Moment-generating function zeros in the study of phase transitions

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Partition function zeros play a central role in the study of phase transitions. Recently, energy probability distribution (EPD) zeros were proposed as an alternative approach that solves some of the implementation issues present in the Fisher zeros method by allowing drastic reduction of the polynomial. Here, a formulation based on the EPD zeros that can reduce even more the polynomial degree while maintaining its accuracy is presented. This method has shown to be computationally cheaper than the EPD zeros, allowing the study of systems by using partition function zeros that would be unfeasible otherwise. In addition, the method can be easily extended to study phase transitions in external fields while maintaining all of its improvements.

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I. INTRODUCTION

Systems that undergo phase transitions as a control parameter changes have a nonanalyticity in their free energy at the phase transition point. This behavior is better understood with the concept of the zeros of the function partition, introduced by Yang and Lee in their seminal papers [1,2]. In these papers, by making a complex extension of the fugacity to the complex plane, they showed that all the system thermodynamic information is contained in the partition function zeros density. More specifically, they showed that as the system size goes to the thermodynamic limit, this density of zeros approaches the real axis signaling that a phase transition occurred. The zeros that pinch the real axis are called dominant zeros and they are responsible for the free energy nonanalyticities. Furthermore, the partition function zeros are considered a cornerstone of statistical physics and were applied to a variety of systems [3–5] and have even been determined in experiments [6–8]. It was also extended by Fisher [9] to the canonical ensemble where a complex extension of the temperature is made.

Although the Fisher zeros were applied to diverse models [3,10,11] and have been determined in experiments [8], this method has two main problems in its practical implementation. To apply this method it is necessary to know the density of states (DOS), a quantity difficult to find, and solve a high degree polynomial with coefficients given by the DOS that can span over many orders of magnitude. Recently [12], some of these issues were solved by the energy probability distribution (EPD) zeros. In the EPD zeros approach, the polynomial coefficients are given by an energy probability distribution, a quantity much simpler to obtain numerically than the DOS, and its degree is reduced by recognizing that states with low probability to occur at a given temperature can be discarded without losing relevant thermodynamic information in the vicinity of the considered temperature. This method was successfully applied to systems that undergo discontinuous, continuous, and topological phase transitions [12–14]. Despite that, although the EPD zeros solve most of the issues of the Fisher zeros method, it is still necessary to solve a high degree polynomial with the degree increasing as the system size increases. Moreover, as will be shown, the EPD zeros method is not very efficient in reducing the polynomial degree for systems that undergo discontinuous phase transitions. In other methods, such as the one proposed by Alves *et al.* [15], there is no need to solve a polynomial, but the knowledge of the DOS for all energy states, a quantity difficult to obtain for very large systems, is still demanded. Last, the method recently proposed by Sarkanych *et al.* [16] seems to be promising, deserving further investigations and comparisons with the mentioned methods.

In this paper, we present an approach to study phase transitions in which, instead of using the partition function zeros, the moment-generating function (MGF) zeros are used. This approach is based on the EPD zeros, but it has several improvements such as the smaller dependence of the polynomial degree on the system size, absence of discretization requirements, lower polynomial degree than the EPD zeros approach, and coefficients that are given by simple thermodynamic averages. In addition, it is computationally faster than the EPD zeros. In what follows we briefly review the Fisher and EPD zeros, introduce the MGF zeros, and apply it to the two-dimensional (2D) Ising and six-state Potts models. Furthermore, estimates of the computational time spent to analyze simulations of the three-dimensional (3D) Ising model using EPD and MGF zeros is shown, highlighting the fact that the present method allows the study by zeros of the partition function of systems that would be otherwise unfeasible.

