The impact of fluctuations on the zeros of the energy probability distribution

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Abstract. In this communication we explore the possible effects of statistical fluctuations on the use of the Energy Probability Distribution (EPD) zeros to study phase transitions. In the EPD zeros technique one has to find the roots of a polynomial whose coefficients are given by the EPD - a histogram of energy values obtained in a Monte Carlo simulation, for example. Phase transitions are signaled by the presence of a zero that approaches the point (1,0) in the complex plane. Once the EPD estimations are usually subject to statistical fluctuations and polynomial roots are known to be sensitive to modifications in its coefficients, we have compared the roots of a given polynomial with the roots of a perturbed one, searching for possible impacts on the method. Our results show that although the overall map of zeros is modified, the location of the dominant zero, the one that indicates the presence of a phase transition, is not affected. Indeed, even for 30\% perturbation only small modifications in the dominant zero location is observed.

1. Introduction

Phase transitions always attracted the interest of researchers of the most diverse areas since they have applications in many different fields such as engineering, medicine, economy and even agriculture. In great part this is due to the sudden changes that the system’s properties face in a phase transition. Perhaps, the most famous examples, besides trivial solid-liquid-gas transitions, are the existence of superfluid\(^1\) and superconducting\(^2\) transitions that lead to physical states that may be widely used in industrial applications. In addition, magnetic transitions\(^3\) also play a very important role once magnetic materials have widespread use in the most diverse technological applications.

Despite their possible technological applications, the theoretical characterization and understanding of phase transitions is not an easy task. A good example is the Hubbard model\(^4\), which is believed to capture the physics behind high \(T_c\) superconductors\(^5\)\(^6\), but yet has not a fully known phase diagram\(^5\)\(^6\). The most common approach to find transition points rely in the previous knowledge of an order parameter - a quantity that assumes different values in each phase. Examples of known order parameters include the magnetization of the Ising model\(^7\) or a complex wave function in type I superconductors\(^8\). However, the proper identification of an order parameter may be controversial in complex systems and in the absence of a standard way to define it for different systems, methods based on it may give results that are sensitive to different choices.
However, there is a method capable to identify a phase transition that is not based on the definition of an order parameter. This method, introduced by Yang and Lee [9] in the grand-canonical ensemble is based on writing the grand-canonical partition function as a polynomial and using its complex roots (zeros) to study a phase transition. These zeros are called the Yang-Lee zeros and, as the grand-canonical partition function, encodes all thermodynamical informations about the system. This method, together with its canonical counterpart introduced by Fisher [10], has been applied to the most diverse systems such as polymers [11, 12], magnetic systems [13–16], out-of-equilibrium systems [17–19], and has been even experimentally measured [20]. Nevertheless, despite allowing the identification of phase transitions without the use of an order parameter, these methods rely in the full knowledge of the partition function, a hard to obtain quantity.

The Fisher zeros [10] in special have a complicated analytical treatment once exact solutions for the density of states are rare. Even with the help of numerical methods such as the Wang-Landau algorithm [21, 22], which is capable to estimate the density of states in the whole energy range with good precision, we face the problem of numerically solve a very high degree polynomial. In order to better understand this problem, consider for instance the Ising model on a square lattice of lateral size \( L = 150 \). In this system we have a polynomial of degree 22500 whose coefficients range from 2 to \( 10^{6744} \). In this condition one may expect severe numerical issues that may put on suspicion the results.

Recently our group proposed a method [23] capable to alleviate some of these numerical issues related to the Fisher zeros approach. With this method, the Energy Probability Distribution (EPD) zeros, one does not need to define an order parameter as in the Fisher zeros approach and can drastically reduce the polynomial degree (\( \sim 90\% \)) and the range of coefficients (to about 4 orders of magnitude) and yet obtain very precise results [23]. The “magic” here is that instead of using as coefficients of the polynomial the density of states, as is the case in the Fisher zeros approach, one considers the EPD at a given temperature as coefficients, allowing the reduction of the energy range by discarding states with very low probabilities to occur at the considered temperature. In addition, the method is iterative, allowing approaching the transition temperature at will.

In this communication we investigate the impact on the EPD zeros of fluctuations on its coefficients and how the presence of fluctuations may impair the phase transition location. The main motivation for that is that usually the EPD (coefficients of the polynomial to be solved) is obtained by means of Monte Carlo simulations that are subject to thermal fluctuations in its estimates. Also, some polynomials are known to be highly sensitive to modifications in its coefficients. Indeed, as shown by Wilkinson in 1963 [24], a very small change in one coefficient of a polynomial of degree 20 whose original roots were integer numbers from 1 to 20, was capable to induce the appearance of complex roots and change the values of other roots. Thus, if a small modification in a “small” polynomial has this undesired impact, what should we expect for the impact of the statistical or numerical fluctuations of the coefficients of very high degree polynomials such as those used in the EPD zeros? That is what we want to address in this communication.

