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Exact partition function zeros and the collapse transition of a two-dimensional lattice polymer

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We study the collapse transition of the lattice homopolymer on a square lattice by calculating the exact partition function zeros. The exact partition function is obtained by enumerating the number of possible conformations for each energy value, and the exact distributions of the partition function zeros are found in the complex temperature plane by solving a polynomial equation. We observe that the locus of zeros closes in on the positive real axis as the chain length increases, providing the evidence for the onset of the collapse transition. By analyzing the scaling behavior of the first zero with the polymer length, we estimate the transition temperature T_θ and the crossover exponent ϕ. © *2010 American Institute of Physics*. [doi:10.1063/1.3486176]

I. INTRODUCTION

The hydrophobic interaction and the excluded volume effect are two main interactions that determine the conformation of a polymer in a dilute solution, in space dimension $d < 4$.[1] In the good solvent regime, the repulsive excluded volume effect is the dominating factor and the mean end-to-end distance R_N of a polymer chain with N monomers asymptotically grows as $\langle R_N^2 \rangle \sim N^{6/(d+2)}$, the behavior of a self-avoiding random walk. On the other hand, the poor solvent regime is defined by the property that the attractive hydrophobic interaction between monomers dominates, where the scaling behavior is $\langle R_N^2 \rangle \sim N^{2/d}$. The situation is usually described by the statement that the polymer adopts a swollen conformation in a good solvent and the collapsed one in a poor solvent. The solvent where the repulsive and attractive interactions cancel each other is called the theta solvent, with the corresponding temperature being called the theta temperature, or the Flory temperature, T_θ.[2] T_θ is the temperature where the condition of the solvent changes from good to poor or *vice versa* and the collapse transition occurs. The collapse transition has been studied and the critical exponents have been calculated using various theoretical and computational methods,[3–24] including lattice models.[9–24] In particular, the self-avoiding walk on a square lattice has been extensively studied as a model for the polymer in two dimensions, and its collapse transition has been studied using exact enumeration[11,12] and Monte Carlo samplings.[9,10,15–24]

Alternatively, phase transitions can be studied by calculating partition function zeros. The study of partition function zeros was initiated by the seminal paper of Yang and Lee,[25] where the zeros in the complex fugacity plane were studied to give a new insight on the phase transition. Subsequently the zeros in the complex temperature plane were studied by Fisher.[26] With the recent advancement of computational power, the study of partition function zeros became one the most popular methods for studying the phase transition and critical phenomena,[27] and was used to study helix-coil transition of polyalanine[28] and folding transition of a simple model protein.[29] However, it was rarely used for the study of lattice polymers, although some preliminary qualitative results on collapse transition were reported for both homopolymers[30] and heteropolymers.[29,31]

The power of the partition function zeros method lies in its sensitivity to the onset of a phase transition. When the energy takes discrete values, the partition function Z is expressed as

$$Z = \sum_E n(E) e^{-\beta E}, \tag{1}$$

with $n(E)$ being the number of states with energy E. When Z is a function of $y \equiv e^{\beta\epsilon}$ with some interaction parameter ϵ, such as when E values are integer multiples of ϵ, the partition function can be expressed in the form

$$Z(y) = A(y) \prod_i (y - y_i), \tag{2}$$

where $A(y)$ is a function which is analytic in the whole complex plane and y_is are the complex roots of the equation $Z(y)=0$, called the partition function zeros. Since Z is real, y_i's form conjugate pairs except for the real-valued ones. By taking log and derivatives, one obtains the specific heat,

$$C_N(T) = \frac{k_B}{N} (\ln y)^2 \left[\sum_i \left\{ \frac{y}{y - y_i} - \left(\frac{y}{y - y_i} \right)^2 \right\} + \left(y \frac{d}{dy} \right)^2 \ln A(y) \right], \tag{3}$$

where N is the size parameter of the system such as the particle number. For a system with the phase transition at

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$y = y_c$, the locus of the zeros close in toward the positive real axis to intersect it at $N = \infty$, and the singularity of $C_N(T)$ appears in this limit. It is clear from Eq. (3) that the leading behavior of such a singularity is due to the pair of partition function zeros closest to the real axis, called the first zeros. Therefore, by calculating the partition function zeros and examining the behavior of the first zeros as $N \to \infty$, the critical behavior can be much more accurately analyzed than examining the behavior of $C_N(T)$ for real values of the temperature, which is plagued by the noise due to the subleading terms containing zeros other than the first ones.