II. FISHER ZEROS

The Fisher zeros [9] approach is developed in the same way as the Yang-Lee zeros approach [1,2], but instead of

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considering a complex extension of the fugacity to the complex plane, the temperature is extended. Thus, the canonical partition function is written as

$$Z = \sum_E g(E)e^{-\beta E} = e^{-\beta\varepsilon_o}\sum_n g_n z^n, \tag{1}$$

where $z = e^{-\beta\varepsilon}$, $\beta = 1/k_BT$ is the inverse temperature, k_B is the Boltzmann constant, $g(E)$ is the DOS, and the energy E was discretized by setting it to $E_n = \varepsilon_o + n\varepsilon$ [17] with $n \in \mathbb{N}$. ε_0 is the ground state energy, ε is the energy bin, and $g_n = g(E_n)$. As the temperature, and consequently z, is seen now as a complex quantity, this polynomial has complex conjugate roots (zeros) and any real root must be negative since $g(E) \geqslant 0$. Moreover, in the thermodynamic limit, one expects that the dominant zero touches the real positive axis, signaling that a phase transition occurs at the temperature that corresponds to the point it touches the real axis. Indeed, this is the signature of the nonanalyticity present in the free energy at a phase transition. For finite systems, however, the dominant zero lies close to the real positive axis, once there is no nonanalyticity in finite systems, and can be used to find the pseudocritical temperature $T_c(L)$, where L is the system lattice size. Of course, proper finite size scaling must be done to confirm the presence of a phase transition.

III. THE ENERGY PROBABILITY DISTRIBUTION ZEROS

The EPD zeros [12] method is obtained by rescaling the Fisher zeros. To see this, note that if we multiply Eq. (1) by $e^{-\beta_oE}e^{\beta_oE} = 1$ and write Z as a polynomial, we find

$$Z = \sum_E g(E)e^{-\beta_oE}e^{-\Delta\beta E} = e^{-\Delta\beta\varepsilon_o}\sum_n h_{\beta_o}(n)x^n, \tag{2}$$

where $\beta_o = 1/k_BT_o$ is an arbitrary inverse temperature, $\Delta\beta = \beta - \beta_o$, $x = e^{-\Delta\beta\varepsilon}$, and $h_{\beta_o}(n) = g_ne^{-\beta_oE_n}$ is the nonnormalized energy probability distribution function at β_o. Note that so far no approximation was made and since $x = z/e^{-\beta_o\varepsilon}$, the set of roots $\{x_i\}$ are only the Fisher zeros roots $\{z_i\}$ rescaled. Thus, because the coefficients of the above polynomial are given by the energy probability distribution, a threshold h_t can be defined so that states with low probabilities to occur can be discarded without losing relevant thermodynamic information in the neighborhood of β_o. It is this discarding process that drastically reduces the polynomial degree when compared with the Fisher zeros approach once most of the energy states are not relevant at β_o.

Nonetheless, the EPD zeros have a distinctive characteristic: the dominant zero is always close to point (1,0) for $\beta_o(L) \approx \beta_c(L)$, where $\beta_c(L)$ is the inverse critical temperature and L is the system lattice size. To understand this, remember that the EPD zeros are just the Fisher zeros rescaled and, therefore, for $\beta_o = \beta_c$ the Fisher dominant zero $z_c = e^{-\beta_c\varepsilon}$ will be rescaled to $x_c = z_c/e^{-\beta_c\varepsilon} = 1$. Furthermore, this can be used as a criterion to identify for which values of β_o a phase transition occurs. Therefore, in Ref. [12] an algorithm was proposed to iteratively estimate β_c. Using the dominant zero $x_c(L)$ and the finite lattice critical temperature $T_c(L)$, the critical temperature T_c and the critical exponent ν can be found by applying the finite size scaling equations [12,18].

IV. MOMENT-GENERATING FUNCTION ZEROS

Before introducing the MGF zeros method, it is better to remember that if we know all the moments $m_k = \langle X^k\rangle$ of a random variable X, it is possible to reconstruct the entire probability distribution $P(X)$ [19]. Therefore, all the information contained in $P(X)$ is also contained in its moments, in such a way that one can use the MGF instead of the actual probability distribution to write the partition function [20].

