HOTRG study on partition function zeros in the p-state clock model

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Outline

1. Fisher zero characterization of a phase transition

— Numerical methods of computing the partition function

— BKT transitions in the p-state clock model?

2. Monte Carlo: Numerical issues due to the stochastic nature

[D.-H. Kim, PRE 96, 052130 (2017)]

— How large systems can we consider for Fisher zeros?

→ **It depends on the type of phase transition: BKT has an issue.**

3. Higher-Order Tensor Renormalization Group

[S. Hong and D.-H. Kim, arXiv:1906.09036]

— Characterization of the two BKT transitions in the p-state clock model

— Finite-size scaling analysis: logarithmic corrections

— Fisher-zero determination of the BKT transition temperature

Emergent symmetry in the 2D p-state clock model

p-state clock model in square lattices

$$\mathcal{H}_p = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

$p \to \infty$

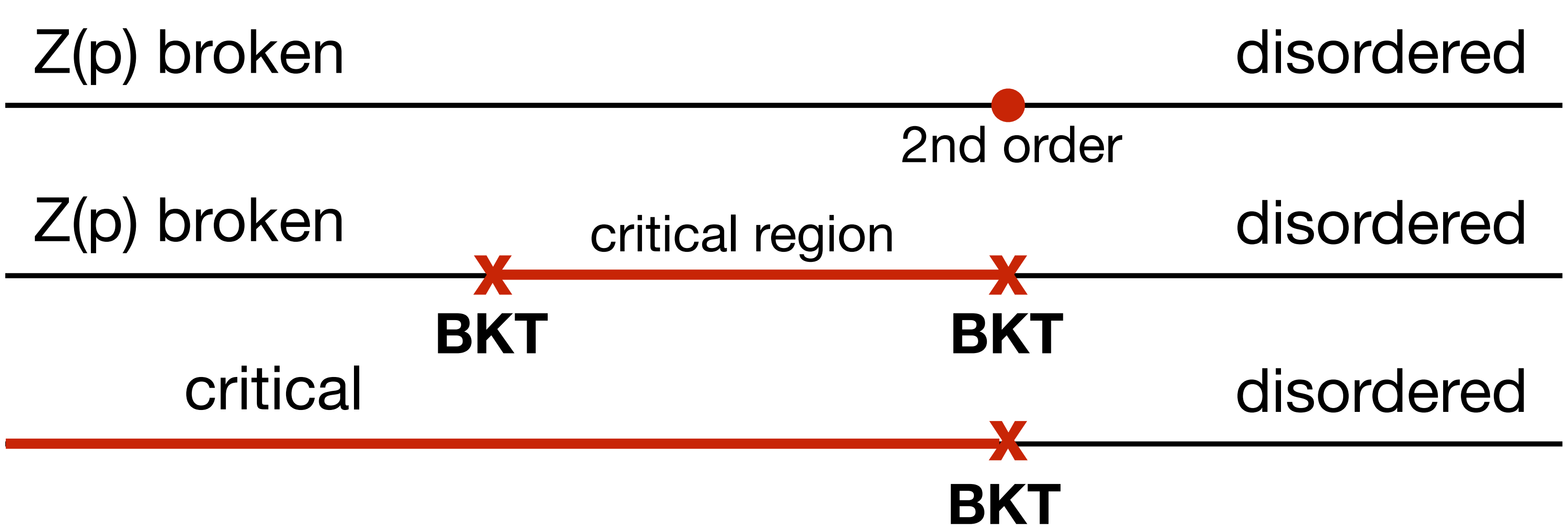
Z(p) symmetry

$$\theta = \frac{2\pi n}{p} \quad : \text{“clock” spin}$$

$$n = 0, 1, 2, .., p-1$$

XY model: U(1) symmetry → **B**erezinskii-**K**osterlitz-**T**houless transition

Emergent U(1) symmetry: BKT transition occurs even at finite p!



$2 \le p \le 4$

$5 \le p < \infty$

$p \to \infty$

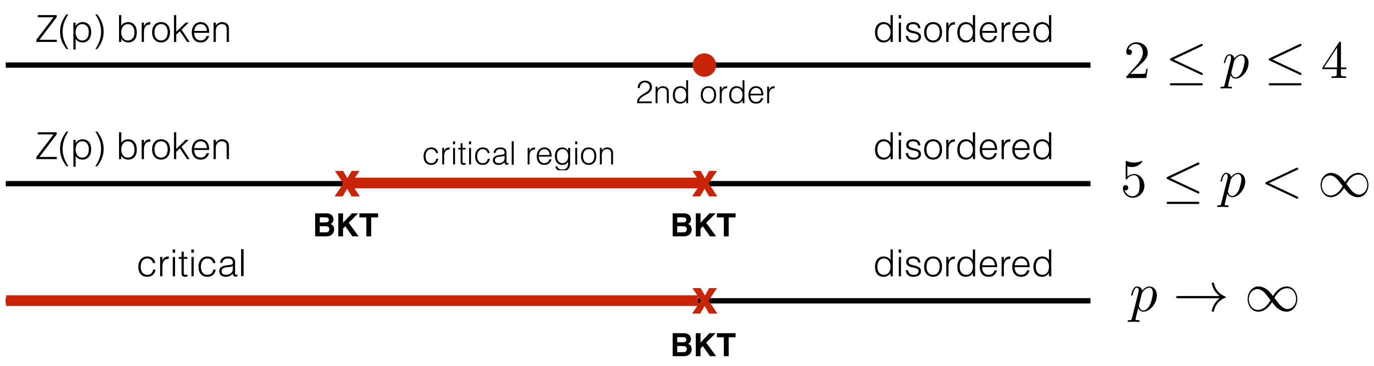
Review: “40 years of BKT theory”, ed. by J. V. Jose

Debates and remaining issues

There are approximations involved!

(Villain approximation, self-dual, …)

; *see* Borisenko *et al.*, PRE 83, 041120 (2011).
review: "40 years of BKT theory", ed. by J. V. Jose



Numerical results with the "exact" p-state clock model:

(mainly for the high-T transition)

Lapilli/Pfeifer/Wexler, PRL 2006:

(**helicity modulus**)

It's not the BKT transition for p < 8!

Hwang, PRE 80, 042103 (2009):

(Fisher zero study) ⟵ ?

Indeed, it doesn't look like BKT for p=6.

Baek/Minnhagen/Kim PRE 2010:

(**helicity modulus**, more rigorously)

Noop, IT IS the BKT for p = 6!

but…

Baek/Minnhagen PRE 2010:

p = 5 looks strange…

Borisenko et al, PRE 2011.

Baek et al, PRE 2013.

Kumano et al, PRE 2013.

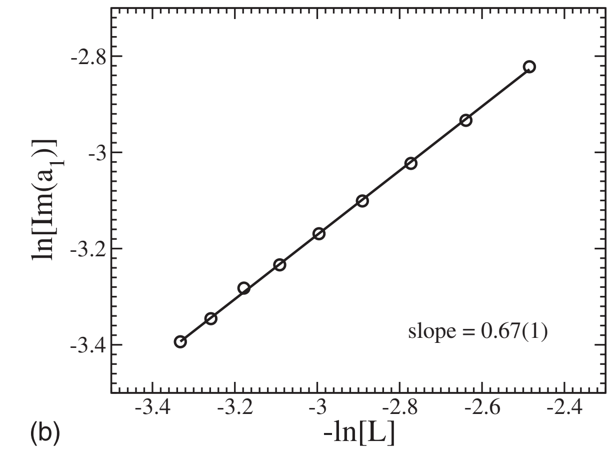
Chatelain, JSM 2014: DMRG

Fisher zero test on p=5 and 6 ?

Hwang, PRE 80, 042103 (2009): the first Fisher zero calculation for p=6

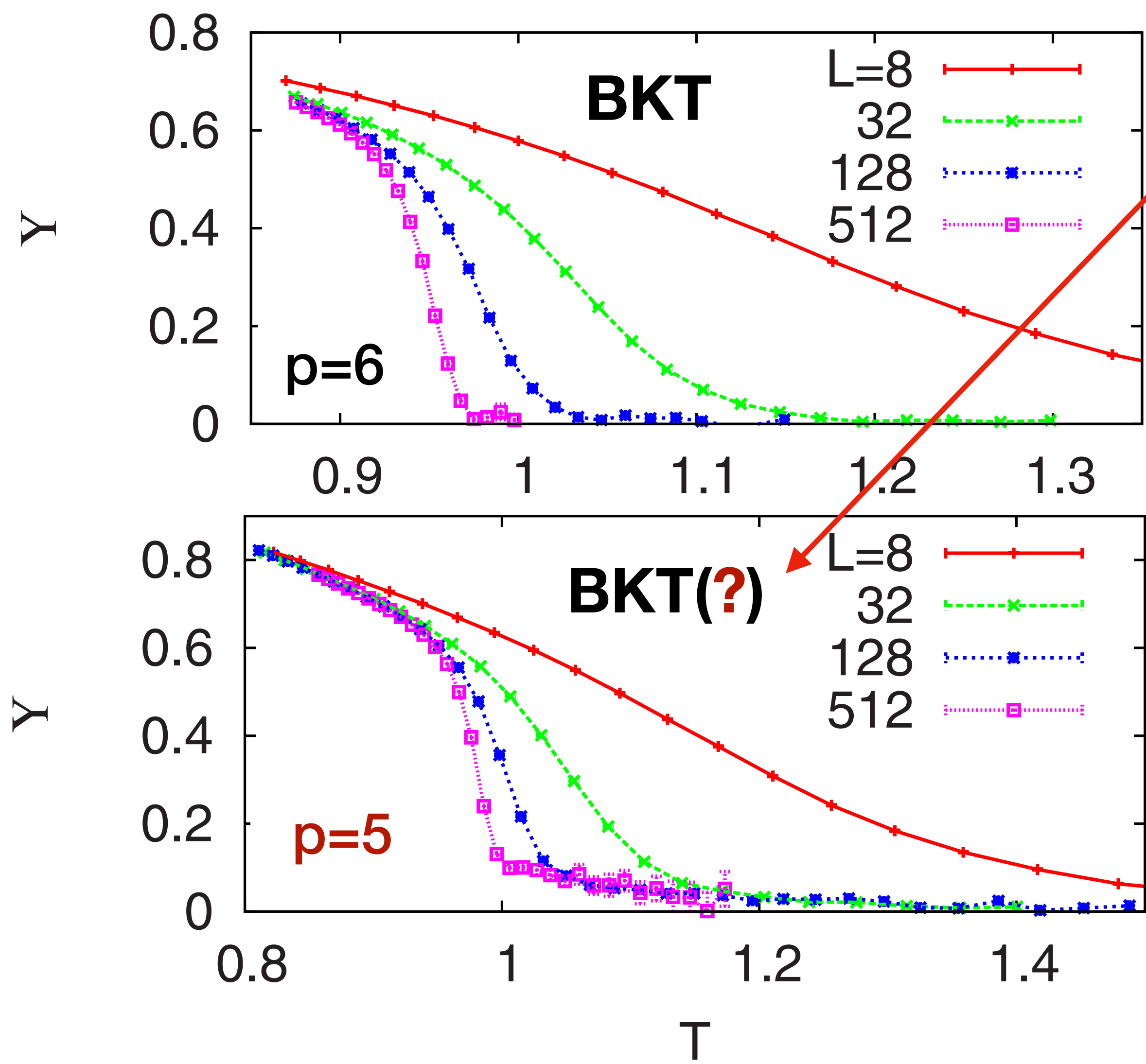
Wang-Landau Monte Carlo calculations **up to L=28**

said it looks like the **second-order(!)** transition.



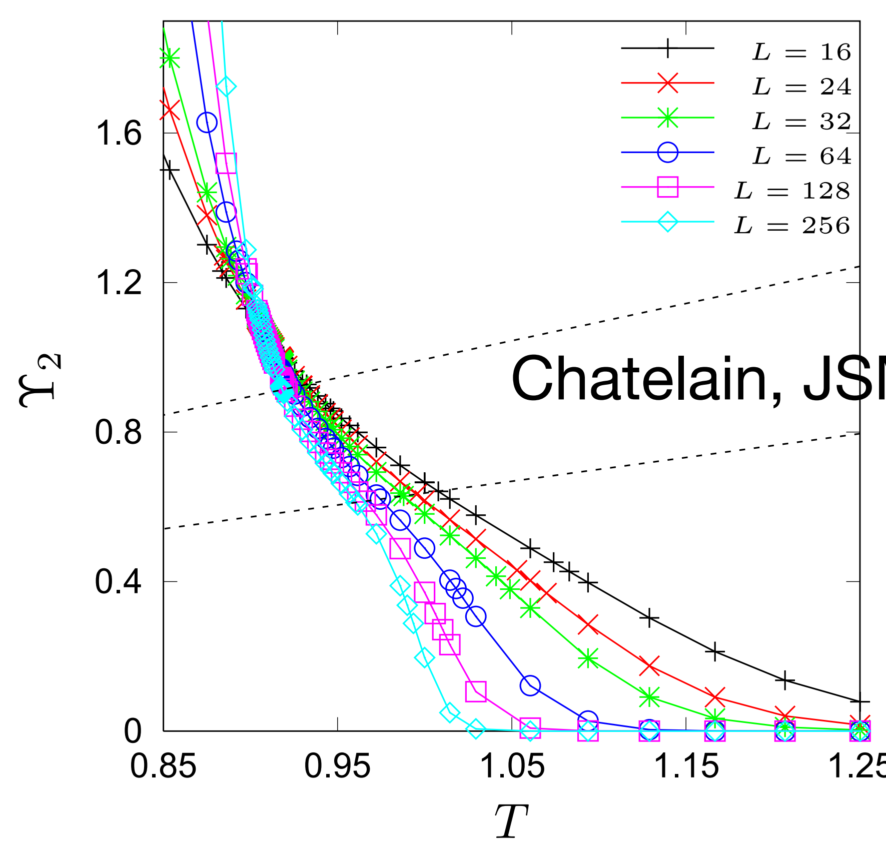
No, it's BKT at p=6 (helicity modulus).

