Cumulants, Zeros, and Continuous Phase Transition

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This paper explores the use of a cumulant method to determine the zeros of partition functions for continuous phase transitions. Unlike a first-order transition, with a uniform density of zeros near the transition point, a continuous transition is expected to show a power law dependence of the density with a nontrivial slope for the line of zeros. Different types of models and methods of generating cumulants are used as a testing ground for the method. These include exactly solvable DNA melting problem on hierarchical lattices, heterogeneous DNA melting with randomness in sequence, Monte Carlo simulations for the well-known square lattice Ising model. The method is applicable for closest zeros near the imaginary axis, as these are needed for dynamical quantum phase transitions. In all cases, the method is found to provide the basic information about the transition, and most importantly, avoids root finding methods.

I. INTRODUCTION

Phase transition has been a major playground of statistical mechanics. A phase transition is generically defined as a point of non-analyticity of any quantity of interest, like the free energy for an equilibrium system and developing an understanding of phase transitions is associated with keywords like critical exponents, order parameter, correlation length etc. and not the least the transition point \cite{1}. One of the innovative ways of locating and finding the nature of a transition is the method of finding the zeros of the partition function by allowing the temperature or similar intensive field like quantities to be complex. This method was first incorporated by Lee and Yang to study the liquid-gas phase transition in the complex fugacity plane and the 2d Ising model in the complex magnetic field plane \cite{2,3}. The failure of the cluster expansion method by Mayer and coworkers in describing the properties of the liquid phase, motivated Lee and Yang to study the liquid-gas phase transition. Of late, studies of zeros of partition functions, or its equivalents, have become relevant in many fields, like quantum dynamics, polymers, QCD, and analysis of experimental data, to name a few \cite{4–6}. The method of Lee-Yang zeros are not only confined to cases of equilibrium systems but have also been applied to systems out of equilibrium successfully \cite{7}.

Finding the zeros of the partition function analytically using numerical techniques is not always possible in the thermodynamic limit, due to the increasing level of memory requirement. The zeros can be found as curves, can cover some planar region or can occur in some other complicated fashion. Although the pattern of the zeros can be visually appealing, it is only the zeros near the positive real axis (or the imaginary axis in case of Dynamical Quantum Phase Transition (DQPT) \cite{4}) that bears useful information. Recently, a cumulant method has been proposed to locate the leading zero taking the first order transition of the zipper model of DNA as an example \cite{8}. Although things seem to be pretty well behaved in case of first order transition, it calls for more detailed analysis for cases where zeros simply do not distribute uniformly. It is difficult to realize complex parameters in experiments, which made it hard to observe the Lee-Yang zeros experimentally for quite some time \cite{9–10}. Recently there have been attempts to explore the Lee-Yang zeros of an Ising type spin bath \cite{9}. It has been shown that for continuous transitions, the angle at which the zeros approach the real axis near the limit point, is related to the critical exponent for diverging length, the ratio of specific heat amplitudes on either side of the critical point, and the specific heat exponent \cite{12}.

We look into a detailed study of different types of continuous transitions to study the effectiveness of the cumulant method from different types of data generated such as by exact methods or from Monte Carlo simulation to see to what extent they can provide us with fruitful information. This work is divided in the following order. In Sec. \textsuperscript{11} and Sec. \textsuperscript{11} we have defined our model of dsDNA on the hierarchical lattice and the cumulant method, showing how good it is possible to estimate the critical temperature $\beta_c$ from closest zeros of some lower generations (or smaller system sizes). The second closest zeros are found with some less accuracy and finally, the exponent for diverging length is calculated. In Sec. \textsuperscript{15} we have probed into the problem of a binary random disorder (motivated from the fact that the energy of the two types of bonds in a dsDNA is not the same), by introducing two types of interaction energies randomly. Then, the critical temperature no longer remains unique and forms a distribution. By observing how the width of the distribution varies with the system size, we concluded that there is a unique $T_c$ in the thermodynamic limit. Finally, in the Sec. \textsuperscript{14} and Sec. \textsuperscript{4} we have checked the known results for the well studied Ising model in 2d and discussed how to find the closest zero which meets...
the imaginary axis for Ising model in 1d.

\[ Z = n_{b} \prod_{j=1}^{n-1} y_{j}^{-1} e^{\beta \epsilon_{j}} = n_{b} \prod_{j=1}^{n-1} y_{j}^{-1} \exp \left( \beta \epsilon_{j} \right). \]

FIG. 1: (Color online) The recursive construction of the hierarchical lattice for \( b = 2 \) and \( n = 0, 1, 2, \ldots \) generations.