Considering that the MGF equation is given by

$$M_X(t) = \sum_{k=0}^{\infty}\frac{\langle X^k\rangle t^k}{k!} = \sum_{k=0}^{\infty}\frac{m_kt^k}{k!}, \tag{3}$$

where t is an arbitrary variable, and its moments are defined by

$$m_k = \left.\frac{d^kM_X(t)}{dt^k}\right|_{t=0}, \tag{4}$$

it is easy to show that with a series expansion of the exponential in the partition function,

$$Z(\beta) = \sum_E h_{\beta_o}(E)e^{-\Delta\beta E}, \tag{5}$$

it can be written as

$$Z(\beta) = Z(\beta_o)\sum_{k=0}^{\infty}\frac{m_k(\beta_o)}{k!}y^k, \tag{6}$$

where $Z(\beta_o)$ is a constant, $y = -\Delta\beta$, and $m_k(\beta_o) = \langle E^k\rangle_{\beta_o} = (\sum_E h_{\beta_o}(E)E^k)/Z(\beta_o)$ are the moments of the energy. Notice that the term within the summation is the definition of an MGF, Eq. (3), with $t = y$. Therefore, since $Z(\beta_o)$ is only a constant, the zeros of the canonical partition function and the zeros of the MGF contain the same information [20].

The main improvement of this method when compared to the EPD zeros is that the polynomial degree can be reduced by a series truncation at $k_{\max}$, instead of the introduction of an arbitrary discard threshold as in the EPD zeros method. Indeed, a series truncation is a much more elegant and controllable way to approximate the partition function. Moreover, in this approach, since only some of the energy moments, $\langle E^k\rangle_{\beta_0}$, are necessary, one does not need to impose a discrete energy spectrum, eliminating arbitrary parameters such as the energy bin ε.

Note that the EPD zeros and the MGF zeros are related by the transformation $x = e^{y\varepsilon}$ and it is straightforward to expand some properties of the EPD zeros to the MGF zeros. For instance, since the EPD dominant zero is at $x_c = 1$ for $\beta_o = \beta_c$, the MGF dominant zero must be at the point (0,0) for $\beta_o = \beta_c$. Furthermore, it is possible to adapt the EPD zeros algorithm presented in Ref. [12] to the MGF zeros. With this in mind, the following modified algorithm can be used to estimate $\beta_c(L)$ considering a truncation at a sufficiently large value $k_{\max}$:

(1) Find the energy moments $m_k(\beta_o) = \langle E^k\rangle$ at $\beta_o^j(L)$.

(2) Find the zeros of the polynomial with coefficients given by $m_k(\beta_o^j)/k!$.

(3) Find the dominant zero, $y_c^j(L)$.

(a) If y_c^j is close enough to the point (0, 0), stop.

(b) Else, make $\beta_o^{j+1}(L) = \beta_o^j(L) - \mathrm{Re}\{y_c^j(L)\}$ and go back to step 1.

Notice that the MGF zeros are related to the Fisher zeros because we chose to make a complex extension of the control parameter β. However, we can make a complex extension of other control parameters, such as the magnetic field, and make a relation with the Yang-Lee zeros. This development is presented in Appendix A.

V. DOMINANT ZERO SCALING

Close to a continuous phase transition we may argue (see Appendix B) that the MGF dominant zeros follow the scaling law given by

$$\frac{y_c}{L^{-1/\nu}} = \frac{\mathrm{Re}\{y_c\} + \mathrm{Im}\{y_c\}i}{L^{-1/\nu}} = g(x) + f(x)i, \tag{7}$$

where $g(x)$ and $f(x)$ are scaling functions. And, since $\mathrm{Re}\{y_c\} = 0$ close to the critical point, the imaginary part scaling is given by

$$\mathrm{Im}\{y_c\} = L^{-1/\nu} f(x). \tag{8}$$

This scaling behavior may be expected since the EPD zeros scale in the same way [12]. To find the critical temperature T_c and the critical exponent ν using the MGF zeros, the following finite size scaling equations are used:

$$\ln \mathrm{Im}\{y_c(L)\} \sim b - \frac{1}{\nu}\ln(L) \tag{9}$$

and

$$T_c(L) \sim T_c + aL^{-1/\nu}. \tag{10}$$

VI. MODELS

In this work, we applied the MGF zeros method and the EPD zeros method to the six-state Potts model and to the 3D and 2D Ising models. Except for the 3D Ising model, the other models are benchmarks for studying continuous and discontinuous phase transitions since exact results for the critical temperature and critical exponents are known. The 3D Ising model is used only to highlight the MGF zeros method efficiency in contrast with the EPD zeros method. In what follows, we briefly present these models.

