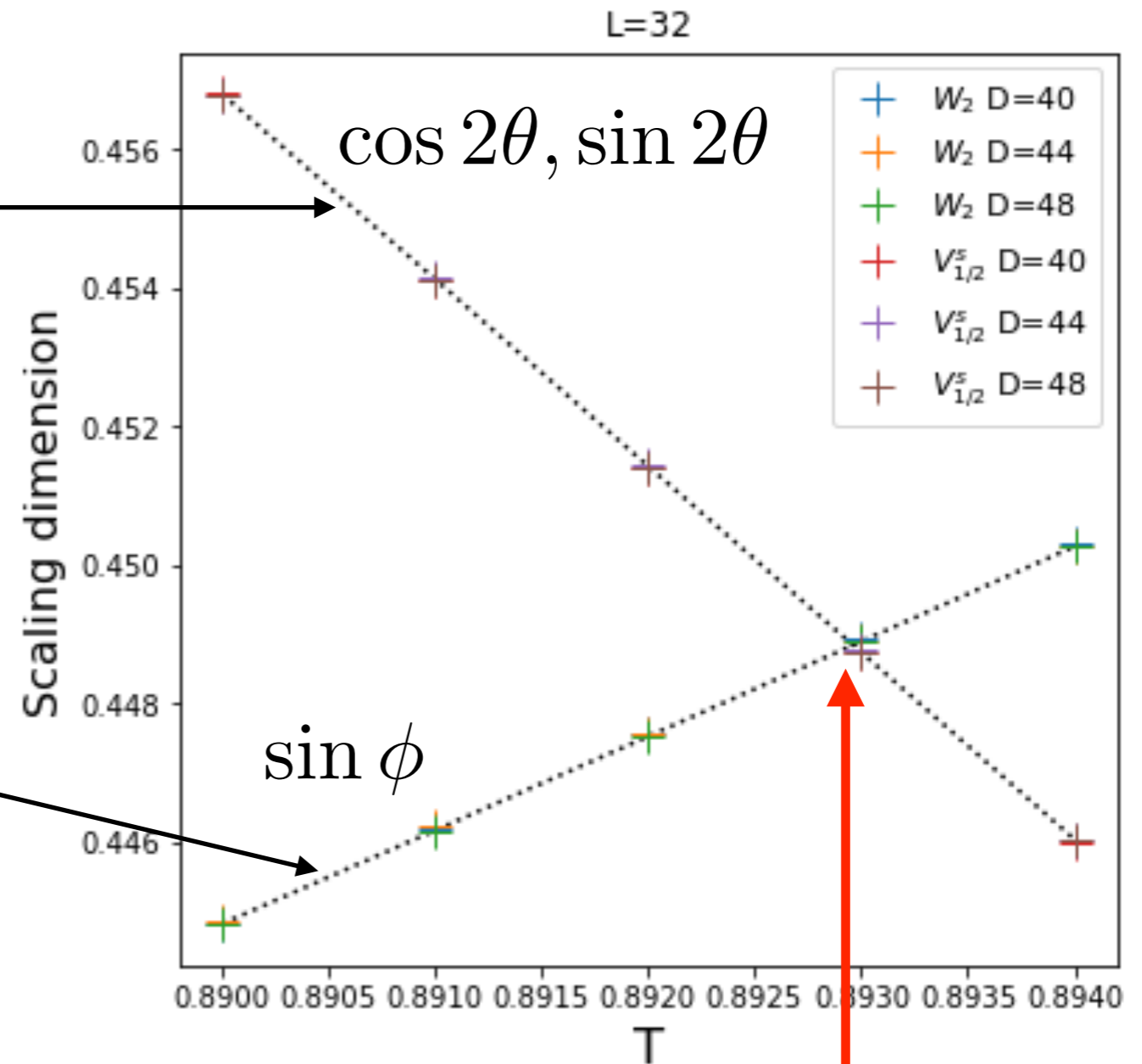


$$\lambda_i = e^{-LE_i(L)}$$

# Identifying $T_c$ with Level Crossing

“spin-wave”  
excited states  
under periodic b.c.

ground state under  
antiperiodic b.c.

