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The zeros of the Energy Probability Distribution - A new way to study phase transitions -

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Abstract. We describe an iterative method to study the critical behavior of a system based on the partial knowledge of the complex Fisher zeros set of the partition function. The method is general with advantages over most conventional techniques since it does not need to identify any order parameter a priori. The critical temperature and exponents can be obtained with great precision. To test the method and to show how it works we applied it to the $2D$ Ising and $6 - states$ Potts models. The strategy can easily be adapted to any model, classical or quantum, once we can build the corresponding energy probability distribution.

1. Introduction

In this communication, we present a new, general and efficient method based on the partial knowledge of the energy probability distribution (*EPD*) conjugated with an analogue of the Fisher zeros expansion of the partition function that allow us to precisely determine the transition temperature and exponents for a given system. In order to present the method we first introduce shortly the Fisher's zeros approach. Next we describe how it can be combined with the *EPD* to obtain the critical behavior of a given system. To demonstrate the robustness of the method and its reliability our calculations are compared with the exact results for the $2D$ Ising model and the exactly known critical temperature for the $2D$ $6 - states$ Potts model.

2. Fisher Zeros

Fisher has shown how the partition function can be written as a polynomial in terms of the variable $x = e^{-\beta\epsilon}$, where $\beta = 1/k_B T$ is the inverse of the temperature, T , k_B is the Boltzmann



constat, and ϵ is the energy difference between two consecutive energy states [1, 2, 3]. For a finite system, all roots of the polynomial lie in the complex plane. The coefficients of the polynomial are real implying that their roots appear in conjugate pairs. If the system under consideration undergoes a phase transition at a temperature T_c , the corresponding zero, x_c , must be real in the thermodynamic limit. To make those statements clearer we recall that the partition function is given by

$$Z = \sum_{\mathbf{E}} g(\mathbf{E}) e^{-\beta \mathbf{E}} = e^{-\beta \epsilon_0} \sum_{n=1}^N g_n e^{-\beta n \epsilon}, \quad (1)$$

where it is assumed that the energy, \mathbf{E} , can be written as a discrete set $\{\mathbf{E}_n = n\epsilon\}; n = 0, 1, 2, \dots$ and ϵ_0 is some constant energy threshold.

As pointed above, if the system undergoes a phase transition at T_c the corresponding zero $x_t(L)$ moves toward the positive real axis as the system size grows. From now on this zero will be named dominant or the leading zero. In Fig. 1 it is shown a partial view of the distribution of zeros for the 2D Ising model in a square lattice of size $L = 32$. The dominant zero is identified in the figure. We observe that surprisingly the zeros do not appear in conjugated pairs as expected.

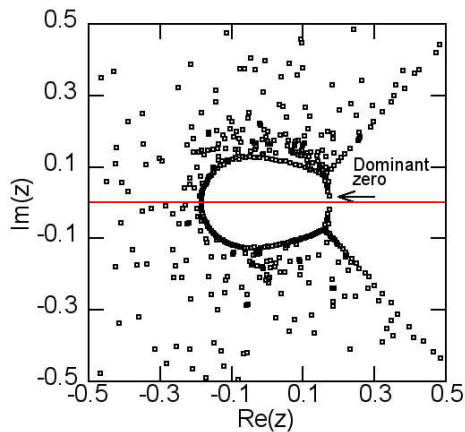


Figure 1. Partial view of the Fisher zeros distribution for the two dimensional Ising model for a 32×32 square lattice. We used the Mathematica's R solve package to get the zeros. Surprisingly, the expected conjugate pairs of zeros were not found. A discussion is found in the text. The arrow marks the dominant zero.

A closer analysis of Z shows that the polynomial coefficients span over many orders of magnitude. For instance, for a lattice size 96×96 in the 2D Ising model one has 9217 possible energy values with the smallest and largest polynomial coefficient being $g(-18432) = 2$ and $g(0) = 2.304 \times 10^{2772}$ respectively. The large ratio between the coefficients turns the zeros finding into a formidable task even for known good algorithms. It should be interesting if we could focus our attention only onto the region where the dominant zero is located. This, in fact, can be done in a systematic way.

