Complex temperature zeros in the partition function of the 3D Ising model

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Overview

1 - Introduction

- Model and open problem
- Fisher zeros: definitions

2 - Methodology

- Simulations
- Analysis

3 - Results

- Critical exponent ν from Fisher zeros
- Impact angle and critical amplitude ratio

4 - Conclusions

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Ising Model

- Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j + \sum_i h_i S_i \qquad ; \qquad S_i = \pm 1$$

- Partition function:

$$Z(\beta) = \sum_{\{S_i\}} e^{-\beta \mathcal{H}} \qquad ; \qquad \mathcal{F} = -k_B T \ \ln \mathcal{Z}$$

We can obtain all system's information from it.

- Zero in the partition function → phase transition.

Phase transition in the model

- Depending on the dimension of the system:
  - $D=1$: NO phase transition. Exactly solved.
  - $D=2$: phase transition. Exactly solved.
  - $D=3$: phase transition. Still unsolved?

- Recent claims of an exact solution in 3D:

  J. Kaupuzs, *Ann. Phys NY* 10, 299 (2001)*, arxiv.org:103.0888 (2011).*

  Z. D. Zhang*, Phil. Mag.* **87**, 5309 (2007).

  N. H. March and Z. D. Zhang, *Phys. Lett. A*, **373**, 2075 (2009).

Conflicting present results

- Most recent accepted numerical results:

  A. Pelissetto and E. Vicari, *Physics Reports* **368**, 549 (2002).

  M. Hasenbusch, *Phys. Rev. B* **82**, 174434 (2010).

$$\xi \propto |T - T_c|^{-\nu} \longrightarrow \nu = 0.6301(4)$$

$$C \propto |T - T_c|^{-\alpha} \longrightarrow \alpha = 0.110(1)$$

$$\left.\begin{array}{l} \lim_{T \to T_c^+} C = A_+ |t|^{-\alpha} \\ \lim_{T \to T_c^-} C = A_- |t|^{-\alpha} \end{array}\right\} \longrightarrow A_-/A_+ = 0.536(2)$$

- Following the GFD theory:

  J. Kaupuzs, *Ann. Phys NY* 10, 299 (2001), arxiv.org:103.0888 (2011).

$$\xi \propto |T - T_c|^{-\nu} \longrightarrow \nu = 2/3$$

$$C \propto |T - T_c|^{-\alpha} \longrightarrow \alpha = 2 - \nu D = 0$$

Overview

Partition function zeros

- The partition function is a sum of positive terms:

$$Z(\beta) = \sum_{\{S_i\}} e^{-\beta\mathcal{H}} = \sum_{E} p(E,\beta) e^{-\beta E}$$

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j + \sum_i h_i S_i$$

- We can only obtain its zeros in finite systems by:
  - Analytic prolongation to complex field:

    Lee-Yang zeros

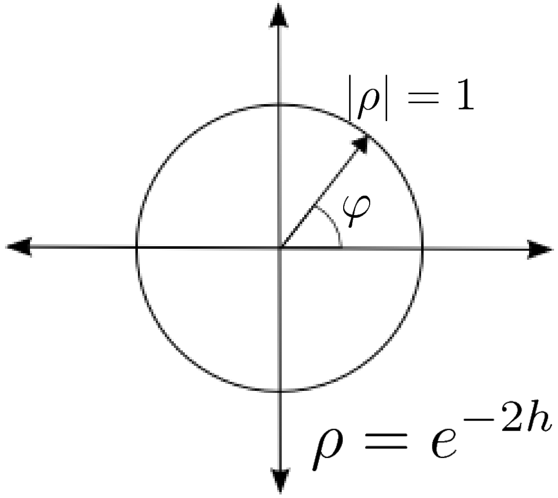
  - Analytic prolongation to complex temperature:

    Fisher zeros

Lee-Yang zeros

- For a uniform external field:

$$Z = \sum_{\{\sigma_i\}} \exp\left(\beta \sum_{\langle i,j \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i\right)$$



Lee-Yang Theorem

The partition function, Z, only vanishes for the purely imaginary magnetic field h.

- The corresponding h values scale with:

$$h_{LY}(t) \propto |t|^{\Delta} \qquad \Delta = \beta + \gamma$$

Fisher zeros: definition

- We define them as complex temperatures β such that:

$$Z(\beta) = Z(\eta + i\xi) = 0 \qquad (i^2 = -1)$$

- As there are some zeros, we order them by their moduli:

$$|\beta^{(1)}(L)| < |\beta^{(2)}(L)| < |\beta^{(3)}(L)| < ...$$

- They will approach the real $\beta_c(\infty)$ as $L \to \infty$.

- It is useful to introduce $u = e^{-4\beta}$ as Z can be expressed as a polynomial in u .

