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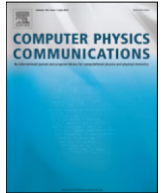For correction or revision of any artwork, please consult http://www.elsevier.com/artworkinstructions.

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Q1 # Using zeros of the canonical partition function map to detect signatures of a Berezinskii–Kosterlitz–Thouless transition

Q2 J.C.S. Rocha [a,b,*], L.A.S. Mól [a], B.V. Costa [a]

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ABSTRACT

Using the two dimensional $XY - (S(O(3)))$ model as a test case, we show that analysis of the Fisher zeros of the canonical partition function can provide signatures of a transition in the Berezinskii–Kosterlitz–Thouless (BKT) universality class. Studying the internal border of zeros in the complex temperature plane, we found a scenario in complete agreement with theoretical expectations which allow one to uniquely classify a phase transition as in the BKT class of universality. We obtain T_{BKT} in excellent accordance with previous results. A careful analysis of the behavior of the zeros for both regions $\Re(T) \leq T_{BKT}$ and $\Re(T) > T_{BKT}$ in the thermodynamic limit shows that $\Im(T)$ goes to zero in the former case and is finite in the last one.

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1. Introduction

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The Berezinskii–Kosterlitz–Thouless (BKT) transition already has more than 40 years of history [1] and is still intriguing the scientific community. The nature of this transition is completely different from the common discontinuous (first order) or continuous (second order) phase transitions. Long range order does not exist and the two point correlation function has an algebraic decay at low temperature ($T \leq T_{BKT}$) and an exponential decay for $T > T_{BKT}$ [2]. Here T_{BKT} is known as the BKT temperature, and a model displaying a BKT transition has an entire line of critical points for $T \leq T_{BKT}$. In addition to that, the corresponding free energy, which is a C^{∞} function, is not analytical in this region. Besides these striking features, the correlation function has a characteristic universal exponent decay $\eta(T_{BKT}) = 1/4$ at the transition temperature. Its phenomenology relies on the belief that it is driven by a vortex–antivortex unbinding mechanism [3,4]. Another proposition that also describes the transition is based on a polymerization of domain walls [5]. Many systems, e.g., superfluid films, Coulomb gases and crystal surface roughening, undergo transitions that can be classified as belonging to this universality class [6]. More recently, Berker et al. [7] found that a BKT transition can occur in a scale free network.

Although the BKT transition is well known, the characterization of an unknown phase transition as being in the BKT universality class is not an easy task since there is no standard method to do so. The lack of a criterion capable of determining the nature of a transition beyond any reasonable doubt is a problem discussed by Bramwell and Holdsworth [8]. They pointed out that to be able to see the transition the system under investigation should be very large. They estimate that for "a system with atomic spacing of 3 Å the area should correspond to the size of a postage stamp". From the analytical point of view, the renormalization group approach is able to describe the main features associated with the transition. However, the approximations involved in the study of a given model may hinder the discovery of its real nature.

In this paper we present an algorithm for the systematic analysis of the Fisher zeros of the canonical partition function [9–11] for the 2D XY model (with spin symmetry $O(3)$) looking for possible signatures of the BKT transition. It was Fisher [11], in 1964, who proposed considering the partition function zeros in the *complex temperature plane* to study phase transitions. As known, the thermodynamic behavior of a given physical system is encoded by its partition function, Z, and all thermodynamic quantities can be obtained as derivatives of the free energy, $F = -k_B T \ln Z$. The basic assumption of the Fisher zeros approach to study phase transitions is that a system undergoes a phase transition at a given (real) temperature, T_c, if $Z(T_c) = 0$, reflecting the non-analyticity of F at T_c [12]. Since in a BKT transition there is an entire line of critical points for $T \leq T_{BKT}$, one should expect that a map of the Fisher zeros in the complex temperature plane exhibits an entire line of

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zeros in the real temperature axis for $T \leq T_{BKT}$, signaling the *BKT* behavior of the transition, while for $T > T_{BKT}$ the zeros should not touch the real positive axis, emphasizing the analytical behavior of thermodynamic functions at high temperatures. Of course, these considerations apply only to the thermodynamic limit. We warn the reader that the Fisher zeros studied here should not be confused with the Yang–Lee zeros [9,10] defined on the complex fugacity plane instead of the temperature plane [13–15]. In what follows we will analyze the Fisher zeros map for the *XY*-model.