The Ising model Hamiltonian is given by

$$H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - h\sum_i \sigma_i, \tag{11}$$

where J is a coupling constant, h is an external field, σ_i is a spin at site i with value ± 1, and $\langle i, j\rangle$ means a sum over nearest neighbors and $M = \sum_i \sigma_i$ is the system magnetization. In this paper we consider the 2D and 3D Ising models in a square and cubic lattice, respectively, with $J = 1$, $k_B = 1$, and $h = 0$. Both lattices have continuous phase transition, but only the 2D Ising model has exact results known for the critical temperature $T_c = 2/\ln(1+\sqrt{2})J/k_B$ and critical exponent $\nu = 1$ [21].

For the q-states Potts model, the Hamiltonian is given by

$$H = -J\sum_{\langle i,j\rangle}\delta(\sigma_i, \sigma_j), \tag{12}$$

where J is a coupling constant, σ_i is on site i with values ranging from 1 to q, δ is the Kronecker delta, and the sum is taken over the nearest neighbors. For a 2D Potts model with $J > 0$, the model has a continuous or discontinuous phase transition depending on the value of q. For $q > 4$ it has a discontinuous phase transition and for $q \leqslant 4$ it has a continuous phase transition. Its critical temperature is given by $T_c = 1/\ln(1+\sqrt{q})J/k_B$ [21]. In the following, we considered the Potts model with $q = 6$, $J = 1$, and $k_B = 1$.

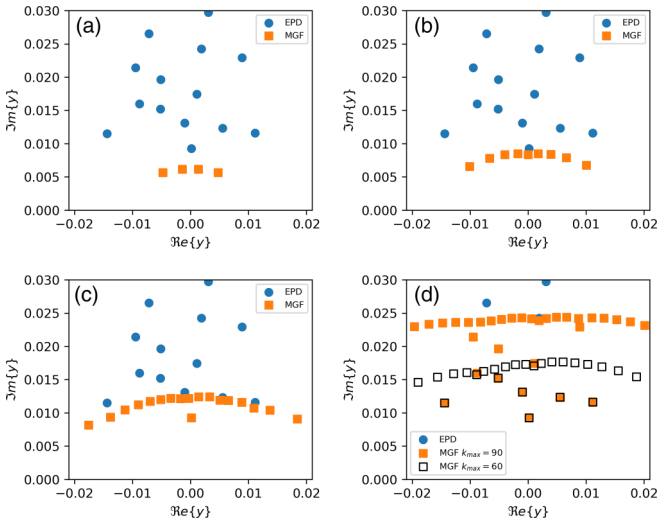

FIG. 1. EPD zeros (circles) with $h_t = 10^{-4}$ and the MGF zeros (squares) for (a) $k_{\max} = 9$, (b) $k_{\max} = 19$, (c) $k_{\max} = 37$, and (d) $k_{\max} = 60$ and $k_{\max} = 90$, for the Ising model at $T = 2.2793$ and lattice size $L = 90$. Notice that the MGF zeros emerge close to point (0,0) for lower $k_{\max}$ and expand towards the EPD zeros as $k_{\max}$ increases. To allow comparison among them we draw the EPD zeros, x, in the same scale of the MGF zeros using the relation $y = \ln x/\epsilon$, such that the unit of the MGF zeros is k_B/J.

VII. RESULTS

First we present a preliminary analysis of the MGF zeros for the 2D Ising and six-state Potts models. We used conventional Monte Carlo simulations for square lattices of sizes $L = [90, 120, 150, 180]$ using 10^6 Monte Carlo steps (MCS) and five different simulations for each simulated temperature. For the Ising model, 3 temperatures close to the critical one were simulated [22] while for the Potts model 15 temperatures were used [23]. A multiple histogram reweighting technique [24] was used to estimate the EPD and moments of energy at β_o. In fact, it is more convenient to use central moments $m_k(\beta_o) = \langle E - \langle E\rangle\rangle^k$ than the moments $m_k(\beta_o) = \langle E\rangle^k$ as the MGF coefficients. This change can be done without any further modification in the method. Statistical errors were estimated by averaging results over these five sets of simulations.