In this work, we calculate the exact partition function zeros of the polymers on the square lattice up to the length $N = 36$, and make extrapolation of the first zero positions to estimate the collapse transition temperature T_θ and the crossover exponent ϕ (see the next section for the definition). The fact that our calculation is exact, along with the sensitivity of the partition function zeros method, allows us to estimate these quantities with reasonably high accuracy.

II. THE SCALING BEHAVIOR AND THE CRITICAL EXPONENT

The collapse transition is described by the scaling behavior of R_N near the critical temperature,[6]

$$\langle R_N^2 \rangle \sim N^{2\nu} f(\tau N^{\phi}), \tag{4}$$

where $\tau \equiv (T - T_\theta)/T_\theta$ is the reduced temperature and $f(x)$ is a function with the property

$$f(0) = 1,$$

$$f(x) = \begin{cases} x^{\mu_+} & (x \to \infty) \\ x^{\mu_-} & (x \to -\infty), \end{cases} \tag{5}$$

with $\mu_\pm$ being exponents that reproduce the scaling behavior of R_N^2 in the good and poor solvent regime,

$$\mu_+ = \frac{6/(d+2) - 2\nu}{\phi},$$

$$\mu_- = \frac{2/d - 2\nu}{\phi}. \tag{6}$$

In most of the studies on lattice models, the transition temperature and the critical exponents were usually obtained by examining the behavior of $\langle R_N^2 \rangle$ as a function of N and T and fitting to Eq. (4), but they could also be obtained from the scaling behavior of the specific heat,[17,24]

$$C_N(T) \sim N^{\alpha\phi} g(\tau N^{\phi}), \tag{7}$$

with

$$g(x) = \begin{cases} A^{+} x^{-\alpha} & (x \to \infty) \\ \text{const} & (x = 0) \\ A^{-} x^{-\alpha} & (x \to -\infty). \end{cases} \tag{8}$$

The crossover exponent ϕ measures how rapidly the system undergoes the transition as the temperature approaches the critical temperature T_θ. As will be shown later, it is directly related to the exponent that measures how rapidly the first zeros approach the positive real axis as $N \to \infty$.

III. THE MODEL

A conformation of a polymer chain with N monomers is modeled as a two-dimensional self-avoiding chain of length N on a square lattice. The position of the monomer i is given by $\mathbf{r}_i = (k, l)$, where integers k and l are the Cartesian coordinates relative to an arbitrary origin. Chain connectivity requires $|\mathbf{r}_i - \mathbf{r}_{i+1}| = 1$, i.e., bond length is unity. Due to the excluded volume, there can be no more than one monomer on each lattice site, $\mathbf{r}_i \neq \mathbf{r}_j$ for $i \neq j$. The attractive hydrophobic interaction is incorporated by assigning the energy $-\epsilon < 0$ for each nonbonded contact between monomers. The resulting Hamiltonian is

$$\mathcal{H} = -\epsilon \sum_{i<j} \Delta(\mathbf{r}_i, \mathbf{r}_j), \tag{9}$$

where

$$\Delta(\mathbf{r}_i, \mathbf{r}_j) = \begin{cases} 1 & (|i-j| > 1 \quad \text{and} \quad |\mathbf{r}_i - \mathbf{r}_j| = 1) \\ 0 & (\text{otherwise}). \end{cases} \tag{10}$$

