Thermal Behavior of the Lee-Yang zeros in the O(3) model

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STATISTICAL PHYSICS in EXTREMADURA

Overview

1 - **Introduction**

- Lee-Yang zeros
- Model and observables

2 - **Methodology**

- Simulations
- Analysis

3 - **Results**

- Scaling of the LY zeros
- Behavior of the zeros density

4 - **Conclusions**

Partition Function zeros

- Typical Spin Model Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + \sum_i \mathbf{h}_i \mathbf{S}_i$$

- Partition function:

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

We can obtain all system's information from it.

- Zero in the partition function $\longrightarrow$ phase transition.

Lee Yang zeros

- With a purely imaginary magnetic field:

$$Z(\beta,h) = \sum_{\{S_i\}} \exp\left(\beta \sum_{\langle i,j\rangle} \mathbf{S}_i\mathbf{S}_j + i\mathbf{h}\sum_i \mathbf{S}_i\right)$$

$$= [\langle\cos(\mathbf{hM})\rangle + i\langle\sin(\mathbf{hM})\rangle] \times \mathcal{Z}(\beta,\mathbf{h}=0) \qquad ; \quad \mathbf{M} = \textstyle\sum_i \mathbf{S_i}$$

- The singularities will only arise from the zeros of: $\langle\cos(\mathbf{hM})\rangle$

- In this way we can define a sequence of ordered zeros:

$$r_1(\beta,L) > r_2(\beta,L) > r_3(\beta,L) > r_4(\beta,L)\ldots$$

- The following relation can be obtained:

$$r \propto \frac{1}{\sqrt{V\chi_{NC}}} \qquad\qquad \chi_{NC} = \frac{1}{V}\langle\mathcal{M}^2\rangle$$

Non-connected susceptibility

Lee Yang zeros

- From the zeros we can extract the critical exponent Δ:

$$h_{LY} \propto |T - T_c|^{\Delta} \quad \text{related with:} \quad \Delta = \beta + \gamma$$

- Or its scaling as a function of the temperature:

$$h_{LY} \propto L^{-c}(1 + dL^{-e})$$

where for:

$$T = T_c \begin{cases} c = \Delta/\nu \\ e = \omega \end{cases} \qquad T < T_c \begin{cases} c = D \\ e = 1 \text{ or } e = 3 \end{cases}$$

Goldstone contribution

- The LY theorem also holds for the O(3) model

T. Asano, PRL , **24**, 1409 (1970).

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Model and observables

- We study the Heisenberg model in 3D

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + \sum_i \mathbf{h}_i \mathbf{S}_i \qquad ; \qquad |\mathbf{S}|_i = 1$$

- The total magnetization is:

$$\mathcal{M} = (M_x, M_y, M_z) = \sum_i \mathbf{S}_i$$

whose thermal average is zero in a finite lattice.

- Therefore we define the order parameter as:

$$M = \langle \sqrt{\mathcal{M}^2} \rangle$$

where the thermal average is denoted by $\langle \cdots \rangle$

Model and observables

- The zeros density can be defined in a system of size L as:

$$G_L[r_j(L)] = \frac{2j-1}{2L^D}$$

W. Janke and R. Kenna, *J. Stat. Phys.*, **102,** 1211(2001).

where j is the index of the zero.

- We expect this to scale as:

$$G_L \sim r^{D/x_1}\left(1 + O(r^{x_2/x_1})\right)$$

$$T = T_c \begin{cases} x_1 = \Delta/\nu \\ x_2 = \omega \end{cases} \qquad T < T_c \begin{cases} x_1 = D \\ x_2 = D \end{cases}$$

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Simulation details

- Cubic systems with $8 \leq L \leq 64$.
- Simulation temperatures: $\begin{cases} T = T_c = 1.443 \\ T < T_c \ : \begin{cases} T = 2/3\ T_c \\ T = T_c/2 \end{cases} \end{cases}$
- We used 10% Metropolis + Wolff cluster method.
- We performed 10^6 measures after equilibration increasing the updates between measures with the system size.
- We simulated 20 pseudo-samples merging their individual MC histories and performing jack-knife with them.