2. Model and methods

Here we study a "fruit fly" model of the *BKT* transition [6], the classical two-dimensional *XY*-model on a square lattice, defined by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y). \qquad (1)$$

The sum runs over the nearest neighbors, J stands for the exchange coupling constant and S_i^α stands for the component $\alpha = (x, y, z)$ of the ith spin. The same Hamiltonian also defines the Planar-Rotator ($O(2)$) model [16,17], whose spins have only two components (one degree of freedom), and can also be viewed as an example belonging to the *BKT* universality class. In spite of the lack of long-range order for the model [2], there is a *non-zero magnetization* for any finite volume [18], resulting in a thermodynamic behavior very similar to that observed at continuous phase transitions. In fact, the behavior can be easily confused with a second order phase transition or something else [19–21]. Thus, distinguishing between continuous and *BKT* behavior in finite systems is difficult and may require system sizes beyond those feasible. Usually, the *BKT* temperature is estimated by using the Binder cumulant, the divergence of the magnetic susceptibility, the correlation functions or the more reliable helicity modulus [6,18], quantities that do not assure the model is in the *BKT* universality class.

In the Fisher zeros approach one starts with a discrete canonical partition function that can be written as $Z = \sum_E g(E) \exp(-\beta E)$, where $g(E)$ stands for the density of states (DOS). For a continuous system one may perform a discretization of the DOS [22]. This can be done by dividing the energy range into M bins of size ε. We can organize the energies inside the interval $[E_0, E_{M-1}]$ by counting the energy of the nth bin as $E_n = E_0 + n\varepsilon$. By defining a variable $x \equiv e^{-\beta\varepsilon}$, we get a discretized version,

$$Z_D = e^{-\beta E_0} \sum_{n=0}^{M-1} g_n x^n = e^{-\beta E_0} \prod_{j=1}^{M-1} (x - x_j), \qquad (2)$$

where $g_n = g(E_n)$, and x_j is the jth zero of the polynomial, usually called Fisher zero. Once g_n is obtained, any reliable zero finder can be used[1] to find the x_j's. As long as $g_n \in \mathbb{R}^+$, Z is an analytical function and has no real positive zeros for finite systems. The zeros show up as complex conjugate pairs. The analysis of Fisher zeros in finite systems is done by considering the special set of zeros $\{x^\star(L) = a(L) + ib(L)\} \in x_j(L)$, where L is the linear size of the system, called first or leading zeros. They have the following properties: $b(L) \to 0$ as $L \to \infty$ while $\lim_{L\to\infty} a(L) = a(\infty)$, a constant value. The leading zeros are very stable against statistical fluctuations, in contrast to non-leading zeros, and are, in general, featured in the map (see, for example, Ref. [23]). They are related to the transition temperature of the system in the thermodynamic limit as $1/k_B T_c = -\ln(a(\infty))/\varepsilon$ [23] and their impact angle
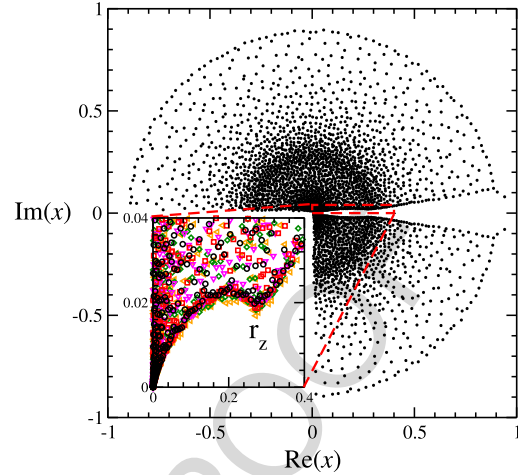

Fig. 1. Fisher zeros map on the $x = e^{-\beta\varepsilon}$ plane for the 2D classical *XY*-model in a 50×50 lattice. The inset shows a zoom on the inner region for five distinct simulations, represented by different symbols. The cusp, r_z, is indicated.

on the real positive axis is directly related to the order of the phase transition [24]. Recent results also suggest that the pattern of zeros as a whole can be used to characterize the order of the transition [25]. In a paper of 1983 Itzykson et al. [26] analyzing the zeros distribution for small lattices, found that some properties of the Ising and gauge models seem to exhibit a universal behavior close to complex singularities. However, it is not clear how to extend their arguments to the *BKT* transition.