Baek, Minnhagen, Kim, PRE 81, 063102 (2010)
Baek, Minnhagen, PRE 82, 031102 (2010)



Yes, it is BKT but with residual symmetry.

Kumano et al., PRE 88, 104427 (2013).
[cf. Baek et al., PRE 88, 012125, (2013)]



Chatelain, JSM P11022 (2014)

Disagreements & Questions

p-state clock model	Helicity modulus	Fisher zero
p=6	**BKT**	2nd. order **?** (WL calc. - Hwang 2009)
p=5	**BKT** (with a **new** definition of helicity modulus)	**?**

The only previous Fisher calculations in the p-state clock models:

Hwang, PRE 80, 042103 (2009): **p=6**, up to **L=28** with **W**ang-**L**andau method

It disagreed with the helicity modulus results but has not been re-examined.

- Wang-Landau method gives very accurate results, usually.
- L=28: too small. WL simulations can be done for much larger ones for p=6;
- cf. Lee-Yang zeros in the XY model: up to L=256 with MC + histogram reweighting.

Q. Are there any fundamental issues with the BKT transition?

In this talk, …

What was wrong with Fisher zeros at the BKT transitions?

⟶ Monte Carlo noises become unbearable, very quickly.

⟶ This is a "**feature**" of BKT; it's *unavoidable within MC*.

Can we improve the situation?

⟶ Yes, with **HOTRG**, to some extent.

⟶ Logarithmic subleading-order corrections are essential.

⟶ Better finite-size-scaling analysis can be done.

Zeros of Partition Function: the "Fisher" zeros

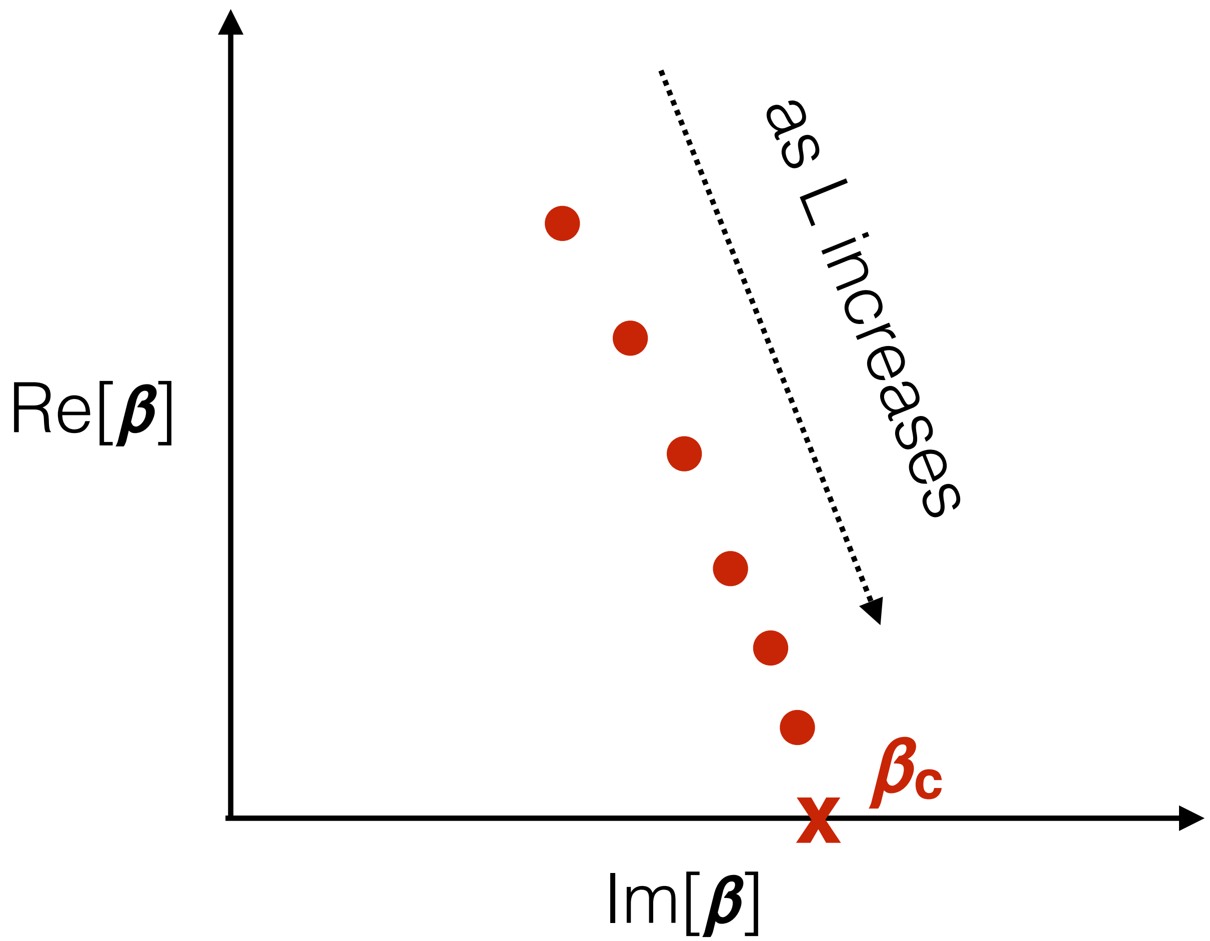
M. E. Fisher (1965)

(**complex temperature**, no external field)

Phase transition: $F = -k_B T \ln \mathcal{Z}$ → **singular free energy!**

At, $\beta = \beta_c$ → $\mathcal{Z}(\beta) = \sum_E g(E) \exp[-\beta E] = 0$

No real solution exists in finite-size systems, but …



Finite-Size-Scaling behavior of the "leading" Fisher zero

$$\mathrm{Im}[z_1] \sim L^{-1/\nu}$$
$$|\mathrm{Re}[z_1] - z_c| \sim L^{-1/\nu^*}$$

↓

A tool to study a phase transition without an order parameter

Lots of works have done. For a review, see Bena et al., Int. J. Mod. Phys. B 19, 4269 (2005).

Numerical strategy to compute Fisher zeros

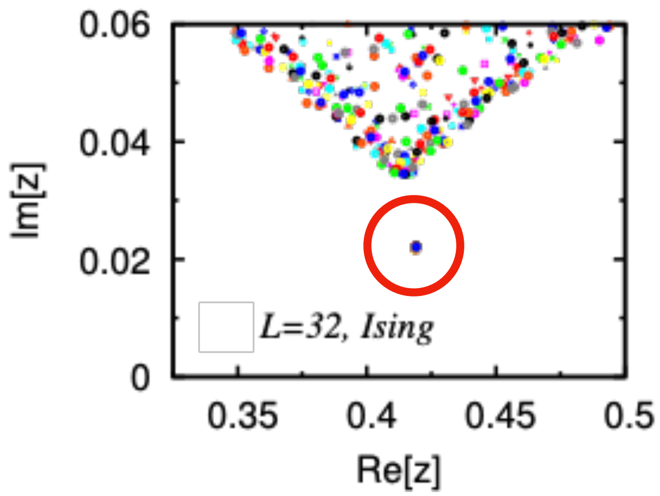
Given that we have g(E) ...

from exact counting,
histogram reweighing,
Wang-Landau, or ...

1. solving polynomial equation

for equally spaced discrete energies

$$\mathcal{Z} = \sum_n g_n e^{-\beta n \epsilon} = \sum g_n z^n \xrightarrow{\text{polynomial solver}} \prod_i (z - z_i)$$



quick and easy, and works the best with exact g(E).

2. graphical solution + minimization

$$\mathcal{Z}(\beta) = \mathcal{Z}_R(\beta) + i\mathcal{Z}_I(\beta)$$

map of zeros   map of zeros

find intersections $\xrightarrow{\text{fine tuning}}$ minimize |Z|

slow, manual-geared, cumbersome,

but allows error analysis!

Numerical strategy to compute Fisher zeros

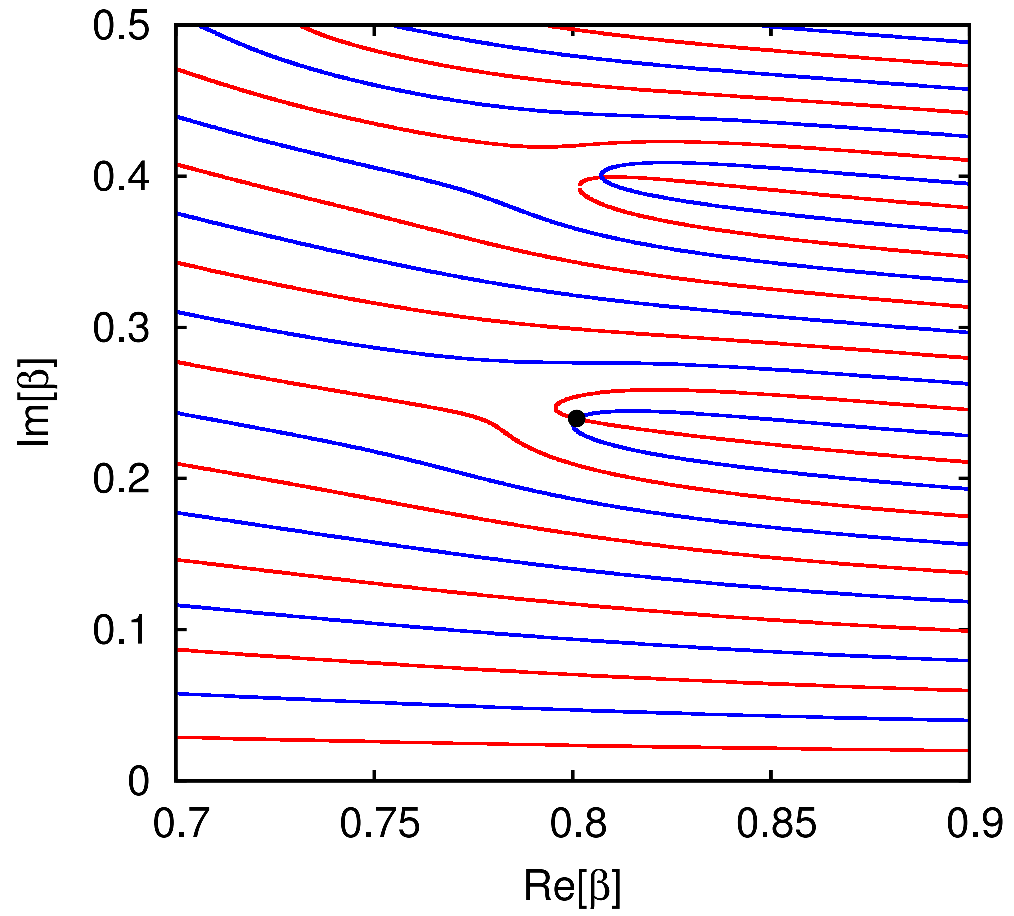
1. solving polynomial equation $\mathcal{Z} = \sum_n g_n e^{-\beta n \epsilon} = \sum g_n z^n \longrightarrow \prod_i (z - z_i)$

2. Graphical search + refinement

$$\tilde{\mathcal{Z}} \equiv \frac{\mathcal{Z}(\beta)}{\mathcal{Z}(\beta_R)}$$

$$\frac{\mathcal{Z}_R(\beta)}{\mathcal{Z}(\beta_R)} = \sum_E P(\beta_R; E) \cos(\beta_I E) \longrightarrow$$ *Find zeros.*

$$\frac{\mathcal{Z}_I(\beta)}{\mathcal{Z}(\beta_R)} = \sum_E P(\beta_R; E) \sin(\beta_I E) \longrightarrow$$ *Find zeros.*



We need the energy distribution at a real T!

Monte Carlo with histogram reweighting

→ **<u>Wang-Landau sampling method</u>**

1. Search for the cross point
2. Minimize |Z| for refinement

Leading Fisher zero behavior vs. type of phase transition

System-size scaling behavior of the leading zero :

Second-order: $\mathrm{Im}[\beta_1] \sim L^{-1/\nu}$ ***well-established!***

First-order: $\mathrm{Im}[\beta_1] \sim L^{-d}$ ***well-established!***

BKT: $\mathrm{Im}[\beta_1] \sim [\ln bL]^{-1-\frac{1}{\nu}}$

(XY: ν=1/2) [Denbleyker et al., PRD 2014]

indirectly examined; only for XY.

Can we compute the leading Fisher zero in a large enough system?