II. DNA ON HIERARCHICAL LATTICES

On untwisting the helical structure of a dsDNA, it takes the shape of a railway track where the ties represent the bonds shared by the two strands. This structure of bond sharing can be mimicked by putting the two strands on a hierarchical lattice with the two endpoints fixed but they can wander at intermediate points. The lattice is generated iteratively by replacing each bond in the \((n-1)\)th generation with a motif of \( \lambda b \) bonds to get the new \( n \)th generation, where \( \lambda \) and \( b \) are the bond scaling factor and bond branching factor respectively. The effective lattice dimension in the thermodynamic limit will be given by \([13]\)

\[ d = \frac{\ln \lambda b}{\ln \lambda}. \tag{1} \]

In this paper we shall choose \( \lambda = 2 \) and \( b = 4 \). Hierarchical lattice with discrete scaling allows exact implementation of the real space renormalization (RG). Thus one can write down recursion relations for the partition function and the zeros of the partition function. The contact energies are defined to be \(-\epsilon (\epsilon > 0)\) when two strands share a bond. This constitutes our DNA model \([13]\).

It is known that dsDNA undergoes a phase transition from a bounded state to an unbounded state (dsDNA melting) under variation of the temperature field, the critical point being known as the duplex melting point. From RG relations the critical point is found to be \( y^* = b - 1 \), with

\[ y = \exp \left( \epsilon \beta \right) \]

being the Boltzmann factor. Exact recursion relations followed by the single chain \( (C_n) \) and double chain \( (Z_n) \) partition functions can be written as

\[ C_n = bC_{n-1}^{2}, \tag{2} \]

\[ Z_n = b(b-1)C_{n-1}^{3} + bZ_{n-1}^{2}, \tag{3} \]

with the initial conditions taken as

\[ C_0 = 1, \quad Z_0 = y. \tag{4} \]

The zeros of the partition function thus follows the following recursion relation

\[ q = \pm \sqrt{b\tilde{q}_j - (b - 1)}, \tag{5} \]

where \( \tilde{q}_j \) is one of the zero of the \((n-1)\)th generation, giving rise to two new zeros in the \( n \)th generation \([13]\).

III. THE CUMULANT METHOD

We can define cumulant-like quantities where we take derivatives of the logarithm of the partition function with respect to the Boltzmann factor i.e. \( y \) instead of \( \beta \) itself, and study the zeros in the complex \( y \) plane. The \( n \)th order cumulant can be defined as

\[ U_n = (-1)^n \frac{\partial^n \ln Z}{\partial y^n}. \tag{6} \]

The partition function of the dsDNA model on hierarchical lattice is of the form

\[ Z_n = a_0 + a_1 y^2 + \cdots + a_n y^{2n}, \tag{7} \]

which being a polynomial with all of its coefficients positive cannot have any of its zeros as real. According to the Weierstrass factorization theorem any entire function can be written in terms of the product of its zeros \([14]\). Thus, the partition function can be written as

\[ Z_n = a_0 \prod_{k=1}^{2^n} \left( 1 - \frac{y}{y_k} \right), \tag{8} \]

where \( y_k \) is the \( k \)th zero in the complex \( y \) plane and these zeros occur in complex conjugate pairs. Thus the free energy becomes a sum over all the zeros

\[ F = -\beta^{-1} \sum_{k=1}^{2^n} \ln \left( 1 - \frac{y}{y_k} \right) + \ln a_0. \tag{9} \]

The \( n \)th order cumulant is completely expressed by the zeros as

\[ U_n = (-1)^{n-1} \sum_{k=1}^{2^n} \frac{(n-1)!}{(y_k - y)^n}. \tag{10} \]

The cumulants are real quantities since the zeros come in complex conjugate pairs. Eq. (10) can be further reduced to

\[ U_n = 2(-1)^{n-1}(n-1)! \sum_{k=1}^{2^n-1} \cos(n\phi_k) \rho_k^n, \tag{11} \]

where \( \rho_k \) is the distance to the \( k \)th zero from the point on the real \( y \) axis at which cumulants are being calculated and \( \phi_k \) is the angle with the real axis from the cumulant
The closest zeros will be dominated by the closest zero contribution in the higher orders. Thus, from four such successive cumulants in the higher orders we can solve for the leading pair of zeros, \( \rho \) and \( \phi \), using the matrix equation

\[
\begin{bmatrix}
1 - \kappa_n^{(+)} & -2\rho_0 \cos \phi_0 \\
1 - \kappa_n^{(-)} & \rho_0^2
\end{bmatrix} = \left[ (n-1)\kappa_n^{(-)} \right] \left[ n\kappa_{n+1}^{(-)} \right],
\]

(13)

where, \( \kappa_n^{(+)} = U_n^{n+1}/U_n \).