Since the energy of the system is $E = -\epsilon K$, where K is the number of monomer-monomer contacts, the partition function is expressed as a polynomial,

$$Z = \sum_{K=0}^{K_{\max}(N)} \Omega_N(K) y^K, \tag{11}$$

where $y \equiv \exp(\beta\epsilon)$, $\Omega_N(K)$ is the number of polymer conformations with contact number K, and $K_{\max}(N)$ is the maximum number of possible contacts, when polymer length is N,[32]

$$K_{\max}(N) = \begin{cases} N - 2m & \text{for } m^2 < N \leq m(m+1) \\ N - 2m - 1 & \text{for } m(m+1) < N \leq (m+1)^2, \end{cases} \tag{12}$$

where m is a positive integer. Therefore the partition function zeros can be obtained by enumerating the number of conformations $\Omega_N(K)$ for each contact number K. The speed of enumeration can be increased by calculating the reduced number of conformations $\omega_N(K)$, where conformations related by rigid rotations, reflections, and translations are regarded as equivalent and counted only once. However, it is assumed that there is an intrinsic direction in the chain so the conformations related by the exchange of labels $i \leftrightarrow N - i + 1$ for all $(i = 1, \cdots, N)$ are considered distinct. We note that since the rigid rotations and reflections in two dimensions form an eightfold symmetry, the total number of conformations generated by rotations and reflections from a given two-dimensional conformation is eight. An exception is the straight chain, a one-dimensional conformation invariant with respect to reflection perpendicular to the chain. Consequently, the total number of conformations generated by rotations and reflections is four in this case. Therefore, the

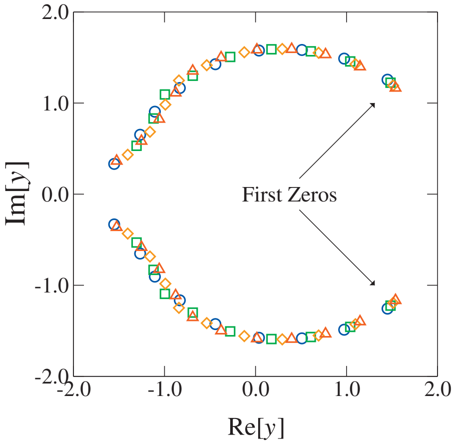

FIG. 1. Positions of the partition function zeros in the complex temperature ($y=e^{\beta\epsilon}$) plane for $N=30$ (circles), 32 (squares), 34 (diamonds), and 36 (triangles). The first zeros are the ones closest to the positive real axis.

number of conformations with rigid rotations and reflections considered distinct, denoted by $\Omega_N(K)$, can be easily obtained by

$$\begin{aligned}\Omega_N(0) &= 8\omega_N(0)-4,\\ \Omega_N(K) &= 8\omega_N(K) \quad (K>0).\end{aligned} \tag{13}$$

Using a parallel algorithm that classifies each conformation according to the size of box it spans,[33] we could calculate $\omega_N(K)$ up to $N=36$. The same quantities were calculated up to $N=28$ in earlier works,[30,32] which agree with the current results.

IV. PARTITION FUNCTION ZEROS

The partition function zeros were obtained by solving the polynomial equation

$$Z=\sum_{K=0}^{K_{\max}(N)} \Omega_N(K)y^K=0, \tag{14}$$

using MATHEMATICA. We observe that the partition function zeros fall on a simple locus, more or less independent of the polymer length N (Fig. 1).

Although there is a relatively large gap between the positive real axis and the first zeros by visual inspection (Fig. 1), the first zeros approach the positive real axis (Fig. 2), and the transition temperature and the crossover exponent can be calculated from their behavior in the $N\to\infty$ limit. However, an oscillatory behavior is observed due to the fact that there are classes of conformations whose numbers depend crucially on the parity of N. For example, there is only one hairpin conformation when N is even, but there are two possible conformations for odd N (Fig. 3). Therefore N's for each parity are used separately when $N\to\infty$ limit is taken so that the large error due to the oscillatory behavior is eliminated.