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Location of the LY zeros: method

- We have to look for: $\langle \cos(\mathbf{hM}) \rangle = 0$

  - We found no different scaling using components or modulus

    $$\mathcal{M} = (M_x, M_y, M_z) \qquad M = \langle \sqrt{\mathcal{M}^2} \rangle$$

  - Iterative method to increase accuracy and decrease analysis time:

    1) Start from $h = 0$ with relatively large Δh.

    2) Estimate zeros from the previous estimations, if any.

    3) Take $\Delta h' = \Delta h / 100$.

    4) Go to 2) until the error bar does not depend on Δh.

Location of the LY zeros: example

- First four LY zeros for different lattice sizes at $T = T_c$

L	$r_1(L)$	$r_2(L)$	$r_3(L)$	$r_4(L)$
8	0.00825415(59)	0.0243727(17)	0.0396287(27)	0.0541716(40)
12	0.00300815(27)	0.00888260(73)	0.0144417(12)	0.0197404(21)
16	0.00147165(14)	0.00434424(34)	0.00706250(50)	0.0096533(9)
24	0.000537193(39)	0.00158625(11)	0.00257895(18)	0.0035250(3)
32	0.000262952(19)	0.000776455(47)	0.0012622695(74)	0.00172516(17)
48	0.0000960985(9)	0.000283759(24)	0.0004612664(37)	0.00063038(6)
64	0.0000470623(4)	0.000138962(10)	0.0002258879(16)	0.00030869(3)

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Scaling of the LY zeros at the critical temperature

- As was stated before: $h_{LY} \propto L^{-\Delta/\nu} = L^{-(D+2-\eta)/2}$

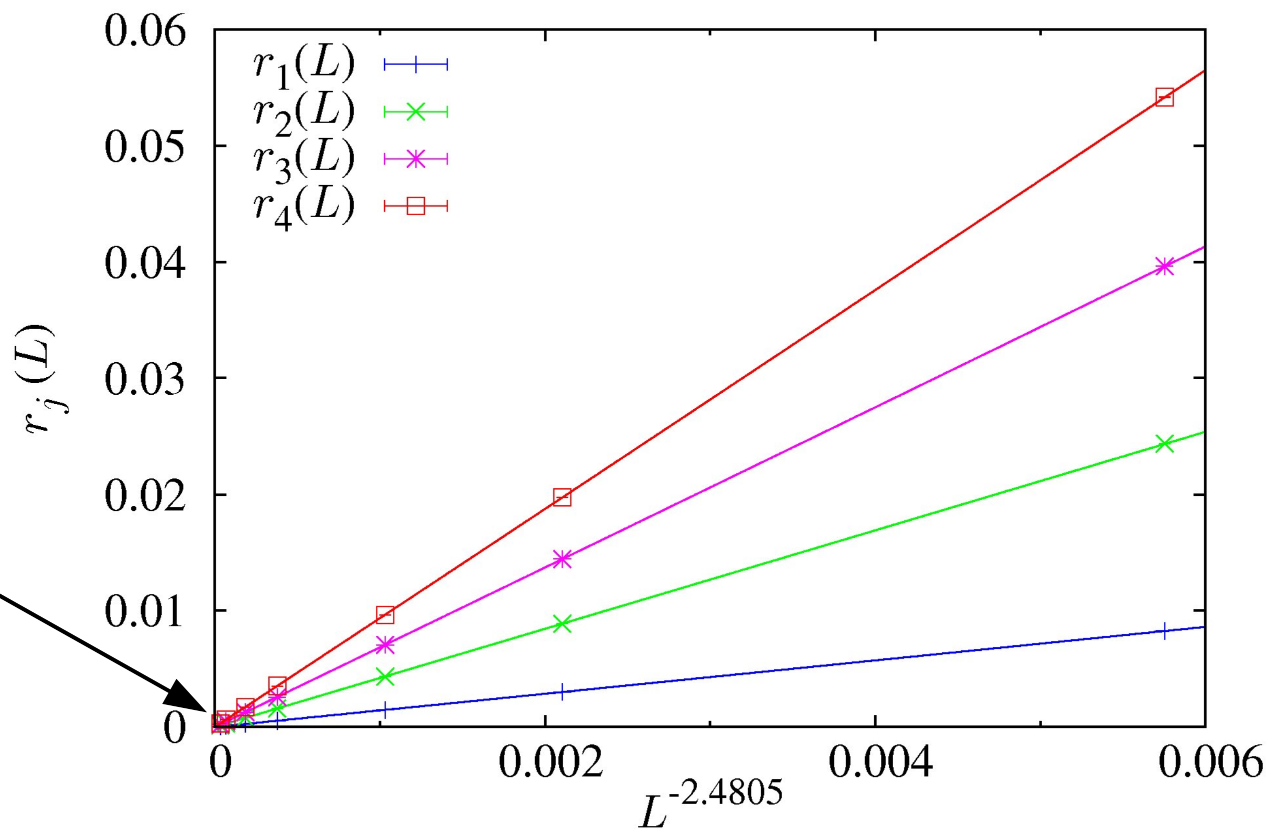
  Using the most recent result: $\eta = 0.0391(9)$