Ising model (2D) : It can be done up to L=256. (my own test, unpublished)

Potts model (2D) : it reached L=128 long time ago. [PRE 65, 036110 (2002)]

XY model : up to L=128 with HOTRG. [Denbleyker et al., PRD 89, 016008 (2014)]

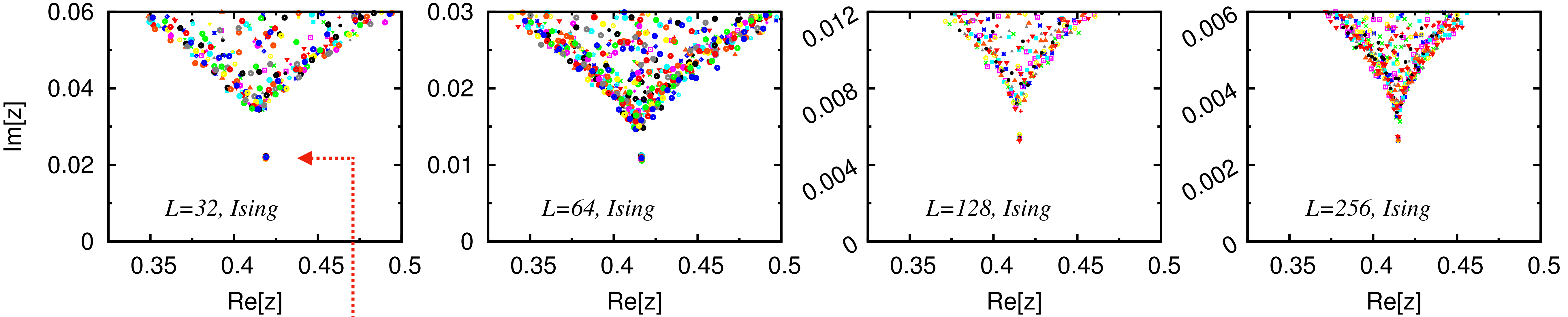
Clock model : up to L=32 with WL. [DHK, PRE 2017]

Test: 2D Ising model

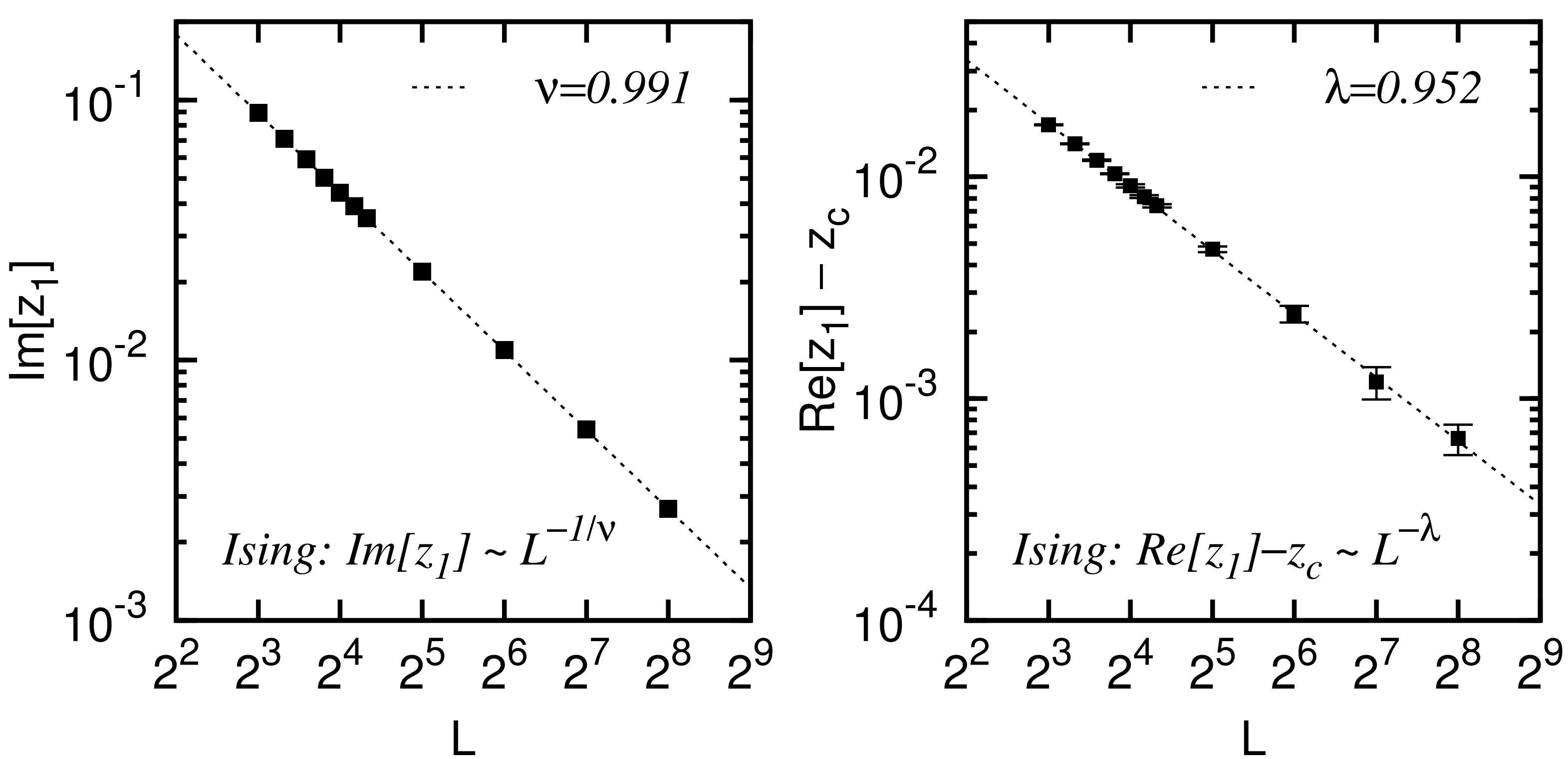
Polynomial Solver + WL density of states

L=256: Parallel replica-exchange WL [Vogel et al., PRL 2013]

$$z = \exp[2\beta]$$



"leading" zero



$$\mathrm{Im}[z_1] \sim L^{-1/\nu}$$

$$|\mathrm{Re}[z_1] - z_c| \sim L^{-1/\nu^*}$$

$$\nu \approx \nu^* \approx 1$$

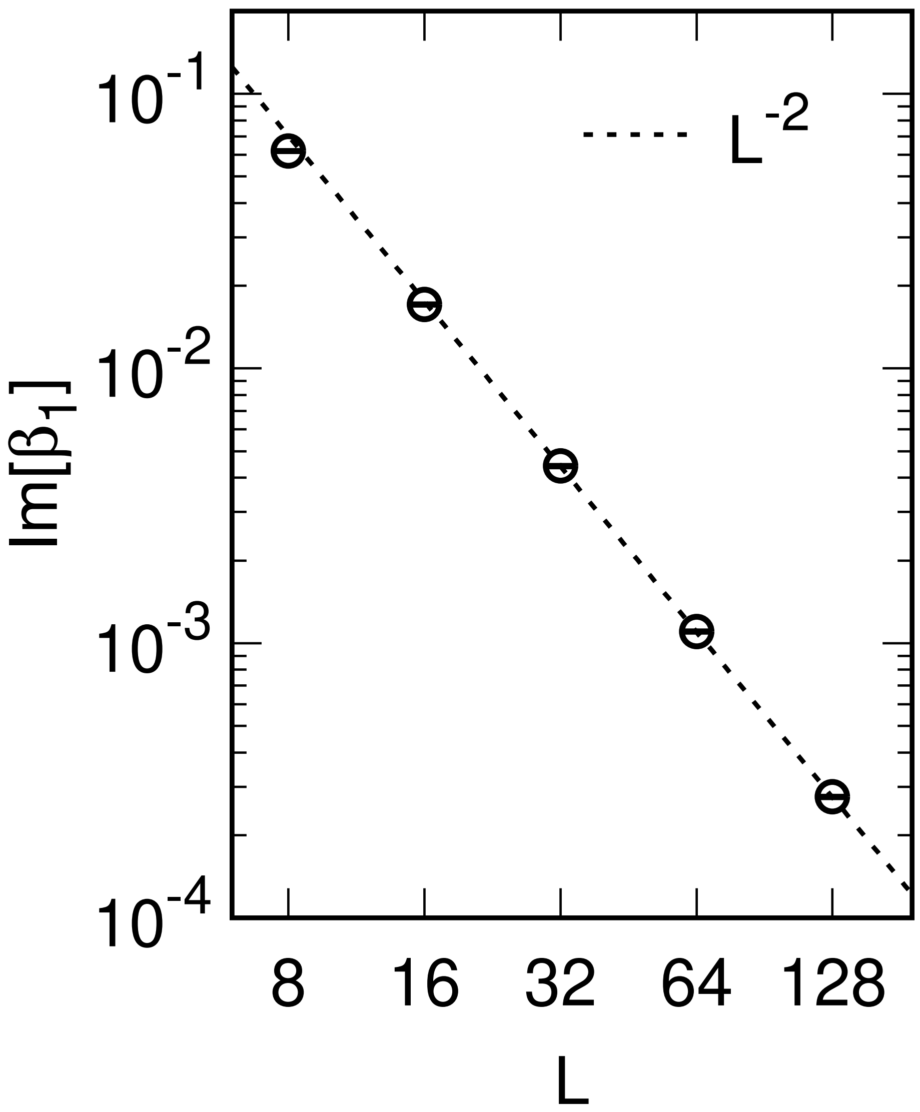
Test: 2D q-state Potts model

Graphical solutions based on WL density of states

q=10

First-order transition

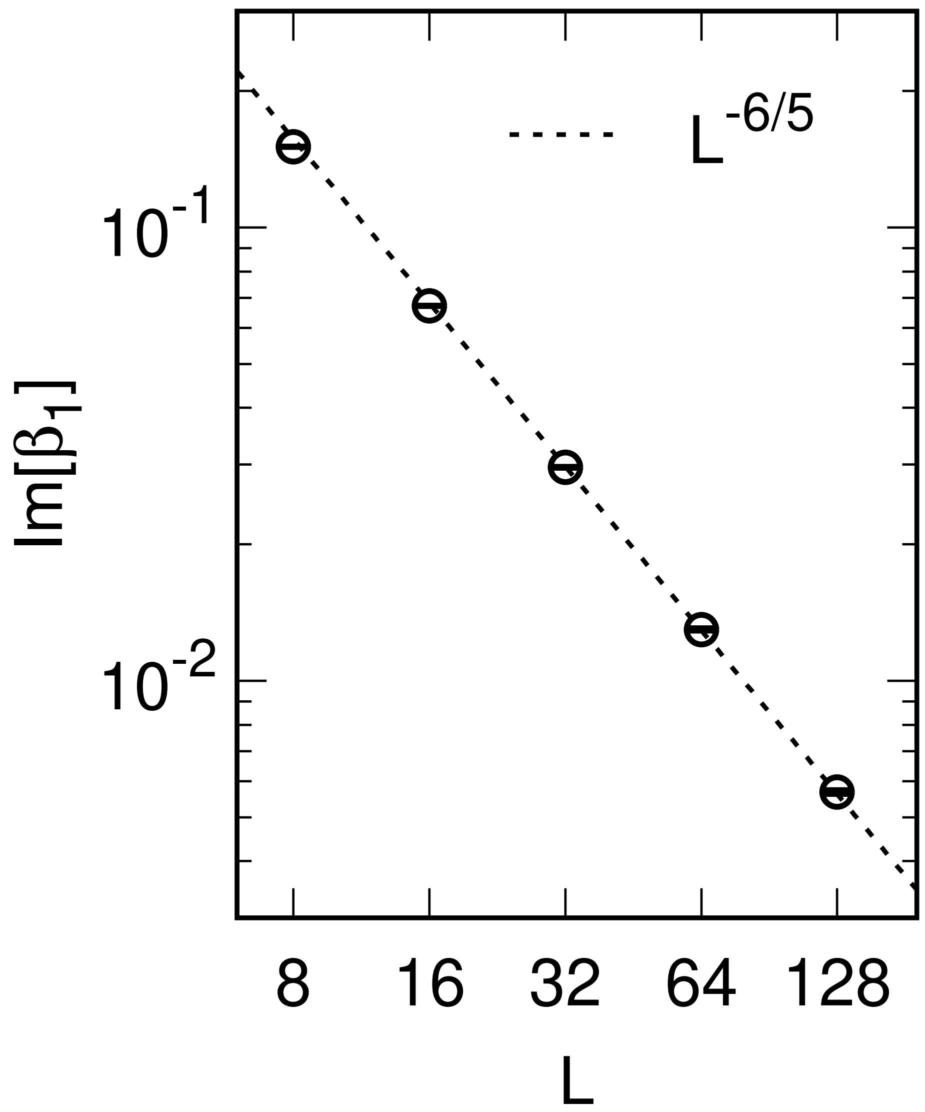
$$\mathrm{Im}[\beta_1] \sim L^{-d}$$



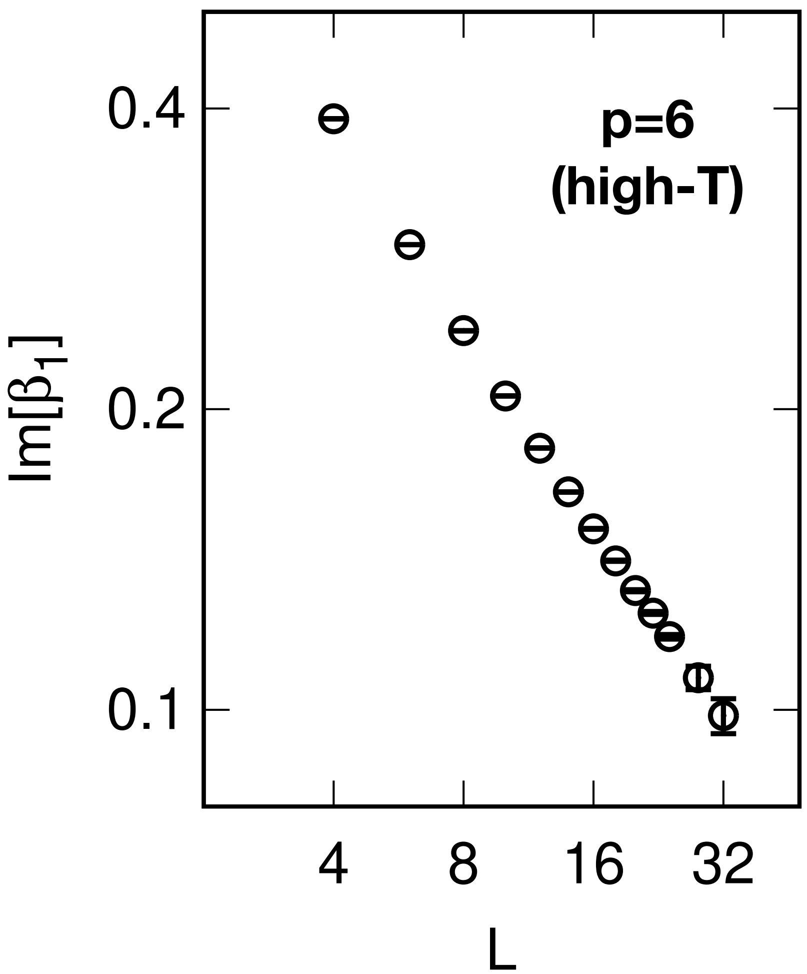
q=3

Second-order transition

$$\mathrm{Im}[\beta_1] \sim L^{-1/\nu}$$



2D p-state clock model



p=6: a usual WL algorithm works fine.