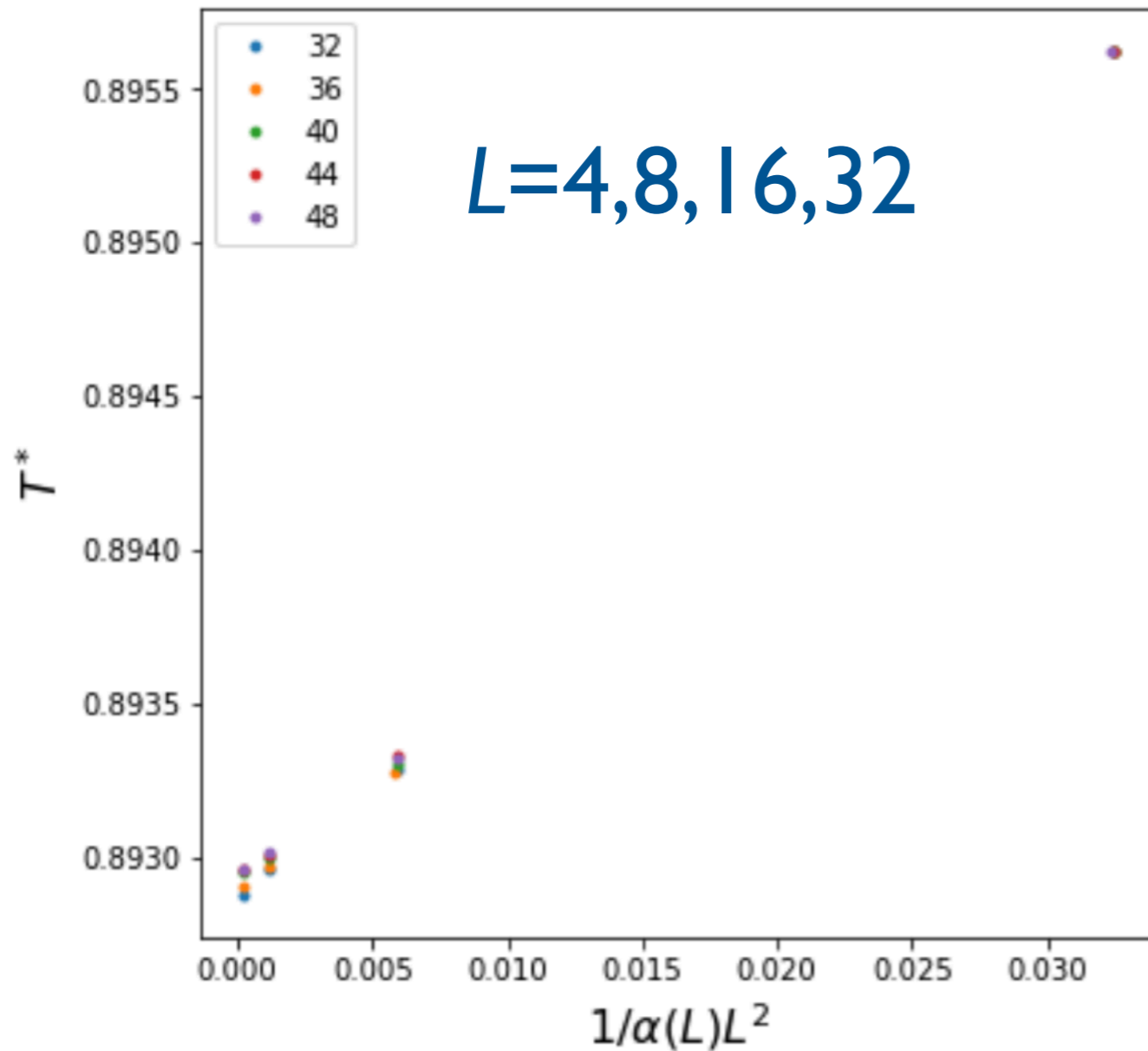


extra degeneracy  
forming SU(2) triplet  
~ BKT transition

This procedure eliminates  
logarithmic corrections  
to all orders in  $g$



# Remaining Finite-Size Effect



Level crossing point  
weakly depends on the  
system size  $L$

Effect of irrelevant  
perturbations

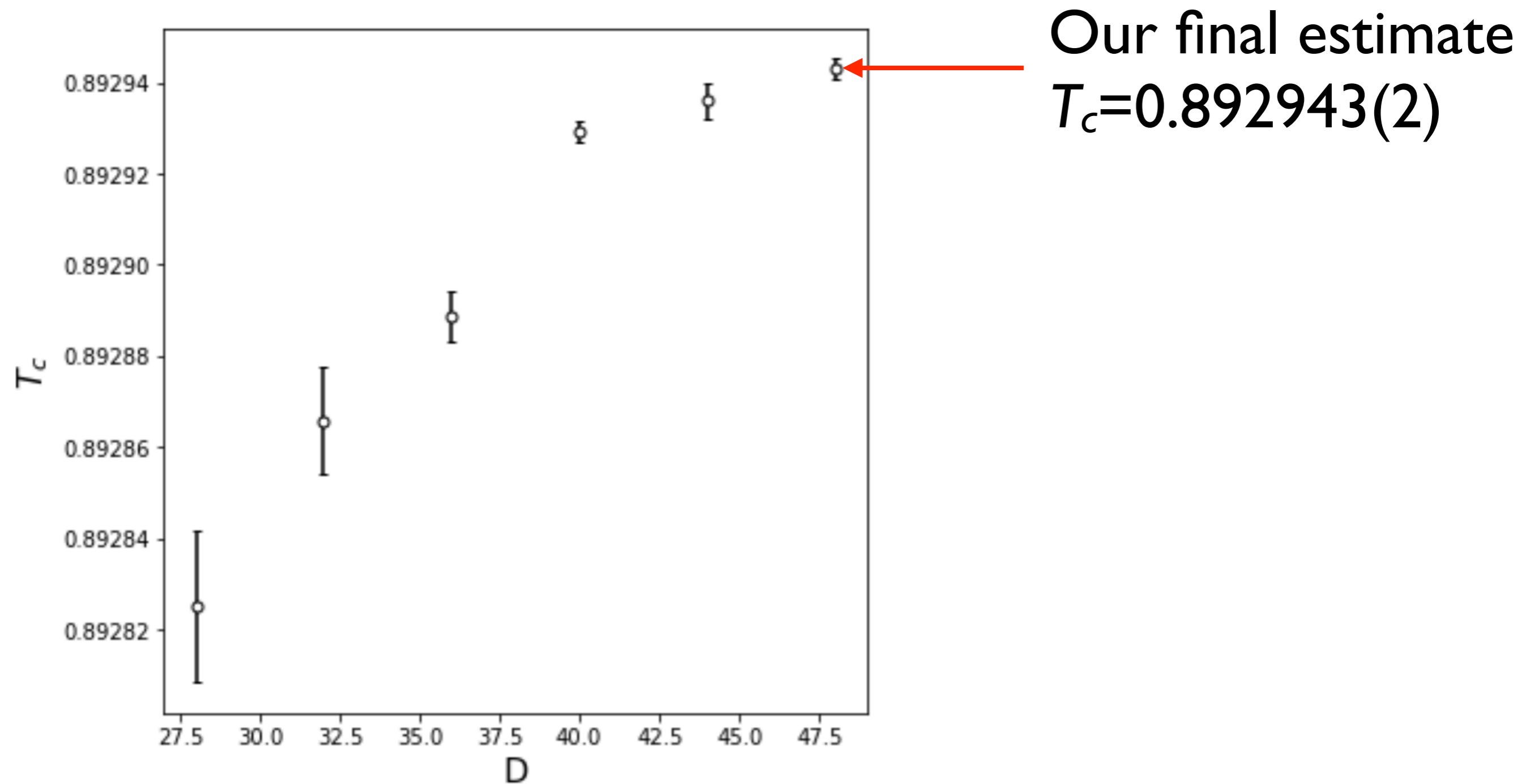
$$T^2, \bar{T}^2, T\bar{T}, \dots$$

$T$ : holomorphic part of the  
energy-momentum tensor

$$T^* \sim T_c + \text{const.} \frac{1}{L^2}$$

Extrapolate to  $L=\infty$

# Dependence on Bond Dimension $D$



# Effect of Finite Bond-Dimension

Finite bond dimension  $D \Leftrightarrow$  finite “correlation length”

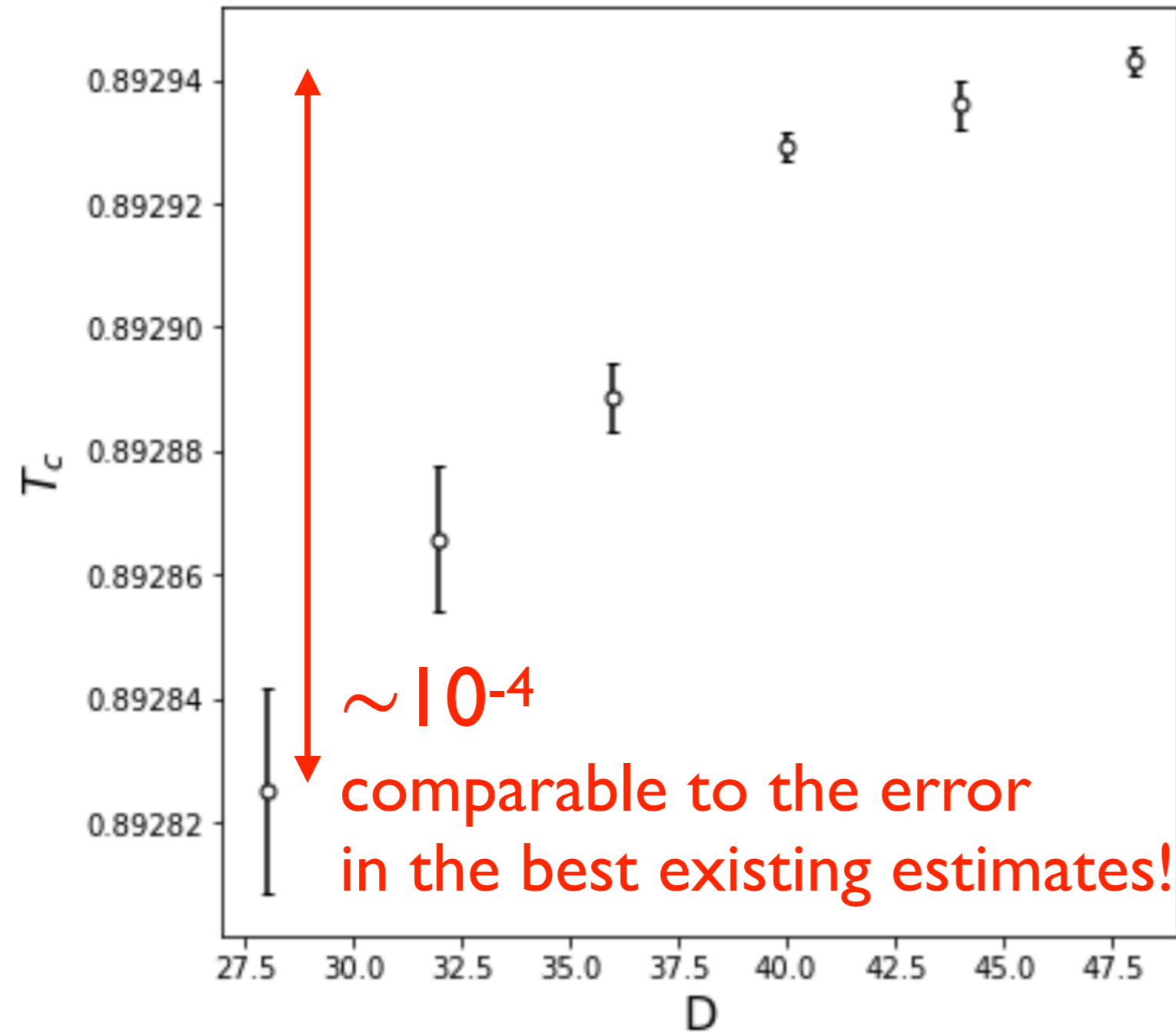
$$\xi_D \sim 0.3D^\kappa$$

$$\kappa = \frac{6}{c \left( \sqrt{\frac{12}{c}} + 1 \right)} \quad \text{[Pollmann et al. 2008]}$$

$\xi_D > L$  low-energy finite-size spectrum almost exact!

$\xi_D < L$  low-energy spectrum still reasonably accurate,  
but some error due to the finite  $D$

# $T_c$ dependence on $D$



$D=48$  gives  $\xi \sim 54$   
enough for up to  $L=32$

$D=28$  gives  $\xi \sim 26$   
too small for  $L=32$   
BUT....

# Error in (Loop-)TNR

(Loop-)TNR is often used to construct the “fixed point” tensor, which would describe the large scale behaviors, by iterating TNR many times

This approach has given accurate results for large systems, but small errors due to the finite bond dimension remain

In our approach, we study the spectrum of finite-size systems with TNR. TNR is almost exact when the system size is less than the effective correlation length.

TNR calculation of the finite-size spectrum  
+ Level Spectroscopy → extremely high accuracy