In order to obtain the DOS of the *XY*-model we used the Replica Exchange Wang–Landau (REWL) method [27–30], a parallel version of Wang–Landau (WL) sampling [31–33], capable of sampling the entire configuration space efficiently in a single simulation. In this scheme the energy range is split into smaller overlapping windows. We considered $e_0 = -1.9J$, $e_{M-1} = 0$, and an overlap of 75%, where $e = E/L^2$ stands for the energy per spin. Several different random walkers are allowed to run in each of these windows following the original WL scheme.[2] We use regular square lattices with sizes ranging from $L = 10$ up to 200. In this work we chose $J = 1$, $S = 1$, $k_B = 1$, and the lattice parameter $a = 1$.

3. Results and discussion

In Fig. 1 we show a typical zeros map of the imaginary and real parts of all x_j's, for a 50×50 lattice. In a continuous phase transition a single leading zero is expected. However, we cannot identify a single point featured in comparison to others. The inset shows in different symbols the zeros for five different simulations for $L = 50$, in order to analyze statistical fluctuations. A leading zero cannot be identified in this picture. Instead, a cusp at r_z is evident and the border line is quite stable against fluctuations.

The size dependence of the internal border of the map pattern as a function of the lattice size is shown in Fig. 2. One should expect the internal border to coalesce into the real axis for $\Re\mathfrak{e}(x) \leq r_z$ and $L \to \infty$, in accordance with the existence of an entire line of critical points at low temperatures. The line for $\Re\mathfrak{e}(x) > r_z$ on the other hand should not touch the real axis. The cusp r_z should, then, give T_{BKT}.

In order to systematically investigate the finite size effects and confirm the above expectations, we opted to work in the complex

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[1] In this work we decided to use: E.W. Weisstein, "Polynomial roots", in MathWorld—A Wolfram Web Resource. http://mathworld.wolfram.com/PolynomialRoots.html.

[2] The considered flatness criteria is $p = 0.7$, the final $\ln f$ value is 10^{-9}, and the acceptance ratio is 60%.
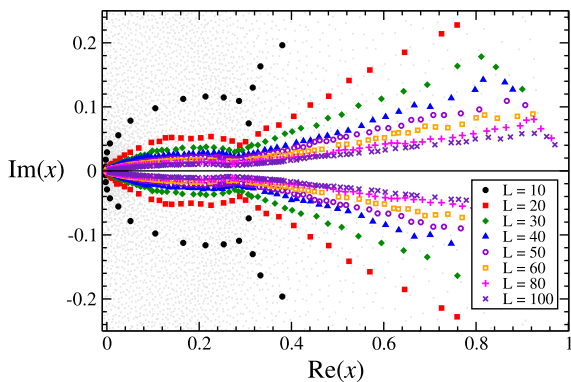
Fig. 2. Zoom on the real positive semi-axis of the zeros maps in the x plane for $L = 10 \to 100$. The zeros on the internal border are highlighted.
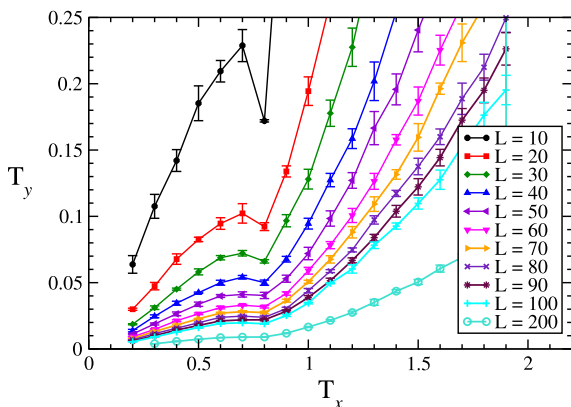

Fig. 3. Internal border of zeros obtained by using the binning process for $L = 10 \to 200$. Here $\Delta T_x = 0.1$ and the error bars represent statistical fluctuations.
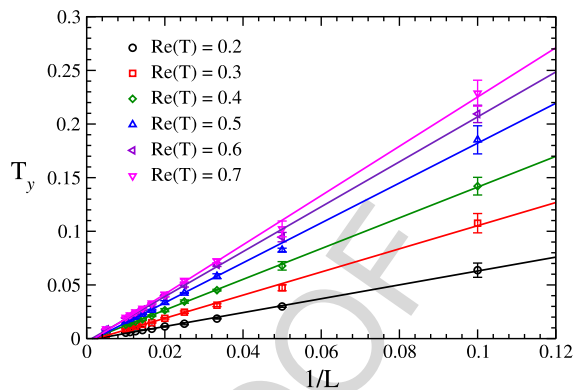

