

A Modern Analysis of Phase Transitions

Using Monte Carlo



This dice was inspired in a figure found in the book
A Guide to Monte Carlo Simulations in Statistical Physics
by Landau & Binder

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Complete Version



Single Histogram

Overview



1. *What is Simulation ?*
2. *Quick Review on Phase Transition*
3. *Fisher Zeros*
4. *The Two Dimensional XY Model*
5. *Finite Size Scaling and The Wang-Landau Technique*
6. *Simulation - Analysis and Interpretation*
7. *Final Remarks*

What is Simulation ?

No single definition of computer simulation is appropriate. In the first place, the term is used in both a narrow and a broad sense. In the second place, one might want to understand the term from more than one point of view.

A Narrow definition

In its narrowest sense, a computer simulation is a program that is run on a computer and that uses step-by-step methods to explore the approximate behavior of a mathematical model. Usually this is a model of a real-world system (although the system in question might be an imaginary or hypothetical one). Such a computer program is a *computer simulation model*. One run of the program on the computer is a computer simulation of the system. The algorithm takes as its input a specification of the system's state (the value of all of its variables) at some time t . It then calculates the system's state at time $t+1$. From the values characterizing that second state, it then calculates the system's state at time $t+2$, and so on. When run on a computer, the algorithm thus produces a numerical picture of the evolution of the system's state, as it is conceptualized in the model.

A Broad Definition

More broadly, we can think of computer simulation as a comprehensive method for studying systems. In this broader sense of the term, **it refers to an entire process. This process includes choosing a model; finding a way of implementing that model in a form that can be run on a computer; calculating the output of the algorithm; and visualizing and studying the resultant data.** The method includes this entire process—used to make inferences about the target system that one tries to model—as well as the procedures used to sanction those inferences. This is more or less the definition of computer simulation *studies* in Winsberg 2003 (111). **“Successful simulation studies do more than compute numbers. They make use of a variety of techniques to draw inferences from these numbers. Simulations make creative use of calculational techniques that can only be motivated extra-mathematically and extra-theoretically. As such, unlike simple computations that can be carried out on a computer, the results of simulations are not automatically reliable. Much effort and expertise goes into deciding which simulation results are reliable and which are not.”** When philosophers of science write about computer simulation, and make claims about what epistemological or methodological properties “computer simulations” have, they usually mean the term to be understood in this broad sense of a computer simulation study.

Partition Function

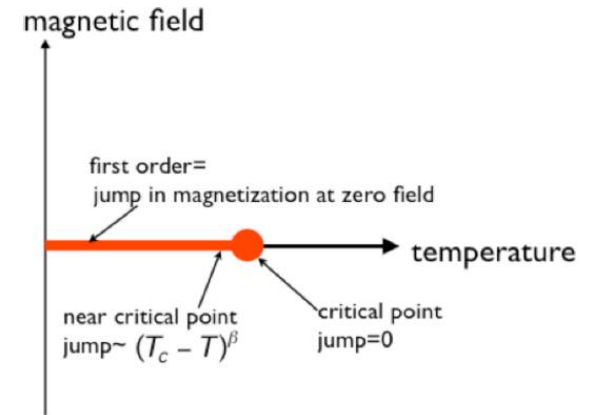
The Partition Function describes completely the equilibrium properties of a thermodynamic system

$$Z \equiv \sum_{\{x\}} e^{-\beta H(\{x\})} \quad \text{or} \quad Z = \sum_E g(E) e^{-\beta E}$$

For example

$\langle E \rangle = -\frac{d}{d\beta} \ln Z$	Energy
$S = k_B (\ln Z + \beta \langle E \rangle)$	Entropy
$\chi = \frac{1}{T} (\langle x^2 \rangle - \langle x \rangle^2)$	Susceptibility

Phase Transitions



Splash and snowflake. This picture is intended to illustrate the qualitative differences between the fluid and solid phases of water. On the left is liquid water, splashing up against its vapor phase. Its fluidity is evident. On the right is a crystal of ice in the form of a snowflake. Note the delicate but rigid structure, with its symmetry under the particular rotations that are multiples of sixty degrees.

Leo P. Kadanoff The Perimeter Institute Waterloo, Ontario, Canada and The James Franck Institute The University of Chicago
<http://jfi.uchicago.edu/~leop/RejectedPapers/ExtraV1.2.pdf>

How to Define a Phase ?

There are various thermodynamic variables one can use to describe matter in thermal equilibrium, some of the common ones being: mass or number density ρ , energy density e , temperature T , pressure P , and chemical potential μ (assuming for simplicity that the material is composed of one pure substance). By definition the states of a “simple” system can be parameterized by two such (independent) variables, in which case the others can be regarded as functions of these.

A thermodynamic phase of a simple material is an open, connected region in the space of thermodynamic states parametrized by the variables T and μ , **the pressure P being analytic in T and μ** . Specifically, P is analytic in T and μ at (T_0, μ_0) if it has a convergent power series expansion in a ball about (T_0, μ_0) that gives its values. Phase transitions occur on crossing a phase boundary.

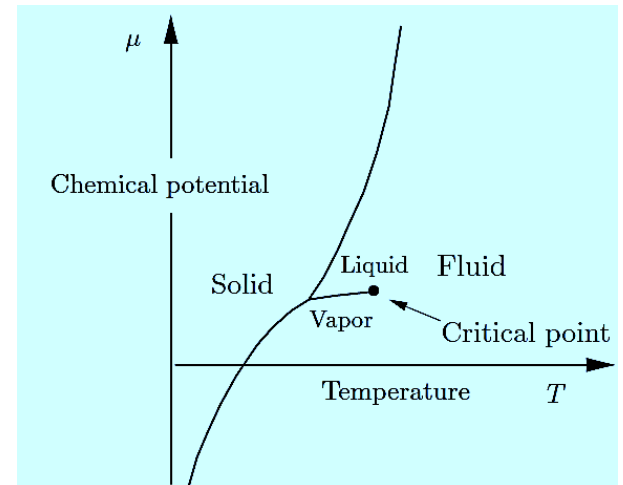
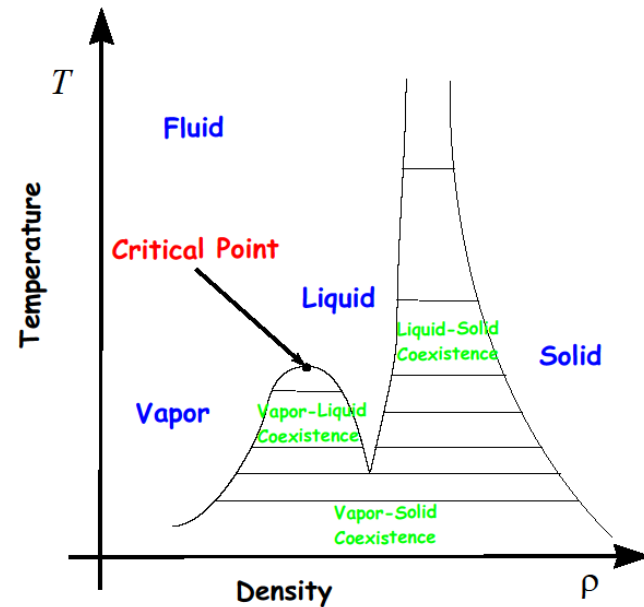


Fig 1. A simple phase diagram in the (μ, T) plane.

From Michael E. Fisher and Charles Radin
(www.aimath.org/pastworkshops/phasetransition.html)

Phase Transitions

Ehrenfest	Fisher
First Order Discontinuity in the first derivative of the Free Energy	First Order Latent Heat
Second order Discontinuity in the second derivative	Continuous Divergent susceptibility Infinite correlation length Power-law decay of correlations near criticality
Third Order (?) Discontinuity in the third derivative	



Non-analyticities in the free energy are central to the theoretical account of phase transitions.

From Michael E. Fisher and Charles Radin
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Analytical Functions

A C^∞ function is a function that has **all derivatives**.

For instance $f(x) = e^{-2x}$ is C^∞ because its n^{th} derivative **exists and is continuous**.

An analytical function is smooth. But a smooth function is not necessarily analytic.

“Analytic” is used to name any function that can be written as a convergent power series in a neighborhood of each point in its domain.

For example:

$$f(x) = \begin{cases} 0, & \text{for } x \leq 0 \\ e^{-1/x} & \text{for } x > 0 \end{cases} \text{ is } C^\infty \text{ but not analytical.}$$

The function can fail to be analytic at a set of discrete singular points or at branch cuts.



Averages - Histograms

Averages are calculated as:

$$\langle A \rangle = \frac{\sum_E A(E)g(E)e^{-\beta_0 E}}{Z}$$

The probability of a configuration E at temperature β_0 is

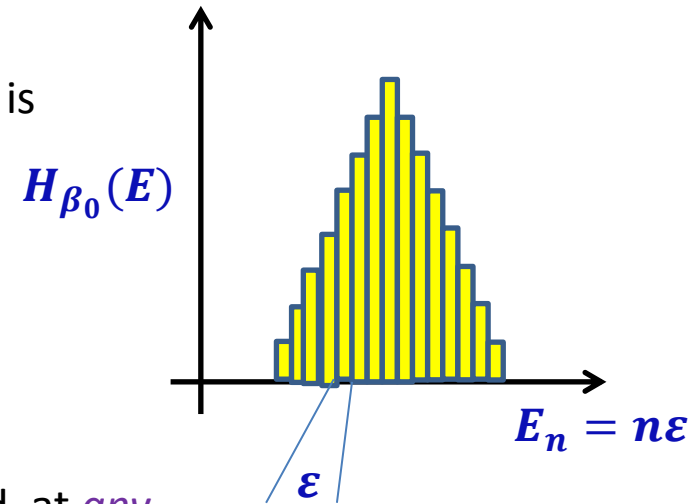
$$P_{\beta_0}(E) = \frac{g(E)e^{-\beta_0 E}}{Z_{\beta_0}},$$

We can generate a histogram $\frac{H_{\beta_0}(E)}{N} \doteq P_{\beta_0}(E)$.

$$g(E) = N^{-1}H(E)Z_{\beta_0}e^{\beta_0 E}$$



With this estimate for $g(E)$ averages $\langle A \rangle$ are obtained at *any temperature*.