  AGG and JRL, *J. Stat. Mech.* , **P06014** (2007).

- We expect:

$$\Delta/\nu = 2.4805(4)$$

Clear extrapolation to zero



Scaling of the LY zeros at the critical temperature

- We obtain:

	$T = T_c$			
	$\|\mathcal{M}\|$		M_x	
	Δ/ν	χ^2/ndf	Δ/ν	χ^2/ndf
$r_1(L)$	2.4774(12)	0.11 / 2	2.4792(7)	2.57 / 5
$r_2(L)$	2.4789(28)	2.52 / 4	2.4845(17)	0.52 / 4
$r_3(L)$	2.4791(3)	5.36 / 4	2.4811(26)	0.89 / 5
$r_4(L)$	2.4793(4)	5.48 / 4	2.4779(52)	4.98 / 5

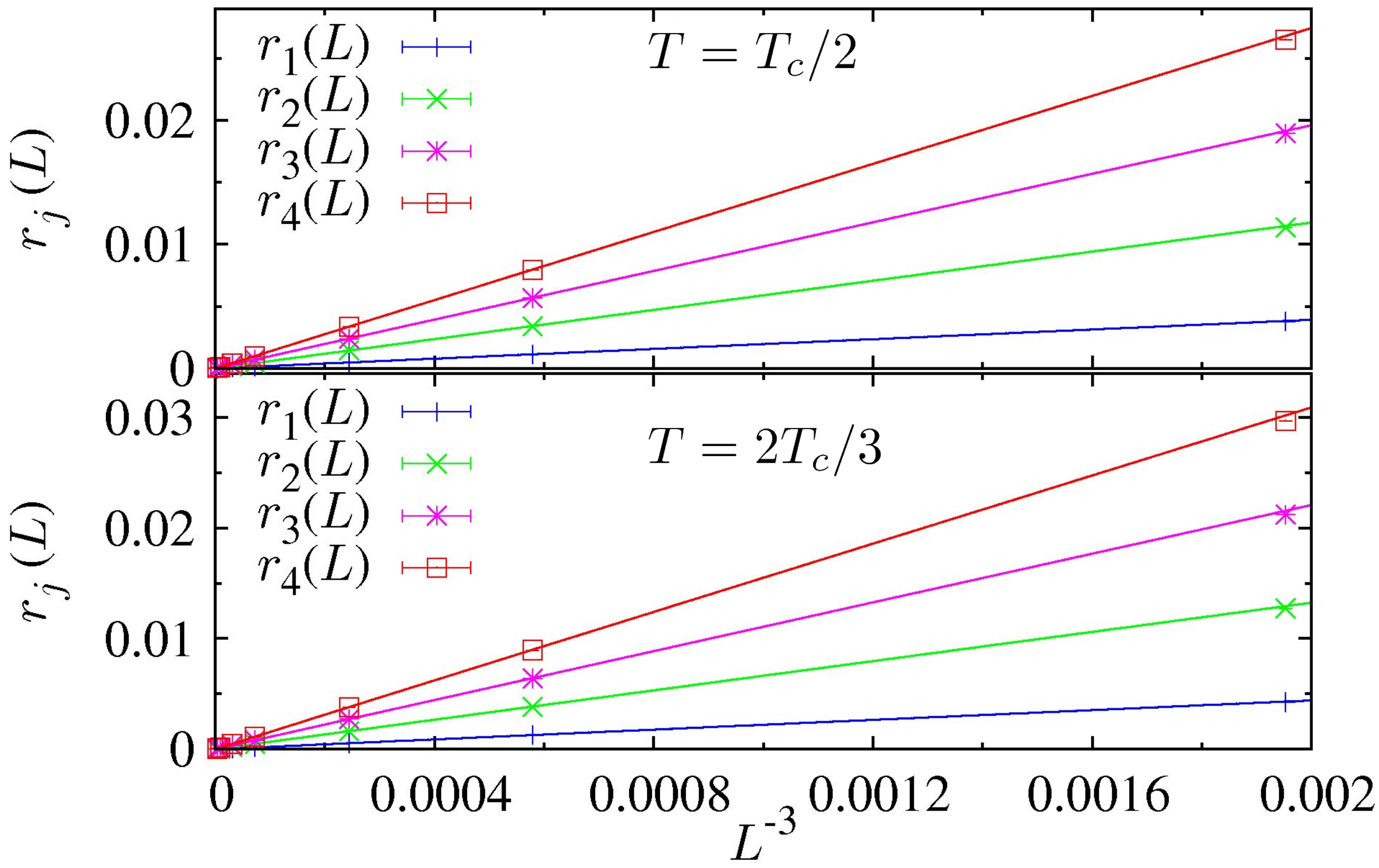
- Very good agreement with the expected value $\Delta/\nu = 2.4805(4)$

- Same scaling from the components or from the modulus of

$$\mathcal{M} = (M_x, M_y, M_z)$$

Scaling of the LY zeros below the critical temperature

- In this case we expect, and clearly obtain: $h_{LY} \propto L^{-D}$



Scaling of the LY zeros below the critical temperature

- In terms of: $h_{LY} \propto L^c(1 + dL^{-e})$

	$T = T_c/2$			$T = 2T_c/3$		
	c	e	χ^2/ndf	c	e	χ^2/ndf
$r_1(L)$	-3.00024(8)	0.962(7)	2.98 / 2	-3.0006(2)	0.949(8)	3.88 / 2
$r_2(L)$	-3.00023(8)	0.963(7)	2.06 / 2	-3.0005(2)	0.952(9)	3.68 / 2
$r_3(L)$	-3.00022(8)	0.964(7)	1.78 / 2	-3.0004(2)	0.956(9)	2.92 / 2
$r_4(L)$	-3.00021(8)	0.965(7)	1.51 / 2	-3.0003(2)	0.962(9)	1.84 / 2

- Therefore we obtain a clear contribution of the Goldstone's modes of the model ($e=1$)