The crossover exponent ϕ can be obtained from examining how fast the first zeros approach the positive real axis as N increases.[34] From the scaling relation Eq. (7), we see that the partition function scales as

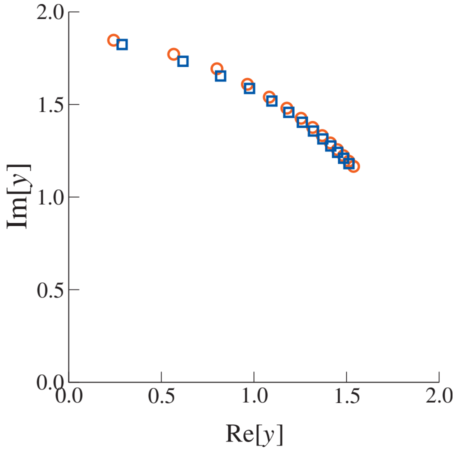

FIG. 2. Positions of the first zeros in the first quadrant of the complex temperature ($y=e^{\beta\epsilon}$) plane for even lengths $N=10,12,14,\ldots,36$ (circles) and for odd lengths $N=11,13,15,\ldots,35$ (squares) from left to right. The first zeros approach the positive real axis as N increases.

$$\ln Z_N(\tau) \sim N^{\alpha\phi-2\phi}g(\tau N^{\phi}) \tag{15}$$

and the equation for the first zero in the first quadrant

$$Z(\tau_1)=0 \tag{16}$$

is invariant with changing N only if

$$\tau_1 \sim N^{-\phi}, \tag{17}$$

which is related to the corresponding complex temperature t_1 as

$$\tau_1 \equiv \frac{t_1-T_\theta}{T_\theta}. \tag{18}$$

In terms of t_1, Eq. (17) is re-expressed as

$$t_1 \sim T_\theta + \text{const} \times N^{-\phi} \tag{19}$$

which is asymptotically equivalent to

$$y_1 \sim y_c + \text{const} \times N^{-\phi} \tag{20}$$

in the large N limit, where $y_1=e^{\epsilon/t_1}$ and $y_c=e^{\epsilon/T_\theta}$. From the imaginary part of Eq. (20),

$$\text{Im}[y_1(N)] \sim N^{-\phi}, \tag{21}$$

the finite-size approximation of the crossover exponent is obtained,

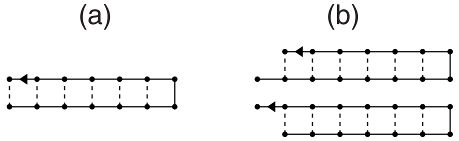

FIG. 3. The hairpin as an example of the class of conformations whose number depends crucially on the parity of N. There is only one conformation for even N (a), whereas there are two possible conformations for odd N (b). Note that there is an intrinsic direction in a chain, indicated by an arrow. The dashed lines indicate the intermonomer contacts.

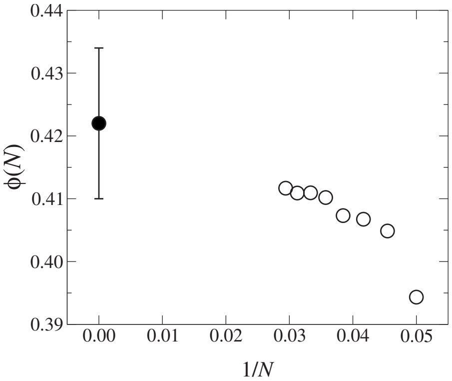

FIG. 4. The finite size approximations of the crossover exponent, $\phi(N)$, are shown as a function of $1/N$ for even N with $N \geq 20$ (open circles), and the value of ϕ at infinite size obtained by the BST extrapolation is indicated by a solid circle with an error bar.

$$\phi(N) = -\frac{\ln\{\mathrm{Im}[y_1(N+2)]/\mathrm{Im}[y_1(N)]\}}{\ln\{(N+2)/N\}}. \tag{22}$$