$$P_{\beta}(E) = \frac{H(E)Z_{\beta_0}}{N} e^{-E(\beta-\beta_0)}$$

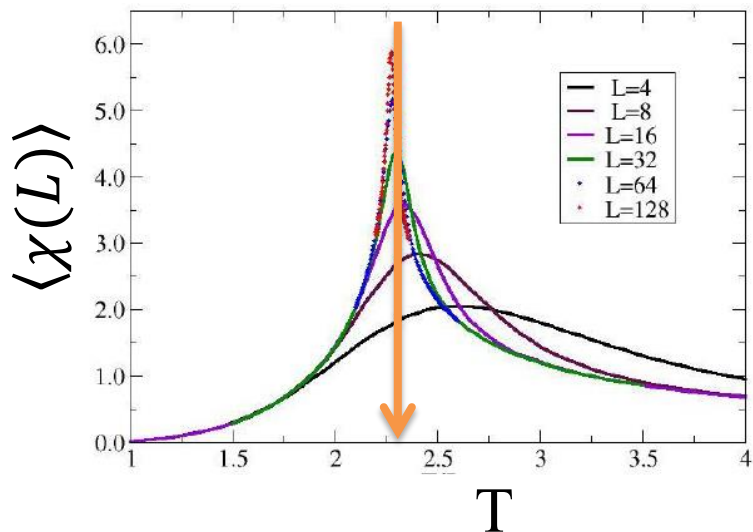
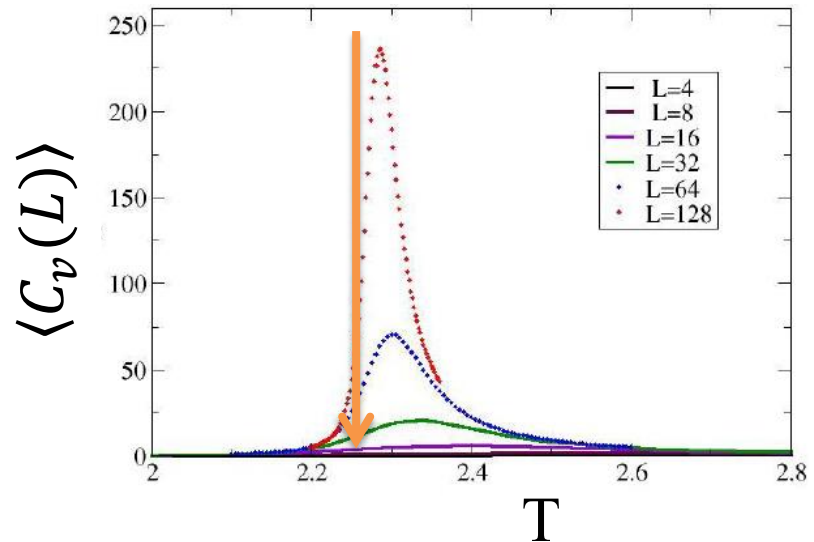
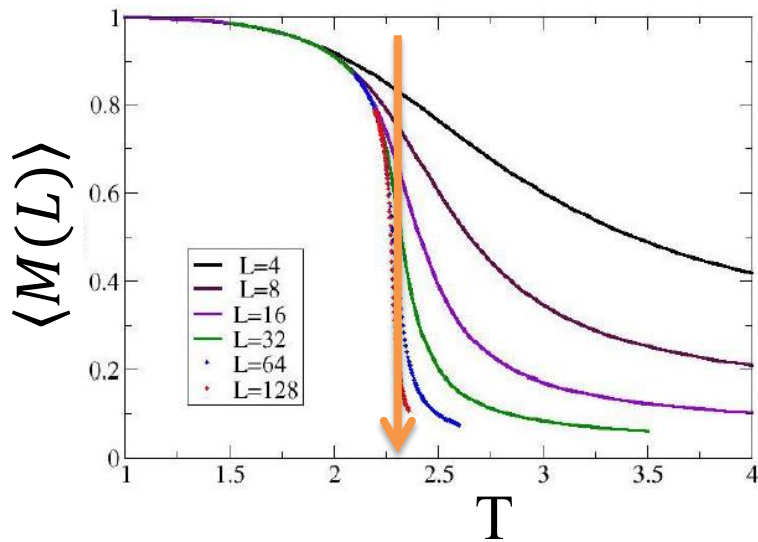


$$Z = \sum_E g(E)e^{-\beta E}$$

Monte Carlo and Equilibrium

Select an initial configuration $\{x_0\}$	Select an initial configuration $\{x_0\}$
1 – Find $E_0 = E(\{x_0\})$	1 – Find $E_0 = E(\{x_0\})$
2 – Move at random $\{x_0\} \rightarrow \{x_1\}$	2 – Move at random $\{x_0\} \rightarrow \{x_1\}$
3 – Find $E_1 = E(\{x_1\})$	3 – Find $E_1 = E(\{x_1\})$
4 – If($E_1 < E_0$)THEN accept $\{x_1\}$ ELSE $\{x_1\}$  ENDIF	4 – If($E_1 < E_0$)THEN accept $\{x_1\}$ ELSE If($E_1 > E_0$) THEN accept $\{x_1\}$ with probability ($r \leq p$) $p = e^{-\beta\Delta E}$, $\Delta E = E_1 - E_0$ ELSE $\{x_1\}$  ENDIF ENDIF
5 – Back to -1-	5 – Back to -1-
Something is missing !	ENTROPY !!!

Finite Size Scaling



For a system of volume \mathcal{V} , make a sequence of simulations

$$\mathcal{V}_1 < \mathcal{V}_2 < \dots < \mathcal{V}_N$$

We expect to recover the thermodynamic limit when $N \rightarrow \infty$.

Universality Class

In [statistical mechanics](#), a *universality class* is a collection of [mathematical models](#) which share a single [scale invariant](#) limit under the process of [renormalization group](#) flow. While the models within a class may differ dramatically at finite scales, their behavior will become increasingly similar as the limit scale is approached. In particular, [asymptotic](#) phenomena such as [critical exponents](#) will be the same for all models in the class.

Close to their critical point, greatly different physical systems exhibit a strong similarity. Various **macroscopic properties turn out to be independent of microscopic details**, but are **solely determined by a small number of global parameters**, such as the **dimensionality of the system and the symmetry and range of the interactions** between the particles. This fascinating phenomenon, universality, is explained by the renormalization-group theory, which was developed in the early seventies by Kenneth G. Wilson (Nobel Prize in Physics 1982). In the last 25 years, the universal properties of a variety of critical systems have been calculated. Many of these predictions have been verified by computer simulations, especially for so-called spin models.

Kadanoff ?

Fisher Zeros and Phase Transitions

Let us describe a finite system with discrete energy spectrum, such that

$$E = n\varepsilon, \quad \text{with} \quad n = 0, 1, 2, \dots, N$$

and the degeneracy of the n^{th} microstate given by $g(n)$

$$Z_N = \sum_{n=0}^N g(n\varepsilon) e^{-\beta n\varepsilon} = \sum_{n=0}^N g(n) z^n$$

Z_N can be factorized as

$$Z_N = z_0 \prod_{n=1}^N (z_n - z)$$

z_n are the N zeros of Z_N and z_0 is a constant.

Since the $g(n)$ are positive the zeros of Z_N can not be real and positive. The zeros z_n lie in the complex plane away from the real axis. In other words Z_N is analytical on the real axis.

Fisher Zeros and Phase Transitions

Clearly this scenario does not allow a phase transition since we identify a transition through the existence of a discontinuity in a derivative of the free energy.

In order to deal with real thermodynamics we must assume that the limit

$$\lim_{N \rightarrow \infty} \frac{\ln Z_N(z)}{N}$$

exists.

The zeros can be written as

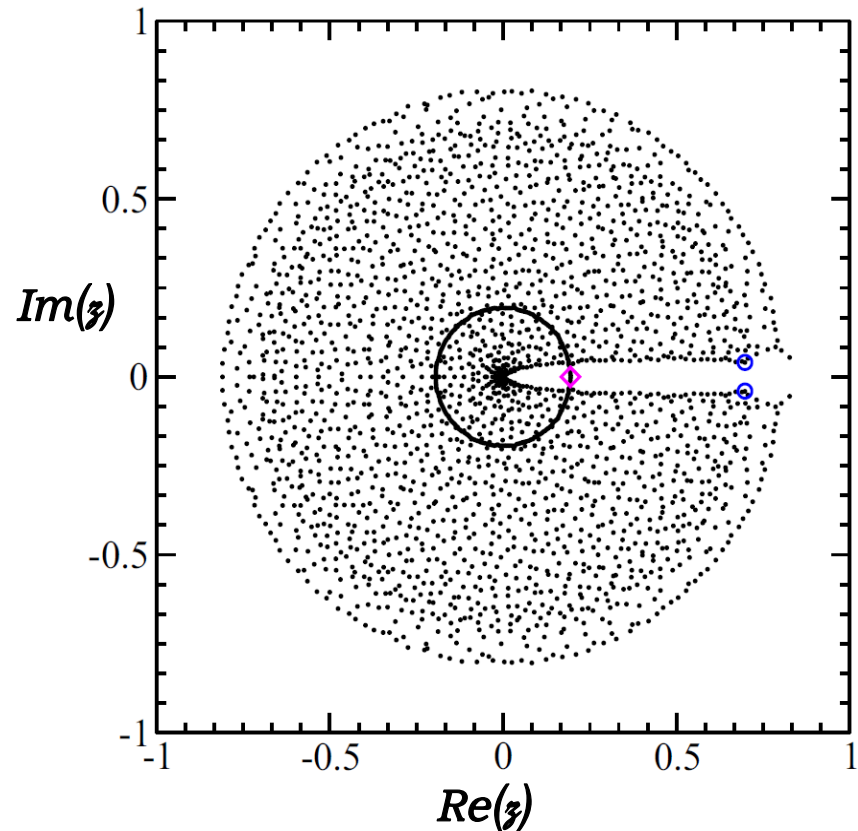
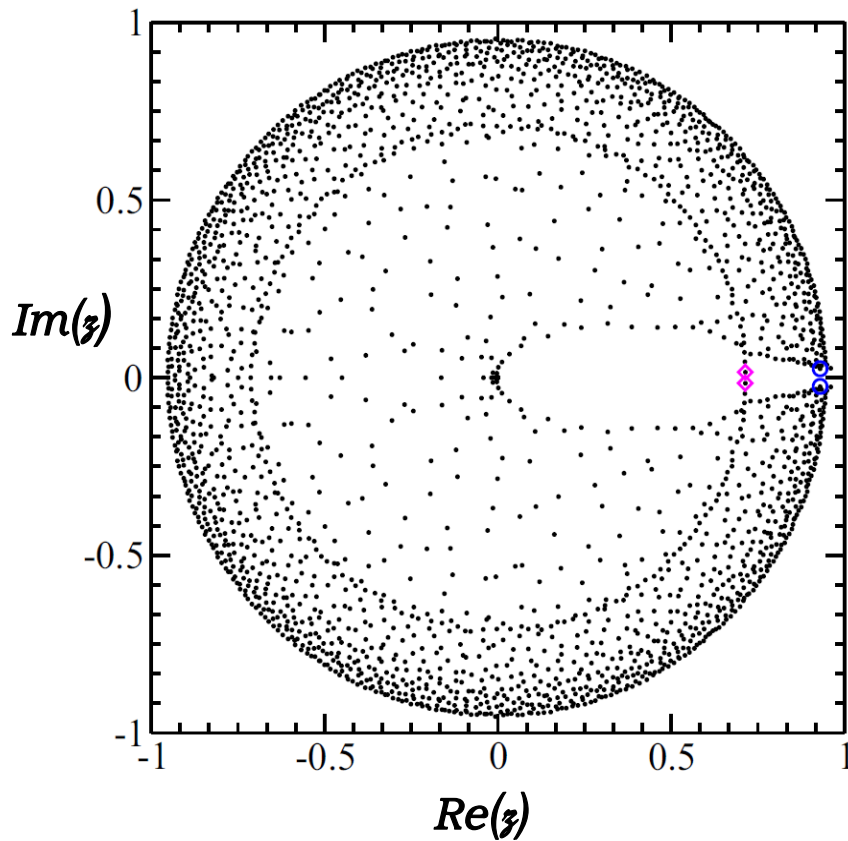
$$z_n = a_n + ib_n$$