(WL DOS is available for up to L=256)

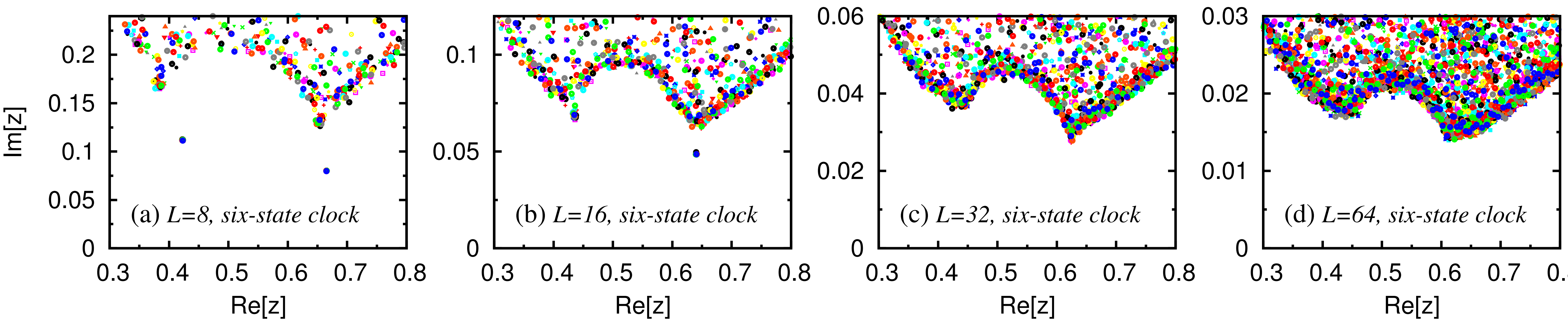
p≠6: [DHK, PRE 96, 052130 (2017): **p=5, 8, 10**, (12)]

(irregular energy spacing problem resolved for WL)

No FSS!

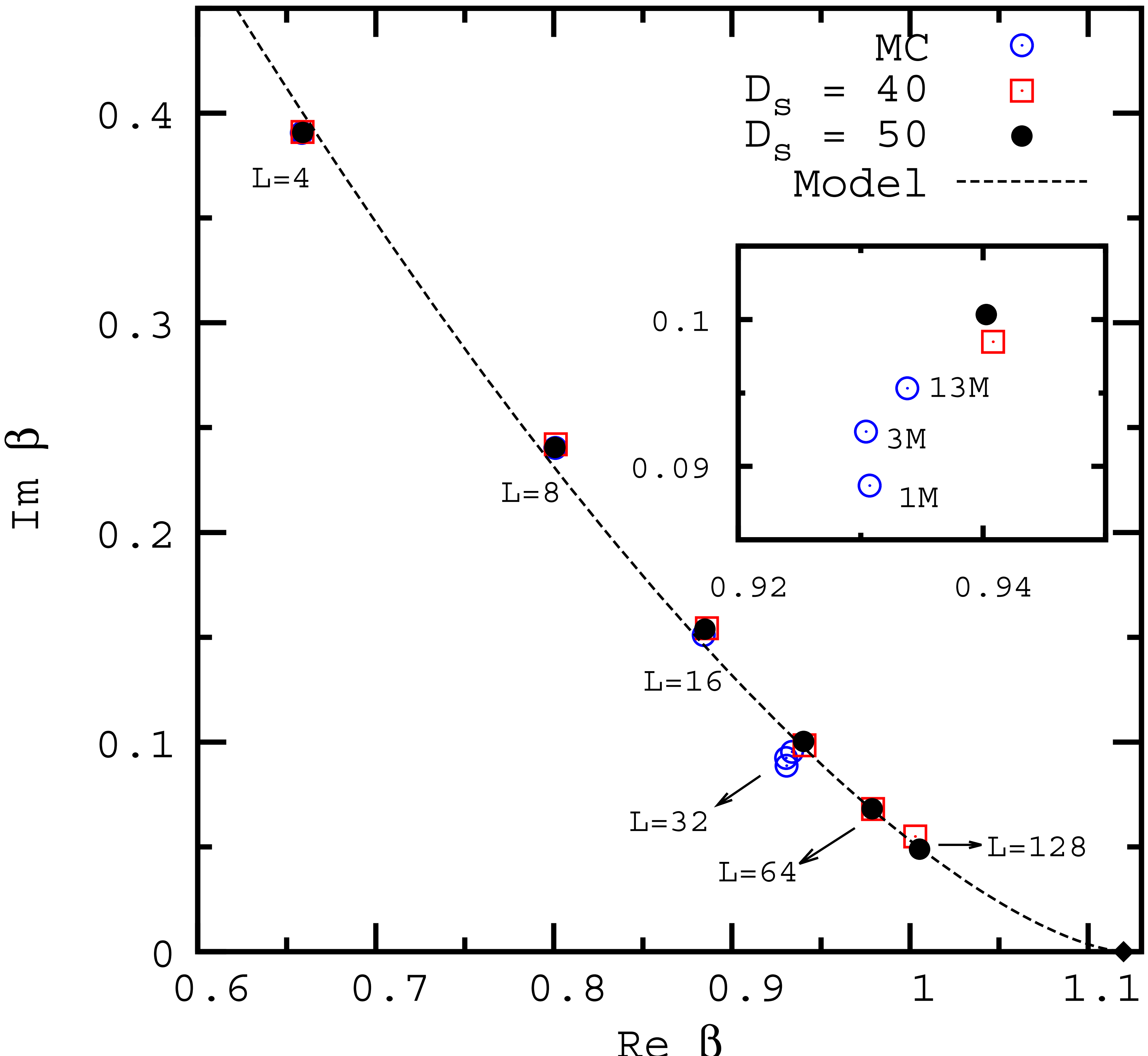
High T: the error blows up for L > 32.

Low T: the error blows up for L > 16.



XY model : leading Fisher zeros calculations using HOTRG

A. Denbleyker, Y. Liu, Y. Meurice, M. P. Qin, T. Xiang, Z. Y. Xie, J. F. Yu, and H. Zou,
Phys. Rev. D 89, 016008 (2014).



For a small Im[β],

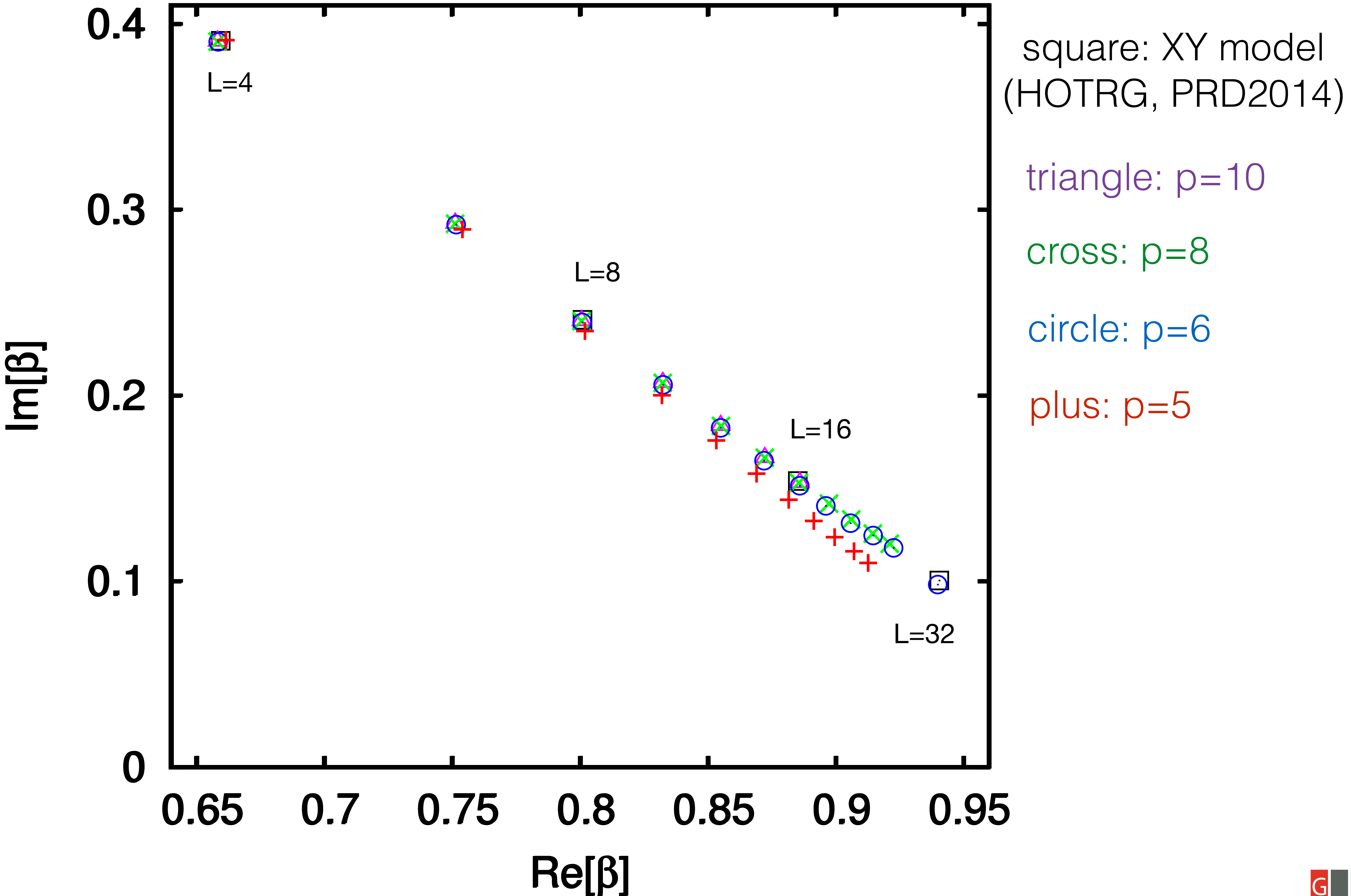
$$\mathrm{Im}[\beta_1] \sim [\ln(bL)]^{-1-\frac{1}{\nu}}$$

$$|\beta_c - \mathrm{Re}[\beta_1]| \sim [\ln(bL)]^{-\frac{1}{\nu}}$$

$$\boxed{\mathrm{Im}[\beta_1] \propto |\beta_c - \mathrm{Re}[\beta_1]|^{\frac{3}{2}}}$$

L = 4, 8, 16, 32, 64, 128

High-temperature transition

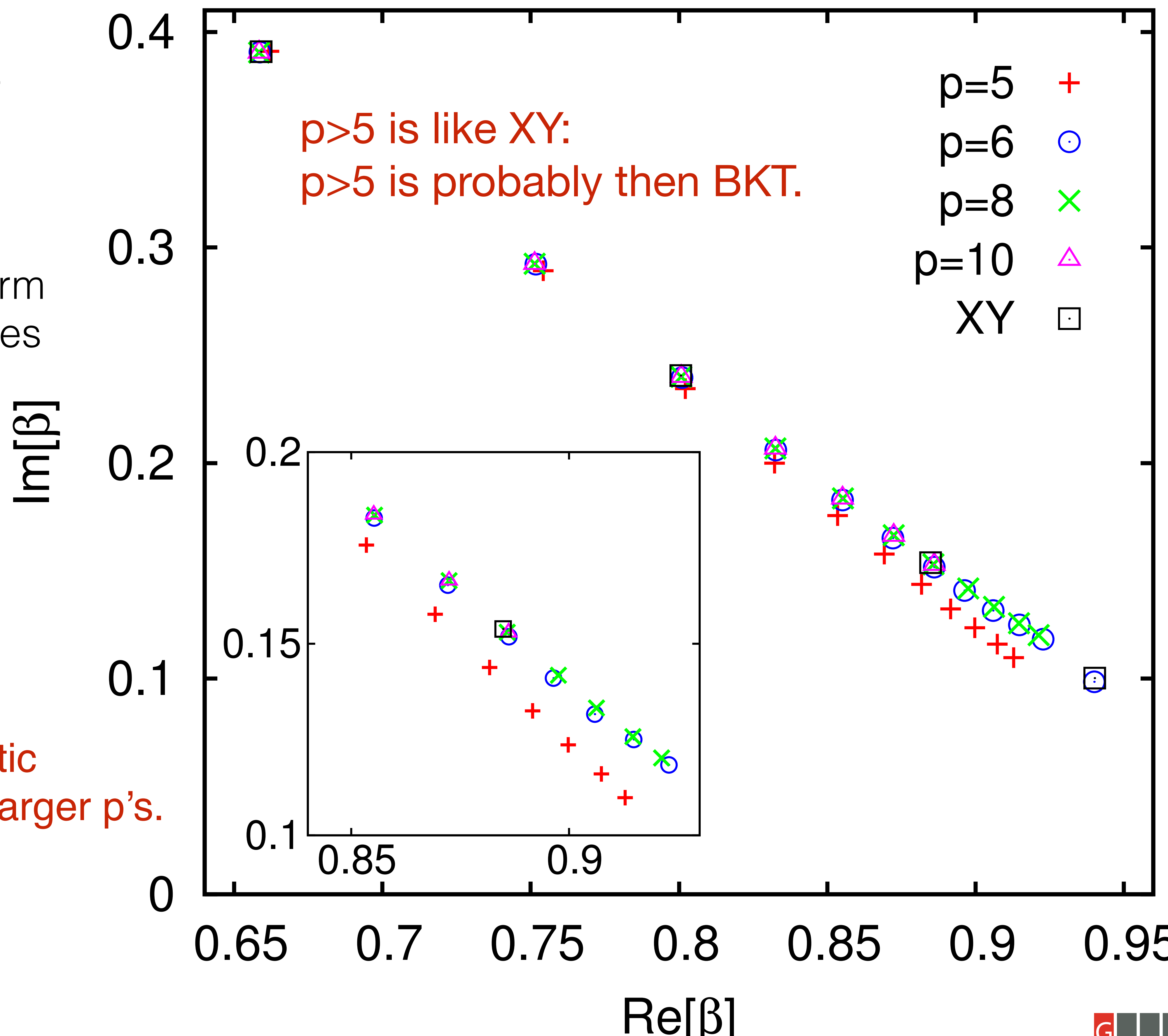


Strong form of universality?

at a high-temperature transition

The leading zeros for p=6,8,10 falls onto those of the XY limit.