Let us first explore the effects of different values of $k_{\max}$ on the map of zeros. A general feature we observed is that for low enough $k_{\max}$ the MGF zeros lie in an almost elliptic curve centered at (0,0). Considering increasing values of $k_{\max}$, this ellipse size increases until some zeros start to deviate from the elliptical pattern, staying fixed in some points as can be seen in Fig. 1. Thus, the EPD zeros distribution is recovered in the limit of sufficiently large $k_{\max}$ values once the zeros that deviate from the elliptical pattern coincide with

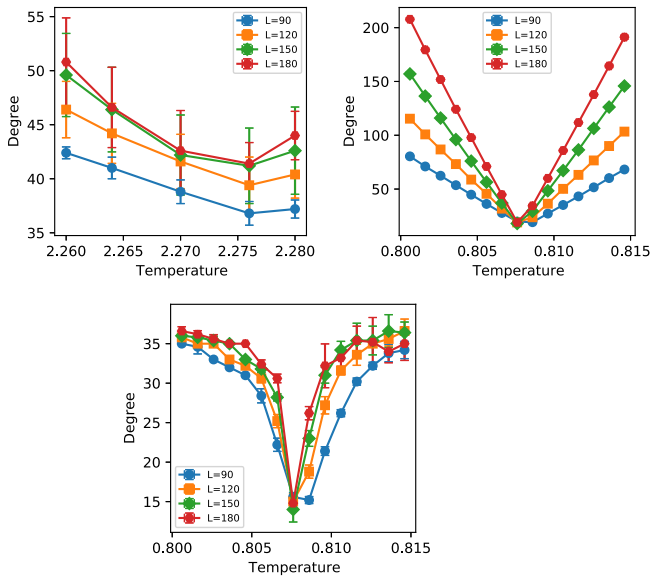

FIG. 2. The minimum degree of the MGF polynomial, $k_{\max}$, necessary to recover the dominant zero of the EPD zero with eight significant figures using the MGF zeros approach. (a) The Ising model considering a threshold in the EPD zeros of 10^{-100}, (b) the Potts model with a threshold of 10^{-100}, and (c) the Potts model with a threshold of 10^{-4}. As can be clearly seen, near the transition temperature (measured in units of J/k_B) the minimum degree is smaller.

the EPD zeros. Although we still do not have an argument for this behavior, it was observed for the Ising and six-state Potts models even far from the transition temperature. We speculate that this may be related to the expansion around the point (0,0) made in the partition function albeit we did not explore it in depth. Thus, the dominant zero, the one closest to point (0,0) for $\beta_o = \beta_c$, can be easily found using small values of $k_{\max}$ as the first one to deviate from the elliptic pattern. In general, it is advisable to use a $k_{\max}$ value large enough to ensure that a good accuracy in the dominant zero location is obtained and that several other zeros are recovered. Remember that as a series expansion truncation, larger $k_{\max}$ implies higher accuracy in the zeros determination. As a rule of thumb one can choose $k_{\max}$ as the smaller value that allows to clearly identify a dominant zero at the temperature where the iterative process begins. During the iterative process this choice can be revisited to reduce the computational effort.

Of course, for β_0 far from β_c large values of $k_{\max}$ must be used in order to obtain the dominant zero with reasonable accuracy. Indeed, as shown in Fig. 2, the polynomial degree, $k_{\max}$, increases when β_0 is not close enough to β_c.

A. 2D Ising model

Now, considering an arbitrary "large" value for $k_{\max}$, the convergence process to the critical temperature obtained from the MGF zeros is compared to the EPD zeros convergence in Fig. 3(a) for the 2D Ising model. Both methods converge to a similar critical temperature, although the number of iterations necessary to achieve the convergence is different for each method. This has a major impact on the computational

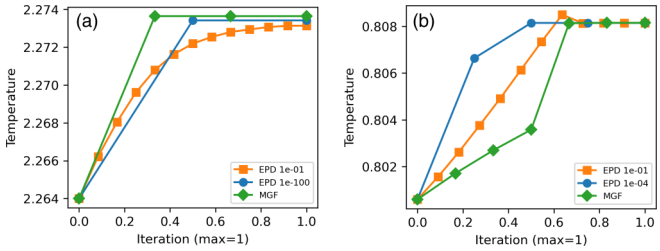

FIG. 3. (a) The convergence process for the MGF zeros with $k_{\max} = 60$ and EPD zeros with $h_t = 10^{-1}, 10^{-100}$ for lattice size $L = 180$ for the Ising model. Both methods converge towards the same critical temperature (measured in units of J/k_B). (b) The convergence process for the EPD zeros with $h_t = 10^{-1}, 10^{-100}$ and MGF zeros with $k_{\max} = 220$ for the six-state Potts model. Both figures were made with $L = 90$.