We should expect that in the thermodynamic limit ($\lim_{N \rightarrow \infty}$) *at the transition*

$$a_n \rightarrow a_c \text{ and } b_n \rightarrow 0$$

Fisher Zeros and Phase Transitions

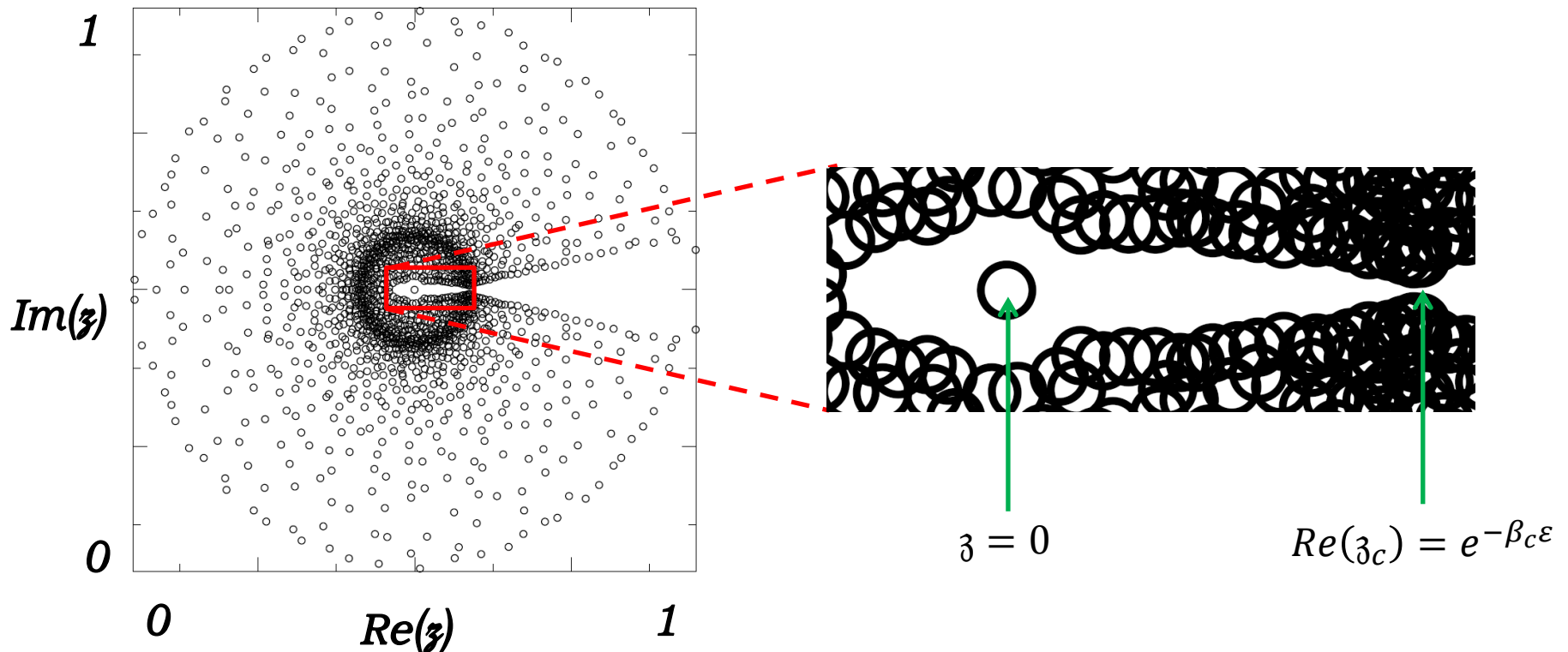
A few examples



Zeros for a flexible polymer chain with N monomers representing first order transitions. Left: $N=55$. Right: $N=300$. (J C. S. Rocha, S. Schnabel, D. P. Landau, M. Bachmann, PHYSICAL REVIEW E **90**, 022601 (2014))

Fisher Zeros and Phase Transitions

A few examples



Characteristic map for a second order phase transition (4 states Clock Model) (Partial results, Laboratório de Simulação)

Fisher Zeros and Phase Transitions

A few comments

In both cases, first and second order phase transitions, the appearing of “leading” zeros is evident.

The zeros, and thus their distribution, do generally depend on the choice of ε , but the transition temperature estimates is unaffected if ε is changed

A striking feature is the observation of an increased accumulation of zeros on a circle containing the pair of the leading zeros associated with the liquid-solid transition. The circular distribution has to be attributed to the self-reciprocity of the partition function polynomial at a phase transition with coexisting phases, in which case the energetic canonical distribution is bimodal and virtually symmetric. Therefore, the circular pattern can be interpreted as the signature of first-order-like transitions.

The XY Model in two Dimensions

$$H = -J \sum_{\langle i,j \rangle} (S_i^x \cdot S_j^x + S_j^y \cdot S_j^y)$$

Planar Rotator

$$\vec{S} = (S^x, S^y)$$

Anisotropic Heisenberg (XY)

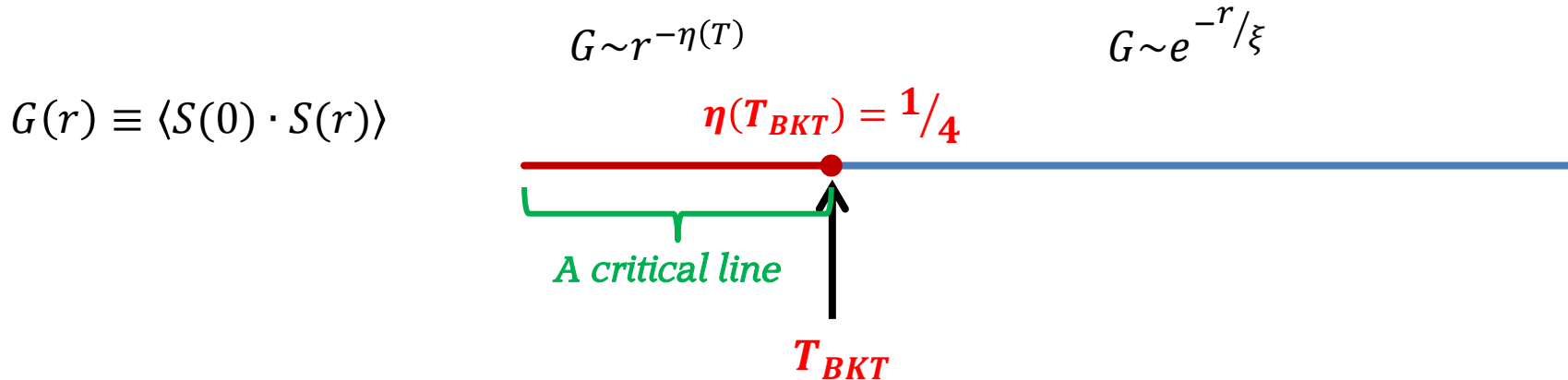
$$\vec{S} = (S^x, S^y, S^z)$$

Mermin-Wagner Theorem

Continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$.

The theorem does not prevent the existence of two regimes of correlation length!

The XY Model in two Dimensions



$$\eta(T_{BKT}) = 1/4$$

$$\xi(T) \approx e^{(bt^{-1/2})} ; t = \frac{T - T_{BKT}}{T_{BKT}}$$

$$m_{XY} \equiv \frac{1}{V} \sum \sqrt{(m_x)^2 + (m_y)^2} = 0$$

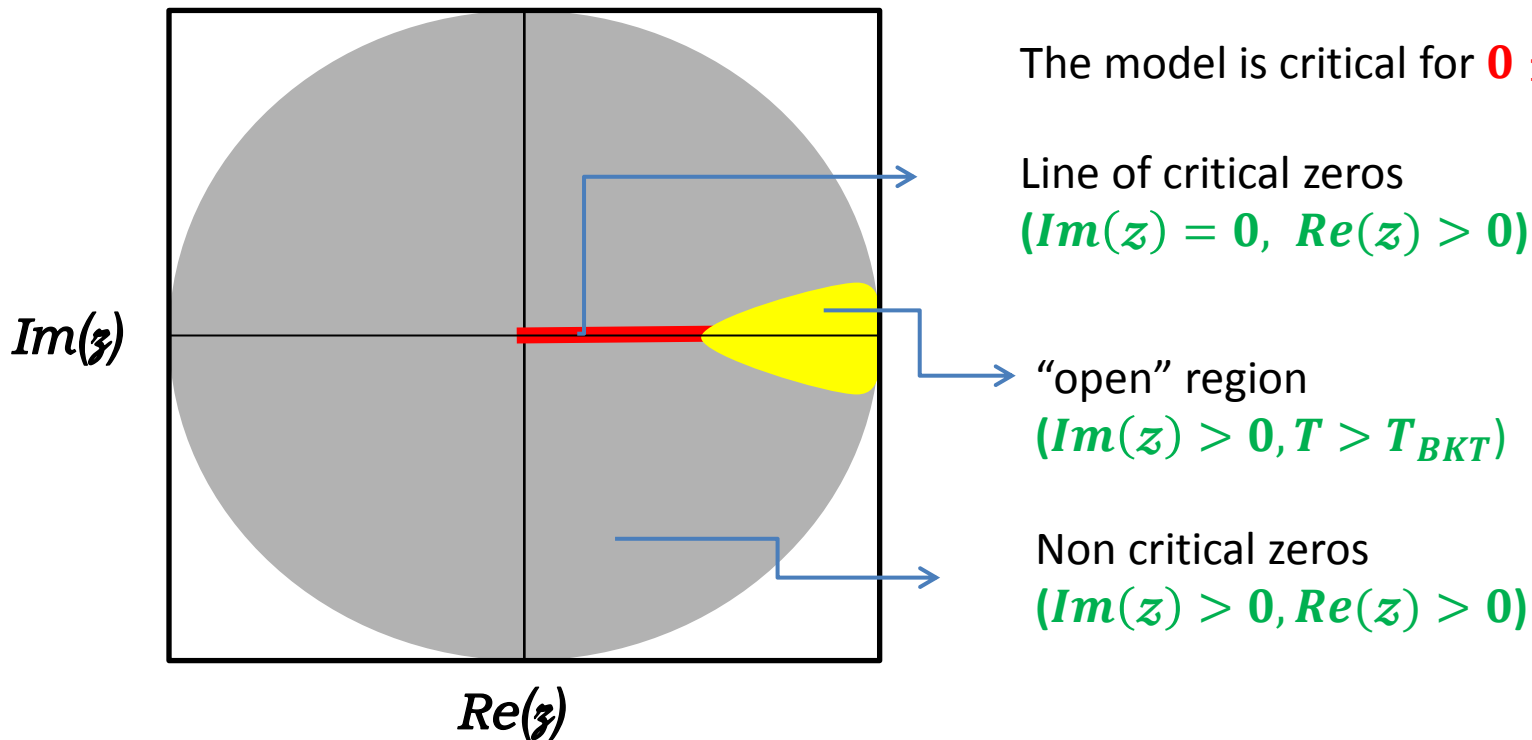
$$\chi_{xy} \equiv \frac{1}{T} (m_{xy} - \langle m_{xy} \rangle)^2 = \begin{cases} \xi^{2-\eta} & , T > T_{BKT} \\ \infty & , T < T_{BKT} \end{cases}$$