The closest zeros found for a few smaller generations are shown in Fig. 2. Once we have the closest pair of zeros we can calculate approximants \( \tilde{U}_n \) of the cumulants using only the closest pair. Now, in the higher order cumulants the closest zero mostly dominates, while in the lower order other zeros should contribute. It must be somewhere in between that the closest zero takes over and just before that the largest contribution must be from the closest and second closest zeros. Thus, we have to look for this crossover region, which will provide us with an upper bound on the second closest zero. The upper bound, will depend upon the error introduced in calculating the closest pair of zeros, which then propagates in the approximate cumulant calculation only from the closest pair of zeros. Let us consider the region where the \( n \)th cumulant consists mainly of the first and second closest zeros. Then, we may write

\[
U_n = (-1)^{n-1}(n-1)! \left[ \frac{1}{(y_0 - y)^n} + \frac{1}{(y_1 - y)^n} \right] + c.c,
\]

(14)

where \( y \) is the point in the complex \( y \) plane at which the cumulant is being calculated, \( y_0 \) and \( y_1 \) being the closest and second closest zeros respectively. Consider,

\[
y_0 = y_0^* + \delta y,
\]

(15)

where \( y_0^* \) is the exact value of the closest zero, and \( \delta y \) is the error introduced when calculated from the exact higher order cumulants. Then, the \( n \)th order cumulant becomes

\[
U_n = (-1)^{n-1}(n-1)! \left[ \frac{1}{(y_0^* + \delta y - y)^n} + \frac{1}{(y_1 - y)^n} \right] + c.c
\]

(16)

\[
U_n \approx (-1)^{n-1}(n-1)! \left[ \frac{1}{(y_0^* - y)^n} \left( 1 - \frac{n\delta y}{y_0^* - y} \right) + \frac{1}{(y_1 - y)^n} \right] + c.c.
\]

(17)
Subtracting the contribution of the closest zero to the cumulant, we get \( \tilde{U}_n \)

\[
\tilde{U}_n = 2(-1)^{n-1}(n-1)! \left[ \frac{\cos(n\phi_1)}{\rho_1^n} - n |\delta y| \cos((n+1)\phi_0 + \psi) \right],
\]

where \( \psi \) is the phase factor coming from the complex \( \delta y = |\delta y| \exp(-i\psi) \). Now, the first term in Eq. (17) dominates when

\[
n \ll \frac{\ln |\delta y|}{\ln \left( \frac{\rho_1}{\rho_0} \right)}.
\]

This signifies that as \( |\delta y| \to 0 \), \( n \to \infty \) i.e. we can have second closest zero contribution in higher orders also.

In Fig. 4(a) and Fig. 4(b) we plot the real and imaginary parts of the second closest zeros calculated at three different temperatures. Clearly, we did not consider very low order points since all the zeros contribute there. There appears to be a crossover region after which there is a constant contribution which corresponds to the first closest zero. In between, there is a flat plateau which is the region of our interest. Thus, we fit our curve such as to get all the points before the crossover region and up to the flat plateau to find our best value of the second closest zero. The thickness of the shaded region in the flat plateau should serve as an error bar to our value. While the closest zeros can be determined with a decent accuracy of four decimal places for smaller generations, the next to closest pair of zeros can be calculated with somewhat less accuracy of one place after the decimal.

Next, we find the angle at which the zeros meet the real axis in the thermodynamic limit; see Fig. 4(c). For this, we have taken the average of the angles made by the first and second closest zeros with the critical point (since the zeros don’t fall in a smooth straight line, in lower generations) and plotted it with the generation number inverse.

**FIG. 4:** (Color online) (a) The real part of the second closest zero of the 4th generation from different cumulant order \( n \) at three different temperatures, the outermost fitting lines encloses the shaded region. (b) The imaginary part of the second closest zero of the 4th generation from different cumulant order \( n \) at three different temperatures, the outermost fitting lines encloses the shaded region. (c) The angle at which the zeros meet the real \( y \) axis. Estimated value is \( \theta_{\text{estimate}} = 53.87 \), the actual value is \( \theta_{\text{exact}} = 52.646 \). (d) Estimated value for the critical exponent for diverging length is \( \nu_{\text{estimate}} = 1.67 \), exact value is \( \nu_{\text{exact}} = 1.7095 \).
The results vary substantially if we do not include the second closest zero.