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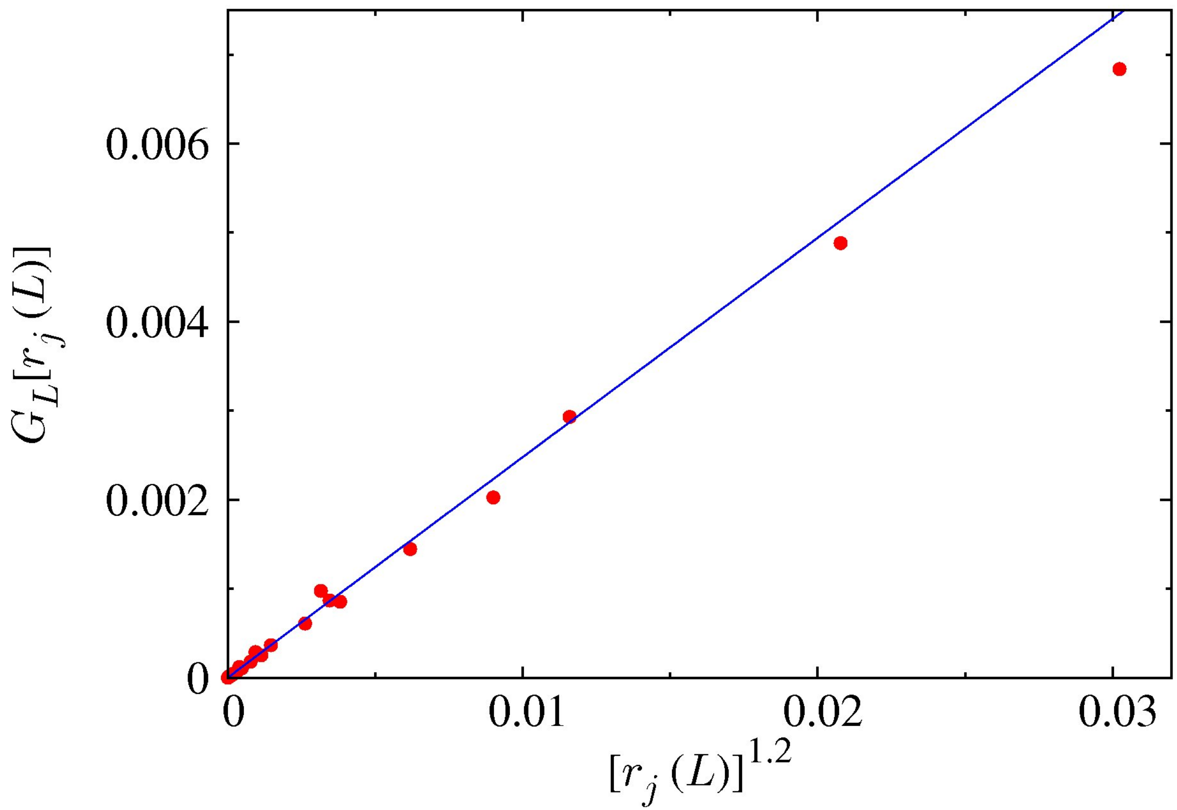
Zeros density at the critical temperature

- We expect the scaling: $G_L[r_j(L)] = a_1[r_j(L)]^{a_2} + a_3$

with: $a_3 = 0$; $a_2 = 2D/(D+2-\eta) = 1.2095(2)$



$$G_L[r_j(L)] = \frac{2j-1}{2L^D}$$

- And we obtain (first zero):