$$C_v \equiv \frac{1}{T^2} (E - \langle E \rangle)^2 \text{ is finite.}$$

The free energy is C^∞

The zeros distribution for the XY Model

What we expect?



The zeros distribution for the XY Model

What we can do

$$Z_N = \sum_{n=0}^N g(n\varepsilon) e^{-\beta n\varepsilon} = \sum_{n=0}^N g(n) z^n$$

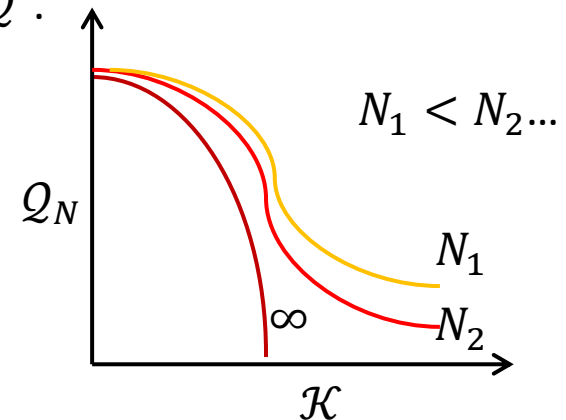
Even for moderate size systems this quantity cannot be calculated

The best we can do is to estimate Z_N for a large sequence of N 's expecting the sequence converges.

$$\lim_{N \rightarrow \infty} \frac{\ln Z_N(z)}{N}$$

$$Z_N = z_0 \prod_{n=1}^N (z_n - z)$$

A finite Size Scaling analysis can give us the behavior of a thermodynamic quantity "Q".



The Wang-Landau Technique

Random walk in energy space with a flat histogram

Our task is to calculate

$$Z = \sum_E g(E) e^{-\beta E}$$

1 - Choose an initial state

2 - Set $g(E) = 1$ and $(f_0 > 1)$

3 - Choose an initial "particle"

Begin with a simple "guess", e.g.

$$g(E) = 1$$

4 - Calculate $\delta = \frac{g(E_1)}{g(E_2)}$

Choose moves according to:

$$p(E_1 \rightarrow E_2) = \min\left(\frac{g(E_1)}{g(E_2)}, 1\right)$$

5 - Generate a random number

$$0 < r < 1$$

6 - If $r < \delta$ accept the move

Following each move, update
 $g(E) \rightarrow f_i g(E)$ (f initially > 1)

7 - Set $g(E_i) \rightarrow f \times g(E_i)$

A histogram of energies is stored,
when it is "flat" the process is
interrupted

8 - (a) If histogram is not "flat" go
to the next move and then to (4)

(b) If histogram is flat, $f = \sqrt{f}$

$$f_{i+1} \rightarrow \sqrt{f_i}$$

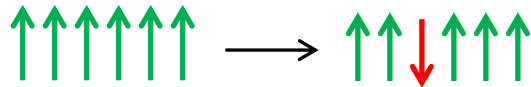
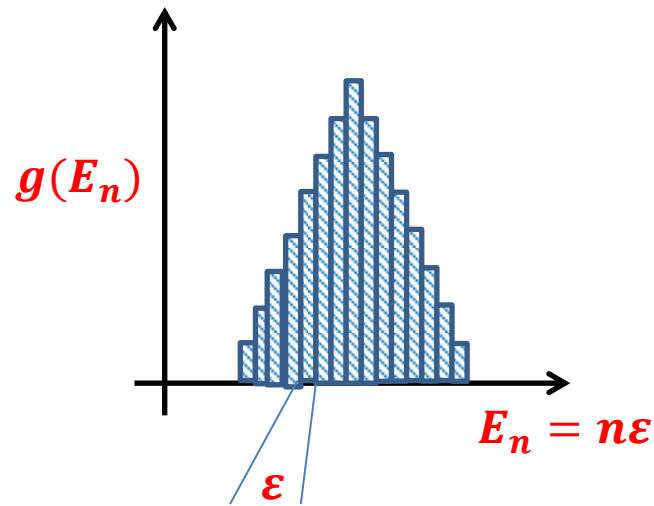
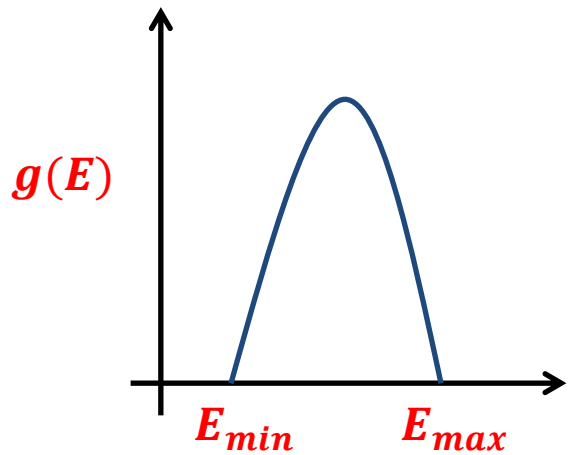
Repeat steps 3 to 9 until $f \leq f_{min}$

Continue the process until $f_i \rightarrow 1$

Done! Calculate properties using
final $g(E)$

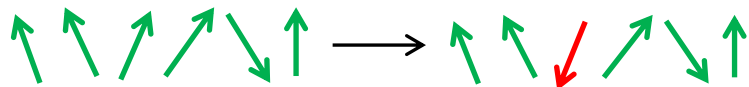
The Wang-Landau Technique

Discrete \times Continuous energy



$$\Delta E = 4J$$

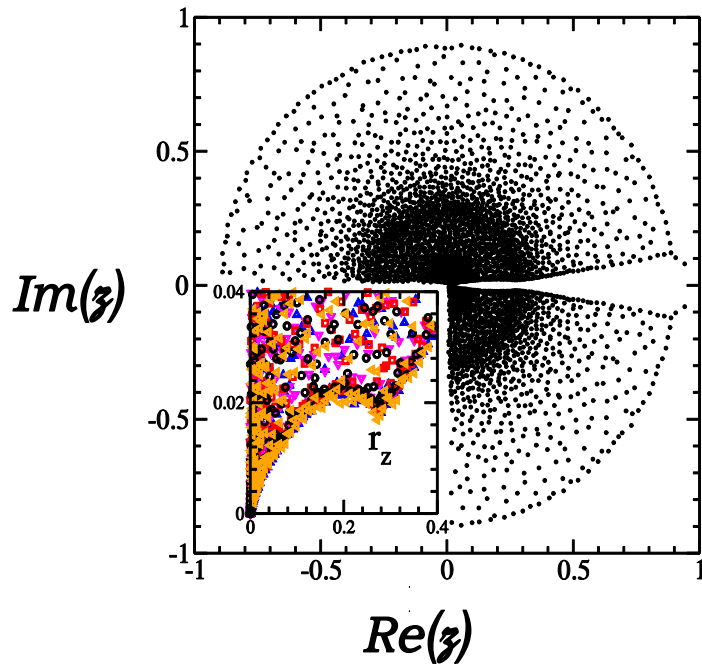
$$H = -J \sum_{\langle i,j \rangle} (S_i^z \cdot S_j^z)$$