3. Energy Probability Distribution Zeros

If we multiply Eq. 1 by $1 = e^{-\beta_0 \mathbf{E}} e^{\beta_0 \mathbf{E}}$ it is rewritten as

$$Z_{\beta_0} = \sum_{\mathbf{E}} h_{\beta_0}(\mathbf{E}) e^{-\mathbf{E} \Delta \beta}, \quad (2)$$

where $h_{\beta_0}(\mathbf{E}) = g(\mathbf{E}) e^{-\beta_0 \mathbf{E}}$ and $\Delta \beta = \beta - \beta_0$. Defining the variable $x = e^{-\epsilon \Delta \beta}$ we obtain

$$Z_{\beta_0} = e^{-\epsilon_0 \Delta \beta} \sum_n h_{\beta_0}(n) x^n, \quad (3)$$

where $h_{\beta_0}(n) = h_{\beta_0}(\mathbf{E}_n)$ is nothing but the non-normalized canonical energy probability distribution (*EPD*), hereafter referred to as the energy histogram at temperature β_0 . There is a one to one correspondence between the Fisher zeros and the *EPD* zeros since they are related through a trivial conformal transformation. Constructing the histogram at the transition temperature, i.e., $\beta_0 = \beta_c$, the dominant zero will be at $x_c = 1$, i.e., $Z = 0$ at the critical temperature ($\Delta\beta = 0$) in the thermodynamic limit. For finite systems, however, a small imaginary part of x_c is expected. Indeed, we may expect that the dominant zero is the one with the smallest imaginary part on the real positive region regardless β_0 . Once we locate the dominant zero its distance to the point $(1, 0)$ gives $\Delta\beta$ and an estimate for β_c .

For temperatures close enough to β_c only states with non-vanishing probability to occur are pertinent to the phase transition. Thus, for $\beta_0 \approx \beta_c$ we can judiciously discard *small* values of h_{β_0} . Therefore, the zeros finder does not have to deal with high degree polynomials with coefficients spanning over prohibitive many orders of magnitude. Moreover, one may speculate that the dominant zero acts as an accumulation point such that even far from β_c fair estimates can be obtained.

With this in mind we can develop a clear criterion to filter the important region in the energy space where the most relevant zeros are located. The idea follows closely the well known *Regula Falsi* method for solving an equation in one unknown. The reasoning is as follows: We first build a normalized histogram $h_{\beta_0^0}$ ($\text{Max}(h_{\beta_0^0}) = 1$) at an initial (False) guess β_0^0 . Afterward, we construct the polynomial, Eq. 3, finding the corresponding zeros. By selecting the dominant zero, x_c^0 , we can estimate the pseudo critical temperature, β_c^0 . Regarding that $\beta_c(L)$ is the true pseudo-critical temperature for the system of size L , if the initial guess β_0^0 is far from $\beta_c(L)$ the estimative β_c^0 will not be satisfactory. Nevertheless, we can proceed iteratively making $\beta_0^1 = \beta_c^0$, building a new histogram at this temperature and starting over. After a *reasonable* number of iterations we may expect that β_c^j converges to the true $\beta_c(L)$ and thus x_c^j approaches the point $(1, 0)$. This corresponds to apply a sequence of transformations, \mathfrak{T} , such that $\beta^{n+1} = \mathfrak{T}\beta^n$. The transition temperature corresponds to the fixed point $\beta_c = \mathfrak{T}\beta_c$. The property $x_c^j \rightarrow (1, 0)$ can be used as a consistency check in this iterative process. An algorithm following those ideas is:

- (i) Build a single histogram $h_{\beta_0^j}$ at β_0^j .
- (ii) Find the zeros of the polynomial with coefficients given by $h_{\beta_0^j}$.
- (iii) Find the dominant zero, x_c^j .
 - a) If x_c^j is close enough to the point $(1, 0)$, stop.
 - b) Else, make $\beta_0^{j+1} = -\frac{\ln(\Re\{x_c^j\})}{\varepsilon} + \beta_0^j$ and go back to 1.

In all our numerical results we observed that the choice of the starting temperature as irrelevant. To build the single histogram we follow the recipe given by Ferrenberg and Swendsen [4, 5]. To specify the energy subspace, the procedure is straightforward dealing with continuous transitions. In a first order transition the probability distribution is bi-modal. The energy distribution between the two peaks may reach low values, even lower than our cutoff criteria. In this case the procedure to define the relevant energy interval is subtler. A general way for dealing with this is to cut the low and high energy tails of the probability density preserving the important intermediate region.

4. Testing the algorithm

4.1. 2D Ising Model

The convergency and accuracy of the method can be tested by using the well-known Ising model

Table 1. Estimate of the pseudo critical temperature for the ferromagnetic $2d$ Ising Model. The last line is the exact value up to five figures.

