Determination of Universal Critical Exponents Using Lee-Yang Theory

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Lee-Yang zeros are complex values of an external control parameter at which the partition function vanishes for a many-body system of finite size. In the thermodynamic limit, the Lee-Yang zeros approach the critical value on the real-axis where a phase transition occurs. Partition function zeros have for many years been considered a purely theoretical concept, however, the situation is changing now as Lee-Yang zeros have been determined in several recent experiments. Motivated by these developments, we here devise a direct pathway from measurements of partition function zeros to the determination of critical points and universal critical exponents of continuous phase transitions. To illustrate the feasibility of our approach, we extract the critical exponents of the Ising model in two and three dimensions from the fluctuations of the total energy and the magnetization in surprisingly small lattices. Importantly, the critical exponents can be determined even if the system is away from the phase transition, for example at a high temperature. As such, our method provides an intriguing perspective for investigations of phase transitions that may be hard to reach experimentally, for instance at very low temperatures or at very high pressures.

Introduction. — Phase transitions are characterized by the abrupt change of a many-body system from one state of matter to another as an external control parameter is varied [1–3]. In their seminal works, Lee and Yang developed a rigorous theory of phase transitions based on the zeros of the partition function in the complex plane of the control parameter, for instance the fugacity or an external magnetic field [4–7]. The crucial insight of Lee and Yang was that the partition function zeros with increasing system size will approach the real value of the control parameter for which a phase transition occurs. These ideas are now considered a theoretical cornerstone of statistical physics, and they have found applications across a wide range of topics, including protein folding [8, 9], percolation [10–13], and Bose-Einstein condensation [14, 15].

Despite these developments, partition function zeros were for a long time considered a purely theoretical concept. This situation is changing now as Lee-Yang zeros have been determined in several experiments [16–23]. Recently, partition function zeros were measured using carefully engineered nano-structures involving the precession of interacting molecular spins [17–19], Cooper pair tunneling in superconducting devices [20–22], or fermionic atoms in driven optical lattices [23]. In parallel with these experiments, several theoretical proposals have been put forward for the detection of partition function zeros [24–28]. These advances motivate a number of questions, which now should be addressed. In particular, it is relevant to ask what we can learn from the determination of partition function zeros in systems of finite size and how future experiments on scalable many-body systems may improve our understanding of phase transitions.

In this Letter, we present a direct pathway from the detection of partition function zeros by measuring or simulating fluctuating observables in systems of finite size to the determination of critical points and universal critical exponents of continuous phase transitions [1–3]. Our method combines ideas and concepts from finite-size scaling analysis [29–32] with the Lee-Yang formalism [4–7] and theories of high cumulants [33–36], and it can be applied in experiments on a variety of phase transitions including non-equilibrium situations such as space-time phase transitions in glass formers [37, 38] and dynamical phase transitions in quantum many-body systems after a quench [39–41]. Specifically, we determine the partition function zeros from fluctuations of thermodynamic observables and find the critical exponents from the approach of the zeros to the critical value on the real-axis. As a paradigmatic application, we determine the critical points and the universal critical exponents of the Ising model from the fluctuations of energy and magnetization in surprisingly small lattices. Unlike most conventional
methods [32], which require the control parameter to be tuned across the phase transition, we can determine the critical exponents even if the system is away from the phase transition, for example at a high temperature. As such, our method provides an intriguing perspective for investigations of phase transitions that may be hard to reach experimentally, for instance at very low temperatures or at very high pressures [42, 43]. Moreover, our method opens an avenue for bottom-up experiments on phase transitions, in which nano-scale structures are carefully assembled, for example by adding single spins to an atomic chain on a surface [44] or by loading individual atoms into an optical lattice one at a time [45], to increase the system size in a controllable manner.

Ising lattice & criticality. — Figure 1a illustrates the Ising lattice that we consider in this work. The lattice has \( N = L^d \) sites, where \( L \) is the linear size and \( d = 2, 3 \) denotes the spatial dimension. Each site hosts a classical spin which can take on the values \( \sigma_i = \pm 1 \). An external magnetic field of magnitude \( h \) can be applied, and neighboring spins are coupled via a ferromagnetic interaction of strength \( J > 0 \). The total energy corresponding to a specific spin configuration \( \sigma = \{ \sigma_i \} \) is then

\[
U(\sigma) = -J \sum_{\langle i, j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i, \tag{1}
\]

where the brackets \( \langle i, j \rangle \) denote summation over nearest-neighbor spins. The thermodynamic properties of the lattice are fully encoded in the partition function

\[
Z(\beta, h) = \sum_{\sigma} e^{-\beta U(\sigma)}, \tag{2}
\]

where \( \beta = 1/(k_B T) \) is the inverse temperature. Phase transitions are signalled by values of the control parameters for which the scaled free energy \( f(\beta, h) = -[\ln Z(\beta, h)]/(N \beta) \) becomes non-analytic in the thermodynamic limit of large lattices [1–3]. The partition function also captures fluctuations of thermodynamic observables. For instance, energy fluctuations can be characterized by the moments \( \langle U^n \rangle = \langle \partial^n_{\beta} Z(\beta, h) \rangle/Z(\beta, h) \) or cumulants \( \langle\langle U^n \rangle\rangle = \partial^n_{\beta} \ln Z(\beta, h) \), which follow upon differentiation with respect to the conjugate variable, here the inverse temperature. The moments and cumulants of the magnetization are given in a similar manner by differentiation with respect to the magnetic field strength.