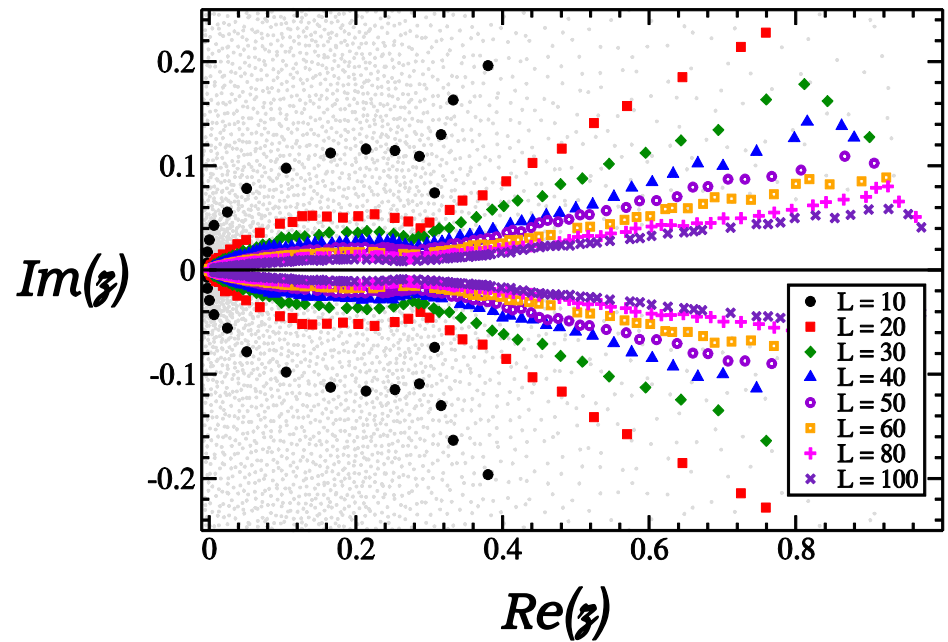
$$\Delta E = 3.284J$$

$$H = -J \sum_{\langle i,j \rangle} (S_i^x \cdot S_j^x + S_j^y \cdot S_j^y)$$

Results

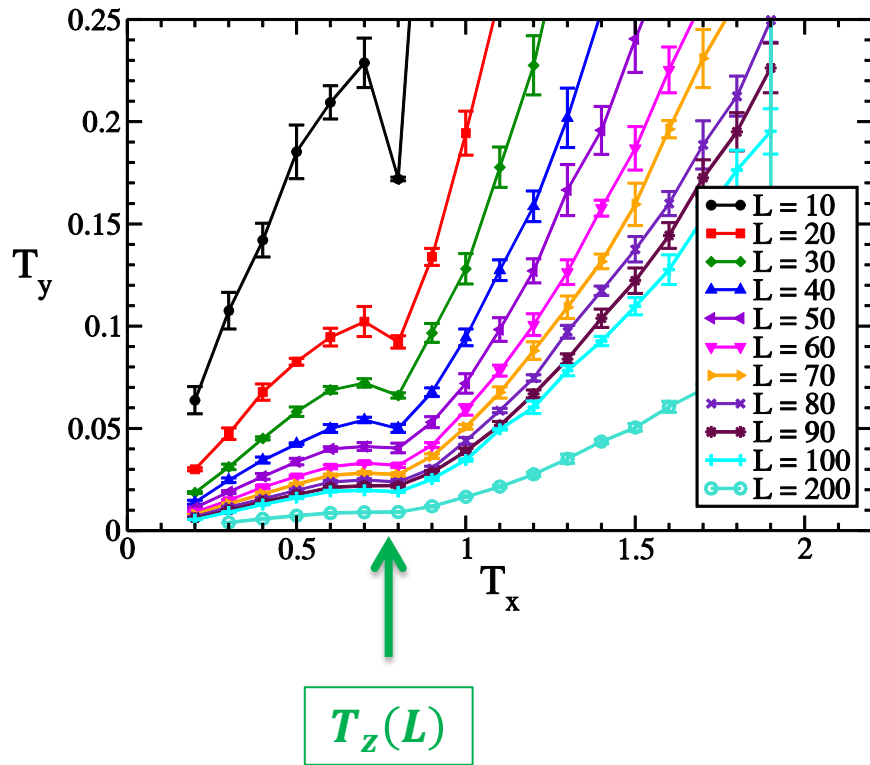


Fisher zeros map in the $x = e^{-\beta\varepsilon}$ plane for the 2D classical XY-model in a 50x50 lattice. The inset is zoom on the inner region for 5 distinct simulations.



Zoom on the real positive semi-axis of the zeros maps in the x plane for $L = 10 \rightarrow 100$. The zeros on the internal border are highlighted.

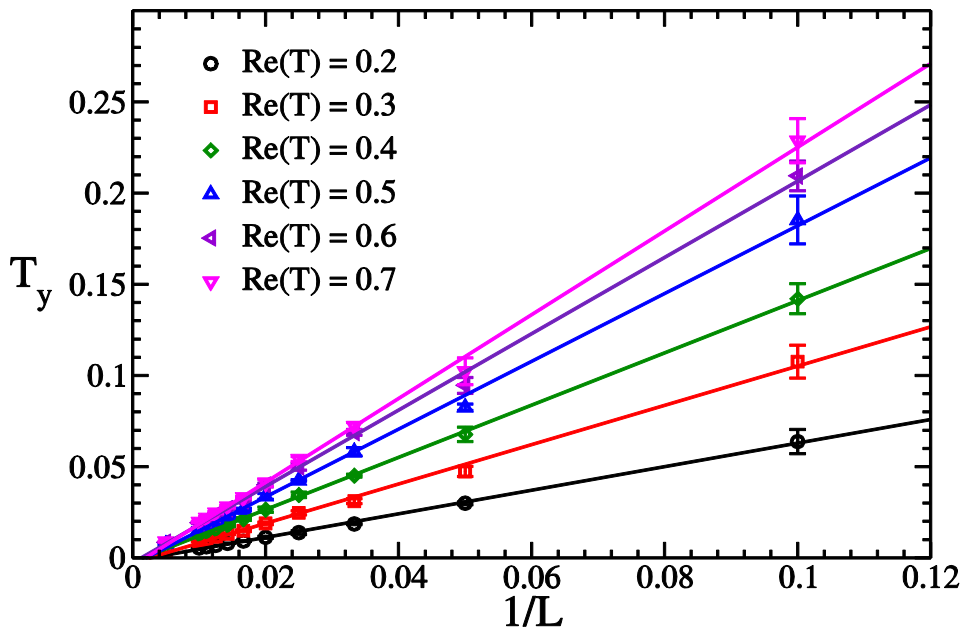
Results



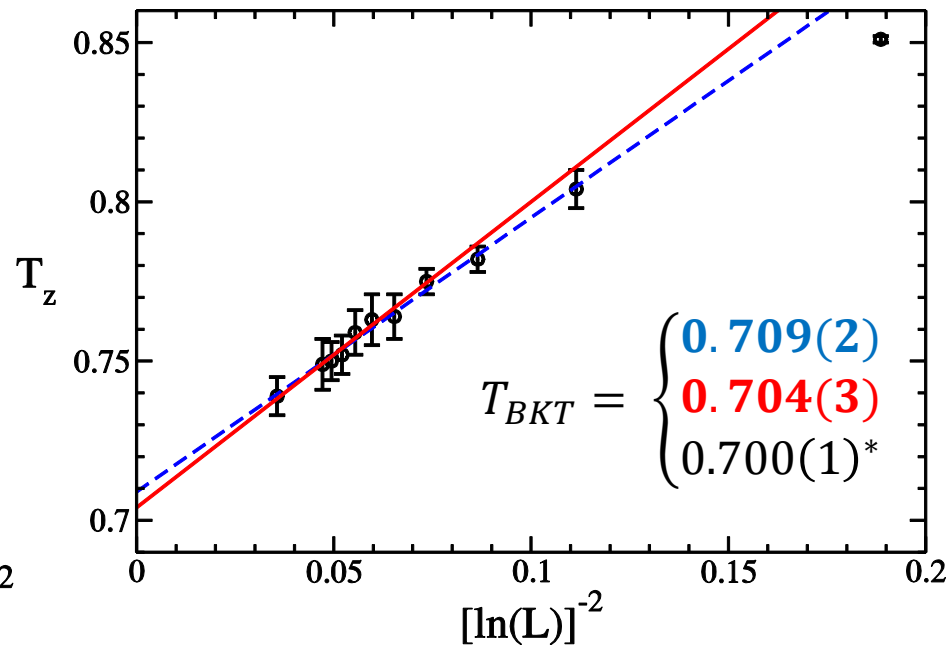
Internal border of the zero distribution obtained by using for $L = 10 \rightarrow 200$.

The location of the inflection point position is $T_z(L)$. $T_z(L) \rightarrow T_{BKT}$ as $L \rightarrow \infty$.

Results



Finite size scaling analysis of the imaginary part of the internal border.



Finite size scaling of the inflection point position, $T_z(L)$. Discarding the point corresponding to $L = 10$ the BKT temperature is estimated as 0.709(2) (dashed blue line) and discarding $L < 40$, $T_{BKT} = 0.704(3)$ (solid red line) in excellent agreement with earlier results.

(*) H.G. Evertz and D.P. Landau, **Phys. Rev. B** 54, 12302(1996)
 B. V. Costa, P. Z. Coura, and S. A. Leonel, **Physics Letters A** 377, 1239 (2013).

A possible pathway to analyze the zeros' map

Consider a function $\mathcal{F}(z)$ that behaves as

$$\mathcal{F}(z) \approx A \left(1 - \frac{z}{z_c}\right)^\gamma ; z \rightarrow z_c, \gamma = \begin{cases} < 0 & \text{a pole at } z_0 \\ = 0 & \text{log or well behaved} \\ > 0 & \text{well behaved} \end{cases}$$

Suppose $\mathcal{F}(z)$ can be represented by

$$\mathcal{F}(z) = \sum_{n=0}^{\infty} a_n z^n$$

with radius of convergence z_0 .

A possible pathway to analyze the zeros' map

If $\lim_{n \rightarrow \infty} (a_n)^{-1/n} = z_0$ the series converges inside the ball $|z| < z_0$, diverges for $|z| > z_0$ and has at least a pole over z_0 .

The “character” of the coefficients are determined by the singularities of $\mathcal{F}(z)$. The singularity closer to the origin determines the asymptotic behavior. (Let us say z_0).

If z_0 is real + $\text{sign}(a_n) = \text{sign}(a_m)$

If z_0 is real - $\text{sign}(a_n) = -\text{sign}(a_{n+1})$

If z_0 is \mathbb{C} $\text{sign}(a_n)$ is irregular

A possible pathway to analyze the zeros' map

$$\mathcal{F}(z) \approx A \left(1 - \frac{z}{z_c}\right)^\gamma = A \sum_{n=0}^{\infty} (-1)^n \binom{\gamma}{n} (z_c)^n z^n$$

The amplitude is given by

$$A = \lim_{z \rightarrow z_c} \frac{\mathcal{F}(z)}{\left(1 - z/z_c\right)^{-\gamma}}$$

Comparing with the Taylor expansion

$$a_n = A(-1)^n \binom{n + \gamma - 1}{n} (z_c)^{-n}$$

Taking the quotient

$$\mu_n = \frac{a_n}{a_{n-1}} = \frac{A \binom{n + \gamma - 1}{n} (z_c)^{-n}}{A \binom{n + \gamma - 2}{n-1} (z_c)^{-n+1}} = \frac{\Gamma(n + \gamma)\Gamma(n)}{\Gamma(n + \gamma - 1)\Gamma(n + 1)} (z_c)^{-1}$$

For n large enough ... $\mu_n \sim z_c^{-1} \left[1 + \frac{\gamma-1}{n} + O(1/n^2)\right]$

A possible pathway to analyze the zeros' map

It does not work !

Why? Because we do not have the TRUE series for the free energy.

Only in the thermodynamic limit (*Volume* $\rightarrow \infty$) our $\mathcal{F}_V(z)$ has a GOOD asymptotic behavior.

Is there any way to explore $\mathcal{F}_V(z)$ to get the asymptotic behavior?
Probably, but we do not know how!

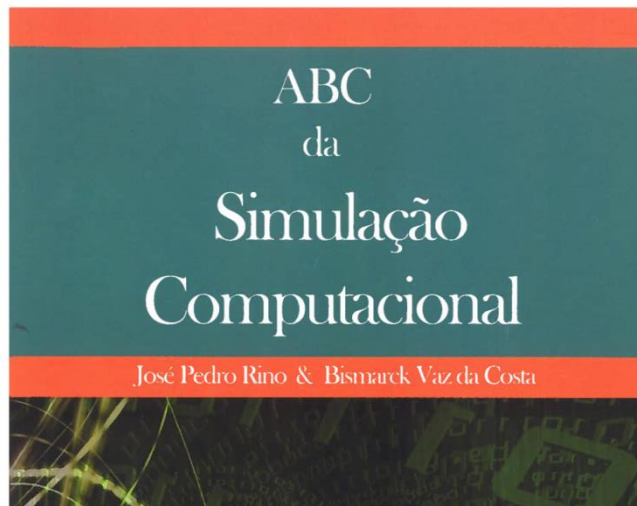
Final Remarks

1. The Study of Phase Transitions is a Challenge. Its Importance ranges from Cosmology, Appearing of Life (Conscience?), Proteins, Magnetism, Quantum Phase Transitions and much more.

