Partition Function Zeros in Two-Dimensional Lattice Models of the Polymer 0-Point

Vladimir Privman* and Douglas A. Kurtze

Department of Physics, Clarkson University, Potsdam, New York 13676.
Received February 21, 1986

ABSTRACT: We report studies of the partition function zeros in lattice models of interacting self-avoiding walks on the triangular and square lattices. The complex Boltzmann factor-plane zeros show a pattern similar to isotropic lattice spin models. For increasing length of the walks, zeros approach the real axis along a unique locus at the point which can be identified with the "tricritical" singularity, particularly by its location, which is consistent with the 0-point values found in other numerical studies.

We report studies of the partition function zeros in the self-avoiding walk (SAW) model with nearest-neighbor bond interactions on the square (SQ) and triangular (TR) lattices. This lattice model1 is believed to have a "tricritical" 0-point transition.2,3 Let c(N,B) denote the number of N-step SAW having exactly B nearest-neighbor-site pairs. The partition function for fixed N is defined by

\[ Z_N = \sum_B c(N,B) B^{-N} \quad (1) \]

where \( B \) runs from \( N \) to some \( N \)-dependent maximum value. The Boltzmann factor \( \epsilon > 0 \) is assigned per each nearest-neighbor bond contact in excess of the \( N \) bonds of the walk itself. It is expected that as \( N \to \infty \), thermodynamic quantities become singular at the 0-point value, \( \epsilon_0 > 1 \). For \( 0 < \epsilon < \epsilon_0 \), the swollen, proper SAW behavior is anticipated. For \( \epsilon > \epsilon_0 \), the chains would be collapsed, globular. Near the borderline value, \( \epsilon_0 \), "tricritical" scaling forms have been proposed2,3 and substantiated by several field-theoretical epsilon-expansion studies.4,5

Numerical efforts to verify the theoretical picture have encountered technical difficulties. Since \( d = 3 \) is the upper critical dimension,4 logarithmic factors complicate \( d = 3 \) scaling behaviors. Monte Carlo (MC) studies seem more or less consistent with the theory: see ref 8-10 and literature cited therein. However, series analyses by Rapaport4 generally contradicted the "tricritical" theory: he found no exponent universality in the SAW and the collapsed regimes. More recently, attention has turned to the two-dimensional systems, which have no "logarithmic" complications. The interest in the physics of the 0-point in \( d = 2 \) is more than academic: \( d = 2 \) polymeric systems in the semicollapsed regime have been realized and studied experimentally.12-15 It seems, however, that the experimental data available to date do not fit well within the "tricritical" theoretical picture. Numerical MC16-18 and transfer matrix19 studies of the SQ-lattice model of interacting SAW described above are generally consistent with tricritical scaling predictions. However, the exponent estimates18,19 obtained by these techniques and also by series analysis methods20,21 are rather spread and inconsistent with some of the experimental13 or analytic22 values.

Our study of the zeros in the complex-\( \epsilon \) plane of the partition function, \( Z_N(\epsilon) \), is intended mainly to establish that their pattern is of a typical form observed for several isotropic lattice spin models with a unique transition, in the complex temperature plane: see ref 23-29 and literature cited therein. For a review of the Yang–Lee zeros in the complex-\( T \) plane, see ref 30 and 31. For anisotropic models, the pattern is distinctively different.23,24 For the interacting SAW model in three dimensions, Rapaport21 calculated location of zeros but could not draw definite conclusions from their \( N \) dependence. However, these complex-plane sequences were far the most regular set of approximants that he11 calculated. We find, in \( d = 2 \), that the partition function zeros behave much more smoothly than other sequences of approximants to various quantities used in ref 20 and 21. The zeros can be used to estimate \( \epsilon_0 \). Unfortunately, accurate estimation of other, universal critical-point quantities, which is theoretically possible,28 seems unfeasible with the existing data.

The values of \( c(N,B;SQ) \) are listed in ref 20 for \( N \leq 20 \), while \( c(N,B;TR) \) have been enumerated21 to order \( N \leq 16 \). We generated the SQ-lattice data to order 21: in Table I we list \( c(21,B;SQ) \). (We actually obtained \( c(SQ) \) for all \( N \leq 21 \).) We used these computer-generated values, checking only a few representative ones against ref 20.) Generally21 the TR-lattice data provide better approximant sequences, in view of the presence of strong even-odd oscillations in the SQ-lattice results. The value of \( \epsilon_0(\text{TR}) \) has been estimated:21

\[ \epsilon_0(\text{TR}) = 1.5 \pm 0.1 \quad (2) \]

For \( \epsilon_0(\text{SQ}) \), the phenomenological renormalization estimate19 \( \epsilon_0(\text{SQ}) = 2.02 \pm 0.04 \), the MC range17 \( \epsilon_0(\text{SQ}) = 2.15 \pm 0.075 \), and the series analysis suggestion20 \( \epsilon_0(\text{SQ}) \sim 2.1 \) are partially inconsistent. We will assume for reference the range

\[ 1.98 < \epsilon_0(\text{SQ}) < 2.22 \quad (3) \]