This angle contains the information about the order of the phase transition. The angle at which the zeros meet the real $y$ axis is related to the specific heat exponent as

$$
\tan(\phi \nu) = -\tan(\pi \alpha) + \frac{A_-}{A_+} \csc(\pi \alpha),
$$

where $\phi$ is the angle between the tangent of the zeros at the limit point and the real axis of $y$, $\nu$ is the critical exponent for diverging length, $\alpha$ is the specific heat exponent and $A_\pm$ are the amplitudes of the specific heat on the low and high $y$ side of the transition [12]. For our problem with double stranded DNA, it is known that $\frac{A_-}{A_+} \to \infty$ as $A_+ = 0$. Therefore, the angle is given by

$$
\phi = \frac{\pi}{2\nu},
$$

Once we have $\phi$, we can find the critical exponent $\nu$. But in general we need to know $\nu$ separately. To determine $\nu$ one can make use of the RG transformation properties of the Hamiltonian to see how the partition function would change under a scaling [12], and obtain the following scaling equation of the distance of the $k$th zero from the critical point

$$
\Delta_k = k^{\frac{1}{d}} L^{-\frac{1}{\nu}} F^{-1},
$$

where $d$ is the dimension, $\Delta_k$ is the distance of the $k$th zero from the critical point, $L$ is the size of the system and $F^{-1}$ is a constant. To determine $\nu$ we plot $\ln \Delta_k$ vs $\ln L$, for the closest zeros ($k = 1$) for generations $n = 5, 6, 7, 8$; see Fig. 4(d).

Our estimate of the length exponent $\nu_{\text{estimate}} = 1.67$ compares reasonably well with the independent estimate from Eq. (21) which also gives $\nu = 1.67$. The exact value of $\nu_{\text{exact}} = 1.70951$. It might be possible to improve the accuracy of the result by iterative inclusion of other zeros.
The randomness only depends on the longitudinal direction. A simpler situation is a random sequence where the interaction energy is randomly chosen from a specified distribution. With the introduction of randomness, the obvious question is whether a critical point for melting exists. Since the partition function is different for the different random samples and our estimated value from the partition function zeros (black dot) with the boxes (green and red) along the β axis representing the uncertainty. In the thermodynamic limit, the melting temperature is estimated to be βc = 1.23 ± 0.004 from the extrapolation of the closest zeros. Whereas the intersection of the specific heat curves gives the melting temperature to be βc = 1.35 ± 0.03. Although it can be confirmed that there is a unique melting point in the thermodynamic limit, the melting point predicted from the distribution of zeros is different from that calculated from the intersection of specific heat curves for successive generations (Fig. 4(e)).

V. ISING 2D

In the previous sections III and IV we determined the closest zeros as well as the second closest zeros from the higher energy like cumulants of the partition function. There we had the privilege of finding the exact cumulants since the partition function is known exactly. But in simulations, the higher energy cumulants can be calculated more easily, albeit approximately, than finding the partition function. One such example is the two dimensional Ising model. The Hamiltonian for 2d Ising model with interaction between the nearest neighbours in the
absence of an external magnetic field is

$$\beta \mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j,$$  \tag{23}$$

where $\sigma_i \in \{-1,1\}$ is the spin at site $i$, $J$ is the coupling constant between neighboring spins and $\langle ij \rangle$ indicates nearest neighbors. It is known that for such a two-dimensional spin system there is a phase transition from paramagnetic to ferromagnetic phase at finite temperature. The energy cumulants were calculated from the energy moments which in turn was calculated from Monte-Carlo simulation and then using Mathematica \cite{14}, we found the expression for $n$th order cumulant in terms of the moments. Since our aim throughout this work had been to determine quantities in the thermodynamic limit by studying the zeros of small system size, we have calculated the zeros for $n \times n$ square lattices with $n = 5, 6, 7, 8, 9, 10, 11$, on the complex $\beta$ plane and then extrapolated the results to the infinite limit. To find the zeros we have calculated up to 30th moment of energy using quadruple precision data type.

Fig. \textbf{6}a) shows the transition point of the 2d Ising model in the absence of any external magnetic field in the thermodynamic limit on the complex inverse temperature plane $\beta_c$. Fig. \textbf{6}b) shows that the imaginary part of the closest zero goes to zero in the thermodynamic limit indicating a phase transition. Fig. \textbf{6}c) shows how the distance between the closest zeros and the transition point scales with the system size. The inverse of the slope of the fitting line gives the critical exponent $\nu$ for the diverging correlation length according to the Eq \text{(22)}.