The same singular form of free energy emerges for p>5.



p=5 shows systematic difference from the larger p's.

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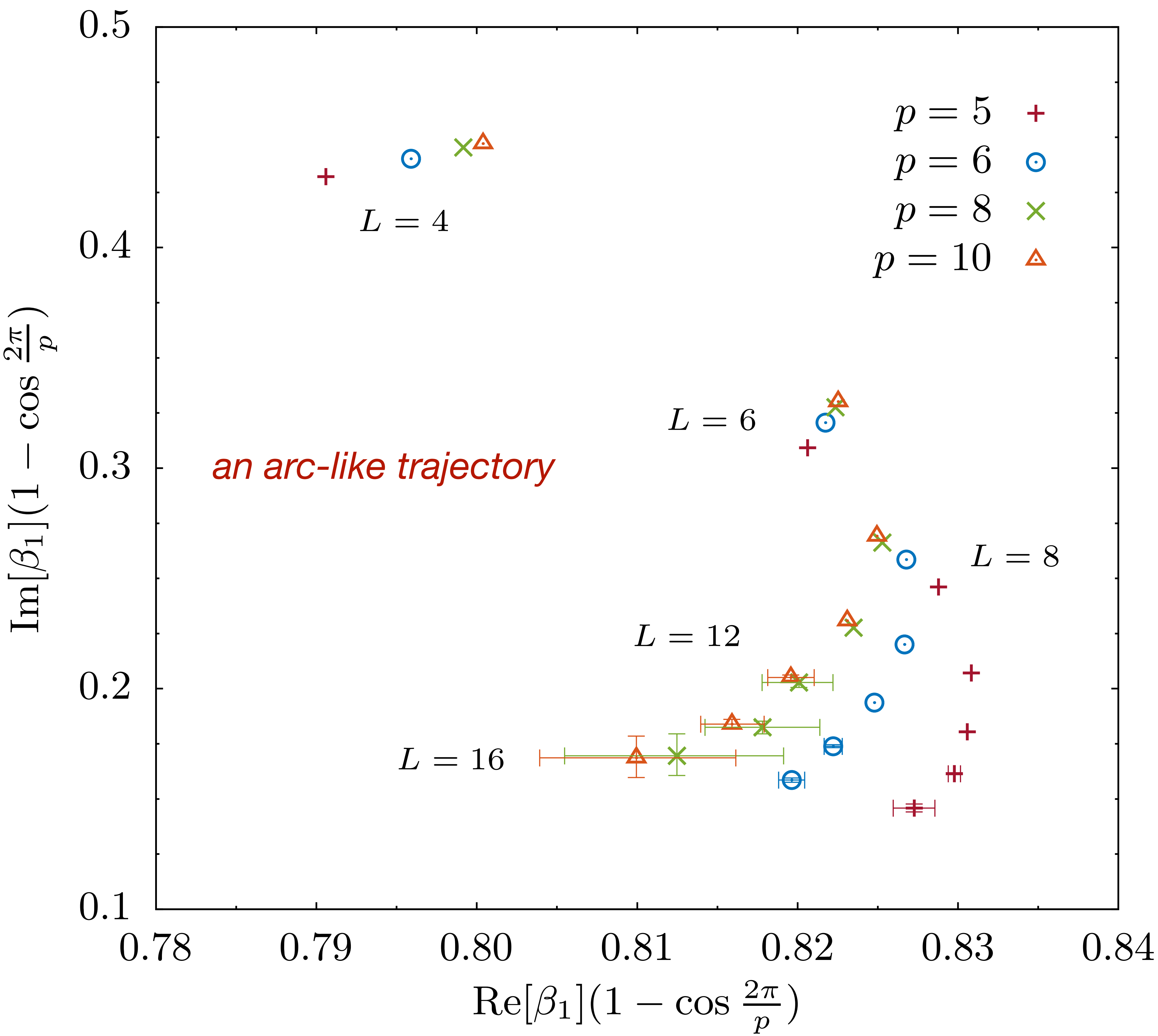
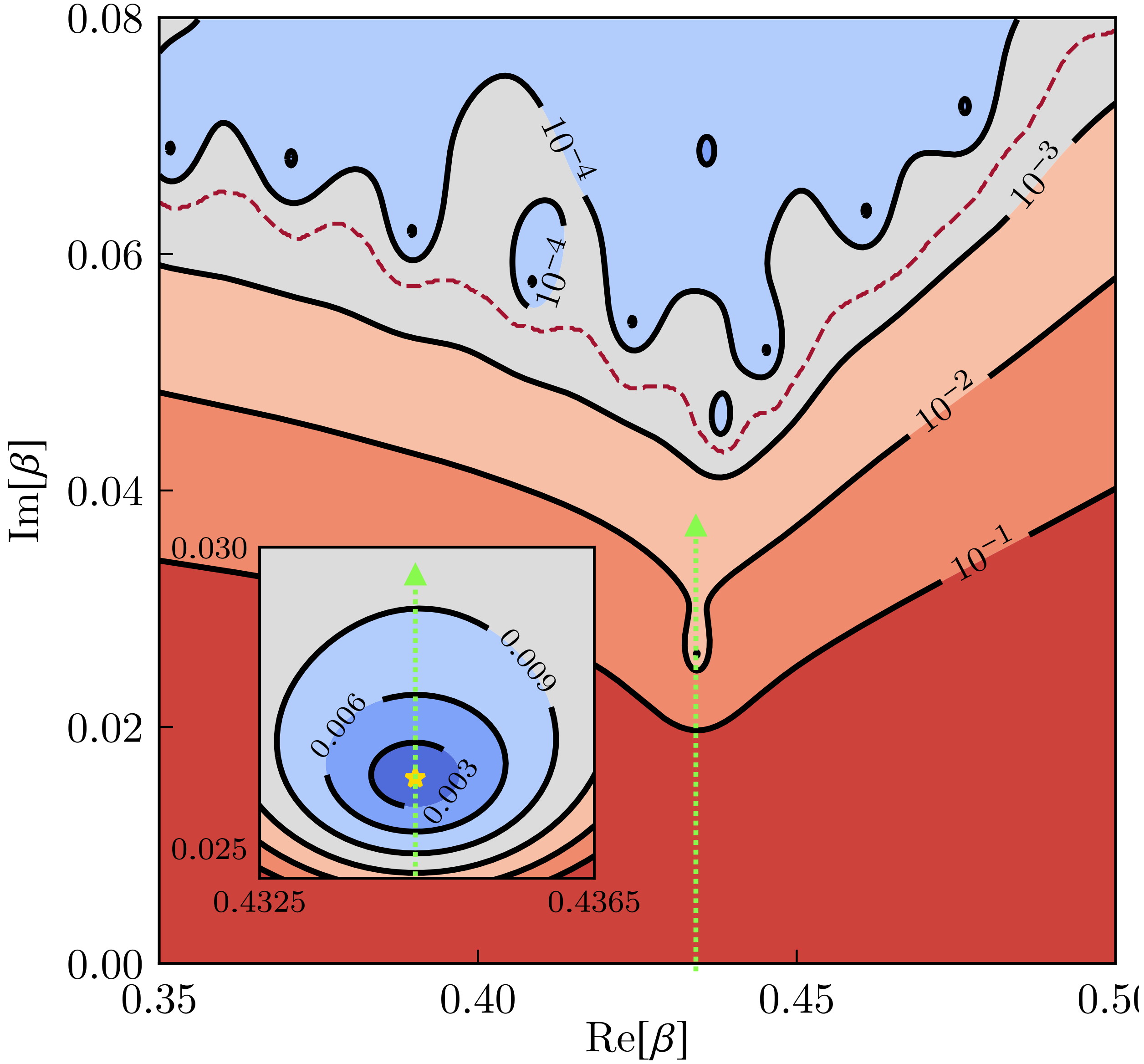
Low-temperature transition