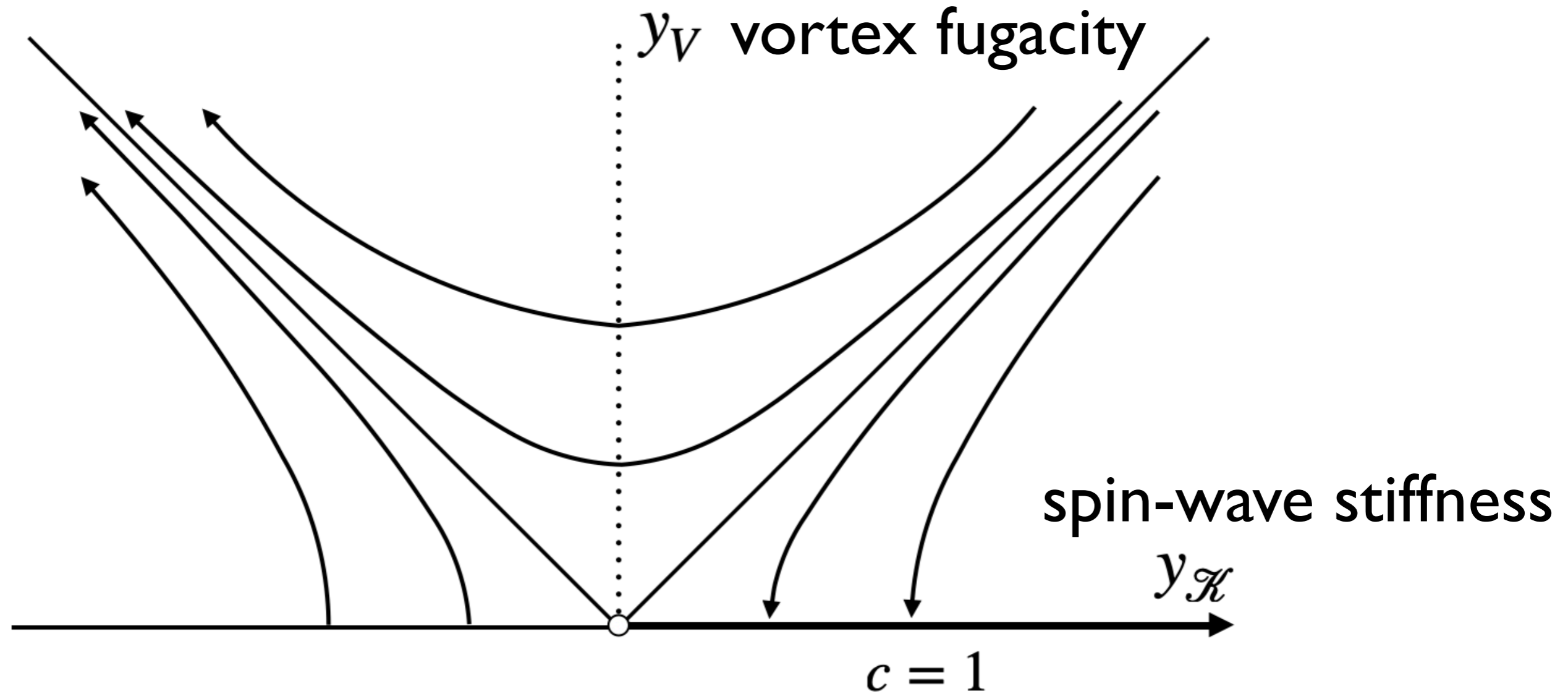
# Estimates of $T_c$

Monte Carlo(1979)[35]	0.89
Monte Carlo(2005)[36]	0.8929
Monte Carlo(2012)[37]	0.89289
Monte Carlo(2013)[38]	0.8935
Series expansion(2009)[39]	0.89286
HOTRG(2014)[40]	0.8921
VUMPS(2019)[41]	0.8930
HOTRG(2020)[42]	0.89290(5)
present work	0.892943(2)

TABLE I. Comparison of the estimated critical temperature of the 2D classical XY model.

# Kosterlitz RG Flow

You must have seen this diagram many times....



*but have you **really** seen the RG flow?*

# Low energy effective Hamiltonian for the $XXZ$ spin chain

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Received 19 February 1998; accepted 18 March 1998

“vacuum energy” under the twisted boundary condition  
with the twist angle  $\theta$  [notation clash...]

$$\begin{aligned} \delta^{\text{RG}} = & -\frac{1}{12} \left\{ 1 + \frac{3}{8} g_{\parallel} g_{\perp}^2 \right\} + \frac{s^2}{2} \left\{ 1 - \frac{g_{\parallel}}{2} + \frac{1}{4} g_{\perp}^2 - \frac{7}{32} g_{\parallel} g_{\perp}^2 \right\} \\ & + \frac{|s|}{16} \left\{ 2g_{\perp}^2 - g_{\parallel} g_{\perp}^2 \right\} + \frac{\theta^2}{2} \left\{ 1 + \frac{g_{\parallel}}{2} + \frac{g_{\parallel}^2}{4} - \frac{g_{\perp}^2}{4} + \frac{g_{\parallel}^3}{8} - \frac{g_{\parallel} g_{\perp}^2}{32} \right\} + O(g^4), \end{aligned} \quad (4.6)$$



# Energy Levels up to 2nd Order

- split between  $x_{V_{1/2}^s}, x_{V_{1/2}^c}$  should be odd in  $y_V$
- SU(2) triplet should be formed on  
the BKT transition line  $y_K = y_V$

⇒ uniquely determines the energy levels up to  $O(y^2)$

$$x_{W_{\pm 2}} = \frac{1}{2} - \frac{y_K}{4} + \frac{1}{4}y_V^2,$$

$$x_{V_{1/2}^s} = \frac{1}{2} + \frac{y_K}{4} - \frac{y_V}{2} + \frac{1}{8}(y_K^2 + 2y_K y_V - y_V^2),$$

$$x_{V_{1/2}^c} = \frac{1}{2} + \frac{y_K}{4} + \frac{y_V}{2} + \frac{1}{8}(y_K^2 - 2y_K y_V - y_V^2),$$

# Obtaining Running Coupling Constants

$$\begin{aligned}x_{W_{\pm 2}} &= \frac{1}{2} - \frac{y_{\kappa}}{4} + \frac{1}{4}y_V^2, \\x_{V_{1/2}^s} &= \frac{1}{2} + \frac{y_{\kappa}}{4} - \frac{y_V}{2} + \frac{1}{8}(y_{\kappa}^2 + 2y_{\kappa}y_V - y_V^2), \\x_{V_{1/2}^c} &= \frac{1}{2} + \frac{y_{\kappa}}{4} + \frac{y_V}{2} + \frac{1}{8}(y_{\kappa}^2 - 2y_{\kappa}y_V - y_V^2),\end{aligned}$$



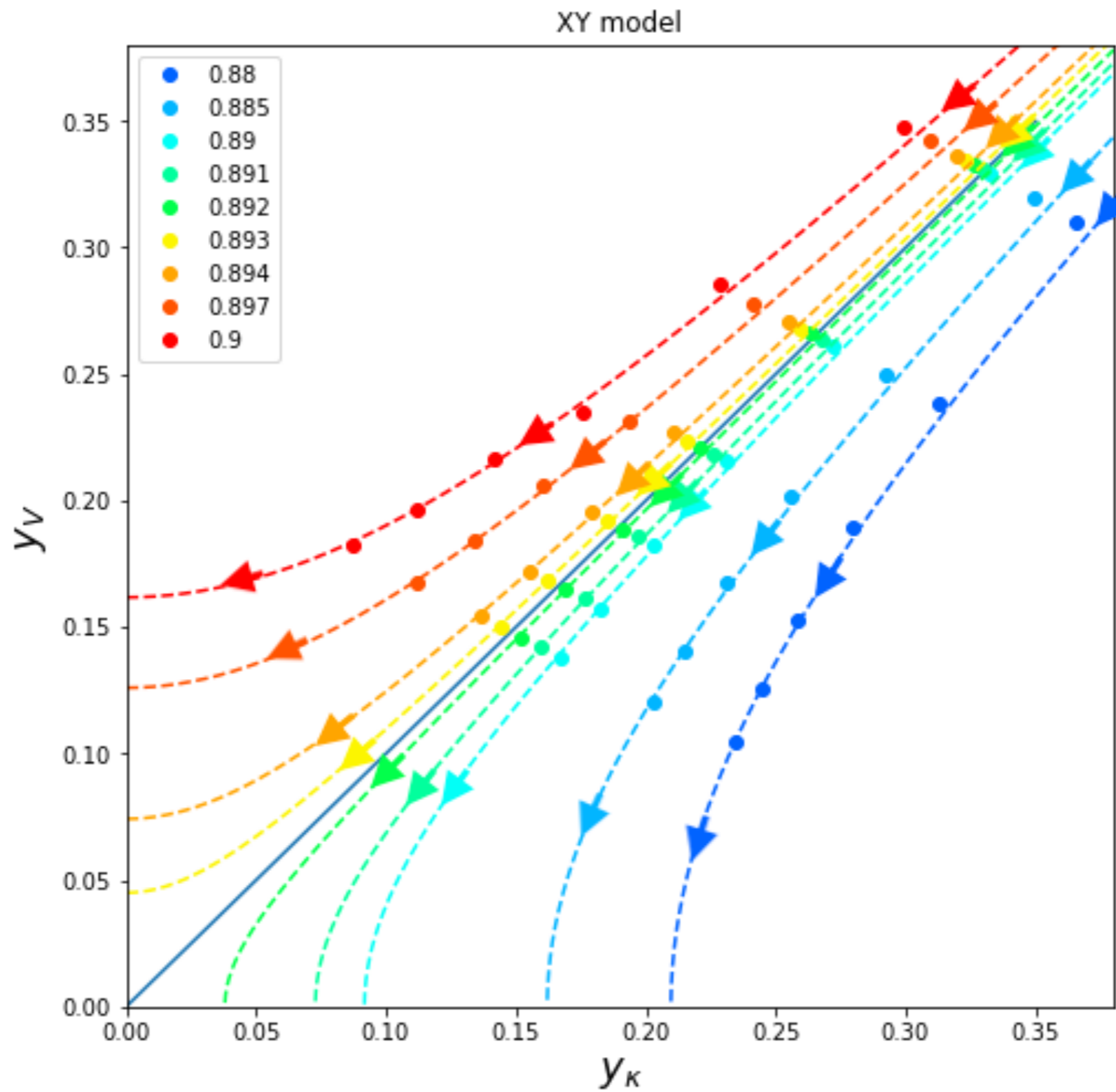
$$y_{\kappa} \sim 2 - 4x_{W_{\pm 2}} + (x_{V_{1/2}^c} - x_{V_{1/2}^s})^2,$$

$$y_V \sim (x_{V_{1/2}^c} - x_{V_{1/2}^s}) / (1 - \frac{1}{2}y_{\kappa}),$$

We can estimate  $y_{\kappa}$  &  $y_V$  from the finite-size energy levels

Less accuracy than  $T_c$ , but we can apply to larger systems  
(up to  $L=512$ )

# Visualization of Kosterlitz RG Flow!



$L=16$   
32  
64  
128  
256  
512

# Revisiting Ising Model

— to clarify the “origin” of the finite- $D$  effect

$$\mathcal{H} \sim \mathcal{H}_{\text{CFT}} + g_\sigma \int dx \sigma(x) + g_\epsilon \int dx \epsilon(x) + g \int dx (T^2(x) + \bar{T}^2(x))$$