The Ising model exhibits a continuous phase transition, which close to the critical inverse temperature \( \beta \simeq \beta_c \) can be completely characterized by a few critical exponents that are independent of microscopic details and are determined solely by general features such as the dimensionality of the problem and its universality class [1–3]. As such, the determination of critical exponents is of key importance in statistical mechanics. In the vicinity of the critical point, we may assume that the probability distribution for the total energy obeys the scaling relation

\[
P_L(U) = L^{-1/\nu} f_{\infty}(UL^{-1/\nu}), \tag{3}
\]

function and the critical exponent \( \nu \) describes the divergence of the correlation length as we approach the critical temperature [29–32]. After some algebra, we then obtain scaling relations for the cumulants of the form

\[
\langle\langle U^n \rangle\rangle = L^{n/\nu} u_n, \tag{5}
\]

where the \( u_n \)'s depend only weakly on the system size. As we will see, these relations carry over to the partition function zeros and their approach to the critical point.

Partition function zeros & finite-size scaling. — Following the seminal ideas of Lee and Yang, we consider the zeros of the partition function in the complex plane of the control parameter [4–7]. For finite-size lattices, the partition function is analytic and it can be factorized as

\[
Z(\beta, h) = Z(0, h) e^{\beta c} \prod_k (1 - \beta / \beta_k), \tag{4}
\]

where \( \beta_k \) are the zeros in the complex plane of the inverse temperature and \( c \) is a constant. The zeros come in complex conjugate pairs, since the partition function is real for real values of \( \beta \). Often these zeros are referred to as Fisher zeros, while zeros for complex external fields are known as Lee-Yang zeros. With increasing system size, the partition function zeros approach the real value of the control parameter for which a phase transition occurs in the thermodynamic limit. From the definition of the cumulants, we now obtain the relation [20–22]

\[
\langle\langle U^n \rangle\rangle = (-1)^{(n-1)} \sum_k \frac{(n-1)!}{(\beta_k - \beta)^n}, \tag{5}
\]

between the cumulants and the partition function zeros. We then see that the high cumulants are mainly determined by the pair of Fisher zeros, \( \beta_0 \) and \( \beta_0^* \), that are closest to the actual inverse temperature \( \beta \) on the real-axis. The contributions from other zeros are suppressed with the distance to \( \beta \) and the cumulant order \( n \) [33–36]. Moreover, close to criticality, we expect the scaling relations (3) to hold and thus that the leading zeros must approach the critical inverse temperature as [46–48]

\[
|\beta_0 - \beta_c| \propto L^{-1/\nu}, \tag{6}
\]

and

\[
\text{Im}[\beta_0] \propto L^{-1/\nu}, \tag{7}
\]

since the critical inverse temperature is real. These relations are important as they allow us to obtain the critical exponent \( \nu \) from the partition function zeros.

Fisher zeros & critical exponents. — Partition function zeros have recently been experimentally determined [16–23]. Lee-Yang zeros have been determined by measuring the quantum coherence of a probe spin coupled to an Ising-type spin bath [17–19], and Fisher zeros have
been extracted for a dynamical phase transition involving fermionic atoms in a driven optical lattice [23]. Partition function zeros have also been obtained from the fluctuations of the number of transferred particles in an experiment on full counting statistics of Cooper pair tunneling [20–22]. Here, we first determine the Fisher zeros of the Ising lattice from fluctuations of the energy, since the energy is conjugate to the inverse temperature. To this end, Eq. (5) can be solved for high orders, $n \gg 1$, to yield the expression

$$\left[ -2\text{Re}[\beta_0 - \beta] \right] \frac{1}{|\beta_0 - \beta|^2} = \left[ \frac{1}{1 - \frac{n\kappa_n^{(-)}}{n+1}} \right]^{-1} \left[ \frac{(n-1)\kappa_n^{(-)}}{n \kappa_n^{(-)}} \right]$$

for the position of the leading partition function zeros, $\beta_0$ and $\beta_0^{\pm}$, in terms of the ratios $\kappa_n^{(\pm)} \equiv \langle |U_n^{\pm}|^2 \rangle / \langle |U_n|^2 \rangle$ of cumulants of subsequent orders.