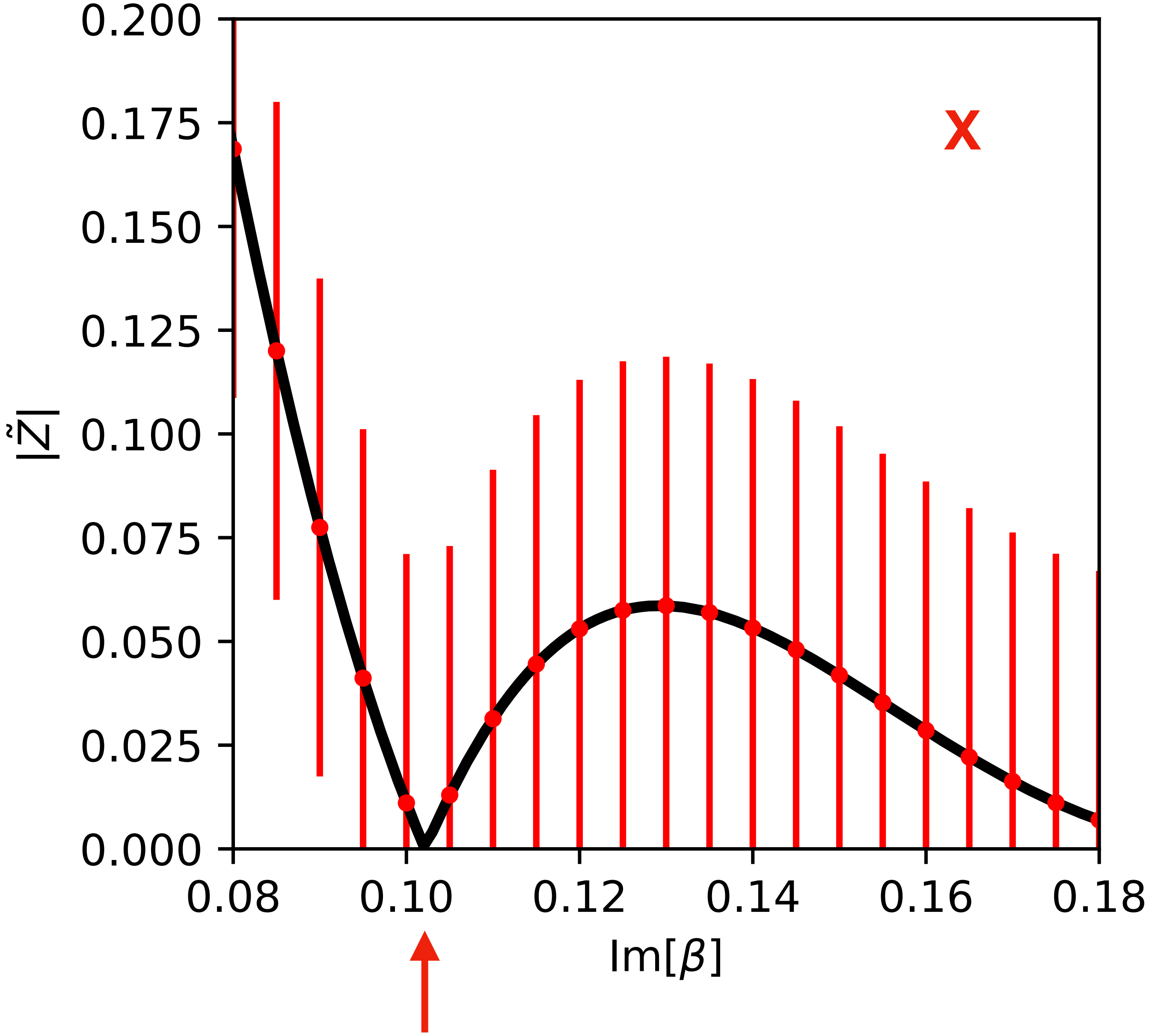
Still, no clues for what they are…



Numerical visibility of Fisher zeros

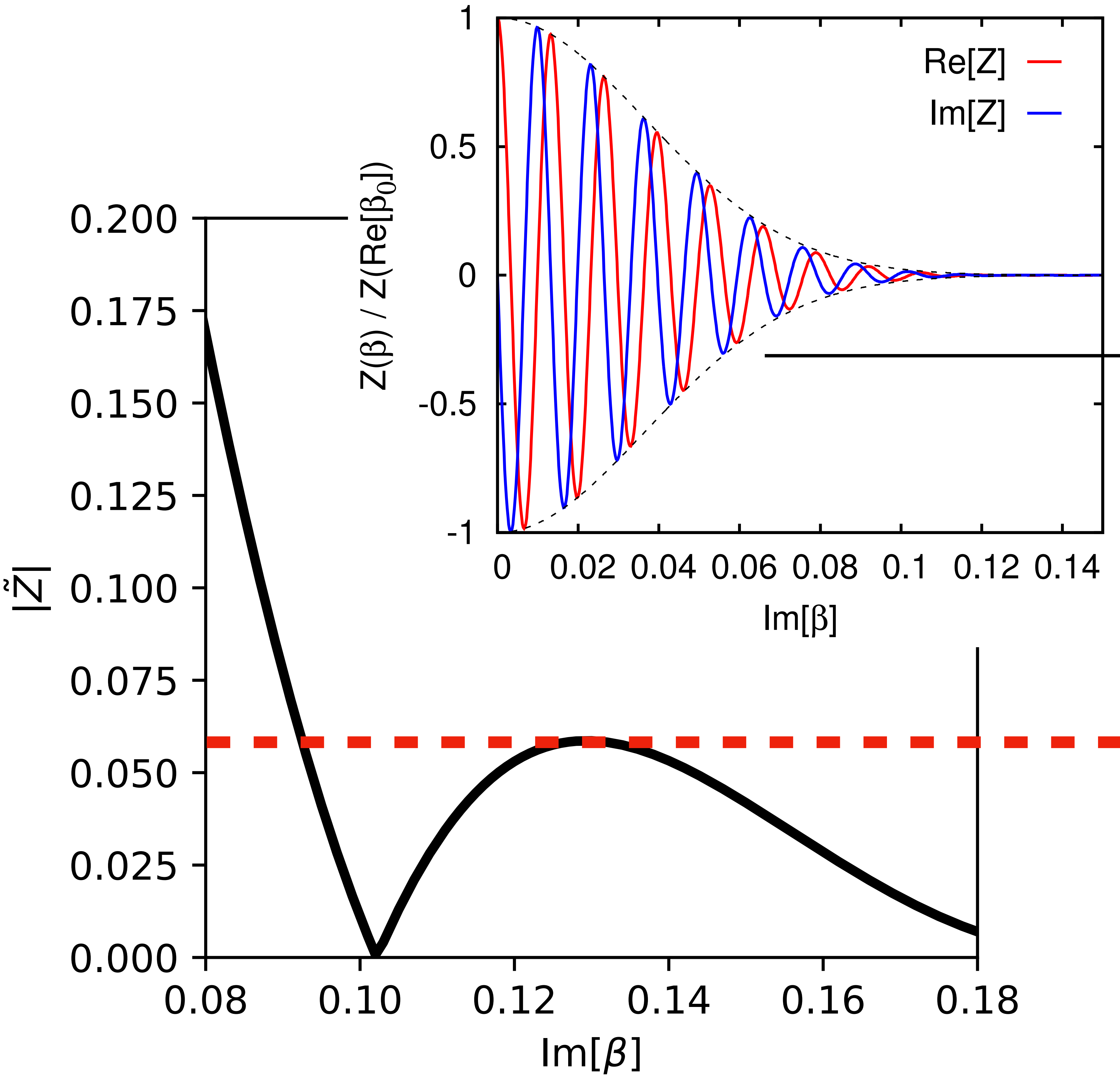
$\left|\tilde{\mathcal{Z}}\right|$ **: amplitude of a normalized partition function**





The leading Fisher zero

Scaling behavior of the tolerable error level



Envelope function (Gaussian DOS)

$$\exp[-\frac{1}{2}\sigma_E^2\beta_I^2]$$

approx.

~ Max. tolerable error

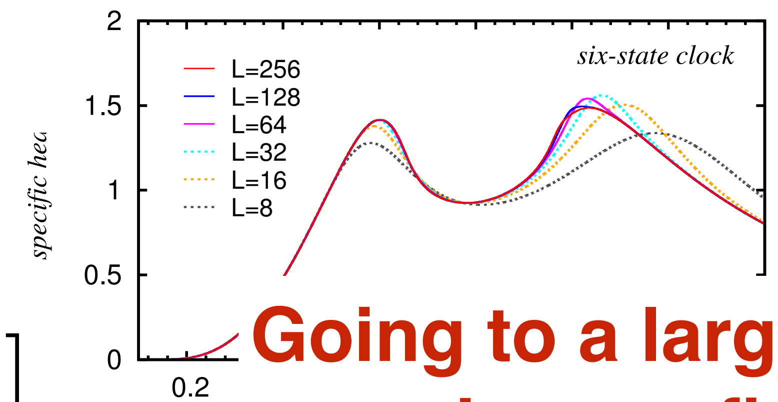
Scaling behavior of the tolerable error level

approx. max. error tolerance vs. Wang-Landau fluctuations

$$\exp[-\frac{1}{2}\sigma_E^2\beta_I^2] \rightarrow \exp[-\frac{L^d c_L^* \beta_I^2}{2\beta_R^2}]$$

at a pseudo-transition point

$$constant$$



Going to a large L is not possible under any finite fluctuations

BKT: $\sim \exp[-L^2(\ln bL)^{-6}]$

(exponential decay)

1st order: $\sim \exp[-L^{2d}L^{-2d}] = \mathcal{O}(1)$

2nd order: $\sim \exp[-L^{d+\alpha/\nu}L^{-2/\nu}] = \mathcal{O}(1)$

Ising model:

$\sim L^{-a}$

weak 2nd. order:

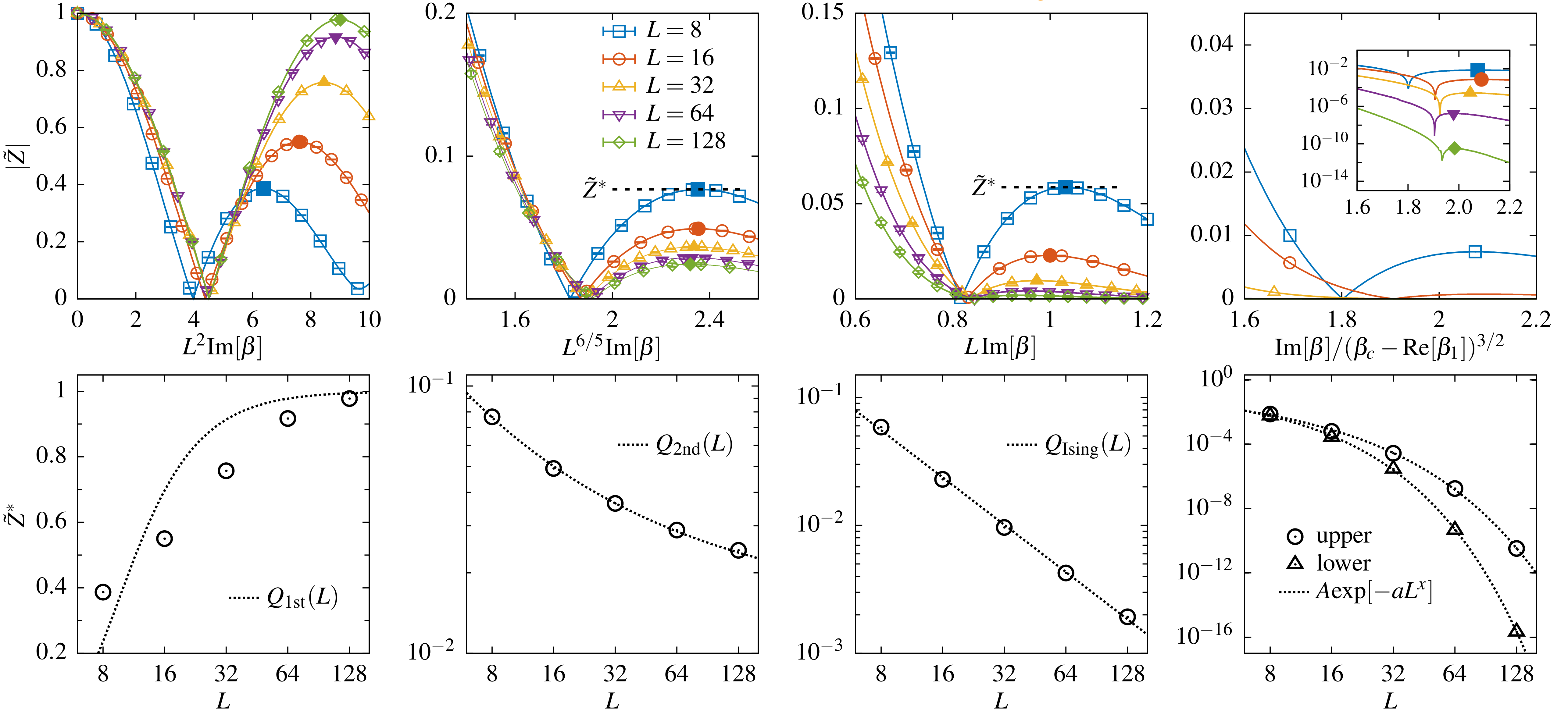
$\sim \exp[aL^{-\omega}]$

1st vs. 2nd. vs. BKT transitions

[S. Hong and D.-H. Kim, arXiv:1906.09036]

System-size scaling of numerical visibility of the leading Fisher zero.

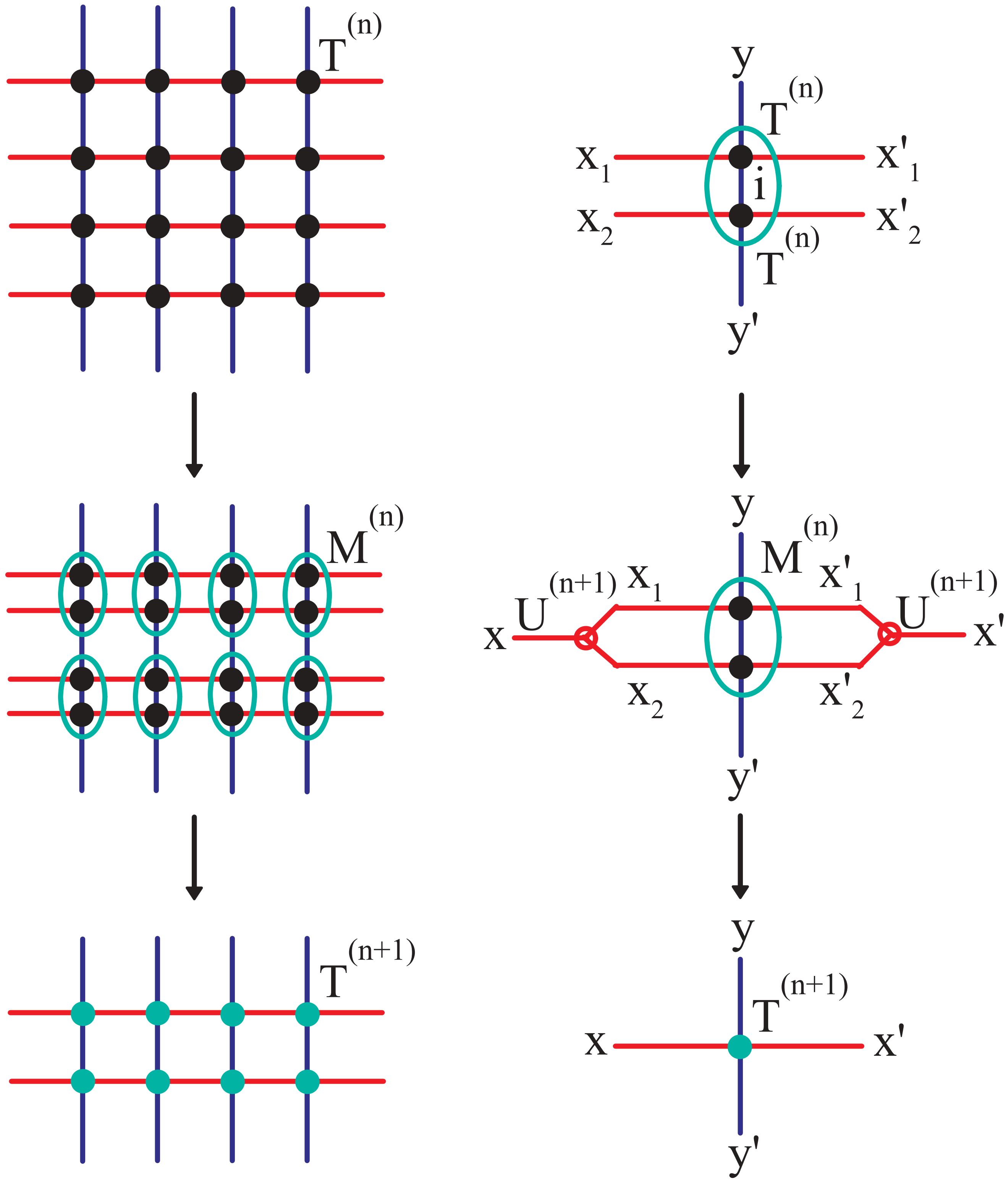
Potts (q=10) | Potts (q=3) | Ising | Clock (p=5); HOTRG



$\sim \exp[aL^{-\omega}]$ $\sim L^{-a}$ $\sim \exp[-aL^{-x}]$

Higher-Order Tensor Renormalization Group (HOTRG)

Xie, Chen, Qin, Zhu, Yang & Xiang, PRB **86**, 045139 (2012).