time for the algorithms to estimate the critical temperature. In addition to that, the computational time is largely impacted by the degree of the polynomial to be solved. Indeed, considering a discard threshold of 10^{-1} for the EPD method and $L = 180$ the polynomial degree is about 600, while in the MGF method it was 60 [25]. Thus, this difference in the polynomial degree together with the smaller number of iterations necessary to achieve the transition temperature leads to a reduction in the computational time spent to estimate the critical temperature of about two orders of magnitude (from 0.13 CPU min in the EPD method to 0.0012 CPU min in the MGF method). We considered in this calculation the time spent to achieve convergence from a given temperature, including the time spent reconstructing the histogram, the polynomial coefficients, and its roots.

It is also worthy of note that the polynomial degree increases with the system size in the EPD method as more energy values become accessible to the system while it can be kept almost size independent in the MGF method. As a consequence, the speedup we observed is larger for larger lattice sizes.

To estimate the critical temperature T_c and the critical exponent ν, the finite size scaling equations described earlier were used. Using the EPD zeros method with discard thresholds at $h_t = 10^{-1}, 10^{-100}$ [26], we found for the critical temperature $T_c = 2.2692(9), 2.2692(5)$ and for the critical exponent $\nu = 1.02(2), 1.07(1)$. The estimates for the MGF zeros using $k_{\max} = 60$ are $T_c = 2.2687(8)$ and $\nu = 1.02(2)$. Both methods gave results in good agreement with the exact values $\nu = 1$ and $T_c = 2.2691$.

B. Six-state Potts model

The six-state Potts model has a more complex energy probability distribution due to its discontinuous phase transition, with the energy probability distribution showing two larger peaks (see, for example, Fig. 2 of Ref. [12]). Because of that, and considering that states between the two peaks cannot be discarded [12], the EPD zeros method has problems reducing the polynomial degree. However, the MGF zeros are not limited by the shape of the histogram; its discard process is made by a series truncation and showed no problem in reducing the polynomial degree. Indeed, we found that at the

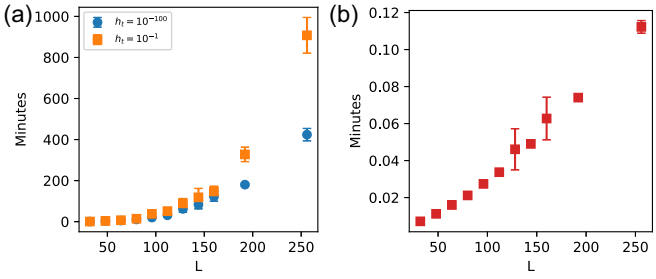

FIG. 4. Computational time spent in the convergence process of the EPD (a) and MGF (b) methods for the 3D Ising model starting at $\beta = 0.221654$. The data were averaged over five samples and we used a 2.80 GHz Intel CoreTM i7 CPU with 16 GB RAM and the package MPSOLVE [30,31], configured to use eight cores in parallel.

phase transition temperature a polynomial of degree about 12 is sufficient to find the dominant zero. Despite the difference in the polynomial degree, both methods converge to the same critical temperature as can be seen in Fig. 3(b).

The critical temperature was found using the finite size scaling equations shown earlier. For the EPD zeros method with $h_t = 10^{-1}, 10^{-100}$ and the MGF zeros method with $k_{\max} = 220$ the results were shown to be the same, $T_c = 0.80763(3)$. This value is in good agreement with the exact one of $T_c = 0.80761$.

Again, huge speedups can be obtained. Indeed, the MGF method has been shown to be at least 290 times faster than the EPD method for the largest lattice size considered ($L = 180$). This is understandable, since the EPD method has a polynomial with degree close to 10 000 while the MGF has a polynomial with degree 220.