$T, \bar{T}$ : energy-momentum tensor

$$x_\sigma(L) \sim \frac{1}{8} + \alpha_\sigma^\sigma g_\sigma^2 + \pi g_\epsilon + \alpha_\sigma^\epsilon g_\epsilon^2 - \frac{7\pi}{768} g + \dots$$

$$x_\epsilon(L) \sim 1 + \alpha_\epsilon^\sigma g_\sigma^2 + \alpha_\epsilon^\epsilon g_\epsilon^2 + \frac{7\pi}{48} g + \dots$$

We can eliminate the effects of leading irrelevant  $g$  by

$$x_\sigma(L) - \frac{1}{8} + \frac{1}{16} (x_\epsilon(L) - 1) \sim \pi g_\epsilon + \left( \alpha_\sigma^\epsilon + \frac{1}{16} \alpha_\epsilon^\epsilon \right) g_\epsilon^2 + \left( \alpha_\sigma^\sigma + \frac{1}{16} \alpha_\epsilon^\sigma \right) g_\sigma^2 + \dots$$

# 1

$$x_\sigma(L) - \frac{1}{8} + \frac{1}{16} (x_\epsilon(L) - 1) \sim g_h^2 + g_t$$

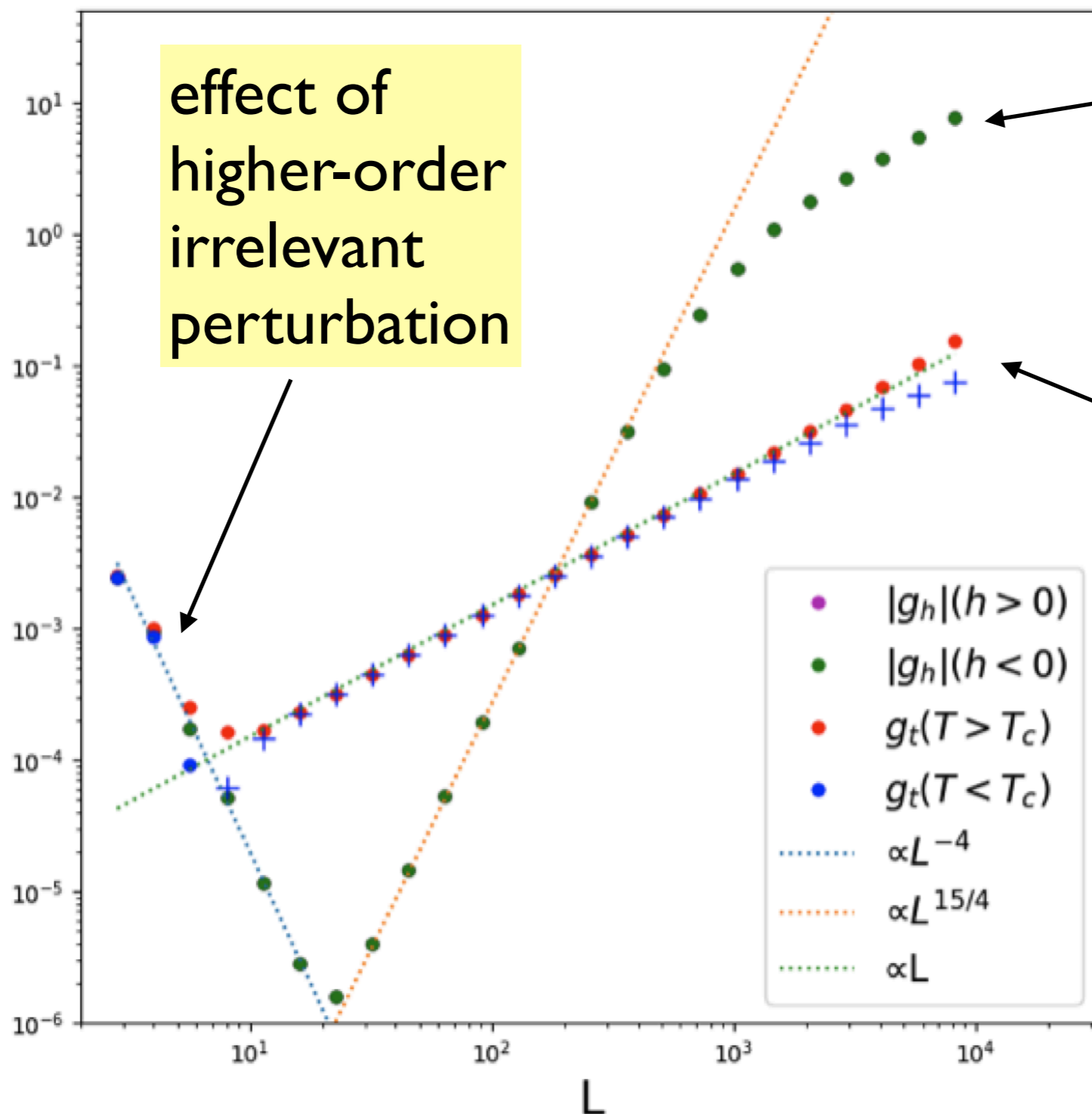
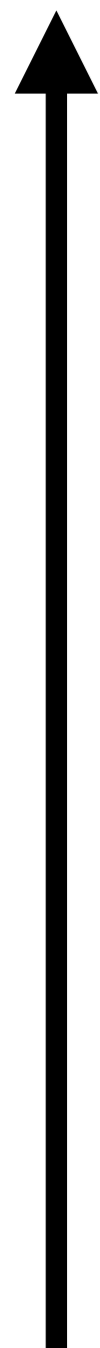
$$g_h \propto g_\sigma, g_t \propto g_\epsilon$$

$h=10^{-5}$   
at  $T=T_c$

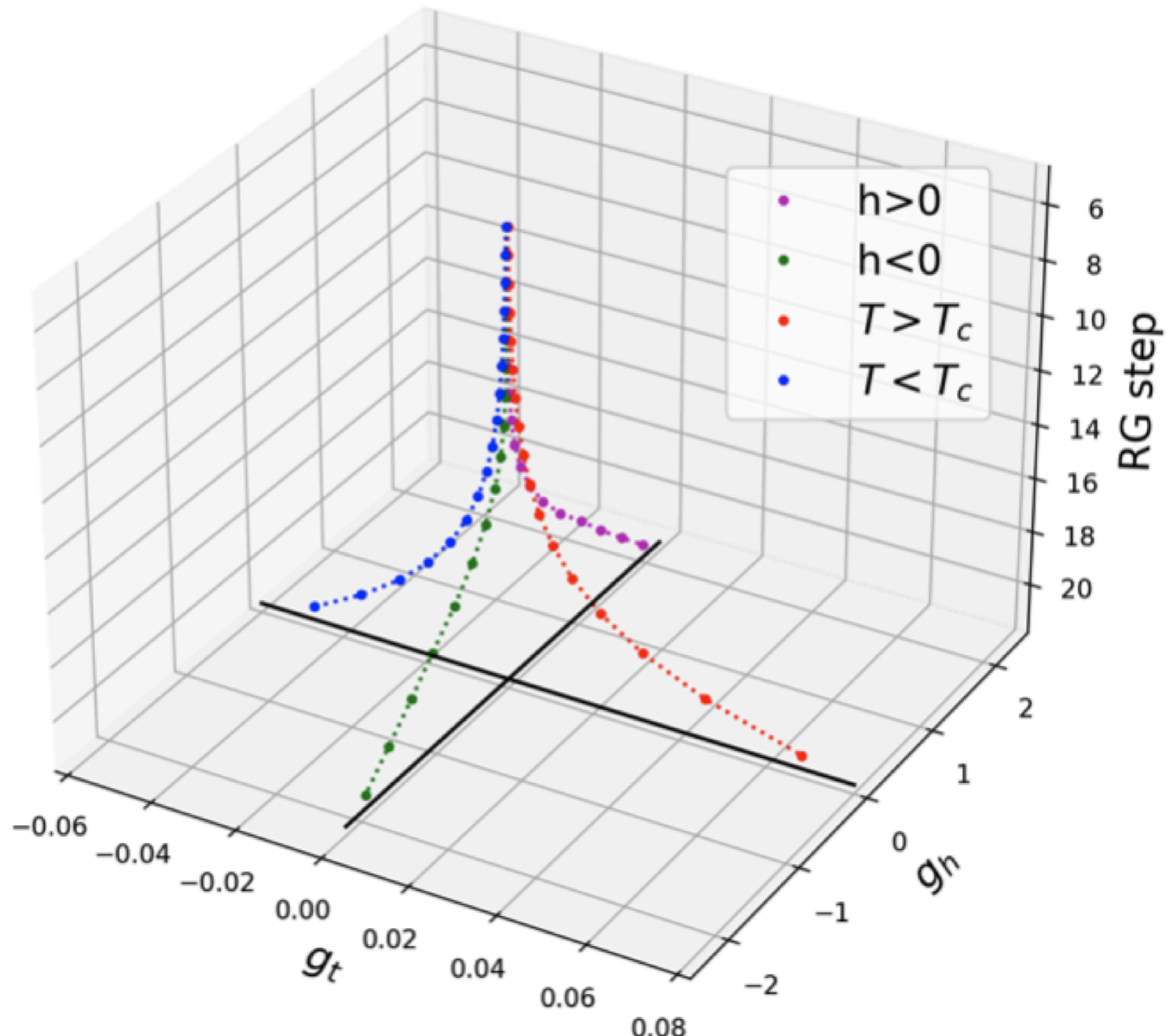
$$g_h^2 \propto \left(L^{2-\frac{1}{8}}\right)^2 = L^{15/4}$$