1. Analytical results are restricted to a few Toy Models

2. Computer Simulations play an (the most ?) important role in describing the physics of Phase Transitions.

Thank you



A Modern Analysis of Phase Transitions

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Overview

1. Introduction
 - a. Partition Function
 - b. Single Histogram
 - c. Wang-landau
 - d. Fisher Zeroes
2. Filtering Zeroes
 - a. High Precision Determination of T_t
3. Examples
4. Final Remarks



Partition Function

The Partition Function describes completely the equilibrium properties of a thermodynamic system

$$Z \equiv \sum_{\{x\}} e^{-\beta H(\{x\})} \quad \text{or} \quad Z = \sum_E g(E) e^{-\beta E}$$

For example

$\langle E \rangle = -\frac{d}{d\beta} \ln Z$	Energy
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$\chi = \frac{1}{T} (\langle x^2 \rangle - \langle x \rangle^2)$	Susceptibility

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The probability of a configuration E at temperature β_0 is

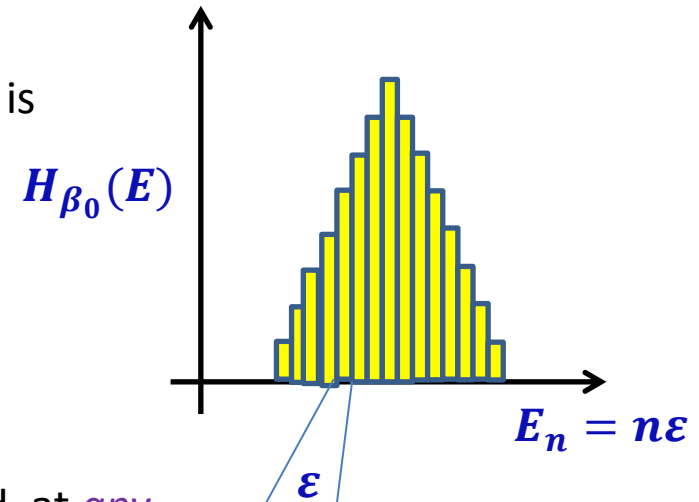
$$P_{\beta_0}(E) = \frac{g(E)e^{-\beta_0 E}}{Z_{\beta_0}},$$

We can generate a histogram $\frac{H_{\beta_0}(E)}{N} \doteq P_{\beta_0}(E)$.

$$g(E) = N^{-1}H(E)Z_{\beta_0}e^{\beta_0 E}$$

With this estimate for $g(E)$ averages $\langle A \rangle$ are obtained at *any temperature*.

$$P_{\beta}(E) = \frac{H(E)Z_{\beta_0}}{N} e^{-E(\beta-\beta_0)}$$



$$Z = \sum_E g(E)e^{-\beta E}$$

The Wang-Landau Technique

Random walk in energy space with a flat histogram

Our task is to calculate

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1 - Choose an initial state

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A histogram of energies is stored,
when it is "flat" the process is
interrupted

8 - (a) If histogram is not "flat" go
to the next move and then to (4)

(b) If histogram is flat, $f = \sqrt{f}$

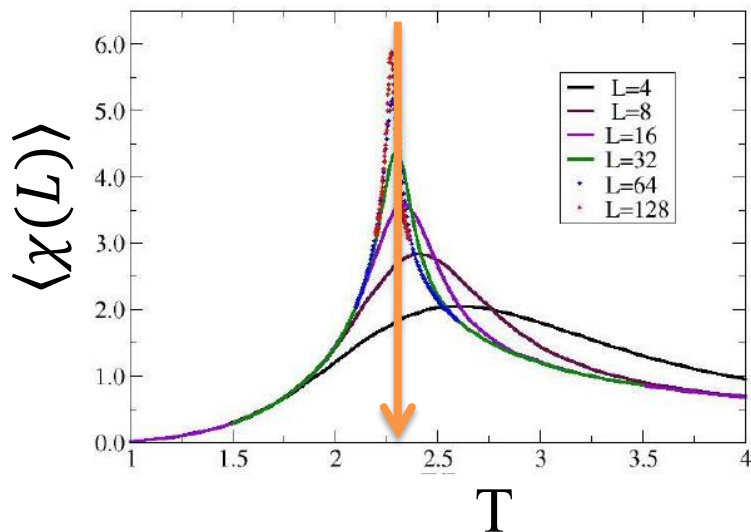
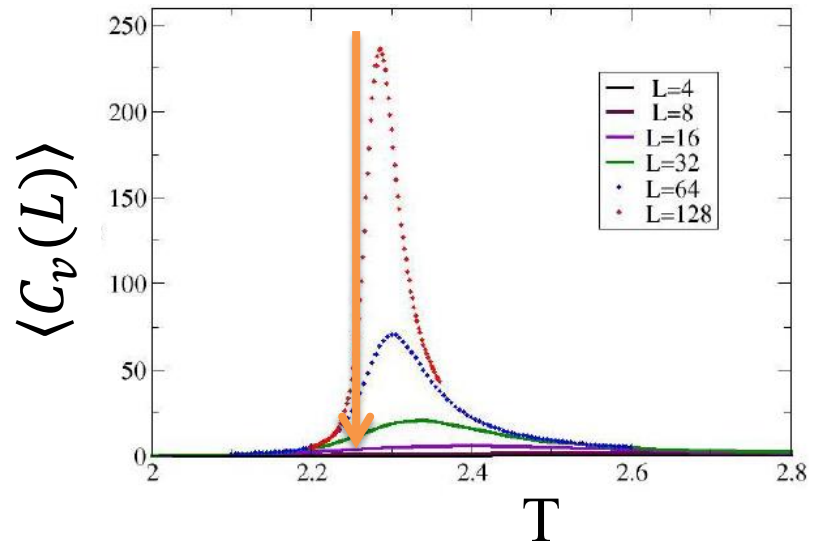
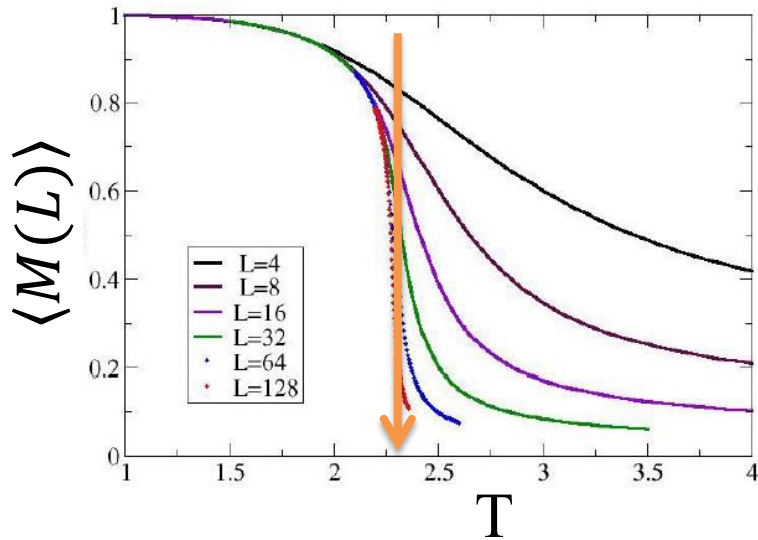
$$f_{i+1} \rightarrow \sqrt{f_i}$$

Repeat steps 3 to 9 until $f \leq f_{min}$

Continue the process until $f_i \rightarrow 1$

Done! Calculate properties using
final $g(E)$

Finite Size Scaling



For a system of volume \mathcal{V} , make a sequence of simulations

$$\mathcal{V}_1 < \mathcal{V}_2 < \dots < \mathcal{V}_N$$

We expect to recover the thermodynamic limit when $N \rightarrow \infty$.

Universality Class

In [statistical mechanics](#), a *universality class* is a collection of [mathematical models](#) which share a single [scale invariant](#) limit under the process of [renormalization group](#) flow. While the models within a class may differ dramatically at finite scales, their behavior will become increasingly similar as the limit scale is approached. In particular, [asymptotic](#) phenomena such as [critical exponents](#) will be the same for all models in the class.

Close to their critical point, greatly different physical systems exhibit a strong similarity. Various **macroscopic properties turn out to be independent of microscopic details**, but are **solely determined by a small number of global parameters**, such as the **dimensionality of the system and the symmetry and range of the interactions** between the particles. This fascinating phenomenon, universality, is explained by the renormalization-group theory, which was developed in the early seventies by Kenneth G. Wilson (Nobel Prize in Physics 1982). In the last 25 years, the universal properties of a variety of critical systems have been calculated. Many of these predictions have been verified by [computer simulations](#), especially for so-called spin models.

Leo Kadanoff (?)

Fisher Zeros and Phase Transitions

Let us describe a finite system with discrete energy spectrum, such that

$$E = n\varepsilon, \quad \text{with} \quad n = 0, 1, 2, \dots, N$$

and the degeneracy of the n^{th} microstate given by $g(n)$

$$Z_N = \sum_{n=0}^N g(n\varepsilon) e^{-\beta n\varepsilon} = \sum_{n=0}^N g(n) z^n$$

Z_N can be factorized as

$$Z_N = z_0 \prod_{n=1}^N (z_n - z)$$

z_n are the N zeros of Z_N and z_0 is a constant.

Since the $g(n)$ are positive the zeros of Z_N can not be real and positive. The zeros z_n lie in the complex plane away from the real axis. In other words Z_N is analytical on the real axis.

Fisher Zeros and Phase Transitions

Clearly this scenario does not allow a phase transition since we identify a transition through the existence of a discontinuity in a derivative of the free energy.

In order to deal with real thermodynamics we must assume that the limit

$$\lim_{N \rightarrow \infty} \frac{\ln Z_N(z)}{N}$$

exists.