L	β	T	$ x $	$\Im m(x)$
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
estimate	0.4404	2.2707	-	-
∞	0.4407	2.2691	-	-

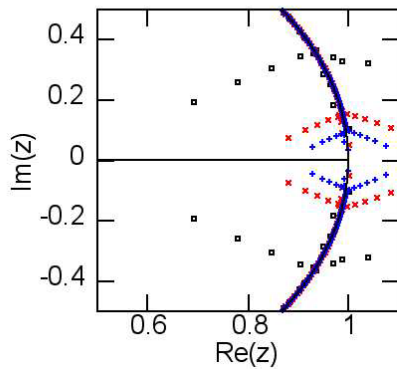


Figure 2. Plot section of the zeros distribution for the Ising model. Lattices sizes are $L = 32, 64, 96$ (\square, \times and $+$ respectively.). The solid black line marks the perimeter of the unit circle and the real axis.

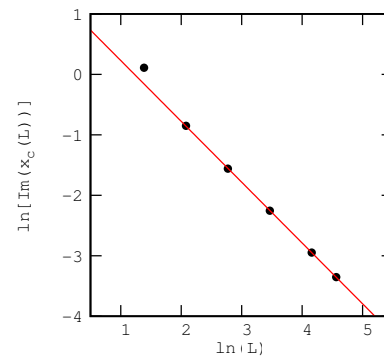


Figure 3. Log-log plot of $\Im m(x_c(L))$ versus L for the Ising model. According to finite size scaling theory we expect the slope to be $\frac{1}{\nu} = 1$. From our data we obtained $\frac{1}{\nu} = 1.006(3)$.

[6] in a square lattice defined by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad (4)$$

where J is a ferromagnetic coupling constant, $\langle i, j \rangle$ means that the summation runs over nearest neighbors on a regular lattice and $\sigma_i = \pm 1$ is the spin variable at site i . The model has a continuous phase transition at $T_c = \frac{2}{\ln(1+\sqrt{2})} \frac{J}{k_B} \approx 2.269 \frac{J}{k_B}$ and was exactly solved in 1944 [6], being thus one of the preferred model for testing new methods on phase transitions. In Tab. 1 we show the results of the application of our method to the Ising model for several lattice sizes ($4 \leq L \leq 96$). The results were obtained by using the exact density of states calculated using the Mathematica[®] software with the code developed in Ref. [7]. The interval of energy used was $[E_{min}, E_{max}]$ chosen in such way that for the normalized $h_\beta(n)$, both $h_\beta(E_{min})$ and $h_\beta(E_{max})$ are of order of 10^{-2} . The zeros of the polynomial were calculated using the Mathematica[®] function *Solve*. In the last two lines of Tab. 1 we show the critical temperature result obtained from finite size scaling and the exact value up to 5 figures. The error is smaller than 0.5%. The zeros distribution is shown in Fig. 2. The critical exponent ν can straightaway be obtained. Finite size scaling theory predicts that $T_c(L) \sim T_c + aL^{-1/\nu}$ [8] and thus, we might expect that $x_c(L) \sim x_c + bL^{-1/\nu}$. Once $\Re\{x_c(L)\} \approx 1$, $\forall L$, the imaginary part of $x_c(L)$ should also scale as $L^{-1/\nu}$. In Fig. 3 a log-log plot of $\Im m(x_c(L))$ versus L is shown for $L = 4, 8, 16, 32, 64, 96$. Discarding the smaller lattice size we obtain $1/\nu = 1.006(3)$, very close to the exact value, 1. Of course, better results for T_c and ν are obtained by diminishing the energy threshold and using larger lattice sizes.

4.2. 2D 6 – states Potts model

The q states Potts Model [9] is defined by the Hamiltonian,

$$H = -J \sum_{\langle i, j \rangle} \delta_{\sigma_i, \sigma_j}, \quad (5)$$

where J is a ferromagnetic coupling constant, $\langle i, j \rangle$ stands for nearest neighbors, $\delta_{\alpha, \beta}$ is the Kronecker delta ($\delta_{\alpha\beta} = 1$ if $\alpha = \beta$, 0 otherwise) and $\sigma_i = 1, 2, \dots, q$ is a spin like variable. The $q = 6$ states Potts model is known to have a first order transition at $T_c = \frac{1}{\ln(1+\sqrt{q})} = 0.80761\dots$. As in the Ising case our method applies straightforwardly. Table 2 shows in detail our results. The finite size scaling in this case has shown to be more subtle. For this weak first order

Table 2. Monte Carlo parameters (N_{term} , N_{MCS} and T_{sim}) and results ($\Im m(x_c(L))$ and $T_c(L)$) for the 6 states Potts model. N_{term} is the number of Monte Carlo steps used to equilibrate the system, N_{MCS} stands for the number of measurements to build the histogram and T_{sim} corresponds to each temperature in the iterative process.