The expression Eq. (22) reduces to the exact value of ϕ in the $N \to \infty$ limit, which is estimated by using the Bulirsch–Stoer (BST) extrapolation.[35–37] For given m data points corresponding to distinct values of N, the BST extrapolation is performed by constructing a rational function of $(1/N)^{\omega}$ that passes through all of these points, under the assumption that the leading finite-size correction is of order $O((1/N)^{\omega})$. Then, the extrapolated value is obtained by evaluating the function at $1/N=0$. The estimated error is defined as[38–40]

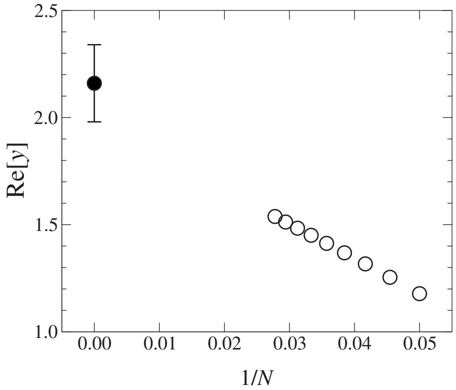

FIG. 5. Values of the real part of the first zeros are shown as a function of $1/N$ for even N with $N \geq 20$ (open circles), and the value for $N \to \infty$ obtained by the BST extrapolation is indicated by a solid circle with an error bar.

$$2|\phi_{-1} - \phi_{-m}|, \tag{23}$$

where ϕ_{-i} is the value of ϕ at $1/N=0$ extrapolated from the data with the eliminated ith point. The estimated error is the measure for the robustness of the extrapolated value with respect to perturbations in the data points, but it has no statistically rigorous confidence level associated with it. The estimated error can be further reduced by removing unreliable data obtained from $N < 20$, and the final result is

$$\phi = 0.422(12) \tag{24}$$

obtained from the data for even N with $20 \leq N \leq 36$. In the absence of additional information, we assumed that the lead-

TABLE I. The critical temperature T_θ and the crossover exponent ϕ obtained in the current work, displayed in the first line, are compared with those in literature. T_θ is displayed only for the model of the current work. The results that agree with ours within the estimated errors are indicated by boldface letters.

Method	Lattice	$N_{\max}$	T_θ/ϵ	ϕ
Exact partition function zeros	Square	36	**1.30(17)**	**0.422(12)**
Field theory[a]	N/A	N/A	⋯	$\frac{7}{11}$(≈0.64)
Renormalization group[b]	N/A	N/A	⋯	$\frac{19}{22}$(≈0.86)
Monte Carlo[c]	Square	160	**1.31(6)**	⋯
Monte Carlo[d]	Square	200	**1.55(15)**	0.6(1)
Transfer matrix[e]	Square	N/A	**1.42(4)**	**0.48(7)**
Series expansion[f]	Triangular	16	⋯	0.64(5)
Coulomb gas method[g]	Hexagonal	N/A	⋯	$\frac{3}{7}$(≈0.43)
Monte Carlo and renormalization group[h]	Square	40	**1.54(7)**	0.52(7)
Monte Carlo[i]	Hexagonal	300	⋯	**0.5(1)**
Scanning simulation[j]	Square	240	1.52(1)	0.530(4)
Recursive enrichment method[k]	Square	2048	1.504(5)	**0.435(6)**
The pruned-enriched Rosenbluth method[l]	Square	256	1.4993(23)	⋯
Interacting growth walk[m]	Square	2000	⋯	**0.419(3)**
Monte Carlo[n]	Square	1600	1.50	0.545(4)
Monte Carlo[o]	Square	300	1.505(18)	⋯
Monte Carlo[p]	Square[q]	20	⋯	**0.436(7)**

[a] Reference 7.
[b] Reference 8.
[c] Reference 9.
[d] Reference 10.
[e] References 11 and 12.
[f] Reference 13.
[g] Reference 14.
[h] Reference 15.
[i] Reference 16.
[j] Reference 17.
[k] Reference 18.
[l] Reference 19.
[m] Reference 20.
[n] Reference 21.
[o] Reference 22.
[p] Reference 23.
[q] A model with explicit solvent molecules. Different from the model studied in this work.

ing finite size correction to ϕ is of order $O(N^{-1})$ when performing the BST procedure, but extrapolated value of ϕ does not seem to depend much on this assumption (data not shown).