The zeros can be written as

$$z_n = a_n + ib_n$$

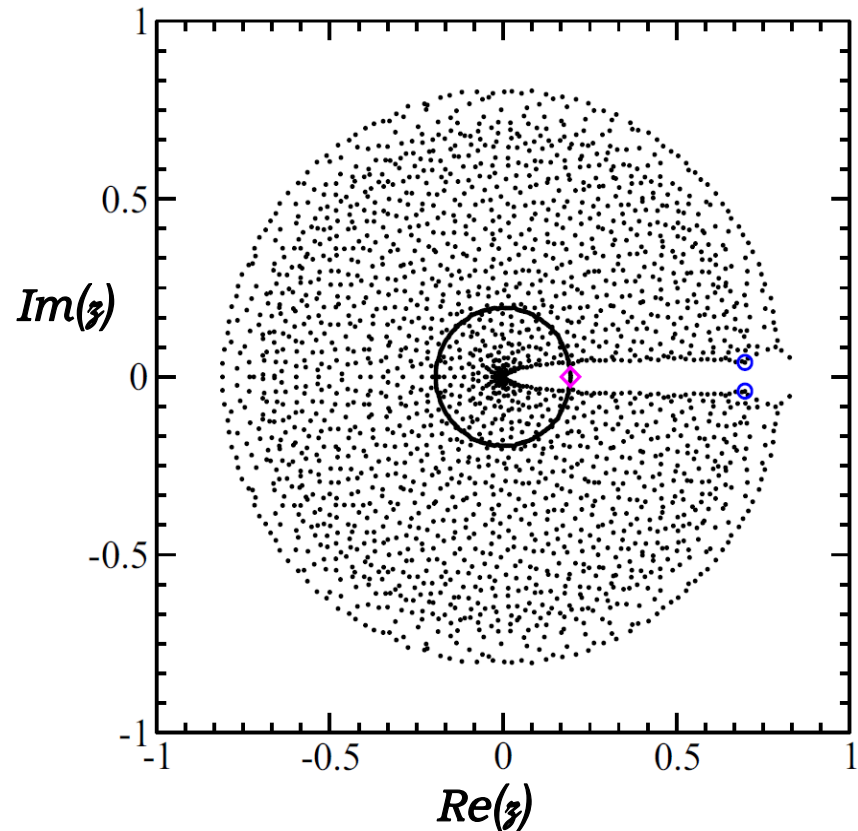
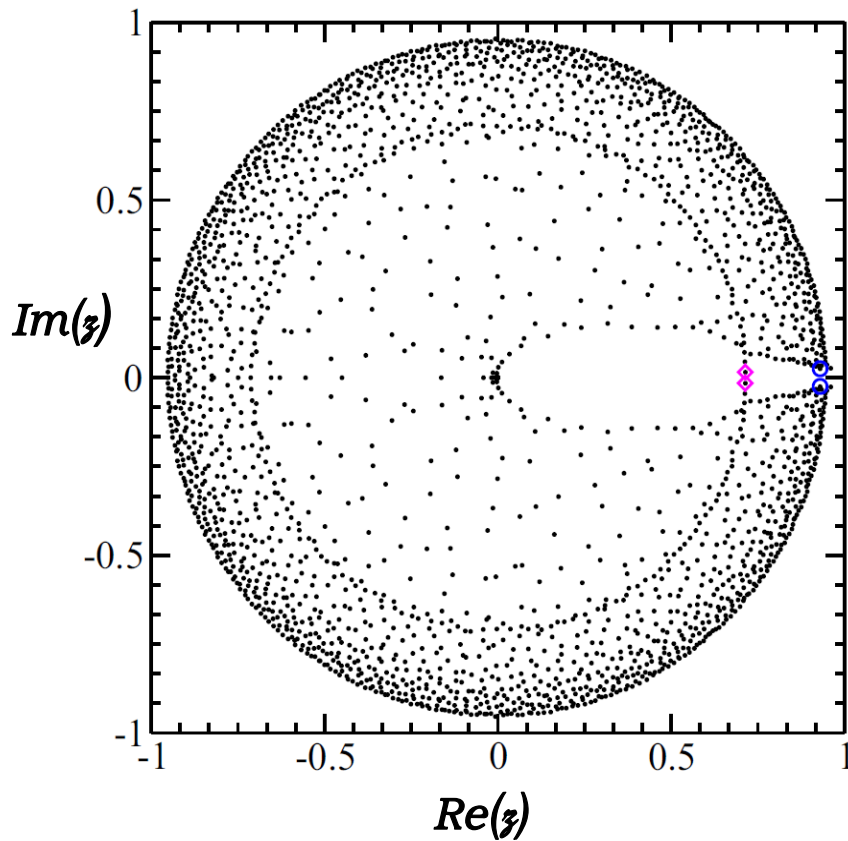
We should expect that in the thermodynamic limit ($\lim_{N \rightarrow \infty}$) *at the transition*

$$a_n \rightarrow a_c \text{ and } b_n \rightarrow 0$$

We'll need this very soon.

Fisher Zeros and Phase Transitions

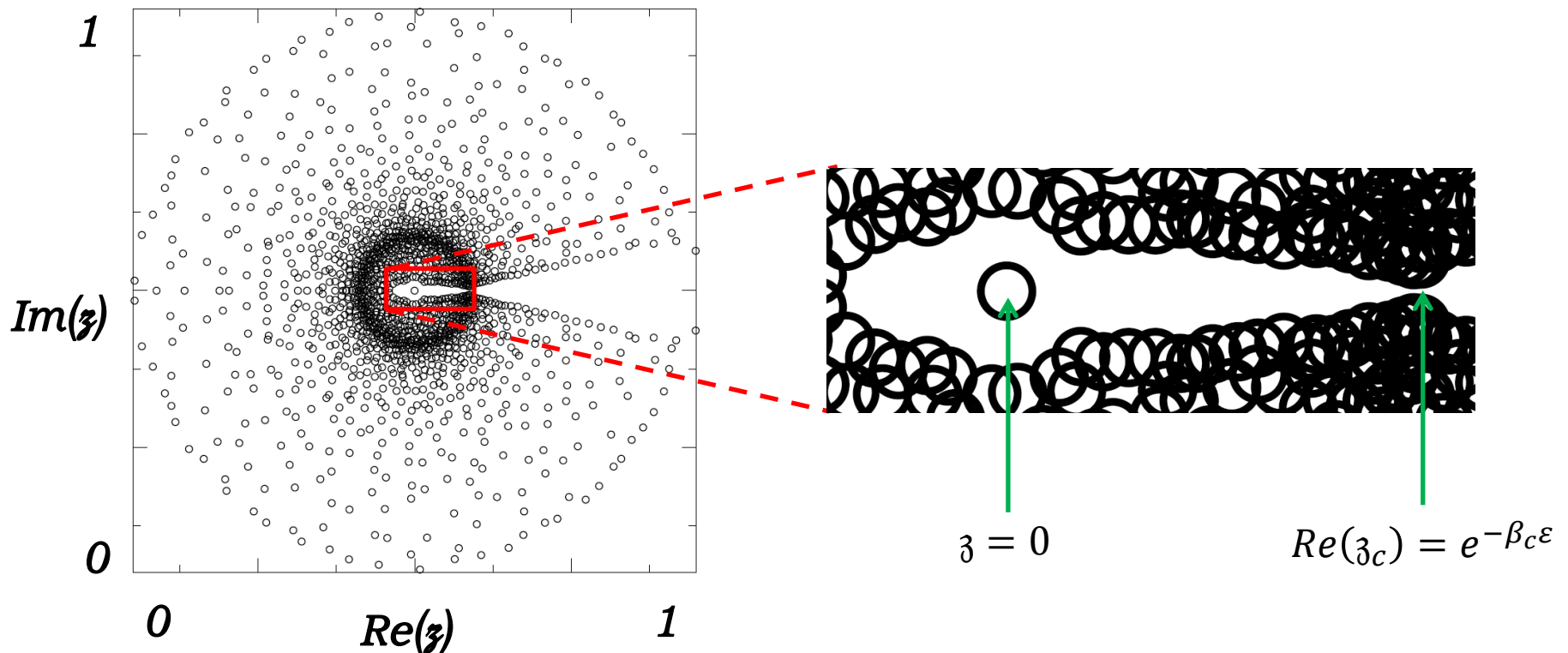
A few examples



Zeros for a flexible polymer chain with N monomers representing first order transitions. Left: $N=55$. Right: $N=300$. (J C. S. Rocha, S. Schnabel, D. P. Landau, M. Bachmann, PHYSICAL REVIEW E **90**, 022601 (2014))

Fisher Zeros and Phase Transitions

A few examples



Characteristic map for a second order phase transition (4 states Clock Model) (Partial results, Laboratório de Simulação)

Fisher Zeros and Phase Transitions

A few comments

In both cases, first and second order phase transitions, the appearing of “leading” zeros is evident. (I name them: dominant zeroes)

The zeros, and thus their distribution, do generally depend on the choice of ε , but the transition temperature estimates is unaffected if ε is changed

A striking feature is the observation of an increased accumulation of zeros on a circle containing the pair of the leading zeros associated with the liquid-solid transition. The circular distribution has to be attributed to the self-reciprocity of the partition function polynomial at a phase transition with coexisting phases, in which case the energetic canonical distribution is bimodal and virtually symmetric. Therefore, the circular pattern can be interpreted as the signature of first-order-like transitions.

Filtering Zeroes

We quickly get in trouble as the system size grows.

WHY?

The coefficients of the polynomial $Z_N = \sum_{n=0}^N g(n\varepsilon)e^{-\beta n\varepsilon} = \sum_{n=0}^N g(n)z^n$ can easily reach prohibitive values

Ising 2d (96x96)

$$\begin{aligned} g(1) &= 2 \times 10^0 \\ g(4632) &= 1.831951704888848 \times 10^{2772} \end{aligned}$$

It turns out impossible to calculate the zeros in a reasonable way.
(In other words, it is impossible to go beyond modest size volumes)

SOLUTION? ...YES...

We can filter the relevant zeroes!