1. Contraction

$$x' = x'_1 \otimes x'_2$$
$$x = x_1 \otimes x_2$$

$$M^{(n)}_{xx'yy'} = \sum_i T^{(n)}_{x_1 x'_1 y i} T^{(n)}_{x_2 x'_2 i y'}$$

(D^2xD^2xDxD)

2. HOSVD

$$M^{(n)}_{xx'yy'} = \sum_{ijkl} S_{ijkl} U^L_{xi} U^R_{x'j} U^U_{yk} U^D_{y'l}$$

U : (D^2 x D_c)

3. Truncation

cutoff

$$T^{(n+1)}_{xx'yy'} = \sum_{ij} U_{ix} M^{(n)}_{ijyy'} U^*_{jx'}$$

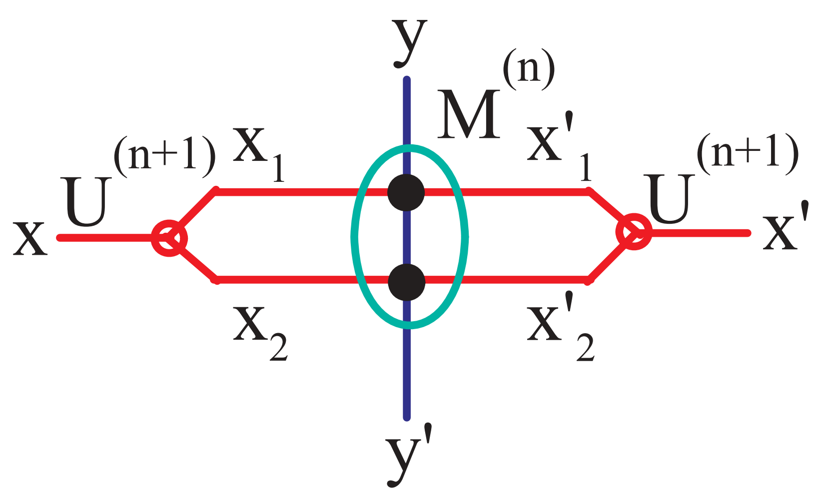
(D_cxD_cxDxD)

$$x \to y \to x \to y \to \cdots$$

HOSVD in practice

$$M^{(n)}_{xx'yy'} = \sum_{ijkl} S_{ijkl} U^L_{xi} U^R_{x'j} U^U_{yk} U^D_{y'l}$$

$$T^{(n+1)}_{xx'yy'} = \sum_{ij} U_{ix} M^{(n)}_{ijyy'} U^*_{jx'}$$



Q. How can we get U?

1. U = U^L (reordering for L)

$$A_{x,x'yy'} \equiv M_{xx'yy'}$$

2. U = U^R (reordering for R)

$$A_{x',xyy'} \equiv M_{xx'yy'}$$

$\longrightarrow$ $$AA^\dagger = U \Lambda U^\dagger$$ ($D^2 x D^2$ matrix diagonalization)

$\rightarrow$ **Pick D_c largest eigenvalues and corresponding eigenvectors for U.**

Between L and R, choose the one with the smaller residual. $\epsilon_{L,R} = \sum_{i>D_c} \Lambda^{L,R}_i$

p-state clock model at a complex temperature

Recipe for XY model: A. Denbleyker et al., PRD **89**, 016008 (2014).

$$Z(\beta) = \prod_i \sum_{\theta_i} \exp\left[\beta \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)\right] = \mathrm{Tr} \prod_i T_{x_i x_i' y_i y_i'}$$

expansion with $e^{\beta \cos\theta} = \sum_{n=-\infty}^{\infty} I_n(\beta) e^{in\theta}$

Initial local tensor:

$$T_{xx'yy'} = \sqrt{I_x(\beta) I_{x'}(\beta) I_y(\beta) I_{y'}(\beta)}\, \underline{\delta_{\mathrm{mod}(x+y-x'-y',p),0}}$$

Invariant under x <-> x' & y <-> y'

c.f. XY : $\delta_{x+y-x'-y',0}$

Issue with complex temperature

$$T^{(n+1)}_{xx'yy'} = \sum_{ij} U_{ix} M^{(n)}_{ijyy'} U^*_{jx'} \longleftarrow$$

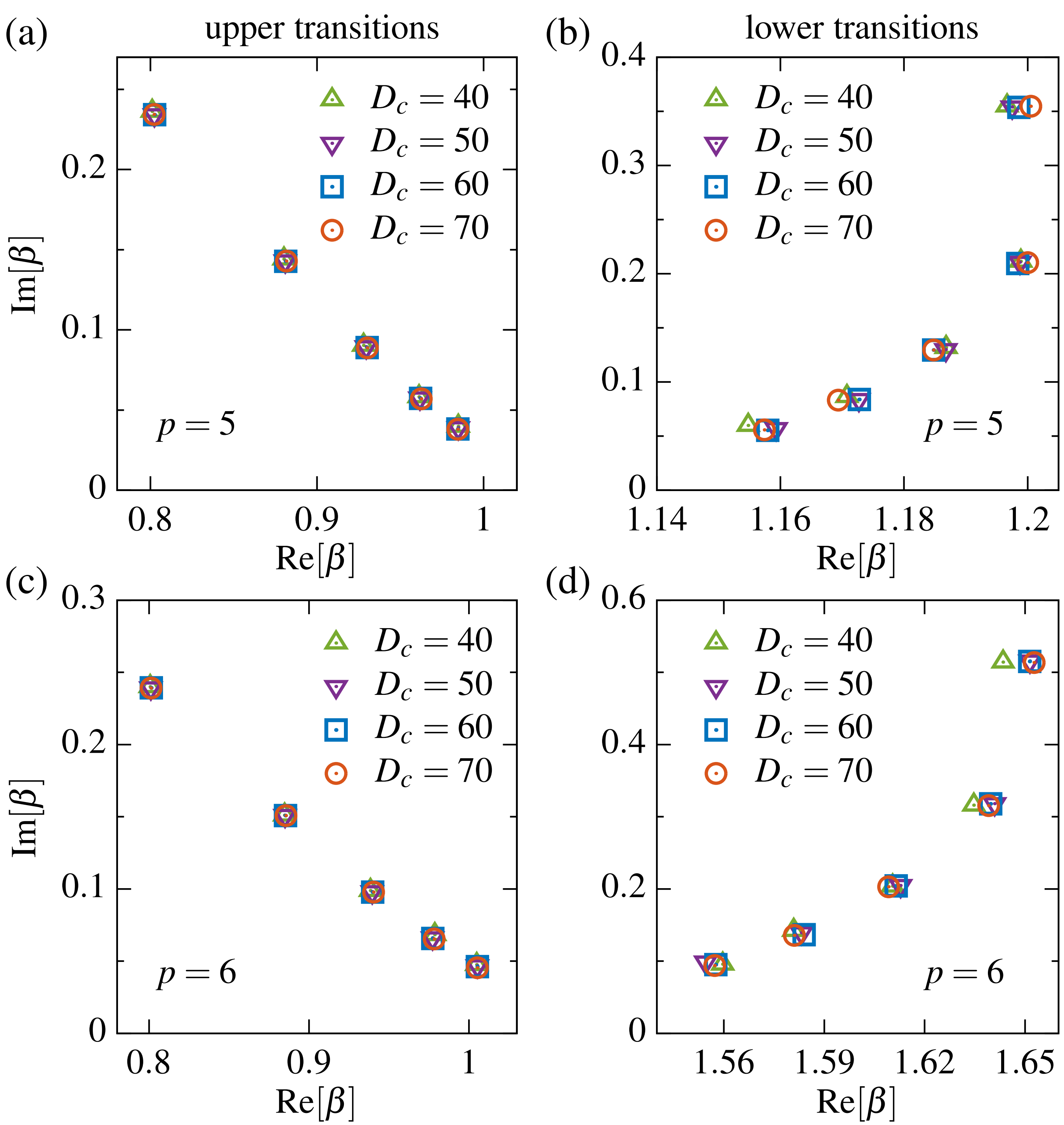
$$\mathrm{Re}[AA^\dagger] = U \Lambda U^T$$

$$\cancel{AA^\dagger = U \Lambda U^\dagger}$$

If U is complex, it breaks the symmetry.

Fix: orthogonal transformation

p-state clock model at complex temperature : leading Fisher zeros



D_c = 40, 50, 60, 70 are tested

L = 8, 16, 32, 64, 128

Are they BKT?

$$\mathrm{Im}[\beta_1] \sim [\ln(bL)]^{-1-\frac{1}{\nu}}$$

$$|\beta_c - \mathrm{Re}[\beta_1]| \sim [\ln(bL)]^{-\frac{1}{\nu}}$$

Leading Fisher zero is like a pseudo-transition (complex) temperature.

$$\frac{\xi_L(\beta)}{L} = a_0$$

BKT correlation length

$$\longleftarrow \quad \xi = A \exp[1/(at^{\nu})]$$

A. Denbleyker et al., PRD 2014.

H. Zou, PhD Thesis 2014.

↓ *limiting case*

$$\mathrm{Im}[\beta_1] \sim [\ln(bL)]^{-1-\frac{1}{\nu}}$$

$$|\beta_c - \mathrm{Re}[\beta_1]| \sim [\ln(bL)]^{-\frac{1}{\nu}}$$

We may need this.

[M. Hasenbusch, JPA 38, 5869 (2005)]

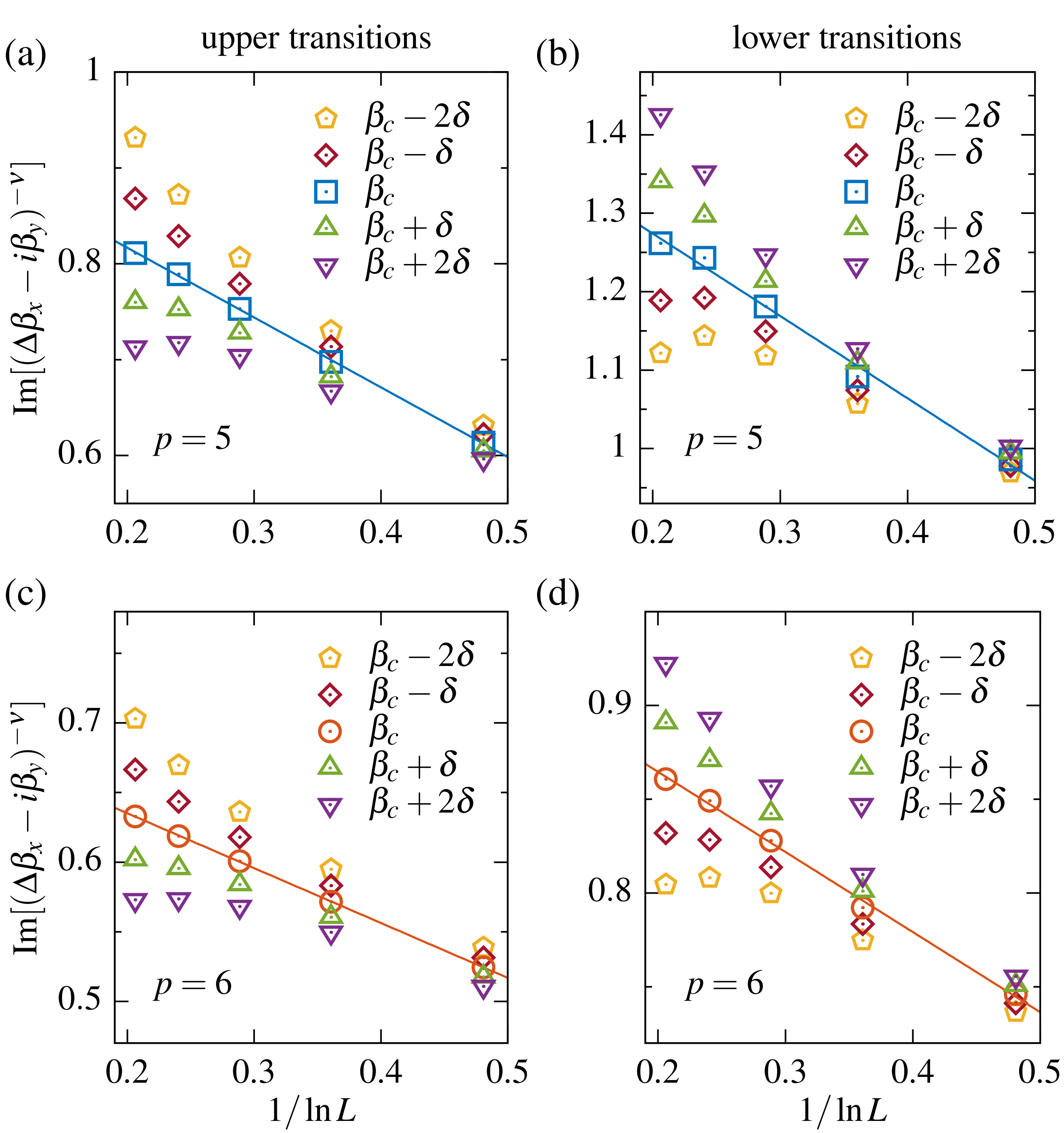
The imaginary part of ξ cannot be constant unless L = ∞.