2. Energy Probability Distribution Zeros

In this section we briefly review the EPD method. More details can be found in Refs. [23, 25–27]. The basic idea behind the Fisher zeros approach is to write the partition function, considering a discrete set of energies \( E_n = E_0 + n\epsilon \) with integer \( n \), as a polynomial:

\[
Z = \sum_E g(E)e^{-\beta E} = e^{-\beta E_0} \sum_n g_n z^n, \tag{1}
\]
where \( z \equiv e^{-\beta \epsilon} \) and \( g_n = g(E_n) \). As already mentioned, by considering the analytic continuation of the temperature, the complex roots of this polynomial contains all thermodynamical informations about the considered system. In special, if the system has a phase transition, we expect to observe a zero (or a set of zeros) touching the positive real axis in the thermodynamic limit as a consequence of the non analyticity of the free energy at a phase transition. Thus, by finding those zeros phase transitions can be studied. The zeros that touch the real axis in the thermodynamic limit are called dominant or leading zeros, and they are expected to be close enough to the real positive axis for finite systems. The main caveat in this approach is the huge degree of the polynomial, i.e., the number of allowed energy states, and the astonishing range of coefficients, i.e., the values of \( g_n \), that spam over many orders of magnitude and impact numerical methods to find the polynomial roots (see the discussion in the introduction).

The EPD method is recovered by multiplying equation (1) by \( 1 = e^{-\beta_0 E_n} e^{+\beta E_n} \) such that the partition function can be written as:

\[
Z_{\beta_0} = e^{-\Delta \beta_0 E_0} \sum_n h_{\beta_0}^n (e^{-\Delta \beta \epsilon})^n = e^{-\Delta \beta_0 E_0} \sum_n h_{\beta_0}^n x^n, \tag{2}
\]

where \( \Delta \beta = \beta - \beta_0 \), \( x \equiv e^{-\Delta \beta \epsilon} \) and \( h_{\beta_0}^n \equiv g_n e^{-\beta_0 E_n} \) is the unnormalized Energy Probability Distribution (histogram) at the inverse temperature \( \beta_0 \). Note that up to this point no approximation was done. However, we may discard states with very low probability to occur at a given (inverse) temperature \( \beta_0 \) without appreciable impact on thermodynamic averages at \( \beta_0 \). Indeed, even for temperatures close enough to \( \beta_0 \) we may expect that thermodynamic quantities would not be too much affected by discarding states with very low probability to occur. As may already be evident, the cern of the method relies on the reduction of the original polynomial degree and range of coefficients by discarding states with very low probability to occur at \( \beta_0 \). Then, one may choose to normalize the histogram at \( \beta_0 \) such that its maximum value is 1. Thus, an appropriate (smaller) energy range is chosen by look for entries with histogram values larger than a given threshold, \( 10^{-6} \), for example\(^1\). In this way, the polynomial degree, i.e., the number of energy entries is drastically reduced as well as the range of polynomial coefficients, which in this example would be only 6 orders of magnitude. Of course, estimates obtained by this approach would be restricted to the vicinity of \( \beta_0 \).

Following the arguments presented in Refs 23–27, when \( \beta_0 = \beta_c \), where \( \beta_c \) is a transition temperature, the dominant zero would be in the point \((1, 0)\) in the thermodynamic limit. For finite systems we may expect that if \( \beta_0 \) is close enough to \( \beta_c \), the zero closest to the point \((1, 0)\) would be the dominant zero. Thus, an algorithm that allows approaching the transition temperature at will is given by:

(i) Build a single histogram \( h_n^{\beta_0} \) at \( \beta_0 \).

(ii) Find the zeros of the polynomial with coefficients given by \( h_n^{\beta_0} \).

(iii) Find the dominant zero, i.e., the zero closest to the point \((1, 0)\), \( x_t^{\beta_0} \).
   a) If \( x_t^{\beta_0} \) is close enough to the point \((1, 0)\), stop.
   b) Else, make \( \beta_0^{\beta_0+1} = -\frac{\ln(Re\{x_t^{\beta_0}\})}{\epsilon} + \beta_0 \) and go back to (i).

3. Methods and Results

When using the EPD zeros method one needs an estimate of the EPD (histogram) at a given temperature. The usual approach to obtain that is to run a conventional Monte Carlo

\(^1\) One should have special care in the vicinity of first order transitions where the valley between the peaks in the probability distribution should not be discarded, see Refs. 23–27 for more details.
(MC) simulation of the considered system using, for example, the Metropolis algorithm [28]. Nevertheless, all MC estimates, including the histogram, are subject to statistical fluctuations. Then, what is the impact of such fluctuations on the roots of the polynomial? In special, is the location of the dominant zero modified by such fluctuations? To address these questions we considered random fluctuations on the coefficients of a given polynomial in order to quantify its impact. This was accomplished by calculating:

$$\left( h_{\beta_0}^\beta \right)^* = h_{\beta_0}^\beta + \varepsilon a h_{\beta_0}^\beta,$$

where $$\left( h_{\beta_0}^\beta \right)^*$$ is the perturbed histogram, $$h_{\beta_0}^\beta$$ the original histogram and $$\varepsilon \in (-1, 1]$$ is a uniform random variable and $$a$$ the percentage of the perturbation.