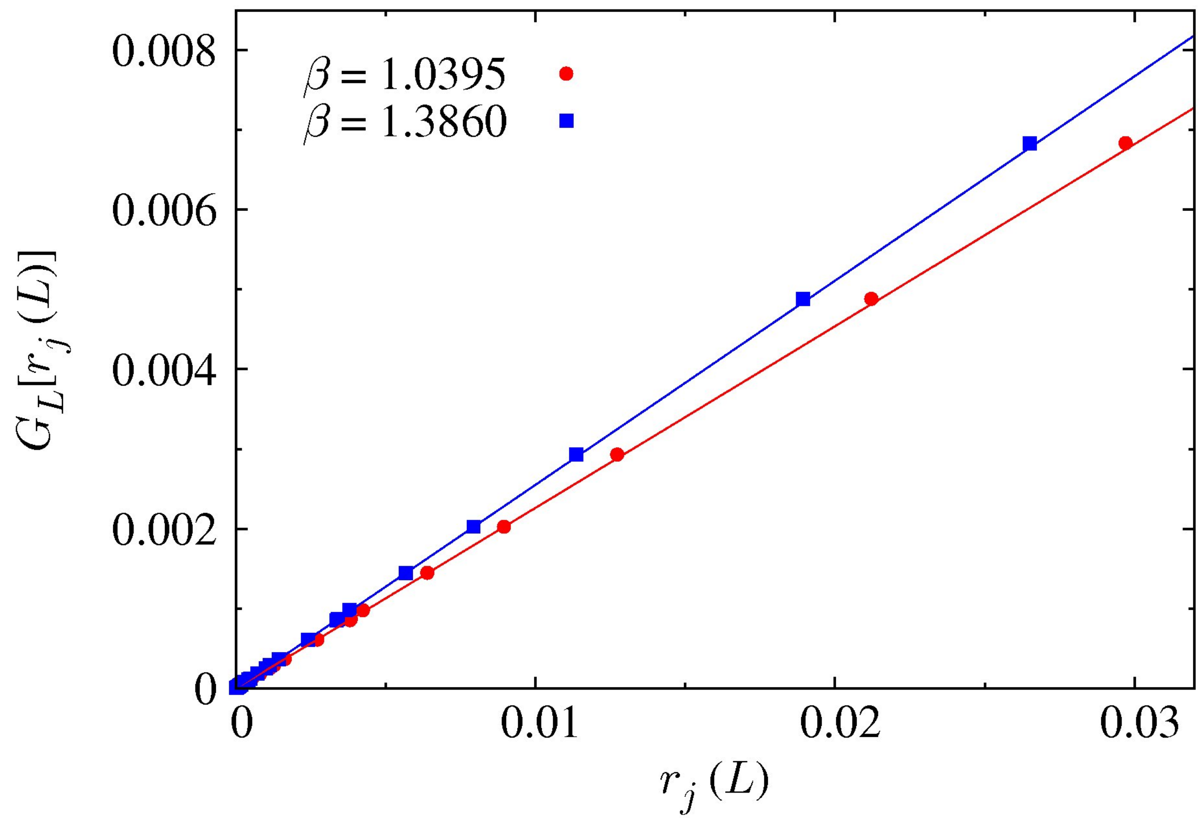
$$a_2 = 1.2097(4) \quad ; \quad \omega = 0.9(3)$$

Zeros density below the critical temperature

- Again we fit to: $G_L[r_j(L)] = a_1[r_j(L)]^{a_2} + a_3$
- In this case we expect:

$$a_1 = M/\pi \quad ; \quad a_2 = 1 \quad ; \quad a_3 = 0$$

Spontaneous Magnetization



Zeros density below the critical temperature

- Very good agreement with the measured values

	$\overline{M}$	
L	$T = 2T_c/3$	$T = T_c/2$
8	0.723070(4)	0.810036(3)
12	0.710792(3)	0.801895(2)
16	0.704728(3)	0.797844(1)
24	0.698713(2)	0.793808(1)
32	0.695724(1)	0.791793(1)
64	0.691257(1)	0.7887771(4)

Measured values for the magnetization

	$\overline{M}$	
L	$T = 2T_c/3$	$T = T_c/2$
8	0.723078(3)	0.810038(3)
12	0.710794(2)	0.801898(2)
16	0.7047315(20)	0.7978451(7)
24	0.6987122(8)	0.7938082(6)
32	0.6957245(5)	0.7917944(3)
64	0.6912572(3)	0.7887785(2)

Fitted values from the zeros density

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Conclusions

- We have numerically studied the O(3) model using the LY zeros at and below the critical temperature.
- We developed an iterative method to obtain fast and accurately the zeros location.
- We obtained the expected scaling (Goldstone) at every simulated temperature.
- We obtained precise estimations for the magnetization of the model from the zeros density.

Just to finish...

Many thanks for your attention!