Fisher zeros: definition

- For the analytic prolongation:

$$Z(\beta) = \sum_E p(E,\beta)e^{-\beta E} = \sum_E p(E,\beta)e^{-(\eta+i\xi)E} =$$

$$= \sum_E p(E,\beta)e^{-\eta E}[\cos(\xi E) - i\sin(\xi E)]$$

- Rescaling with $Z[Re(\beta)]$ we obtain:

$$R = \frac{Z(\beta)}{Z[\mathrm{Re}(\beta)]} = \frac{\sum_E p(E,\beta)e^{-\eta E}[\cos(\xi E) - i\sin(\xi E)]}{\sum_E p(E,\beta)e^{-\eta E}} =$$

$$=< \cos(\xi E) >_\eta -i < \sin(\xi E) >_\eta$$

Fisher zeros: calculation

- Given: $$R =< \cos(\xi E) >_\eta - i < \sin(\xi E) >_\eta$$

we can estimate zeros in Z by:

- looking for the simultaneous conditions:

$$\mathrm{Re}(R) = 0 \quad ; \quad \mathrm{Im}(R) = 0$$ → *Graphical procedure*

- minimizing the function:

$$R^2 =< \cos(\xi E) >_\eta^2 + < \sin(\xi E) >_\eta^2$$

Numerical procedure

Fisher zeros: expected Finite Size Scaling

- Real parts will scale with:

$$\mathrm{Re}(\beta) - \beta_c(\infty) \sim L^{-1/\nu}$$

- While imaginary parts must converge to the real axis with:

$$\mathrm{Im}(\beta) \sim L^{-1/\nu}$$

- They will pin the real axis with an angle φ, being:

$$\tan[(2-\alpha)\varphi] = \frac{\cos\pi\alpha - A_-/A_+}{\sin\pi\alpha}$$

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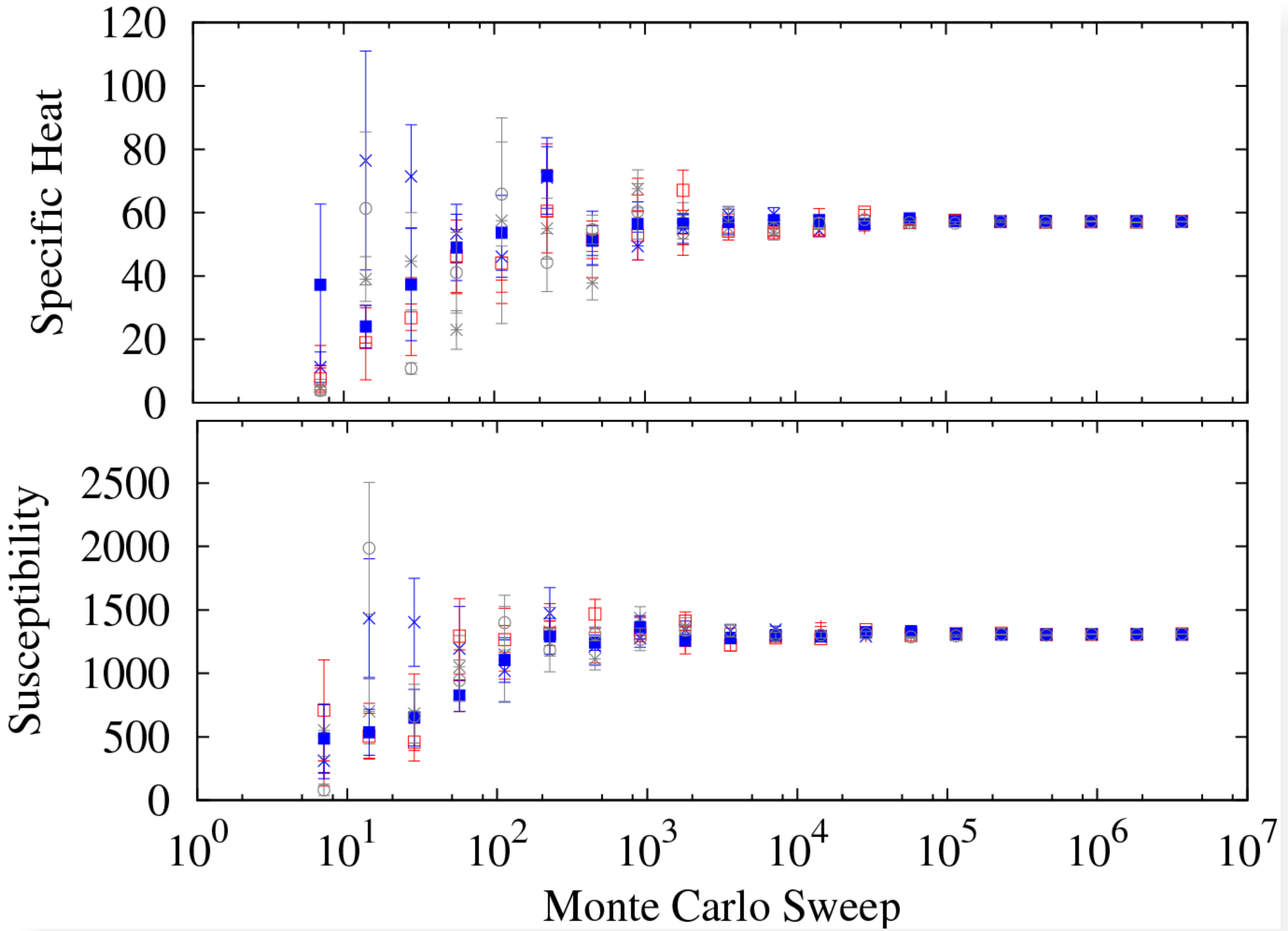
Simulation details