Fig. 4. Finite size scaling analysis of the imaginary part of the internal border according to the *ansatz* $T_y \sim L^{-1}$. The lines represent a linear regression of the data, showing good agreement with the *ansatz* and the convergence to zero or small negative values for $L \to \infty$. We use $\Delta T_x = 0.1$.

temperature (T) plane instead of the complex $x = e^{-\varepsilon/k_B T}$ plane. ¹
This choice is justified by the fact that finite size scaling in terms ²
of the temperature is known [15] and that by doing so our results ³
are almost independent on the chosen bin size, ε. This last point ⁴
is especially important when dealing with bigger lattices. In this ⁵
work we used $\varepsilon = 1$ for $L \leq 100$ and $\varepsilon = 3$ for $L = 200$; we ⁶
noted that small modifications in the bin size did not change our ⁷
results. To determine the limits of the internal border we divided ⁸
the real temperature axis into small bins of size ΔT_x centered at ⁹
$T_x = \mathfrak{Re}(T)$. The border line was identified by looking inside a ¹⁰
given bin for the smallest value of $T_y = \mathfrak{Im}(T)$ that appears. At ¹¹
least five different simulations were used for each lattice size. The ¹²
resulting curves are presented in Fig. 3. Fig. 4 shows T_y as a function ¹³
of L^{-1} for some typical $T_x \leq T_{BKT}$ values. The solid lines are linear ¹⁴
regressions showing that $T_y \to 0$ for $L \to \infty$, i.e., the internal ¹⁵
border coalesces with the real positive axis in the thermodynamic ¹⁶
limit. Other scaling functions and exponents were also tested (not ¹⁷
shown here), but they do not describe our data as well as this ¹⁸
ansatz. ¹⁹

To estimate the critical temperature we used the location of the ²⁰
cusp position, $T_z(L)$. Since the scaling function for the "pseudocrit- ²¹
ical" temperature is given by [15] $T_{BKT}(L) \sim [\ln(L)]^{-2}$ we plotted ²²
$T_z(L)$ as a function of $[\ln(L)]^{-2}$ in the Fig. 6. A linear regression, dis- ²³
carding the point corresponding to $L = 10$, gives $T_{BKT} = 0.709(2)$, ²⁴
and discarding the points for $L < 40$ gives $T_{BKT} = 0.704(3)$, ²⁵
which agrees very well with previous results [34,18], 0.700(5) and ²⁶
0.700(1) respectively. More precise results could be obtained by ²⁷
increasing the number of zeros in the map by reducing ε, increas- ²⁸
ing the precision in the location of the cusp. However, the zeros ²⁹
finder task may become a problem for such a high degree polyno- ³⁰
mial ($>3 \times 10^4$). In any case, conventional methods to locate the ³¹

BKT may be used together with this one to get even more precise ³²
results for T_{BKT}. ³³

From Figs. 2 and 3 one can see that the curves diverge from ³⁴
the positive real axis, in accordance with the expectation that for ³⁵
$T > T_{BKT}$ the imaginary part of the zeros should remain finite. ³⁶
Moreover, since the free energy *has to be* an analytic function at ³⁷
high temperatures, *there can be no real positive zero of the partition* ³⁸
function at high temperatures. ³⁹

To analyze the behavior of T_y in the non-critical region we have ⁴⁰
to be careful. First we have to consider the following. An analysis ⁴¹
based on finite size scaling, as we did in the critical region, is ⁴²
meaningless since the basic assumption of any *FSS* is that the free ⁴³
energy behaves as a homogeneous function. Following Itzykson we ⁴⁴
identify three regions. (1) The region far from T_{BKT} where $L \gg \xi \approx$ ⁴⁵
1, where finite size lattice effects are not relevant. Here ξ is the ⁴⁶
correlation length which for the *XY* model diverges exponentially ⁴⁷
when T_{BKT} is approached from above, remaining infinite in the ⁴⁸
critical region. (2) The region $T \gtrsim T_{BKT}$ where $L \gg \xi \gg 1$. ⁴⁹
The finite lattice exhibits the same scaling behavior as the infinite ⁵⁰
system. And, (3) the region where $L \approx \xi \gg 1$ for which are ⁵¹
observed severe finite size effects. Regions (2) and (3) are scaling ⁵²
regions. With that in mind we content ourselves with an analysis ⁵³
in a region far enough from T_{BKT} where we may expect that the ⁵⁴
border of the zeros map should converge fast to its asymptotic ⁵⁵
limit. For $T > T_{BKT}$ the free energy is an analytical function of ⁵⁶
T so that it can be approximated by a polynomial in T with the ⁵⁷
coefficients depending on the lattice size in powers of $1/L$. Farthest ⁵⁸
we are from T_{BKT} faster will decay the higher coefficients of the ⁵⁹
polynomial, so that, it is reasonable to suppose that in this region T_y ⁶⁰
has a power law $T_y(\infty) + AL^{-\omega}$ behavior. Asymptotic convergence ⁶¹
is assured by the Brouwer fixed point theorem [35]. Reasoning in ⁶²
this way we can plot T_y for the largest lattices of our simulations ⁶³
as a function of $L^{-\omega}$. By varying ω we can find the best value that ⁶⁴
adjusts a linear function to our data. This procedure is shown in ⁶⁵
Fig. 5. It is noteworthy the different "scaling" behavior of $\mathfrak{Im}(T)$ in ⁶⁶
both regions, $T < T_{BKT}$ and $T > T_{BKT}$. As should be expected the ⁶⁷
exponent ω is not universal, depending on T. ⁶⁸