Finite-Size-Scaling Ansatz with Logarithmic Corrections

Corrected FSS form: $$(\Delta\beta_x \pm i\beta_y)^{-\nu} \simeq a \ln bL + i\left(c_0 \boxed{- \frac{c_1}{\ln L}}\right)$$

Determination of Tc! ↓

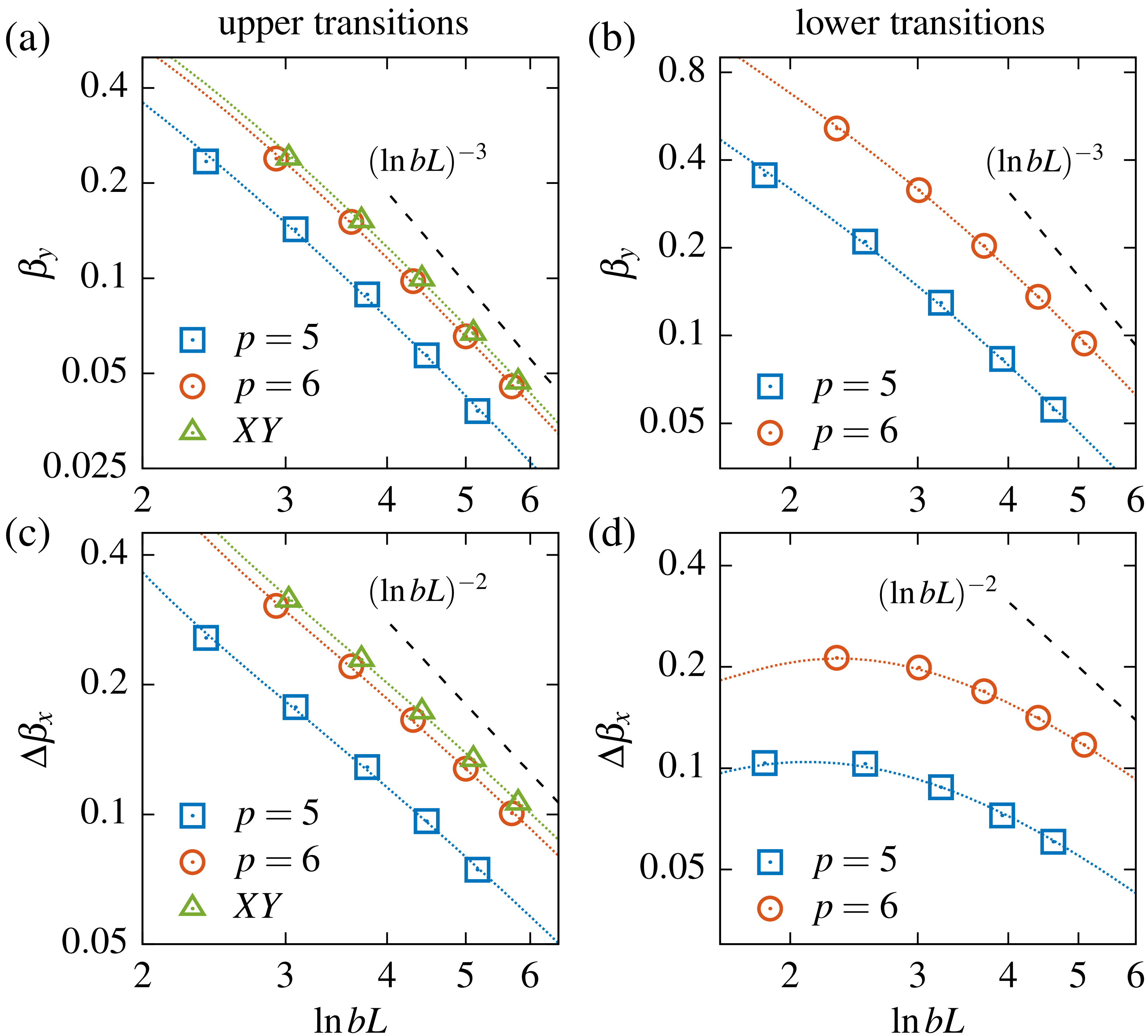
$$\Delta\beta_x = |\beta_c - \mathrm{Re}[\beta_1]| \qquad \beta_y = \mathrm{Im}[\beta_1]$$



$\beta_c^{\mathrm{high}}(p=5)$	$\beta_c^{\mathrm{low}}(p=5)$	$\beta_c^{\mathrm{high}}(p=6)$	$\beta_c^{\mathrm{low}}(p=6)$	reference
		1.088(12)	1.47(4)	[28]
		1.1111	1.4706	[29]
		1.1101(7)	1.4257(22)	[30]
1.0510(10)	1.1049(10)			[31]
		1.1086(6)		[36]
1.0593	1.1013	1.106(6)	1.4286(82)	[37]
1.058(19)	1.094(14)			[38]
1.0504(1)	1.1075(1)			[40]
1.059	1.097	1.106	1.441	$L_{\mathrm{min}} = 8$
1.058	1.101	1.106	1.444	$L_{\mathrm{min}} = 16$

It agrees well with other method.

Finite-Size-Scaling Ansatz with Logarithmic Corrections



Corrected FSS form:

$$\Delta\beta_x = \frac{\psi_L^2(1-\psi_L^2)}{(1+\psi_L^2)^2}\left[c_0 - \frac{c_1}{\ln L}\right]^{-2},$$

$$\beta_y = \frac{2\psi_L^3}{(1+\psi_L^2)^2}\left[c_0 - \frac{c_1}{\ln L}\right]^{-2}.$$

$$\psi_L = \frac{1}{a\ln bL}\left[c_0 - \frac{c_1}{\ln L}\right]$$

Finite-Size-Scaling Ansatz with Logarithmic Corrections

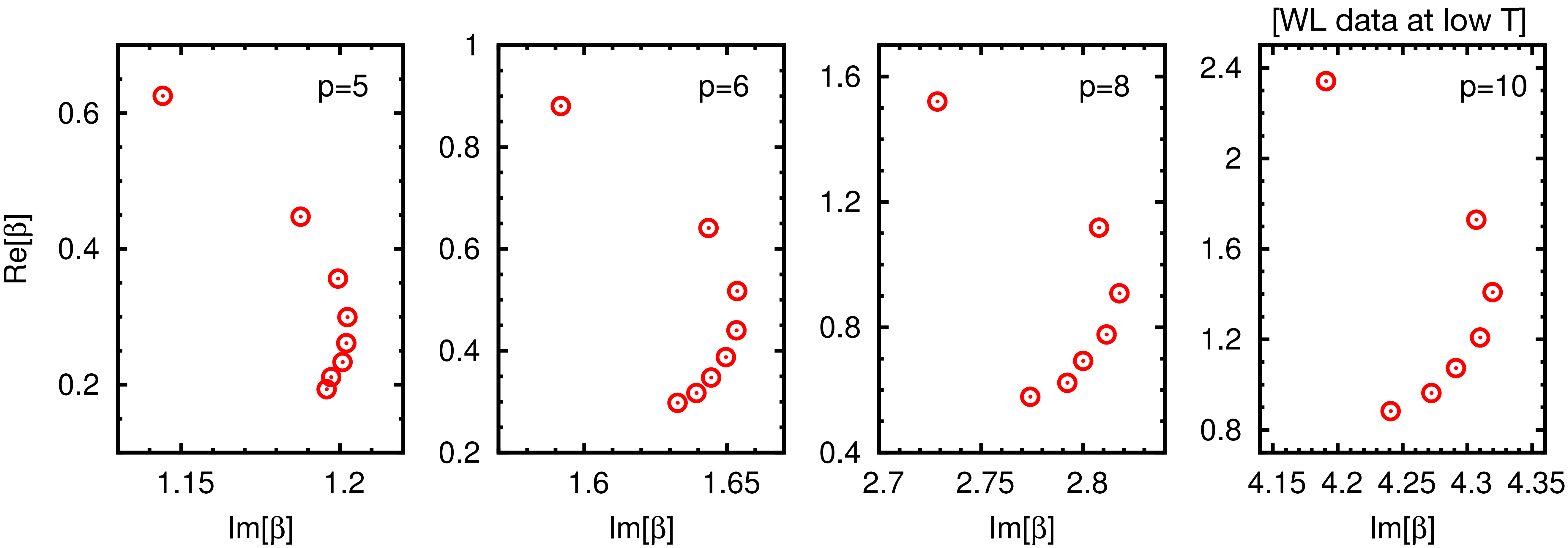
Corrected FSS form:

$$\Delta\beta_x = \frac{\psi_L^2(1-\psi_L^2)}{(1+\psi_L^2)^2}\left[c_0 - \frac{c_1}{\ln L}\right]^{-2},$$

$$\beta_y = \frac{2\psi_L^3}{(1+\psi_L^2)^2}\left[c_0 - \frac{c_1}{\ln L}\right]^{-2}.$$

$$\psi_L = \frac{1}{a\ln bL}\left[c_0 - \frac{c_1}{\ln L}\right]$$

An arc-like trajectory is observed in a certain range of ψ_L.

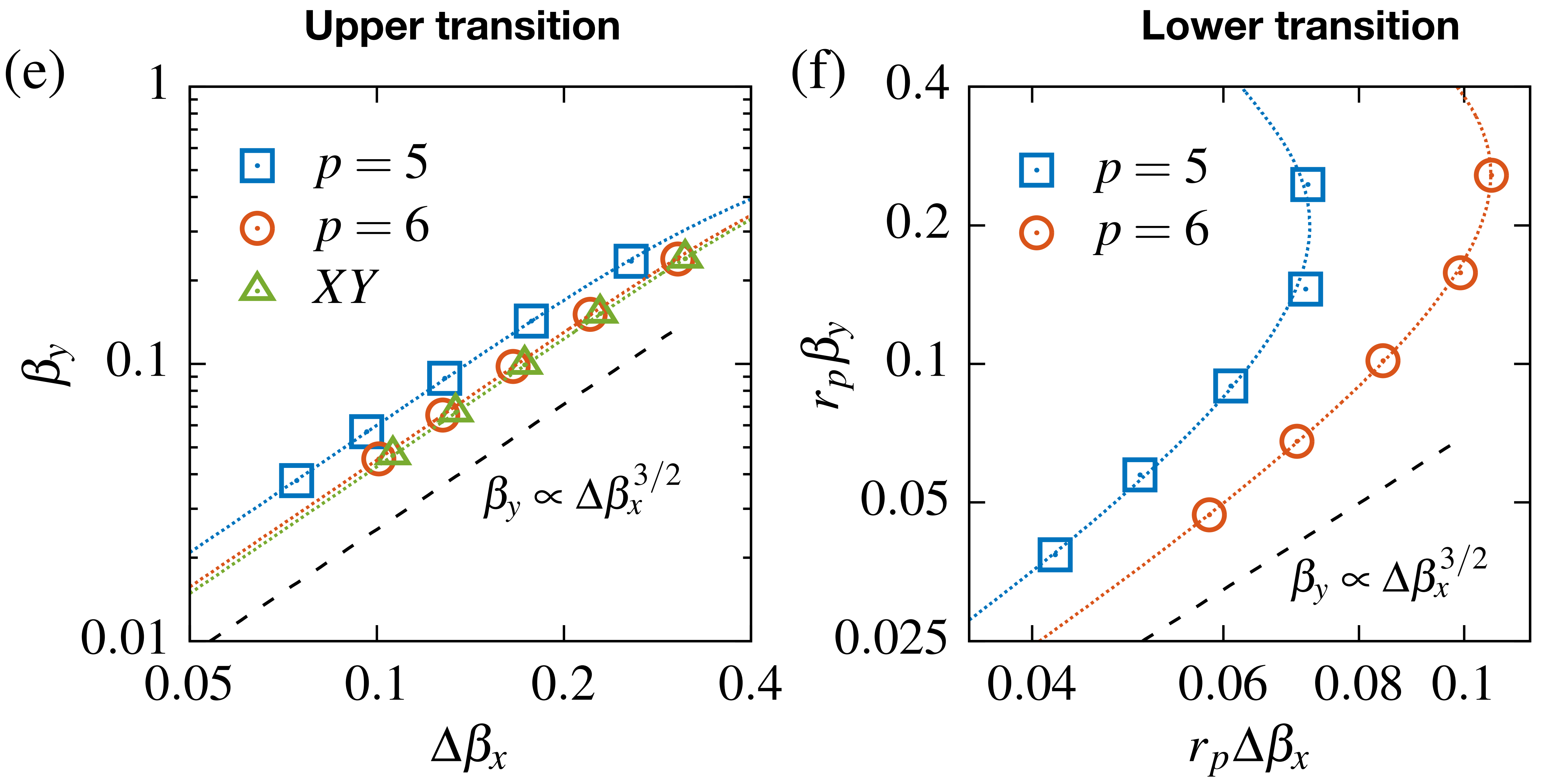


β_y **is monotonically decreasing.** $\Delta\beta_y$ **can be non-monotonic.**

Finite-Size-Scaling Ansatz with Logarithmic Corrections

Correction to the trajectory: $$\Delta\beta_x = w_1 \beta_y^{\frac{1}{1+\nu}} + w_2\beta_y + w_3\beta_y^{2-\frac{1}{1+\nu}} + O\left(\beta_y^{3-\frac{2}{1+\nu}}\right)$$

With HOTRG data, p=5 fits well with the BKT scenario.



Summary and Conclusions

[D.-H. Kim, PRE 96, 052130 (2017)]
[S. Hong and D.-H. Kim, arXiv:1906.09036]

Fisher-zero characterization of phase transitions in the p-state clock model

HOTRG vs. Wang-Landau MC

1. WL MC is destined to fail because of the non-diverging specific heat.

2. HOTRG: Leading Fisher zeros are computed up to L = 128.

— Better FSS analysis is done using more accurate data + ansatz w/ correction.

— BKT transition points are located using the logarithmic scaling behavior.

3. Corrections to the previous WL results:

1. p=5 : it now fits well to the BKT trajectory with HOTRG data

2. The arc-like trajectory at the lower transition is now explained by the BKT ansatz with the finite-size corrections.