We have considered as a benchmark the 2D Ising model in a square lattice of lateral size $$L = 150$$. Metropolis simulations [28] were performed at three different temperatures (in units of $$J/k_B$$) $$T = 2.26, T = 2.28$$ and the estimated critical temperature $$T = T_c = 2.275805$$. 100$$L^2$$ Monte Carlo steps (MCS) were used for thermalization and 10$$^8$$ MCS were used to build the histograms at each temperature. When applying the algorithm to approach the critical temperature histogram reweighting [29] was used. The roots for the original polynomial and perturbed ones were obtained by using the LAPACK [30] package.

![Figure 1](image_url)

**Figure 1.** Map of zeros for three different Monte Carlo simulations at the same temperature $$T = T_c$$. As can be seen, although the location of most zeros does not coincide, the position of the dominant and nearby zeros is almost the same for the three samples.

As a first attempt to quantify the impacts of statistical fluctuations on the location of the zeros we show in Fig. 1 the map of zeros in the complex plane for three different simulations (with different random number sequences) at $$T = T_c$$. As can be seen, the location of the zeros varies a lot while the three zeros that are closest to the point $$(1, 0)$$ have remarkable stability. This is a general feature observed for the EPD and Fisher zeros (see, e.g., Refs. [16, 31]). Fig. 2 shows the original histograms and perturbed ones as well as a portion of the map of zeros in the complex plane. Again, even for 30% perturbation of the coefficients, the dominant and nearby zeros remain almost unaffected, while the rest of the map is highly affected.

In order to better quantify the modifications introduced by perturbations on the location of the dominant zero, the mean distance between the original dominant zero and the perturbed ones ($$R$$) as well as the standard deviation of them ($$\sigma$$) were obtained using 20 different samples of perturbation. This is shown in Fig. 3. As can be seen, although both increase with increasing...
perturbation, their values are remarkably small. Indeed, as can be seen in Fig. 2b, the imaginary part of zeros has a value $\sim 0.02$ while the real part is $\sim 1$. The mean deviation goes up to $1.5 \times 10^{-4}$, two orders of magnitude smaller than the imaginary part of the zero. In addition, closer to the transition temperature, the deviation from the original zeros seems to saturate for large fluctuations.

The impact on the real and the imaginary part is shown in Fig. 4. For both, the mean deviation seems to oscillate around 0, while the standard deviation has an apparent increase with perturbation. These results are strong evidences of the stability of the dominant zero against fluctuations and numerical issues.

The approaching to the critical temperature was also analyzed for different percentages of perturbation and is shown in Fig. 5. To this end, for each iteration of the algorithm the next temperature is chosen by building 20 perturbed histograms, finding the dominant zero for each of them and using its mean value to estimate the new critical temperature. As can be seen in

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**Figure 2.** a) Original EPD without perturbation (black) and other EPDs generated following the equation 3 with $a = [1\%, 5\%, 10\%, 30\%]$. b) Map of zeros for each EPD.

**Figure 3.** a) Mean distance between the original dominant zero position and the position of the dominant zeros of perturbed polynomials for different temperatures as a function of perturbation. b) Standard deviation from the perturbed zeros. Although both $R$ and $\sigma$ grow with perturbations none of them presents great deviations from zero. That is, the dominant zero is highly stable over perturbations.
Figure 4. a) and b) Mean distance and its standard deviation, respectively, for the real part of the zeros. c) and d) shows the same for the imaginary part. The mean distance oscillates around zero while the standard deviation increases with increasing perturbation. This shows that perturbations on the EPD shifts equally the dominant zero in both directions and that the displacement is more pronounced for higher perturbation.

the figure, the algorithm converges to the expected temperature for all analyzed perturbations, while for larger perturbation the estimates oscillate with higher amplitude around the expected value than for lower perturbations. This was to be expected since for larger fluctuations one expect less precise results and consequently a larger error bar for estimates of the transition temperature.

4. Conclusions
As is well known, the roots of polynomials are, in general, highly sensitive to modifications in its coefficients (see for example the seminal work of Wilkinson [24]). However our results indicate that the dominant zero of the EPD is almost unaffected by random fluctuations in its coefficients. This is at the same time an expected and surprising result. While from the pure numerical methods perspective one would be very surprised that the position of one special zero of a 1369 degree polynomial deviates from the unperturbed position by less than $10^{-4}$, from the statistical mechanics point of view, the point that signalizes a phase transition is expected to be very robust against small modifications in the system. For luck and the success of the method, the statistical mechanics characteristic of the coefficients seems to surpass numerical issues related to finding roots of very high degree polynomials. In addition, these results emphasize that the location of the dominant zero is related to general features of the EPD and not to its
Figure 5. Convergence process of the EPD zeros for different strengths of perturbation, \( a = [1\%, 5\%, 10\%, 30\%] \). For each iteration of the algorithm the next temperature is chosen by building 20 perturbed histograms, finding the dominant zero for each of them and using its mean value to estimate the new critical temperature.

Specific details. It seems that the overall shape of the EPD is the main ingredient related to the existence and location of a phase transition.

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