Once the value of ϕ is determined, the transition temperature T_θ can be obtained by estimating the point on the positive real axis where the first zeros approach in the limit of $N \to \infty$, applying the BST extrapolation procedure to the real part of Eq. (20),

$$\mathrm{Re}[y_1(N)] - y_c \sim N^{-\phi}. \tag{25}$$

The resulting value of y_c is 2.16(18), equivalent to $T_\theta/\epsilon = 1.30(17)$, where again, the data for even N with $20 \leq N \leq 36$ were used.

The finite value approximations of ϕ and y_c are displayed in Figs. 4 and 5 as functions of $1/N$, along with their extrapolated values at $1/N=0$. The extrapolated value of y_c in Fig. 5 is larger than obtained by drawing a straight line through the data points because we assumed the leading behavior of $y-y_c$ being proportional to $(1/N)^{0.422}$. There is no change of the extrapolated value of T_θ under the current precision when we use the conjectured exact value of the crossover exponent $\phi=3/7$ (Ref. 14) instead of $\phi=0.422$. The values obtained in the current study are compared with those from the earlier works in Table I. Since T_θ/ϵ is not a universal quantity, it is displayed only for the square lattice polymer with nearest neighbor interaction. The maximum sizes of the polymer studied, $N_{\max}$, are displayed wherever applicable. The results of the current study are given in the first line of Table I. Although there are variations in the results reported earlier, we find that many of them are consistent with ours. Those that agree with our results within the estimated errors are indicated by boldface letters. In particular, it should be noted that the value of ϕ obtained in the current work agrees quite well with the exact value 3/7 obtained by analytic calculation on the polymers on the hexagonal lattice,[14] which is believed to be in the same universality class as those on the square lattice.[18,20,22,23]

V. DISCUSSION

We studied the zeros of the exact partition function of lattice polymers on square lattices up to chain length 36 by exhaustively enumerating the number of all possible conformations. We observed that the first zeros tend to approach the positive real axis as the chain length increases, and estimated the critical temperature T_θ and the crossover exponent ϕ by the BST extrapolation.

In contrast to Monte Carlo approaches where the calculation can be done for polymer lengths up to several hundreds or thousands, the chain length studied in the current study is much shorter, but the exactness of our data allows us to use powerful extrapolation methods, leading to a reasonably accurate estimation of the transition temperature and the crossover exponent. Furthermore, by studying the complex zeros of the partition function zeros, instead of examining the scaling behavior of real-valued quantities such as radius of gyration or specific heat, much more accurate analysis of the phase transition could be performed.

It is of immediate interest to perform the exact enumeration of polymer conformations up to sizes where the approach of the first zeros toward the positive real axis is more visible. An exact enumeration has been performed using a transfer matrix for length up to 72 at infinite temperature,[41] and it would be interesting to see whether it can be generalized to count the number of conformations for each energy without introducing too much extra computational costs in order to calculate the partition function zeros. One could also combine Monte Carlo methods with the partition function zeros to increase the polymer size, at the cost of introducing sampling error. There are indications that the locations of the first zeros are robust with respect to the sampling errors, a point that needs further investigation.[42]

As a final remark, the partition function zeros method may be applied to study the transition behavior of heteropolymers,[29,31] related to the very important and interesting topic of protein folding. In contrast to homopolymers, the definition of large N limit is not so clear for a heteropolymer so the finite size scaling argument such as the one used in the current study cannot be applied directly. Various methods to extract information relevant to the collapse and the folding transition, from the complex partition function zeros, will have to be explored.

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