$T=1.0001T_c$   
 $T=0.9999T_c$   
with  $h=0$

$$g_t \propto L^{2-1} = L$$



# Visualizing RG Flow for Ising



# *What* is Finite- $D$ Effect?

Finite- $D \Leftrightarrow$  Finite correlation length

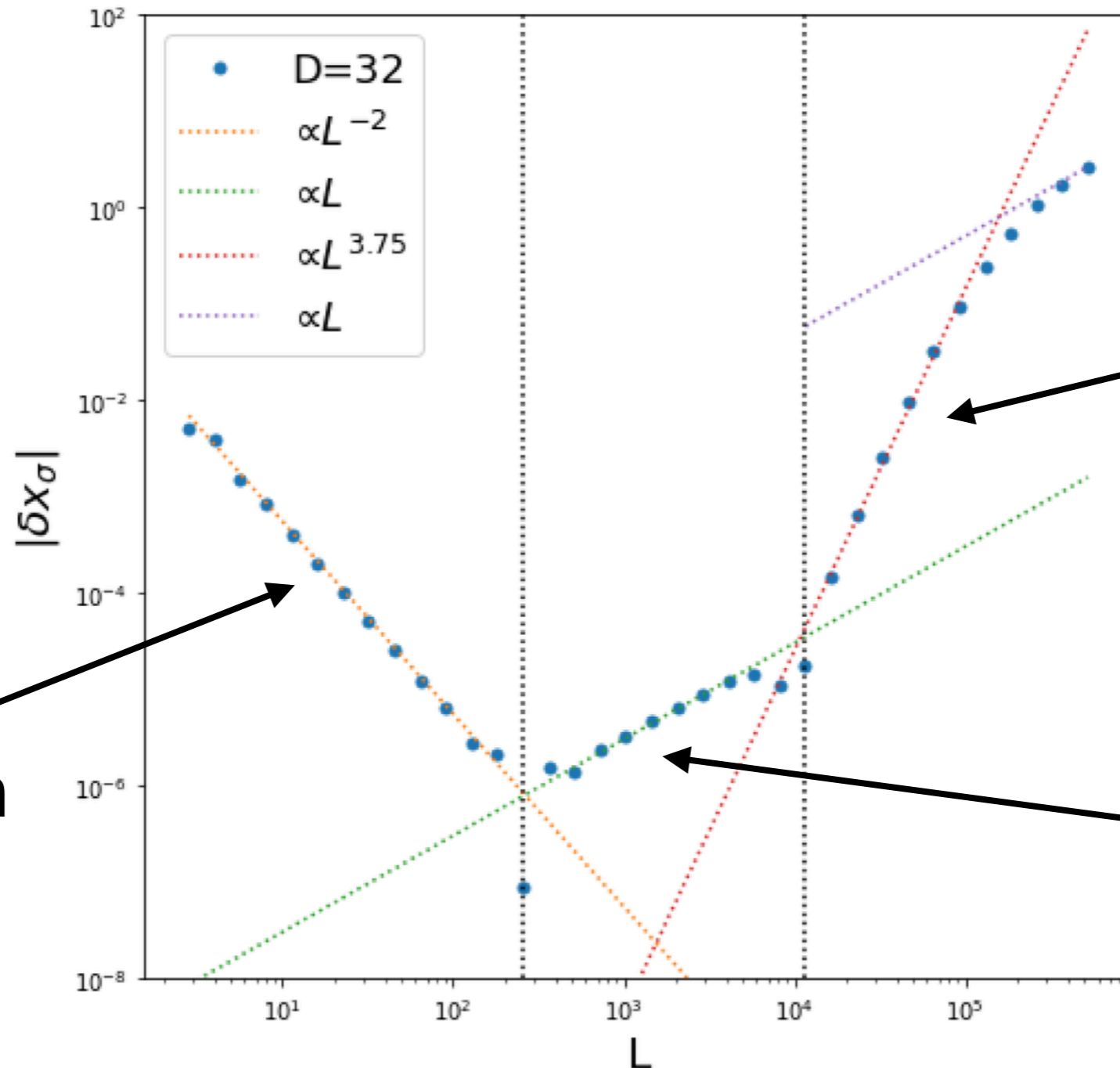
$\Leftrightarrow$  “Massive” field theory due to relevant perturbation

Natural idea, but is this true?

(Are relevant perturbations somehow automatically induced for finite- $D$ ??)

# Finite- $D$ TNR at the Critical Point

$$x_\sigma(L) - \frac{1}{8} \sim -\frac{7\pi}{768}g + g_t + g_h^2 + \dots$$



leading  
irrelevant  
perturbation

$$g \propto \frac{1}{L^2}$$

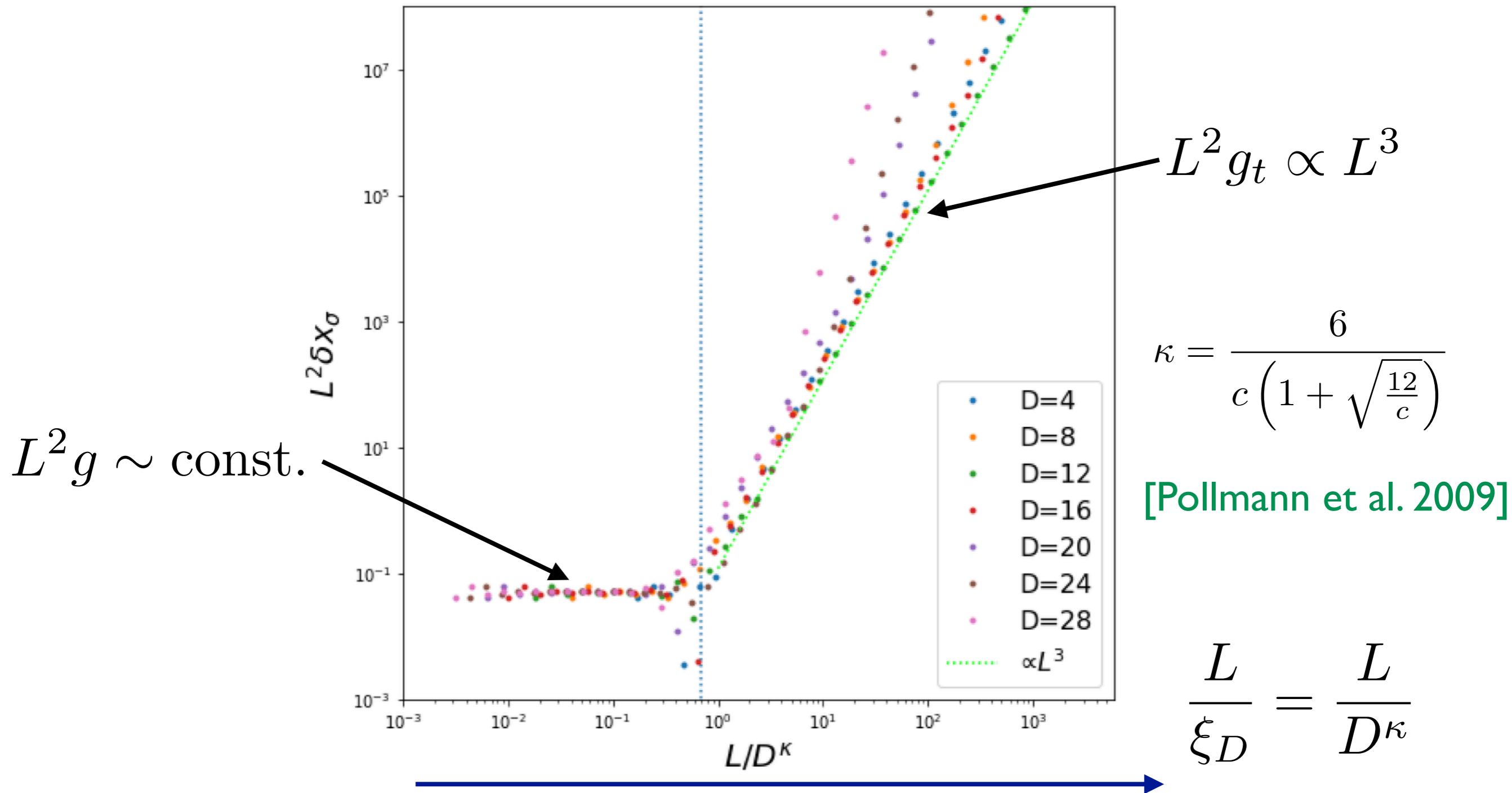
“generated”  
 $g_h^2 \propto L^{15/4}$

“generated”  
 $g_t \propto L$



# Scaling in $L/\xi_D$

$$L^2 \left( x_\sigma(L) - \frac{1}{8} \right) \sim -\frac{7\pi}{768} L^2 g + L^2 g_t + \dots$$



# Conclusions (so far)

**TNR + Level Spectroscopy** (finite size scaling of the transfer-matrix spectra based on CFT)

allows

- visualization of RG flow by **extraction of running coupling constants** from the spectrum
- extremely **accurate determination of the critical point**
- also applicable to continuous valued 2D classical spin systems such as XY model
- **finite bond dimension  $D$**  corresponds to “automatically” **induced (relevant) perturbations**

# Classical Heisenberg Model

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j,$$



continuum limit

$$\mathcal{L} = \frac{1}{2g} (\partial_\mu \vec{n})^2 \quad \vec{n}^2 = 1 \quad \text{O(3) Nonlinear Sigma Model}$$

coupling  $g$  corresponds to temperature

Asymptotic freedom  $\Rightarrow$  disordered at any  $T > 0$

$$\frac{dg}{d \log L} = \frac{g^2}{2\pi} + \dots$$

Supported also by factorizable  $S$ -matrix (Zamolodchikov<sup>2</sup>)

BUT...