- 3D Systems with $4 \leq L \leq 72$, updated using Metropolis+Wolff.
- Simulation temperatures: $\begin{cases} \beta_c(\infty) = 0.2216546 \\ \beta'^{(2)}(L) : \text{estimated second zero location} \end{cases}$
- We performed 10^7 measures after equilibration.
- We simulated 20 pseudo-samples merging their individual MC histories and performing jack-knife with them.

Thermalization test

- Log. binning for the largest system ($L = 72$) and several samples



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Analysis details: graphical estimation

- We can do histogram reweighting with the quantities:

$$< \cos(\xi E) >_\eta = \frac{\sum_E \cos(\xi E) e^{(\eta - \beta_c)\Delta E}}{\sum_E e^{(\eta-\beta_c)E}}$$

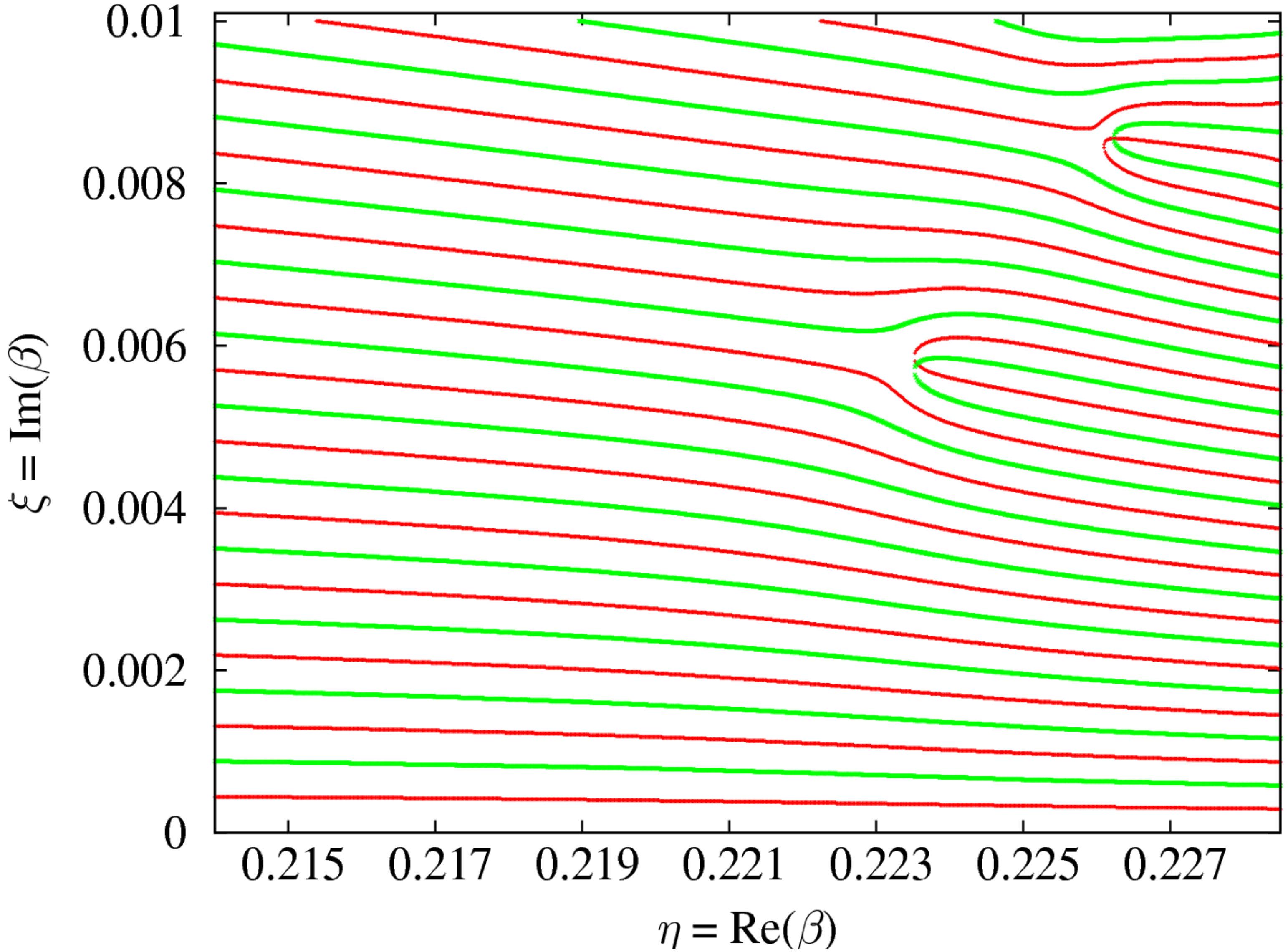
$$< \sin(\xi E) >_\eta = \frac{\sum_E \sin(\xi E) e^{(\eta - \beta_c)\Delta E}}{\sum_E e^{(\eta-\beta_c)E}}$$