4. Conclusion ⁶⁹

In summary, we show that a method of investigating the ⁷⁰
Fisher zeros of the partition function can identify whether or not ⁷¹
the model exhibits a Berezinskii–Kosterlitz–Thouless (BKT) phase ⁷²
transition. By studying the 2D *XY*-model we found a qualitative ⁷³
picture that is completely consistent with expectations for the *BKT* ⁷⁴
transition, i.e., the zeros map is consistent with the existence of an ⁷⁵
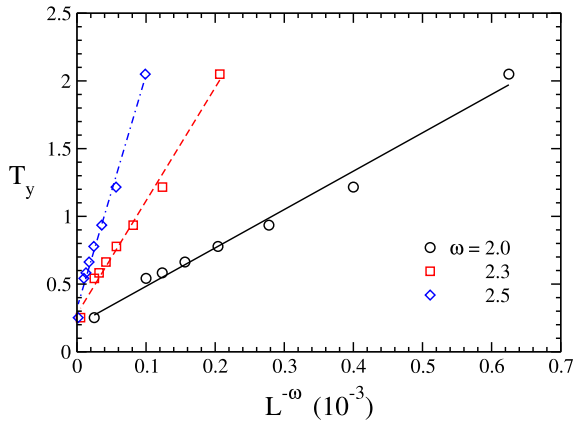entire line of zeros in the real positive axis in the thermodynamic ⁷⁶

Fig. 5. Typical $T_y \times L^{-\omega}$ behavior. Here $T_x = 3.0 > T_{BKT}$. Linear fit gives support to a power law behavior with exponent $\omega \approx 2.4$.
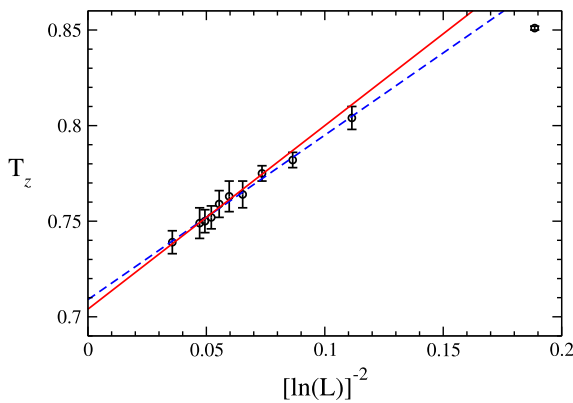

Fig. 6. Finite size scaling of the cusp position, $T_z(L)$, according to the prediction for the *BKT* "pseudocritical" temperature $T_{BKT}(L) \sim [\ln(L)]^{-2}$. Discarding the point corresponding to $L = 10$ the *BKT* temperature is estimated by a linear regression as 0.709(2) (dashed blue line) and discarding $L < 40$, $T_{BKT} = 0.704(3)$ (solid red line).

limit, with different behaviors for points below and above the transition temperature that could be used to signalize the *BKT* transition. Moreover, the *BKT* transition temperature was successfully obtained by considering the location of the cusp that splits regions with different behaviors giving $T_{BKT} = 0.704(3)$, in excellent accordance with previous results [18,34]. Our quantitative analysis shows that for temperatures above T_{BKT} the imaginary part of the zeros converges to finite values. This behavior is in accordance with the fact that the free energy *must be* an analytical function over the real axis at high temperatures, which prevents the existence of any real positive zero at high T.

Acknowledgments

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