# Quasi-long-range ordering in a finite-size 2D classical Heisenberg model

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Received 24 November 2006, in final form 13 February 2007

Published 20 March 2007

Online at [stacks.iop.org/JPhysA/40/3741](http://stacks.iop.org/JPhysA/40/3741)

## Abstract

We analyse the low-temperature behaviour of the classical isotropic ferromagnetic Heisenberg model on a two-dimensional square lattice of finite size. Presence of a residual magnetization in a finite-size system enables us to use a low-temperature approximation, which is however more restricting than the usual spin-wave approximation known to give reliable results for the  $XY$  model at low temperatures  $T$ . For the system considered, we find that the spin–spin correlation function decays as  $1/r^{\eta(T)}$  for large separations  $r$  bringing about the presence of a quasi-long-range ordering. We give analytic estimates for the exponent  $\eta(T)$  in different regimes and support our findings by Monte Carlo simulations of the model on lattices of different sizes at different temperatures.

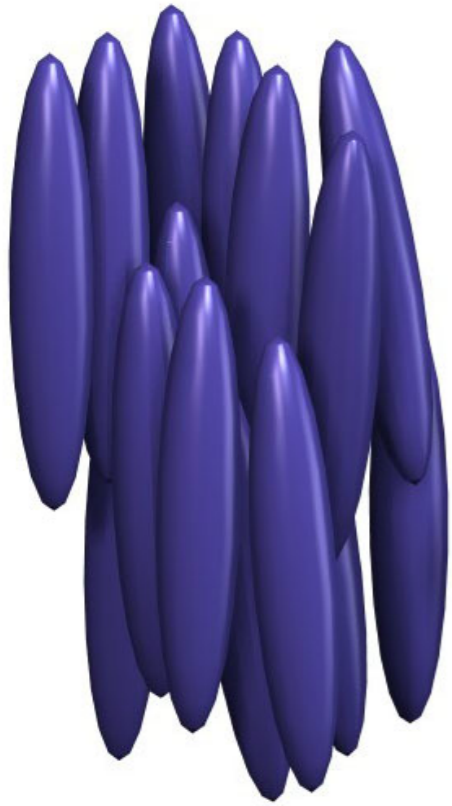
PACS numbers: 05.50.+q, 75.10

Really??

But not easy to  
prove/disprove

difficult to distinguish  
massive with  
very large  
correlation length  
from  
massless...

# $\mathbb{Z}_2$ vortex-driven transition?



Nematic liquid crystal:  
symmetric rod-like molecules  
(no distinction between head & tail)

$$H = -J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j)^2,$$

Lebwohl-Lascher 1972

Kawamura-Miyashita 1984

Target space =  $\mathbb{RP}^2$

$$\pi_1(\mathbb{RP}^2) = \mathbb{Z}_2 \quad \mathbb{Z}_2 \text{ vortex!}$$

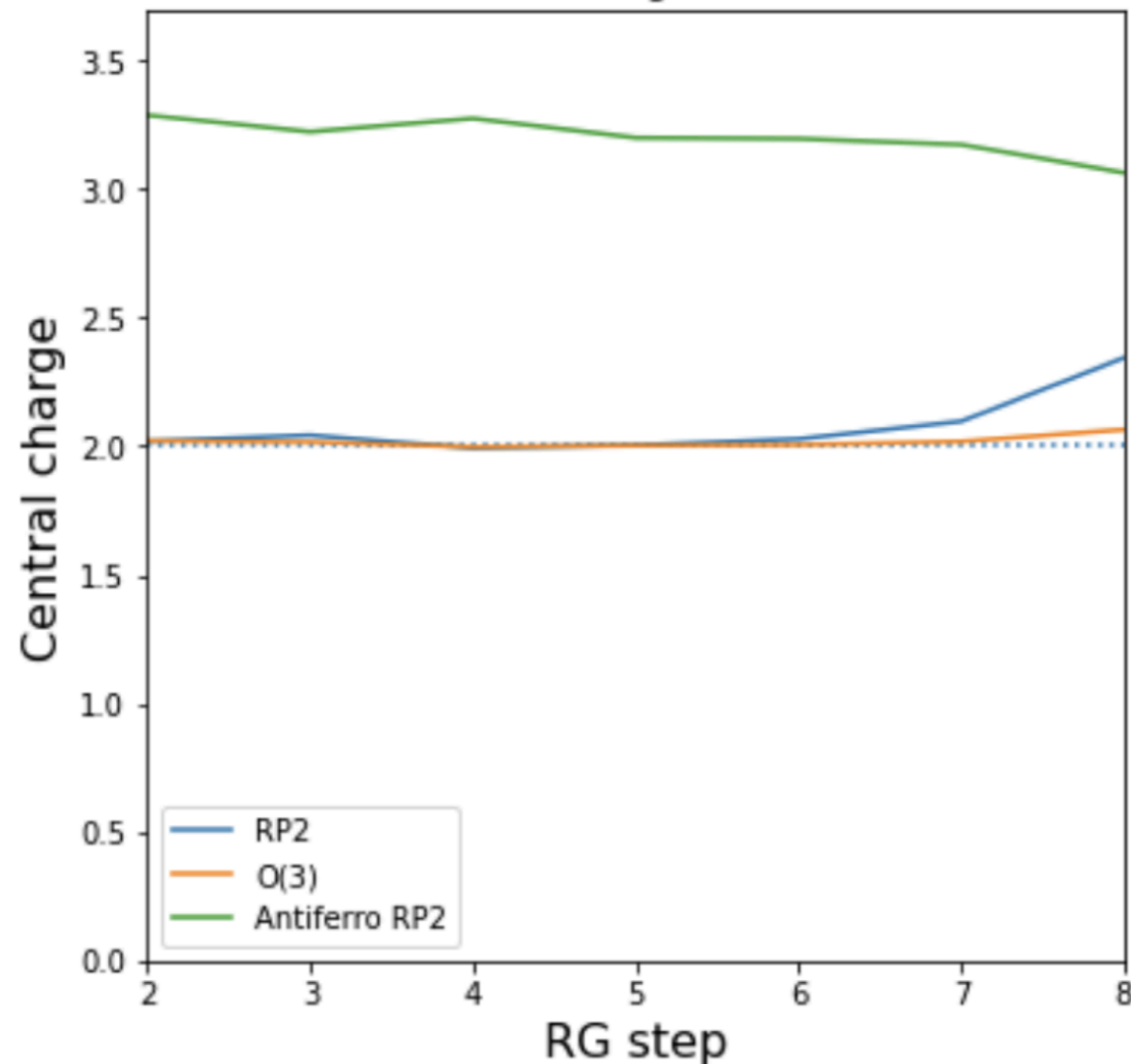
BKT-like transition driven by the  $\mathbb{Z}_2$  vortices?

But the RG equation also implies asymptotic freedom..

# UV Fixed Point

(a)

UV central charge at  $T=0.005$



$T \rightarrow 0$

Spontaneous Symmetry  
Breaking of  $SO(3)$

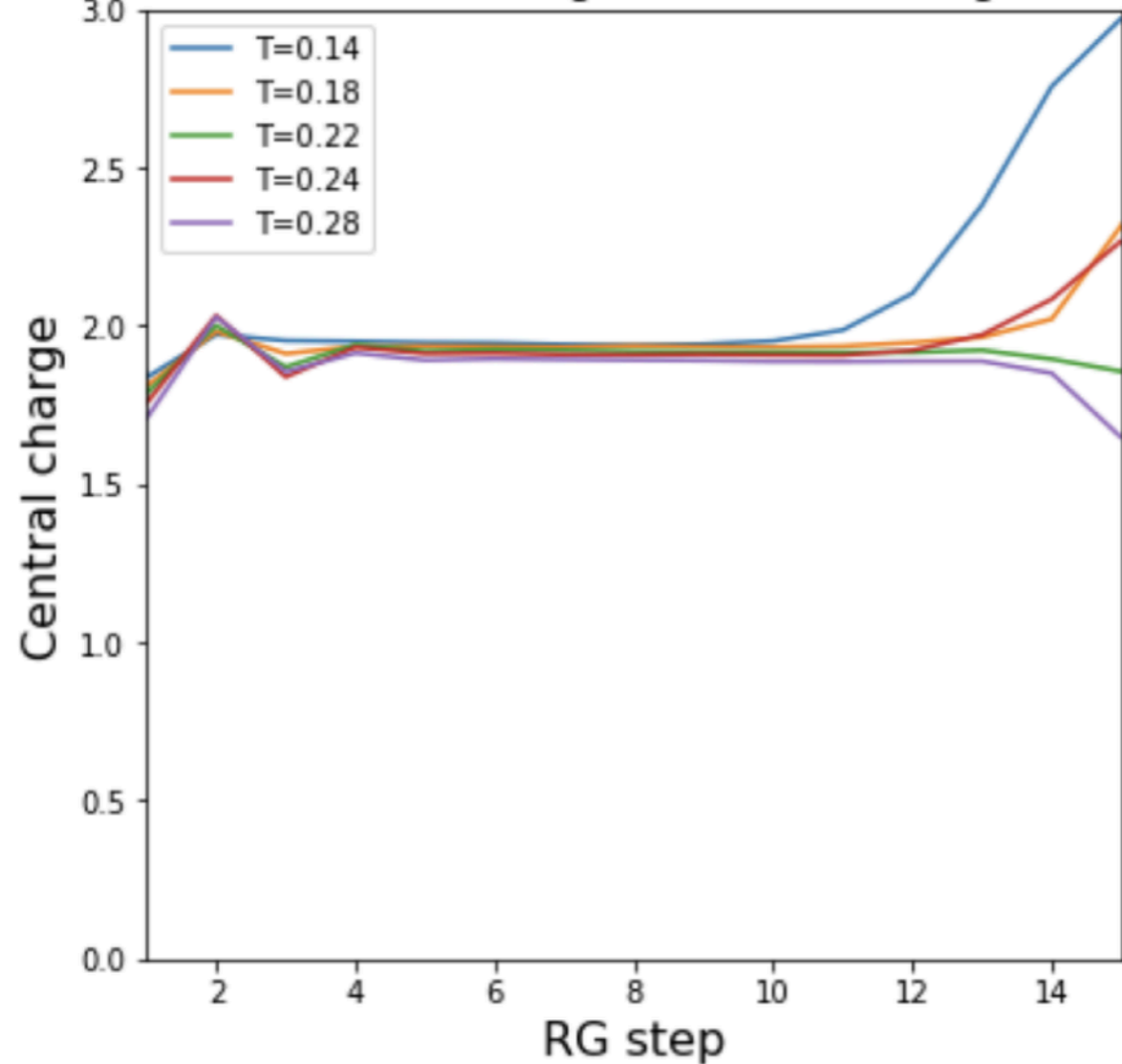
2 independent  
Nambu-Goldstone modes  
 $\Rightarrow c=2$