and then estimate graphically the zeros looking for the crossing of the conditions:

$< \cos(\xi E) >_\eta = 0$ and $< \sin(\xi E) >_\eta = 0$

Graphical location of Fisher zeros

- 1000x1000 extrapolation grid for $L=16$.



Analysis details: minimization procedure

- Graphical procedures are time consuming and not accurate enough.

- They can be used as starting point for a numerical minimization of:

$$R^2 = < \cos(\xi E) >_\eta^2 + < \sin(\xi E) >_\eta^2$$

- We used a downhill simplex method (AMOEBA) to obtain η and ξ .

N. A. Alves et al., *Int. J. Mod. Phys. C* **8**, 1063 (1997).

- We have been able to locate zeros with small relative error bars:

$$\frac{\Delta\eta}{\eta} \sim 10^{-6} \qquad \frac{\Delta\xi}{\xi} \sim 10^{-3}$$

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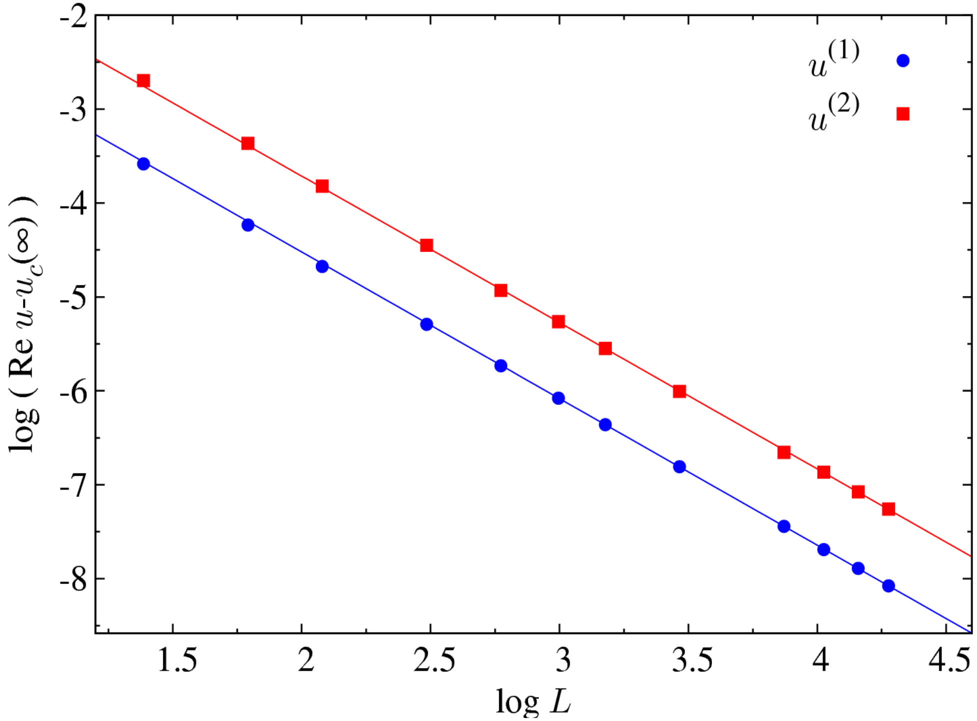
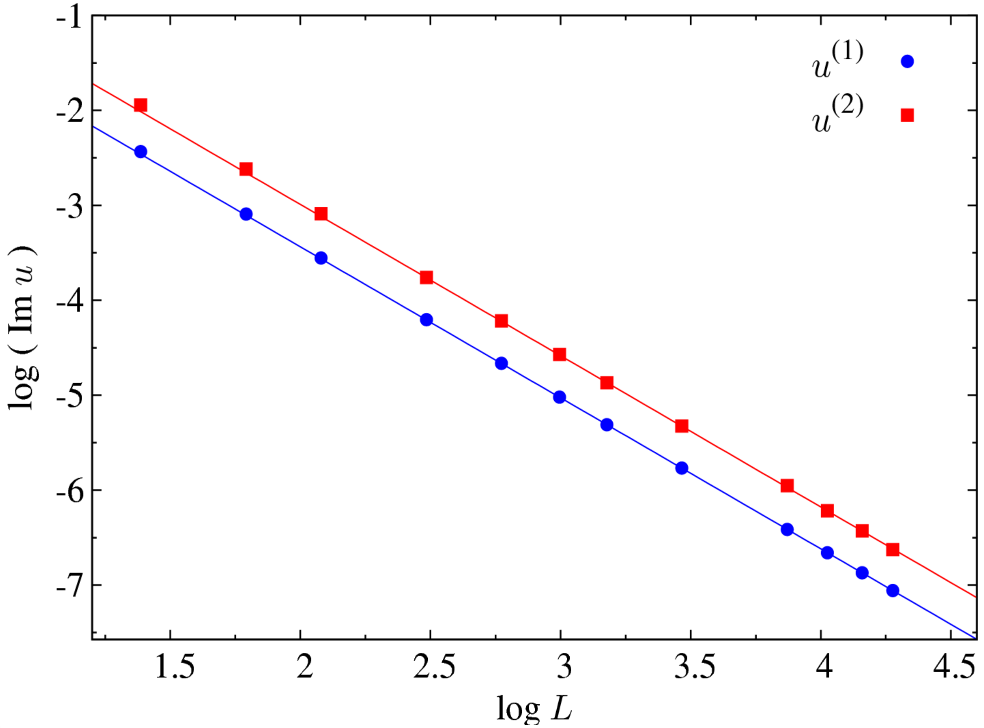
Critical exponent ν from Fisher zeros