Filtering Zeroes

$$Z_N = \sum_{n=0}^N g(n\varepsilon)e^{-\beta n\varepsilon} = \sum_{n=0}^N g(n\varepsilon)e^{-\beta_0 n\varepsilon} e^{-(\beta-\beta_0)n\varepsilon}$$

This equation can be rewritten as

$$Z_{\Delta\beta} = e^{-\varepsilon_0\beta} \sum_{n=0}^N \mathfrak{H}_{\beta_0}(n)\zeta^n, \text{ where now, } \zeta = e^{-(\beta-\beta_0)n\varepsilon},$$

and,

$\mathfrak{H}_{\beta_0}(n) = g(\varepsilon_0+n\varepsilon)e^{-\beta_0(\varepsilon_0+n\varepsilon)}$ is a distribution **at** β_0

Filtering Zeroes

We get a new polynomial

$$Z_{\Delta\beta} = e^{-\varepsilon_0\beta} \sum_{n=0}^N \mathfrak{H}_{\beta_0}(n)\zeta^n = e^{-\varepsilon_0\beta} \prod_{n=1}^N (\zeta - \zeta_n),$$

Where now the coefficients are controlled by the exponential

$$\mathfrak{H}_{\beta_0}(n) = g(\varepsilon_0 + n\varepsilon) e^{-\beta_0(\varepsilon_0 + n\varepsilon)}.$$

Any quantity is easily obtained:

$$\langle E \rangle_{\Delta\beta} = \varepsilon_0 + \frac{\varepsilon \sum_{n=0}^N n \mathfrak{H}_{\beta_0}(n) \zeta^n}{\sum_{n=0}^N \mathfrak{H}_{\beta_0}(n) \zeta^n}$$

$$\langle C \rangle_{\Delta\beta} = \frac{\varepsilon^2 \sum_{n=0}^N \sum_{m=0}^N (n^2 - nm) \mathfrak{H}_{\beta_0}(n) \mathfrak{H}_{\beta_0}(m) \zeta^{n+m}}{\left(\sum_{n=0}^N \mathfrak{H}_{\beta_0}(n) \zeta^n \right)^2}$$

Filtering Zeroes

Observe that if we build the histogram at the transition $(\beta_0 = \beta_t)$, then $\zeta = 1$ for $(\beta = \beta_t)$ and consequently

One, and only one, of the zeroes of the polynomial $IS = 1!$

$$(\zeta = e^{-(\beta - \beta_0)n\varepsilon})$$

$$\langle E \rangle_{\Delta\beta=0} = \varepsilon_0 + \frac{\varepsilon \sum_{n=0}^N n \mathfrak{H}_{\beta_0}(n)}{\sum_{n=0}^N \mathfrak{H}_{\beta_0}(n)}$$

$$\langle C \rangle_{\Delta\beta=0} = \frac{\varepsilon^2 \sum_{n=0}^N \sum_{m=0}^N (n^2 - nm) \mathfrak{H}_{\beta_0}(n) \mathfrak{H}_{\beta_0}(m)}{\left(\sum_{n=0}^N \mathfrak{H}_{\beta_0}(n) \right)^2}$$

Filtering Zeroes

Unfortunately we are not at the thermodynamic limit.

Our zeros have the form: $a_n \rightarrow a_c$ and $b_n \rightarrow 0$

However, the closest zero to $\Re(\zeta)$ ($\min\{\Im m(\zeta)\}$) is a dominant zero. It allow us to write the following algorithm :

1. Build a single histogram $\{\mathfrak{H}_{\beta_0}(n)\}$ (Chose β_0 at your will)
2. Find the dominant zero , $\min\{\Im m(\zeta)\}$
3. Use the corresponding temperature to build a new histogram
4. Go back to the (1)
5. Stop when $|\zeta| = 1$

Some Examples

Table I. 1d Ising Model

L	β	T	$\Re(\zeta)$	$\Im(\zeta)$
100	1.0000	1.0000	4.0122	9.7538
	0.6527	1.5321	4.3043	5.2287
	0.9502	1.0524	4.0424	9.4067
	0.6010	1.6639	3.4254	6.9428
100	2.0000	0.5000	-0.7356	0

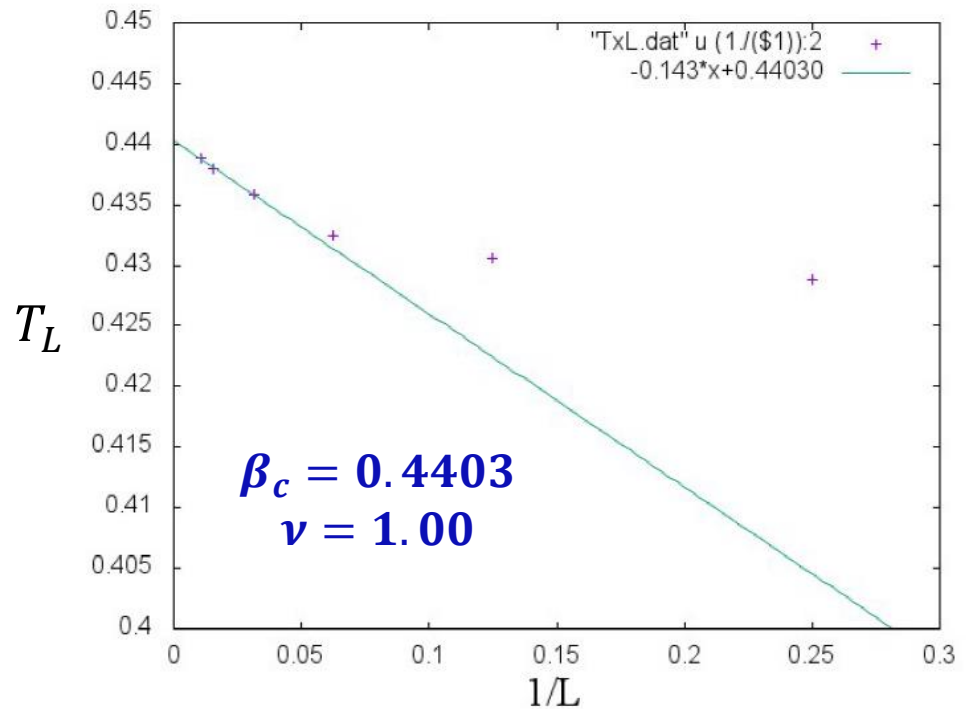
No Transition.

Some Examples

Continuous

Table II. 2d Ising Model

L	β	T	$\Re(\zeta)$	$\Im(\zeta)$
4	0.6667	3.0000	0.6262	0.7652
	0.4504	2.2202	1.1130	1.2180
	0.4236	2.3607	0.9752	1.0939
	0.4299	2.3261	1.0059	1.1218
	0.4284	2.3343	0.9985	1.1150
	0.4288	2.3321	1.00045	1.1168
	0.4287	2.3326	0.9999	1.1159
8	0.4287	2.3326	0.9924	0.4241
	0.4306	2.3223	0.9999	0.4273
16	0.4306	2.3223	0.9923	0.2088
	0.4325	2.3121	0.9999	0.2104
32	0.4325	2.3121	0.9872	0.1035
	0.4357	2.2952	0.9998	0.1049
	0.43575	2.2949	0.9999	0.1049
64	0.43575	2.2949	0.9911	0.0520
	0.4380	2.2831	1.00005	0.0525
96	0.43575	2.2949	0.9967	0.0349
	0.4388	2.2789	0.9999	0.0350
∞	0.4407	2.2692	1	0

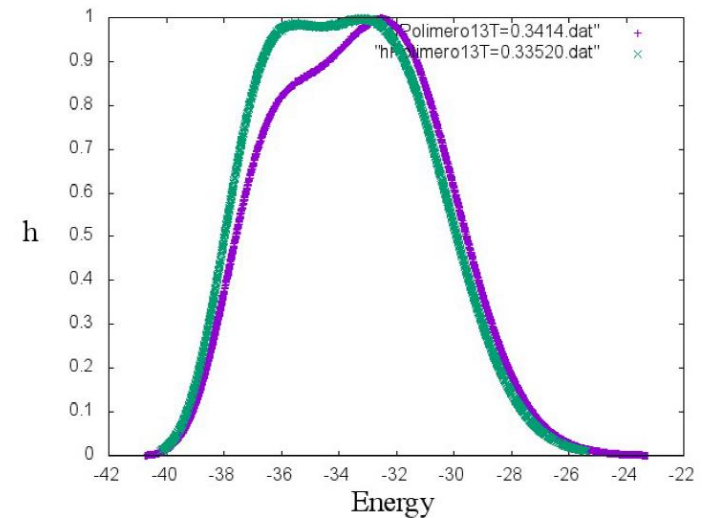


Some Examples

Two Transitions: First order & Continuous

Table III. 13 monomers polymer

L	β	T	$\Re(\zeta)$	$\Im(\zeta)$
13	10.0000	0.10000	1.02230	0.02650
	6.60690	0.15140	1.01414	0.01660
	4.44675	0.22488	1.00855	0.00806
	3.13696	0.31878	1.00135	0.00502
	2.92940	0.34142	0.99965	0.00502
	2.98685	0.33520	1.00002	0.00502
13	0.8333	1.2000	0.99988	0.00425
	0.8487	1.1783	0.99991	0.00423
	0.8625	1.1594	0.99994	0.00421
	0.8717	1.1472	0.99996	0.00420
	0.8779	1.1391	0.99997	0.00420
	0.8825	1.1331	0.99998	0.00420
	0.8856	1.1292	0.99999	0.00419

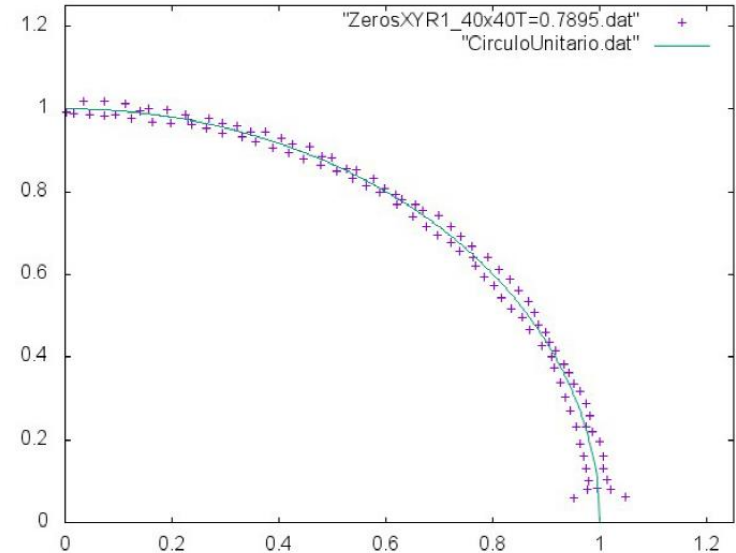


Some Examples

BKT

Table VI. Anisotropic Heisenberg Model

L	β	T	$\Re(\zeta)$	$\Im(\zeta)$
10	0.6667	1.5000	0.8326	0.2590
	8499	1.1766	0.8566	0.2254
	1.0047	0.9953	0.8837	0.1901
	1.1283	0.8863	0.9494	0.2307
	1.1802	0.8473	0.9990	0.2431
	1.1812	0.8466	1.0000	0.2433
20	1.1812	0.8466	0.9439	0.1388
	1.2389	0.8072	0.9999	0.14705
	1.2390	0.8071	1.0000	0.1471
40	1.2390	0.8071	0.9955	0.0830
	1.2666	0.7895	0.9959	0.0826
60	1.2435	0.8042	1.0007	0.0568
	1.2838	0.7789	1.0064	0.0528



Final Remarks

1. We developed a new method to study phase transitions
2. It seems, at least in all our tests, to be of universal application
3. It is easy
4. It is cheap
5. It gives wonderful results for:
 - a. Transition temperatures
 - b. Exponents
6. Allow to “guess” the order of the transition

Thank you so much