C. 3D Ising model

The speedup obtained by using the MGF in comparison with the EPD method can be highlighted by considering the 3D Ising model, where the use of the EPD zeros is shown to be unfeasible. Following the seminal works of Ferrenberg, Xu, and Landau [27,28] we simulated the 3D Ising model using the Wolff cluster flipping algorithm [29] to simulate cubic lattices with linear sizes $L = 24, 32, 48, 64, 80, 96, 112, 128, 144, 160, 192$, and 256 with 5×10^6 MCS for each sample, 500 samples for each lattice size at $\beta = 0.221654$, following closely what was done in Ref. [28] but with smaller lattice sizes and fewer samples. Again, histogram reweighting [24] was used to estimate the EPD and moments of energy at β_o. Here, only a preliminary comparison between the EPD and MGF zeros is presented while a more detailed study of the 3D Ising model using partition function zeros is still in progress and will be presented elsewhere.

The preliminary analysis was focused on the estimate of the computational time that would be spent in the calculation of zeros for both methods to analyze the data for all lattice sizes and samples. In Fig. 4 we compare the time spent to achieve convergence starting at the simulation temperature, $\beta = 0.221654$, for each lattice size, L, for the 3D Ising model averaged over five different samples using both the EPD zeros and MGF zeros. As can be seen, EPD convergence time seems to scale exponentially with lattice size while MGF zeros scale almost linearly. Using this result, we estimated that the time needed to analyze all samples considering the EPD zeros without cutoffs would be ≈ 326 days. Using a cutoff at 10^{-1} the total time was estimated to be 591 days, since in many cases the convergence took more steps as compared to the EPD without cutoffs. In contrast, the total computational time estimated to analyze all the data using the MGF is ≈ 4 hours. It is the huge reduction in polynomial degree provided by the MGF method in comparison to the EPD method that is mainly responsible for this speedup with negligible loss of accuracy as shown, since most of the computational time considered here is spent solving polynomials. Indeed, for the largest lattice size we considered, $L = 256$, the number of EPD zeros is about 70 000, while for the MGF we considered only 100 zeros. In addition, as we were close enough to the transition temperature, a more detailed analysis would permit us to use even fewer zeros, reducing even more the time spent in this analysis. These times were obtained in a 2.80 GHz Intel CoreTM i7 CPU with 16 GB RAM, and the package MPSOLVE [30,31], configured to use eight cores in parallel, was used to solve the polynomials. This result clearly shows that the methodology presented in this paper offers the possibility to analyze through the zeros of the partition function (in this case the zeros of the MGF) systems otherwise inaccessible to this kind of analysis.

VIII. CLOSING REMARKS

In summary, this paper introduced the MGF zeros method, a method to study phase transition that was based on the EPD zeros. The MGF zeros are shown to reproduce the same results of the EPD zeros method with the advantage to consume fewer computational resources. This is achieved because the MGF method can accurately represent the partition function polynomial in the vicinity of the transition temperature with a much lower degree polynomial. Besides that, the EPD zeros method depends on the shape of the energy probability distribution to reduce the polynomial degree, while the MGF zeros reduce its degree by a truncation in a Taylor series expansion of the partition function. This was shown to be a great improvement for studying discontinuous phase transitions, where the EPD zeros method has difficulties to reduce the polynomial degree. In addition, the requirement to discretize the energy spectra present in the Fisher or EPD zeros method is absent in the MGF zeros method.

By considering a preliminary analysis for the 3D Ising model, we have shown that the study of the phase transition by Fisher or EPD zeros is unfeasible. Indeed, the estimated computational time that would be required for the precise determination of the dominant zero location in the EPD method is about 326 days, while using the MGF zeros, the determination of the same information requires only about 4 h. Through the improvement provided by the MGF zeros, the study by means of partition function zeros of large enough systems as a 256^3 3D Ising model becomes feasible. We must remark, however, that methods such as the logarithmic summation procedure proposed in Ref. [15] may allow the study of phase transitions by means of partition function zeros in such a large system provided that the DOS is known. However, the present method can be applied using only the partial knowledge of

the DOS provided by Monte Carlo simulations performed at a single temperature close enough to the transition temperature instead of the full knowledge of the DOS.