- We can obtain it from the scaling of real or imaginary parts, or from the modulus of the zeros.

- We fit to the form: $aL^{-1/\nu}(1 + bL^{-\omega})$





Critical exponent ν from Fisher zeros

- Fixing ω to the best present estimation:

$$\omega = 0.832(6)$$ ← M. Hasenbusch, *Phys. Rev. B*, **82**, 174433 (2010).

we obtain the best fit from $\mathrm{Im}(u^{(1)})$:

$$\nu = 0.63048(32)$$

Good agreement with accepted values

$$\nu = 0.6301(4)$$

- Using hyperscaling relations:

$$\nu d = 2 - \alpha \longrightarrow \alpha = 0.1086(10)$$

Clearly incompatible with $\alpha = 0$ from the conjectured exact solution.

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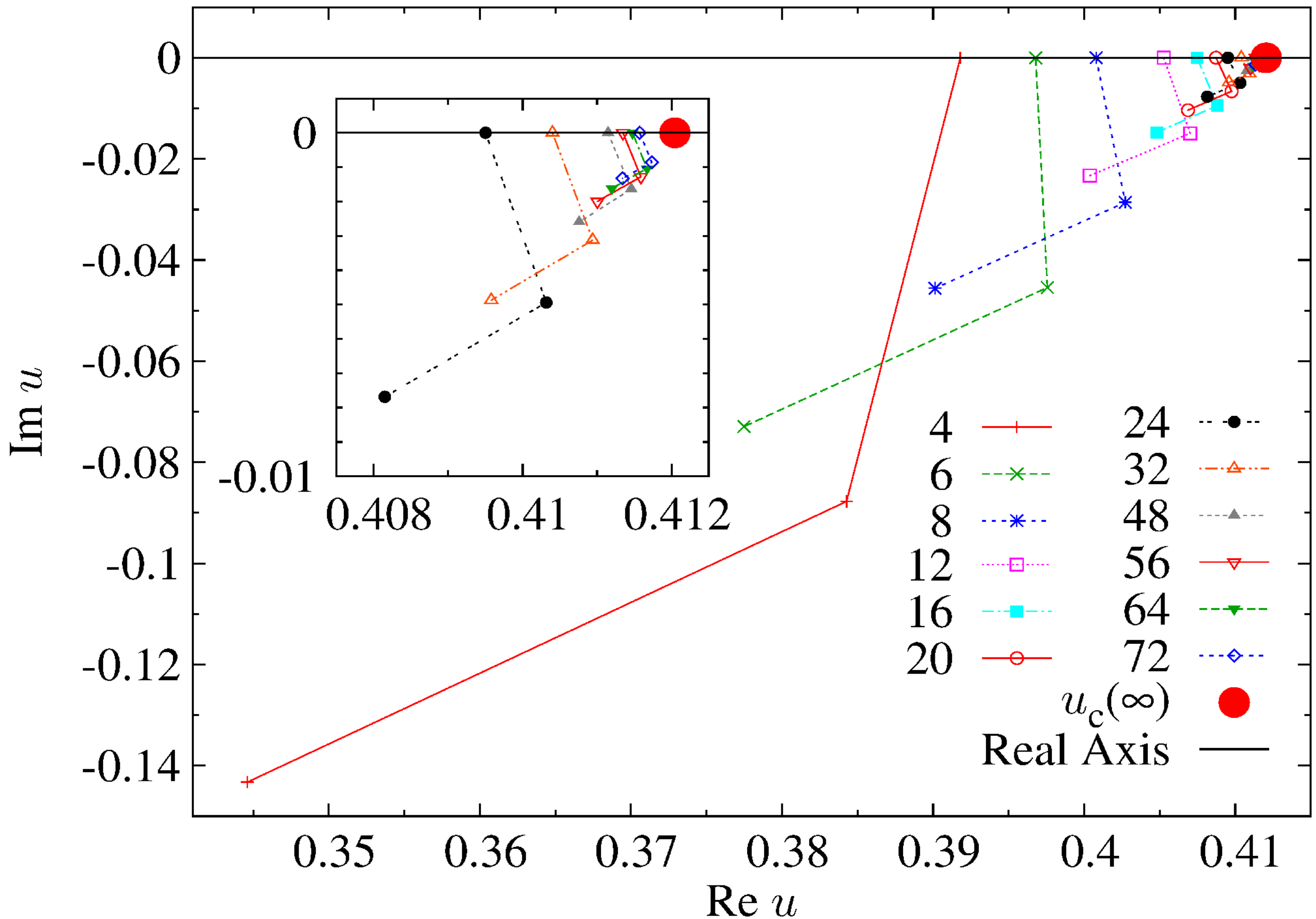
Impact angle and critical amplitude ratio