Results for the 2d Ising model was found to be in excellent agreement with the exact results. Below given is a table for comparison with exact results in the thermodynamic limit.

| | $\mathbb{R}_c\beta$ | $\mathbb{I}_c\beta$ | $\nu$ |
|---|---|---|---|
| Estimated | 0.445 | 0.003 | 1.01 |
| Exact | 0.44068 | 0.0000 | 1.0 |

VI. IMAGINARY ZEROS IN ISING 1D

Motivated by the fact that a phase transition can happen with time as a parameter in case of DQPT where the zeros meet on the imaginary axis, we have found the zeros closest to the imaginary axis, for the 1d Ising model which do not have any transition at any non zero temperature \cite{2}. The partition function of the 1d Ising model is exactly known to be:

$$Z = \lambda_+^N + \lambda_-^N,$$  \tag{24}$$

where $\lambda_\pm$ are the eigenvalues of the transfer matrix and $N$ is the number of spins.

In absence of any external magnetic field, the eigenvalues become

$$\lambda_\pm = e^{\kappa} \pm e^{-\kappa},$$  \tag{25}$$

where $\kappa = \frac{J}{k_B T}$ and the zeros of the partition function on the complex $\kappa$ plane are found to be

$$\kappa = \frac{1}{2} \log \left[-i \tan \left(\frac{(2n + 1)\pi}{2N}\right)\right],$$  \tag{26}$$

with $n = 0, 1, 2 \cdots N - 1$. The zeros in the complex $\kappa$ plane are not distributed symmetrically for all the lengths. Symmetrical distribution about the imaginary axis is only to be found for systems with size $N = 4, 8, 12, 16$. For all other sizes, zeros either fall on
the imaginary axis or distributes asymmetrically. While finding the zeros using the cumulant method at a point on the imaginary $\kappa$ axis, it is found that it works only for zeros with a symmetrical distribution.

Assuming a symmetric distribution about the imaginary axis, since the free energy is a real quantity, we can write

$$F = -\beta^{-1} \ln (ZZ^*),$$

where the $Z$ and $Z^*$ are the partition functions evaluated at a complex temperature and its complex conjugate respectively so that the free energy is real. In terms of zeros of the complex $\kappa$ plane:

$$F = \ln \left[ \prod_{j} (\kappa_j - i\kappa) \prod_{l} (\kappa_l + i\kappa) \right].$$

The $n$-th cumulant expression

$$U_n = (-\partial_{\kappa})^n \ln(ZZ^*)$$

$$= (-\partial_{\kappa})^n \ln \left[ \prod_{j} (\kappa_j - i\kappa) \prod_{l} (\kappa_l + i\kappa) \right]$$

Retaining only the terms of the closest zeros

$$U_n \approx (-\partial_{\kappa})^n [\ln (\kappa_1 - i\kappa) + \ln (\kappa_2 - i\kappa) + \ln (\kappa_1^* + i\kappa) + \ln (\kappa_2^* + i\kappa)]$$

$$U_n = 4(-1)^{n-1} (n-1)! \frac{\cos(n\phi_0)}{(i\rho_0)^n},$$

which requires a little modification of the matrix equation by simply putting $i\rho_0$ instead of $\rho_0$. Here, $\phi_0$ is the angle made by the vector extending from the cumulant calculating point on the imaginary axis to the zero closest to the imaginary axis and the imaginary axis itself. The zeros meet the imaginary axis periodically due to the presence of the $-i$ factor inside log in Eq (26). The schematic diagram on Fig. 8 shows how the determination of the closest zeros along the imaginary axis is possible only if we choose the cumulants calculating point judiciously. The closest zeros for different branches lies at a distance of $\pi/4$ along the imaginary $\kappa$ axis. The shaded regions on Fig. 8 for example represents points along the imaginary $\kappa$ axis where if we choose our cumulants calculating point, would give the closest zero of that particular branch (shown by the blackened top of that shaded region).

VII. SUMMARY

To summarize, we have found the leading pair of zeros of the partition function for a dsDNA on hierarchical lattice where the zeros are exactly solvable as well as for disordered case. We have chosen such a system to have a good comparison with the exact results. The results found out to be matching well enough with the theoretical exact results, thus giving us a new way to look into systems in the thermodynamic limit from smaller system sizes. Although the zeros from the lower generations may not always be helpful, still it proved to be quite a powerful method. Moreover, it is shown that results from Monte Carlo simulation proved to be equally good to reproduce the known results for the critical exponent and critical point estimation for the case of Ising model in 2d and 1d as well, through this cumulant method.

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