Complex zeros of \( Z_{16}(\epsilon;\text{TR}) \) are plotted in Figure 1, where we use the notation

\[ \epsilon = x + iy \quad (4) \]

The pattern here is very typical for all \( N \leq 16 \) and also for the SQ lattice. The \( x \equiv \text{Re} \) (\( \epsilon \)) > 0 ray is always free from zeros since \( c(N,B) > 0 \). For given \( N \), a majority of zeros form a claw-shaped structure enclosing the origin of the \( \epsilon \) plane. The "claw" closes on the part of the real-\( \epsilon \) axis between \( x \sim -1 \) and a point which, theoretically, must be at \( x = \epsilon_0 > 1 \). The two complex conjugate arms which trap part of the real axis "grow" as \( N \) increases. There is, however, a definite locus which remains well away from

0024-9297/86/2219-2377$01.50/0 © 1986 American Chemical Society
This pattern is typical for isotropic spin-lattice models with a unique singularity point. All the zeros of $Z_N(c; TR)$ for $N \leq 16$ (only zeros having $x > -0.5$ are displayed). The $x$ coordinates increase monotonically with $N$ within each sequence. The range of eq 2 is indicated on the real axis.

To see that the trapping occurs at the unique point $x = \epsilon_0$, let us first plot in Figure 2 those zeros of $Z_N(c; TR)$ for $N = 5, ..., 16$ that satisfy $x > -1.5$, $y > 0$. All the $x > -2$, $y > 0$ zeros of $Z_N(c; SQ)$ for $N = 6, ..., 21$ are shown in Figure 3. Indeed, the distribution of zeros in Figures 2 and 3 shows no tendency to approach the $x > 0$ ray, except perhaps by its rightmost end. This pattern is typical for isotropic spin-lattice models with a unique singularity point.

From now on, we concentrate on the rightmost zero (maximal $x$) and the one next to it (next-to-maximal $x$) for each $N$. We will analyze the trend in $x$ and $y$ of these zeros as $N$ increases. The location of this subset of zeros is shown in Figures 4 and 5 for the TR and the SQ lattices, respectively. By using Figures 4 and 5, one can also easily identify these sequences of zeros in Figures 2 and 3. The TR-lattice zeros, shown in Figure 4, behave smoothly and seem to close systematically on the real axis at the location consistent with the $\epsilon_r$ range of eq 2. The SQ-lattice data (Figure 5) have the usual even–odd oscillations; however, the points do seem to move toward the $\epsilon_r$ range of eq 3.

In Figures 6 and 7 we plotted the real parts, $x_N$, of the rightmost and the following zeros vs. $1/N$ for the TR and the SQ lattice, respectively. The data sequences extrapolate linearly to ranges of eq 2 and 3 of $\epsilon_r$. On the other hand, the basic scaling combination at the 3-point, $N^{\phi}(\epsilon - \epsilon_r)$, entails the crossover exponent $\phi$. Extending the scaling ansatz to the complex plane would lead to the convergence laws

$$x_N = \epsilon_1 + AN^{\phi} + ...$$  \hspace{1cm} (5)

$$y_N = BN^{\phi} + ...$$ \hspace{1cm} (6)

The crossover exponent has been estimated\textsuperscript{21} by series analysis techniques

$$\phi = 0.64 \pm 0.05$$ \hspace{1cm} (7)

This range is consistent with epsilon-expansion\textsuperscript{5,6,7} and MC\textsuperscript{10} values ($\phi \approx 0.636$ and $\phi \sim 0.6$, respectively). The observed nearly linear convergence of the real parts, $x_N$, in Figures 6 and 7 suggests that the coefficient $A$ of the leading contribution to $(x_N - \epsilon)$ in eq 5 is small or zero for both lattices. To investigate the "scaling" term in the
imaginary part (eq 6), we plotted in Figure 8, the effective \( \phi \) estimates

\[
\phi_N = \ln \left( y_N/y_{N-1} \right) / \ln \left( (N-1)/N \right)
\]

vs. \( 1/N \), for the TR lattice. The values for \( N \leq 16 \) are below 0.64, but their trend in Figure 8 is consistent with them extrapolating toward the range of eq 7 as \( N \to \infty \). Study of the SQ-lattice data with \( N - 1 \) replaced by \( N - 2 \) in eq 8 produced irregular sequences (all \( \phi_N < 0.64 \) for \( N \leq 21 \)) which, however, show an upward trend similar to the TR-lattice results.

Having an infinite-slope locus is not inconsistent with the trend in Figures 4 and 5. By the general considerations of ref 28, the 90° angle implies equal specific heat divergence amplitudes below and above the \( \epsilon_c \). The available data, however, are not sufficient to conclusively substantiate this possibility.

In summary, our study of the partition function zeros in the \( d = 2 \) O-point lattice model provides a convincing indication of the existence of a unique transition point at the location consistent with that found in other, "real-axis" numerical studies.

Acknowledgment. We acknowledge instructive discussions with Professor L. S. Schulman.

References and Notes

(18) Birshtein, T. M.; Buldyrev, S. V.; Eryashevich, A. M. Polymer 1985, 26, 1814.