Confirmed by TNR

$$E_0(L) \sim \epsilon_0 L - \frac{\pi c}{6L}$$

# Heisenberg Model at Intermediate $T$

Effective central charge of the Heisenberg model

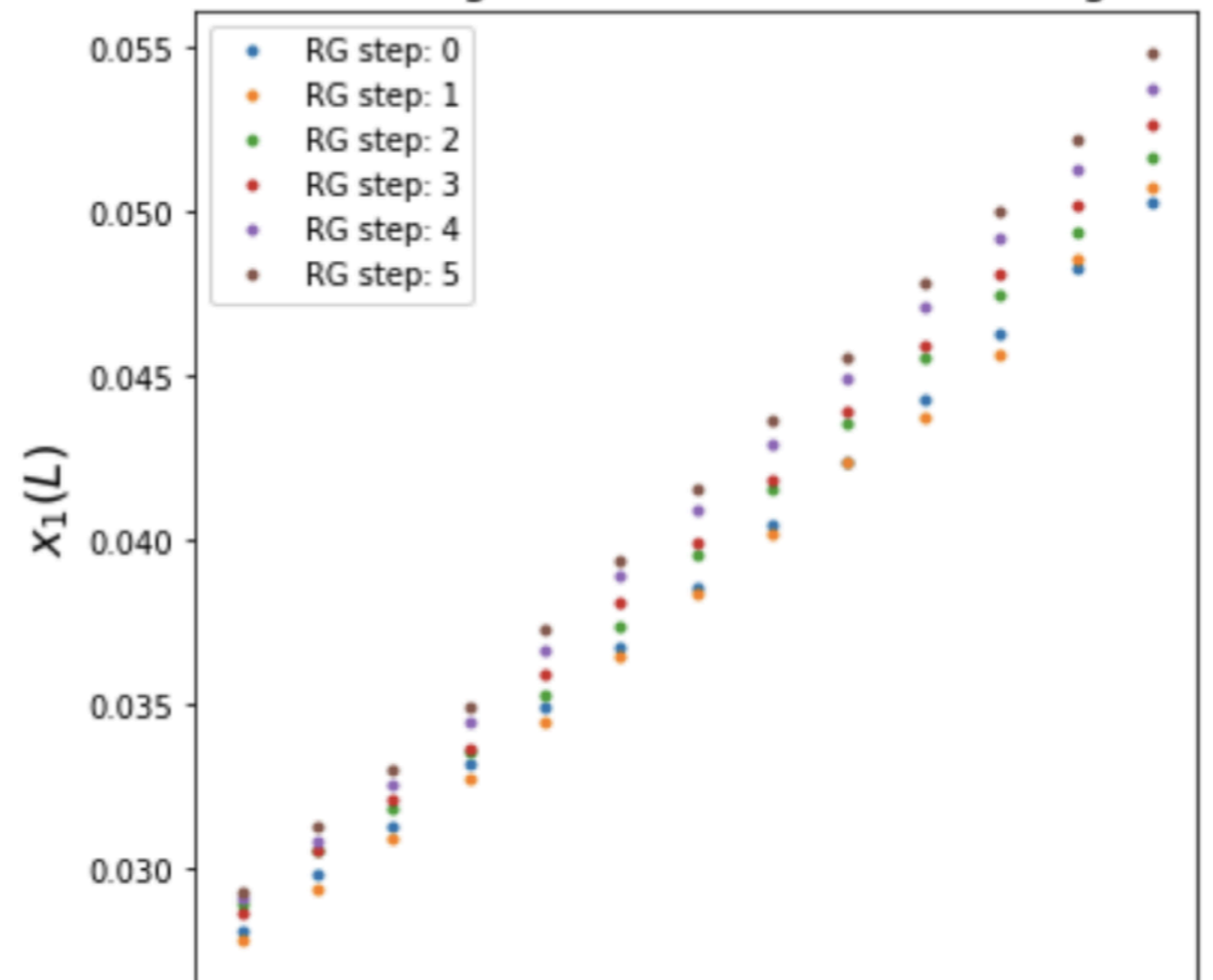


$$E_0(L) \sim \epsilon_0 L - \frac{\pi c}{6L}$$

$c \sim 1.94 < 2$  no candidate CFT

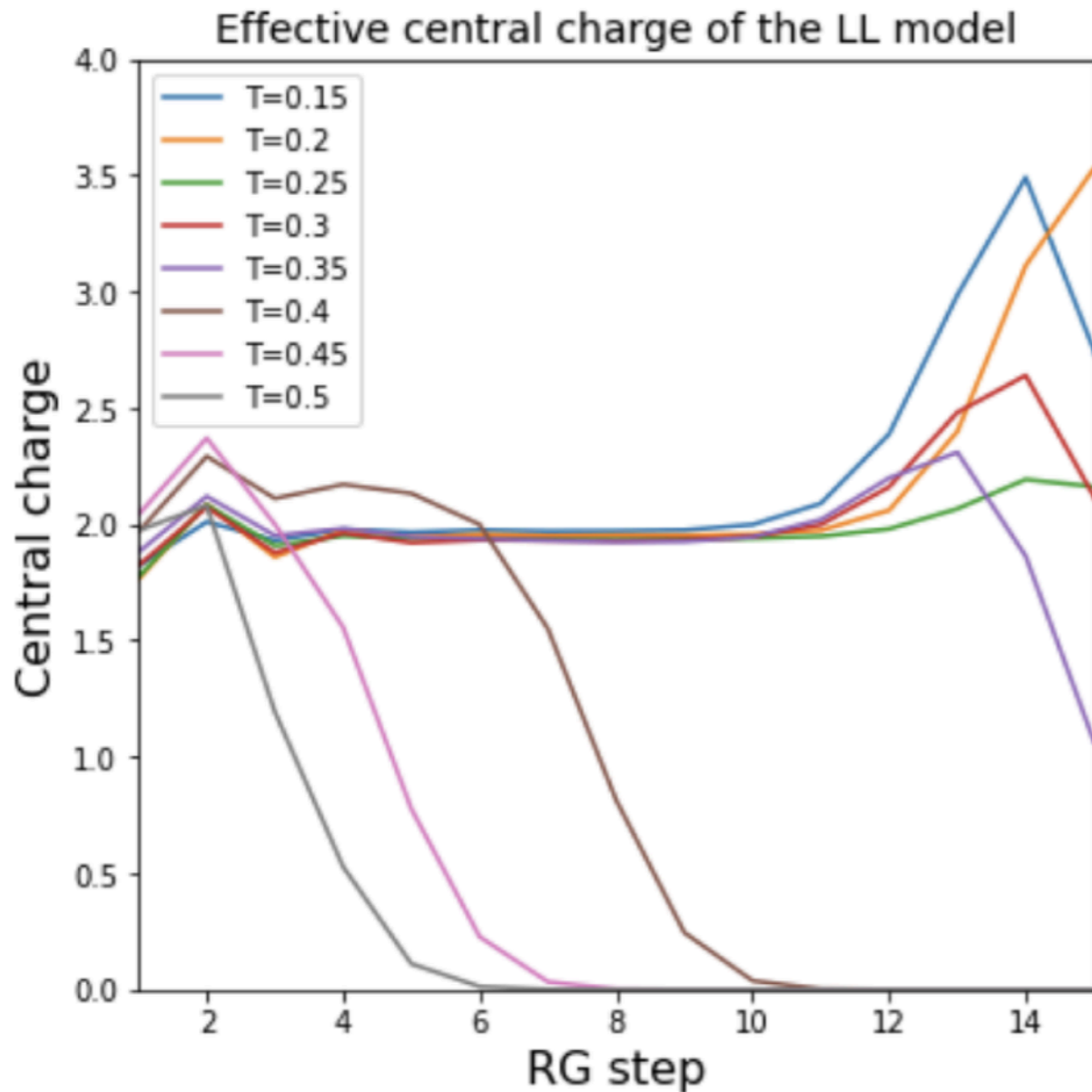
$\frac{2\pi x_n}{L} = E_n(L) - E_0(L)$  does not converge