To mimic an experiment, we perform Monte-Carlo simulations based on the standard Metropolis algorithm [50, 51]. We thereby evaluate the high cumulants of the energy and subsequently obtain the leading Fisher zeros from Eq. (8) with increasing system size. The results of this procedure are shown in Fig. 2a and Fig. 1b for the Ising lattice in two and three dimensions. Already for surprisingly small lattices of linear size $L \lesssim 10$, we clearly see that the Fisher zeros approach the critical inverse temperature on the real-axis. A quantitative analysis is provided in Fig. 2b, where we investigate the finite-size scaling of the imaginary part and extract the critical exponent $\nu$ based on Eq. (7) [50]. Remarkably, the extracted critical exponents are close to the best-known values for the Ising model in two and three dimensions [49], even if obtained for very small lattices. Moreover, in contrast to conventional methods [32], which typically require that the control parameter is tuned across the phase transition, we are here able to determine the critical exponents from the energy fluctuations at a fixed temperature above the phase transition. Having determined the critical exponents, we can also find the critical inverse temperature by extrapolating the position of the leading Fisher zeros to the thermodynamic limit in Fig. 2c. The imaginary part of the Fisher zeros vanishes in the thermodynamic limit, while the real part comes close to the best-known values for the Ising model.

**Lee-Yang zeros & critical exponents.**—Our method can be applied to a variety of phase transitions, not only in equilibrium settings, but also in non-equilibrium situations such as space-time phase transitions in glass formers [37, 38] and dynamical phase transitions in many-body systems after a quench [39–41]. For example, for the Ising model we may also consider the partition function zeros in the complex plane of the magnetic field. These Lee-Yang zeros can be obtained from the fluctuations of the magnetization similar to how the Fisher zeros are determined using Eq. (8). At the critical temperature, the magnetization is assumed to obey the scaling relation $P_L(M) = L^{-d} g_M(ML^{-d})$, where $g_M$ is a scaling function for the total magnetization and the critical exponent $\mathcal{E}$ describes how the average magnetization vanishes as the critical temperature is approached from below [55, 56]. This scaling hypothesis translates into scaling relations for the Lee-Yang zeros of the form

$$|h_c - h| \propto L^{\frac{\varepsilon}{d}}$$

FIG. 2. Fisher zeros & critical exponents. (a) The leading Fisher zeros (blue circles) for the Ising model with $d = 2$ are extracted from the energy cumulants of order $n = 6, 7, 8, 9$. With increasing system size, the Fisher zeros approach the critical inverse temperature $\beta_c J \simeq 0.4404$ (red circle), which is close to the exact result $\beta_{2D} J = \ln(1 + \sqrt{2})/2 \simeq 0.4407$. The simulations were carried out at a temperature above the phase transition, $\beta J = 0.35$ (black circle). For the Ising model in Fig. 1 with $d = 3$, we find $\beta_c J = 0.22169$, which is close to the best numerical estimate of $\beta_{3D} J \simeq 0.22165$. The critical inverse temperatures are determined in panel c. (b) The extracted critical exponents $\nu$ from the finite-size scaling of the imaginary parts are close to the known values for the Ising model, $\nu_{2D} = 1$ (exact) and $\nu_{3D} \simeq 0.630$ (numerics) [49]. (c) In the thermodynamic limit, the imaginary part of the zeros vanishes, and the real parts approach the critical values indicated with red circles in panels a and c.
and

$$|\text{Im}(h_0)| \propto L^{\frac{d}{\nu} - d}, \quad (10)$$

where $h_c$ is the magnetic field strength at which the phase transition occurs. We can now determine the Lee-Yang zeros from the simulated fluctuations of the magnetization. The results of this procedure for the Ising lattice with $d = 2$ are shown in Fig. 3a. Above the critical temperature, the Lee-Yang zeros remain complex in the thermodynamic limit, since there is no phase transition. By contrast, at the critical temperature (and also below; not shown), the Lee-Yang zeros reach the real-axis, and we can proceed with the finite-size scaling analysis in Fig. 3b for $d = 2$ and $d = 3$. Using Eq. (10), we then extract the ratio $B/\nu$ of the critical exponents, also known as the scaling dimension, and again find good agreement with existing estimates. We note that from two independent critical exponents we can obtain all other exponents using the hyperscaling relations derived in renormalization group theory [57]. Finally, in Fig. 3c, we show how both the real and imaginary parts of the leading Lee-Yang zeros vanish in the thermodynamic limit, signaling that a phase transition occurs at zero magnetic field.

Conclusions.— We have presented a direct pathway from measured or simulated fluctuations in finite-size systems to the determination of critical points and universal critical exponents of continuous phase transitions. Our method can be applied to a wide range of equilibrium and non-equilibrium phase transitions, including space-time phase transitions in glass formers and dynamical phase transitions in experiments or simulations of engineered many-body systems of finite size. To illustrate the feasibility of our approach, we have determined the critical points and the universal critical exponents of the Ising model from the fluctuations of energy and magnetization in surprisingly small lattices. The critical behavior of the Ising model depends on the dimensionality of the problem as confirmed by our results. Importantly, we can determine the critical points and critical exponents even if the system is away from the phase transition, for example at a high temperature. As such, our method paves the way for investigations of phase transitions that may be hard to reach experimentally, for instance at very low temperatures or at very high pressures. It also opens an avenue for bottom-up experiments on phase transitions, in which nano-scale structures are carefully assembled to increase the system size in a controllable manner. Extending these ideas to the quantum realm constitutes an exciting theoretical challenge for future work.

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