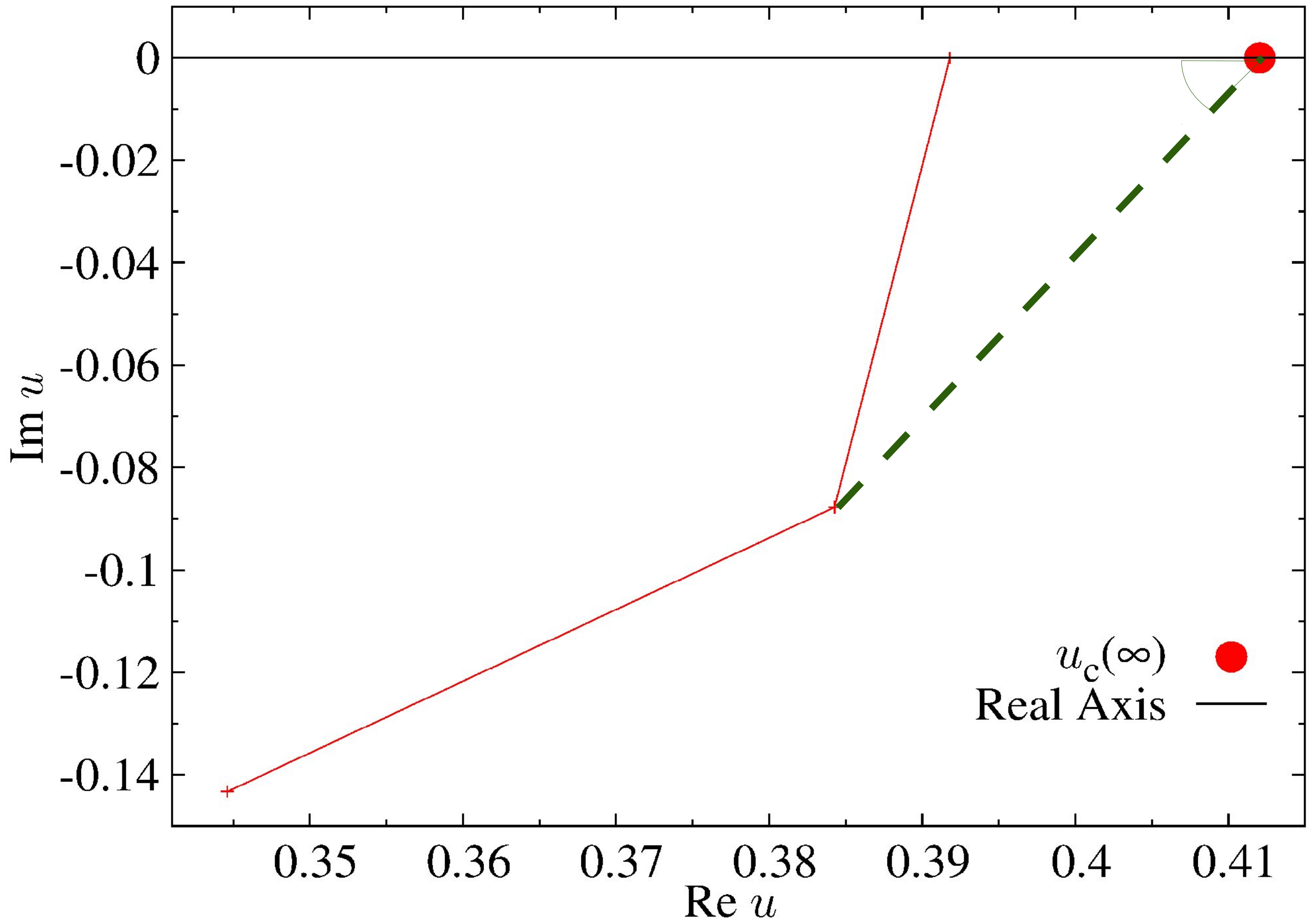
- We can plot the location of the zeros in the complex u plane:



Impact angle and critical amplitude ratio

- Different definitions of the impact angle:

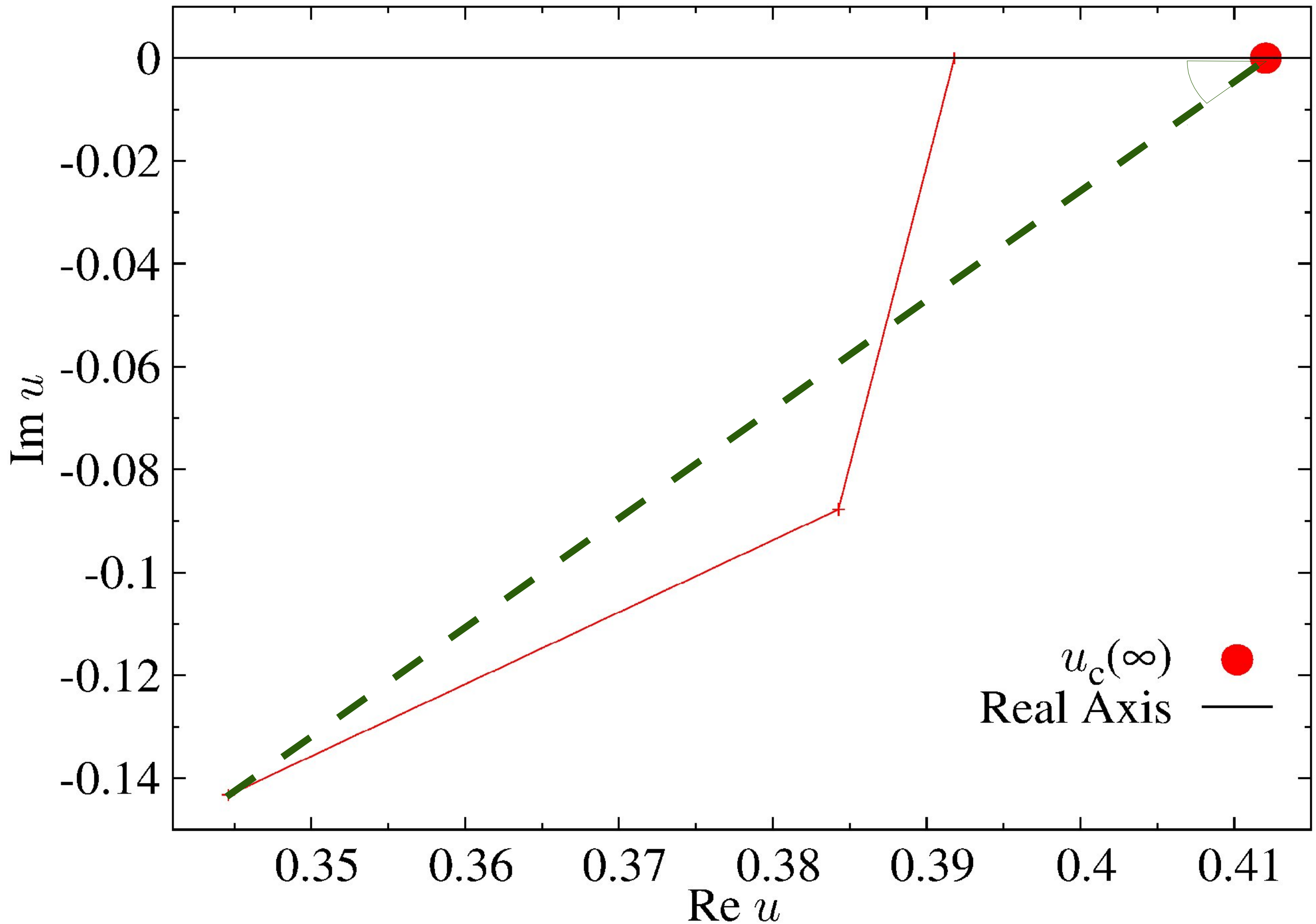
From asymptotic value and first zero



Impact angle and critical amplitude ratio

- Different definitions of the impact angle:

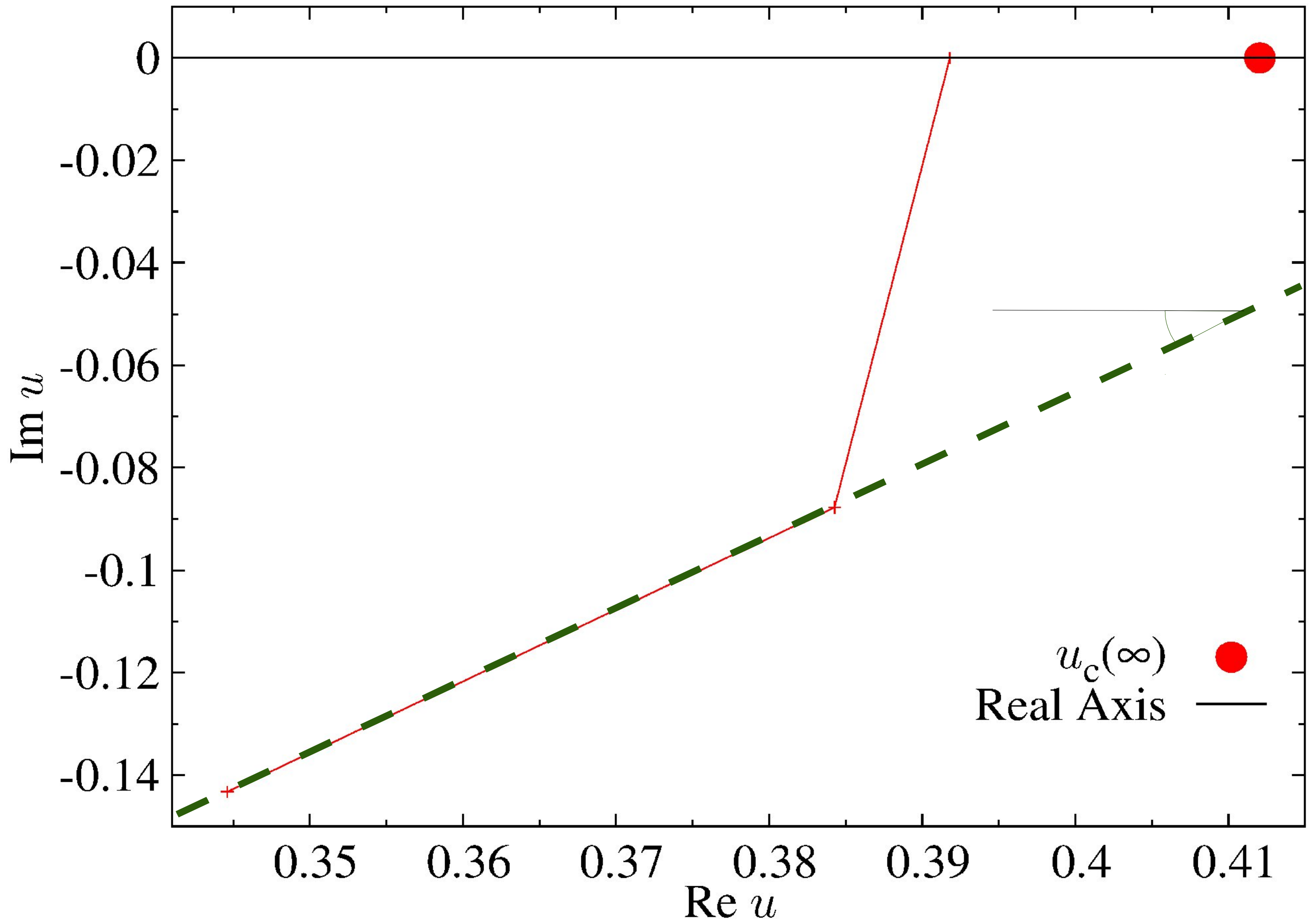
From asymptotic value and second zero



Impact angle and critical amplitude ratio

- Different definitions of the impact angle:

From the first and second zeros



Impact angle and critical amplitude ratio

- We take a conservative approach taking the average between definitions to obtain:

L	Angle Average	$(A_+/A_-)_{\text{average}}$
32	61.3(4)	0.610(9)
48	62(1)	0.63(2)
56	60.5(8)	0.59(2)
64	60.5(7)	0.59(2)
72	59.9(8)	0.58(2)

- Using a correction ansatz we extrapolate to TL with: $\phi(L) = \phi + bL^{-\omega}$

$$\phi = 59.2(1.0)^\circ \longrightarrow \frac{A+}{A_-} = 0.56(3)$$

Good agreement with accepted value: $A_-/A_+ = 0.536(2)$

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Conclusions

- We have studied a typical model from an alternative perspective.
- Only 30-year old measures of the impact angle existed in the literature.
- We updated the measures obtaining good agreement for critical exponents and amplitude ratios.
- Our measures are incompatible with the values claiming exact solution for the 3D Ising model.

Just to finish...

Many thanks for your attention!