Finite-size scaling dimension of the Heisenberg model



likely to support  
“asymptotic freedom”  
RG flow  $c=2 \rightarrow c=0$

# RP<sup>2</sup> Model at Intermediate $T$

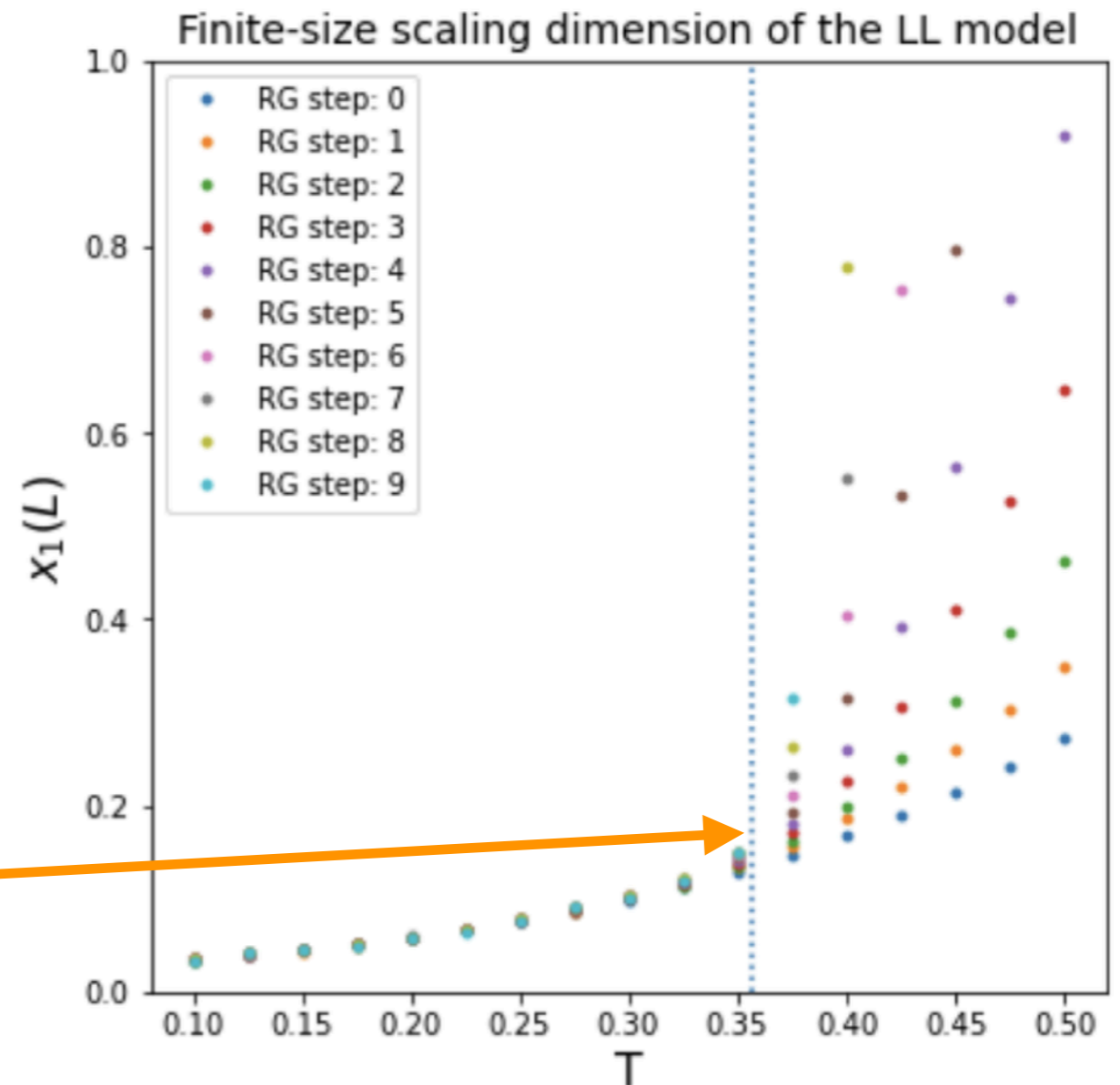


$$E_0(L) \sim \epsilon_0 L - \frac{\pi c}{6L}$$

$c \sim 1.92 < 2$  no candidate CFT

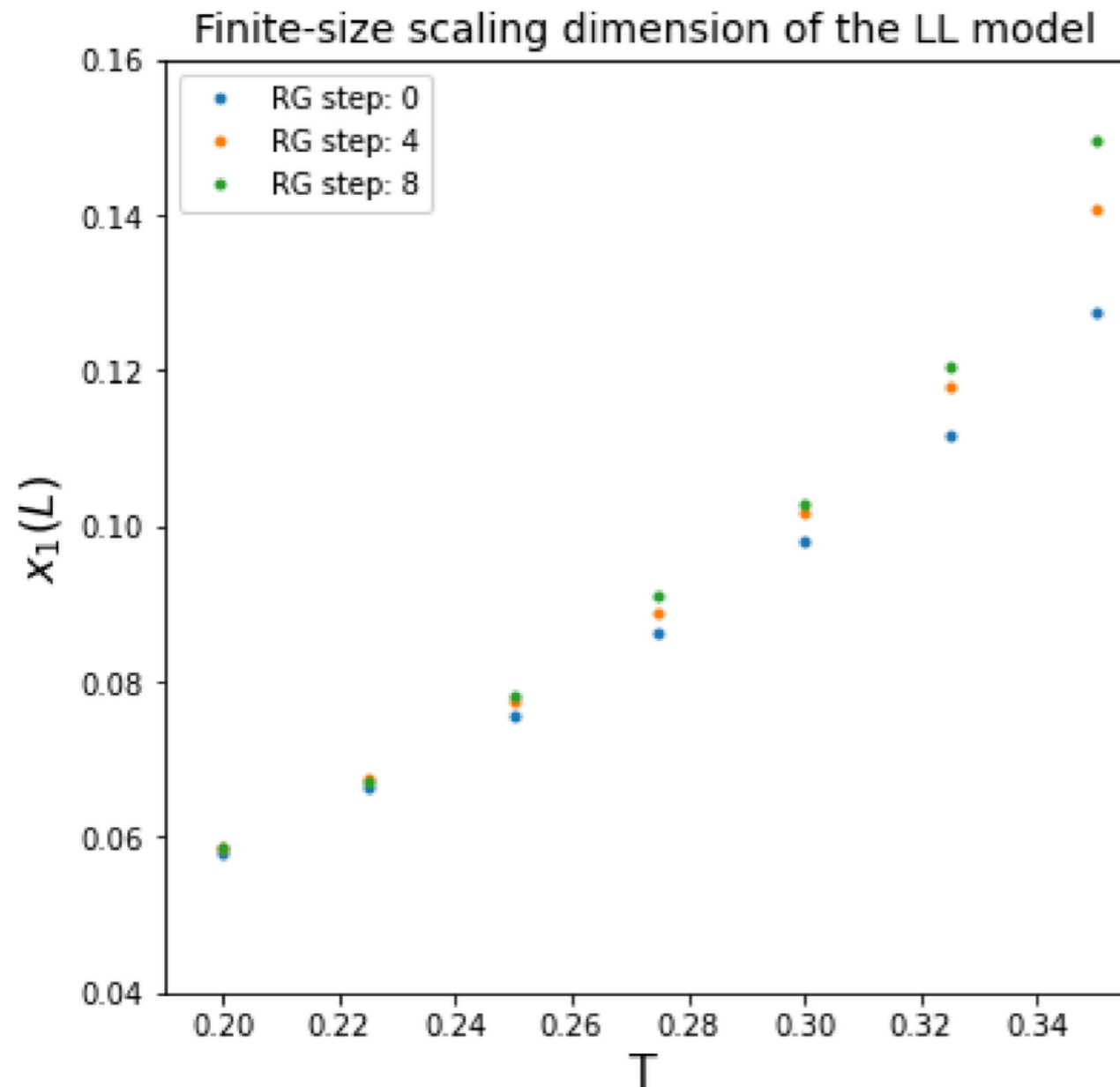
$$\frac{2\pi x_n}{L} = E_n(L) - E_0(L).$$

Z<sub>2</sub> vortex dissociation transition(?)





# RP<sup>2</sup> Model at $T \leq T^*$



Spectrum does not converge well even at  $T \leq T^*$

$$c \sim 1.92 < 2$$

SU(2) level 4

$c=2$  but smallest scaling dim

$$x_{j=1} = \frac{2}{3} = 0.666 \dots \gg 0.2$$

likely to support “asymptotic freedom”

RG flow  $c=2 \rightarrow c=0$ , but with a strong crossover at  $T^*$

# Conclusions (Heisenberg & RP<sup>2</sup>)

Both Heisenberg & RP<sup>2</sup> Models

show  $c=2$  at the UV fixed point for  $T \rightarrow 0$

consistently with 2 (would-be) Nambu-Goldstone modes

At intermediate temperatures, the effective central charge exhibit a “plateau” at  $c \sim 1.9$

but there is no appropriate candidate CFT and scaling dimensions do not converge

Our results support the “asymptotic freedom” scenario with the single disordered phase in  $T > 0$

# Discussion (Heisenberg & RP<sup>2</sup>)

Difficulty in distinguishing very large but finite correlation length from criticality

Even when (system size)  $<$  (correlation length)  
the Hamiltonian/transfer matrix spectrum  
gives useful information!

We do not completely rule out the possibility of the critical point at  $T \sim T_*$  or the critical phase in  $T \lesssim T_*$  suggested in several papers. However, to pursue this viewpoint, one would need to explain the effective central charge and the spectra obtained in the present TNR study, which is perhaps more difficult than simply discussing whether the correlation length diverges or not.

# Conclusions (Overall)

TNR + Level Spectroscopy (finite size scaling of CFT) allows

- super accurate determination of BKT critical point
- visualization of Kosterlitz RG flow by extraction of running coupling constants from the spectrum
- identify the UV fixed point for the Heisenberg &  $RP^2$  models
- clarify(?) the crossover in the Heisenberg &  $RP^2$  models

Future: extension/application to more nontrivial systems & unknown physics