Although the MGF zeros were used to identify the critical temperature, it is not limited to that. The MGF can be used to identify critical points for other control parameters such as an external field, as shown in Appendix A. Moreover, since the MGF polynomial coefficients are given by thermodynamic observables such as the energy moments $\langle E^k \rangle$ or the magnetization moments $\langle M^k \rangle$, this method can be used in any analytical, numerical, or experimental method, provided that it is possible to estimate these thermodynamic means.

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APPENDIX A: BEYOND β AND ENERGY

The MGF zeros method presented here was developed using the energy probability distribution and considering a complex extension of β. However, this method can be extended to other probability distributions with different control parameters. For example, consider the Ising model Hamiltonian with a magnetic field h,

$$\mathcal{H}(J,h) = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - hM. \tag{A1}$$

The canonical partition function is given by

$$Z = \sum_{E,M} g(E,M)e^{\beta J\sum_{\langle i,j\rangle}\sigma_i\sigma_j}e^{\beta hM}, \tag{A2}$$

where M is the system total magnetization and a complex extension of h was made. Multiplying it by $1 = e^{-\beta h_o M}e^{\beta h_o M}$, we find

$$Z = \sum_{E,M} g(E,M)e^{-\beta\mathcal{H}(J,h_o)}e^{\beta\Delta hM}, \tag{A3}$$

where $\Delta h = h - h_o$. Expanding the last exponential in a Taylor series and rearranging the terms, the partition function can be rewritten as an MGF equation,

$$Z = Z_o\sum_{k}^{\infty}\frac{\langle M^k\rangle}{k!}(\beta\Delta h)^k, \tag{A4}$$

where $\langle M^k\rangle$ are the moments of the magnetization at (β, h_o). Therefore, the MGF zeros can be used to find the magnetic field for which a phase transition occurs. Furthermore, a similar approach can be made for the EPD zeros using Eq. (A3) but that is outside the scope of this paper.

APPENDIX B: DOMINANT ZERO SCALING

Close to a continuous phase transition, it is well known that thermodynamic observables follow scaling laws [32] such as

$$c_{\rm v} = L^{\alpha/\nu}F_{C_{\rm v}}(x), \quad \chi = L^{\gamma/\nu}F_{\chi}(x), \tag{B1}$$

where x is a quantity that goes to zero at the critical temperature and F_i is a scaling function that is constant as $x \to 0$; i.e., these functions are independent of the system size L for $x = 0$. Therefore, since the cumulants and moments scale in the same way [33], the moments scale as $m_k = L^{k/\nu}F_k(x)$ [34] and Eq. (6) when properly normalized is given by

$$Z = Z(\beta_o)\sum_{k=0}^{\infty}\frac{F_k(x)}{k!}y_s^k = C\prod_i\left(y_s^i(x) - y_s\right), \tag{B2}$$

where $y_s = \frac{y}{L^{-1/\nu}}$ and y_s^i is the ith rescaled zero. Notice that this polynomial scales as a thermodynamic observable and at the critical temperature it is independent of the system size L. The same is valid for the set of zeros $\{y_s^i\}$; at the phase transition all the zeros are independent of the system size. Therefore, the rescaled MGF dominant zero given by $y_s^c = y_c/L^{-1/\nu}$ must scale as

$$\frac{y_c}{L^{-1/\nu}} = \frac{{\rm Re}\{y_c\} + {\rm Im}\{y_c\}i}{L^{-1/\nu}} = g(x) + f(x)i, \tag{B3}$$

where $g(x)$ and $f(x)$ are scaling functions. And, since ${\rm Re}\{y_c\} = 0$ close to the critical point, the imaginary part scaling is given by

$${\rm Im}\{y_c\} = L^{-1/\nu}f(x). \tag{B4}$$

This scaling behavior is expected since the EPD zeros scale in the same way [12].

Finally, to estimate the critical temperature T_c and the critical exponent ν using the MGF zeros the following finite size scaling equations are used:

$$\ln{\rm Im}\{y_c(L)\} \sim b - \frac{1}{\nu}\ln(L) \tag{B5}$$

and

$$T_c(L) \sim T_c + aL^{-1/\nu}, \tag{B6}$$

where a and b are unimportant scaling constants with no special meaning in this context.

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