L	N_{term}	N_{MCS}	T_{sim}	$\Im m(x_c(L))$	$T_c(L)$
20	10^5	5×10^6	0.8100	0.2118(7)	0.814(2)
40	10^5	5×10^6	0.8100	0.669(3)	0.8098(8)
60	3×10^5	5×10^6	0.810		
	3×10^5	5×10^6	0.809		
	3×10^5	5×10^6	0.808	0.3387(8)	0.80880(5)
80	3×10^5	5×10^6	0.810		
	3×10^5	5×10^6	0.809		
	3×10^5	5×10^6	0.808	0.208(3)	0.8085(5)
120	3×10^5	5×10^6	0.810		
	3×10^5	5×10^6	0.809		
	3×10^5	5×10^6	0.808		
	3×10^5	5×10^6	0.807	0.109(3)	0.808(1)

transition the scaling functions need to be considered in more detail [8]. In Figs. 4 and 5 are shown both the imaginary part of $x_c(L)$ and the pseudo-critical temperature as a function of L^{-d} . A linear adjust does not work in this case, anticipating that a correction is missing in the scaling function. Following Lee and Kostelitz [10] we introduce a L^{-2d} scaling correction which fits quite well our results as seen in figs. 4 and 5. The critical temperature encountered (0.80797(7)) agrees up to 5 figures with the exact value (0.80761).

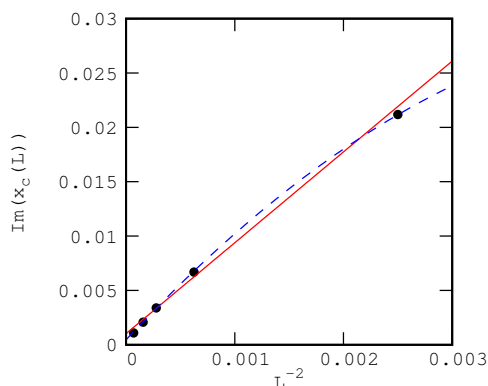


Figure 4. $\Im m(x_c(L))$ versus L^{-2} for the 6 states Potts model. The solid red line is a linear adjust. The dashed blue line is a quadratic fit corresponding to scaling corrections.

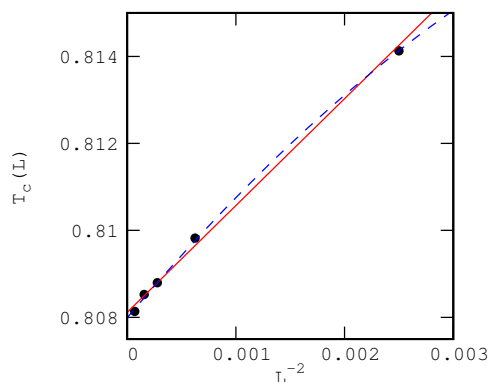


Figure 5. $T_c(L)$ versus L^{-2} for the 6 states Potts model. Solid line is a linear fit. When the quadratic scaling correction is introduced (dashed blue line) the data are very well adjusted. From the adjust we get 0.80797(7) while the exact value is 0.80761.

5. Closing Remarks

In summary, we introduced a novel method to study phase transitions based on the zeros of the energy probability distribution. The method has shown to be fully applicable to the models studied allowing accurate determination of the critical temperatures and the exponent ν as demonstrated by our results in the Ising and Potts models. More general applications are found in the reference by Costa et al [11]. The only criterion we have used was the fact that at the transition temperature the partition function zero goes to the real positive axis in the thermodynamic limit. No *a priori* knowledge of an order parameter is necessary. The method is iterative, so that, the transition temperature can be approached at will. Besides that, the knowledge of the complete density of states is not required since we work in a restricted range of energy. The advantage is that the polynomial representing the partition function has fewer roots with its coefficients ranging in a civilized, narrow region.

Acknowledgments

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