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Worms exploring geometrical features of phase transitions

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Abstract

The loop-gas approach to statistical physics provides an alternative, geometrical description of phase transitions in terms of line-like objects. The resulting statistical random-graph ensemble composed of loops and (open) chains can be efficiently generated by Monte Carlo simulations using the so-called "worm" update algorithm. Concepts from percolation theory and the theory of self-avoiding random walks are used to derive estimators of physical observables that utilize the nature of the worm algorithm. The fractal structure of random loops and chains as well as their scaling properties encode the critical behavior of the statistical system. The general approach is illustrated for the high-temperature series expansion of the Ising model, or O(1) loop model, on a honeycomb lattice, with its known exact results as valuable benchmarks.

Keywords: loop gas, Monte Carlo simulations, worm update algorithm, percolation, fractal structure, critical properties, duality

1. Introduction

The loop-gas approach to lattice spin systems provides an alternative, geometrical description in terms of fluctuating loops which is based on their high-temperature series expansions [1]. The standard approach involves estimating observables (expressed in terms of spins) by sampling a representative set of spin configurations. New configurations are typically generated by means of importance sampling Monte Carlo techniques with each spin configuration weighted according to the probability that it occurs. In contrast, the geometrical loop-gas approach based on the high-temperature series expansion involves line-like objects. Physical observables are no longer estimated by sampling an ensemble of spin configurations, but by sampling a grand canonical ensemble of (mostly closed) lines, known as a *loop gas*, instead. The weight of a given high-temperature graph is typically determined by its total size, the number of intersections, and the number of loops contained in the tangle.

In relativistic quantum field theories formulated on a space-time lattice, the high-temperature expansion is replaced by the strong-coupling expansion, representing the hopping of particles from one lattice site to the next, which is closely connected to Feynman's space-time approach to quantum theory [2].

About a decade ago, Prokof'ev and Svistunov [3] have introduced a Monte Carlo *worm algorithm* that, although based on local updates, does away with critical slowing down almost completely. Its name derives from the property that loop configurations are generated through the motion of the end points of an *open* chain – the "head" and "tail" of a "worm". A loop is generated in this scheme when the head bites the tail, or through a "back bite" where the head erases a piece (bond) of its own body and thereby leaves behind a detached loop and a (possibly drastically) shortened open chain.

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Besides this outstanding technical advantage, the worm algorithm has the additional advantage that the complete set of standard critical exponents can be determined at a stroke. This set is known to split into two, namely the thermal and the magnetic exponents. While the thermal exponents, such as the specific-heat exponent α, pertain to closed lines, the magnetic exponents, such as the magnetic susceptibility exponent γ, pertain to open chains in the geometrical approach. By the nature of the worm algorithm, which features an open chain to update the loops, data for both sectors are generated on the fly. More specifically, the open chains directly sample the spin-spin, or two-point, correlation function.

In this project, which extends previous work by two of us on the subject [4, 5], we describe estimators of physical observables that naturally arise in a loop gas and that allow determining the standard critical exponents. Our approach amalgamates concepts from percolation theory – the paradigm of a geometrical phase transition – and the theory of self-avoiding random walks. To support our arguments we performed Monte Carlo "worm" simulations for the two-dimensional Ising or O(1) loop model on a honeycomb lattice [6]. This model serves as a prototype with its various exact results providing a yardstick for our numerical results and also for the feasibility of our approach.

2. High-temperature graphs

Let us first briefly recall the high-temperature series expansion of the Ising model on an arbitrary lattice or graph with V_s spins $s_i = \pm 1$ and V_b bonds. By a Taylor expansion one readily derives

$$Z = \sum_{\{s_i\}} e^{\beta \sum_b s_i s_j} = \sum_{\{s_i\}} \sum_{\{n_b\}} \prod_b \frac{\beta^{n_b}}{n_b!} (s_i s_j)^{n_b} = 2^{V_s} \sum_{\{n_b\}'} \prod_b \frac{\beta^{n_b}}{n_b!} \quad , \tag{1}$$

where on each bond b the bond variable $n_b = 0, 1, 2, \ldots$ runs over all non-negative integers. The last equality follows by carrying out the summation over all spins s_i, $i = 1, \ldots, V_s$. Since $s_i = \pm 1$ only those bond configurations contribute (a factor of 2) for which $\sum n_b$ is even at each site, so that *no* open lines can occur which is indicated by $\{n_b\}'$. The resulting loop tangle thus contains lines of variable strength $n_b = 0, 1, 2, \ldots$ and hence has a rather complicated interpretation in terms of a loop gas.

A more convenient representation can be derived by noting that for $s_i = \pm 1$ the Boltzmann factor may be rewritten as $\exp(\beta s_i s_j) = \cosh\beta[1 + \tanh\beta s_i s_j]$. The summation over s_i then leads to

$$Z = 2^{V_s} \cosh^{V_b} \beta \sum_{\{n_b = 0,1\}'} K^{N_b} \quad , \tag{2}$$

where $\{n_b = 0, 1\}'$ indicates that again no open lines are allowed, $K = \tanh\beta$, and $N_b = \sum_{b=1}^{V_b} n_b$ is the total number of "active" bonds ($n_b = 1$).

An additional open chain running from site i_0 to j_0 immersed into the background of loops can be introduced using the same arguments by considering the spin-spin, or two-point, correlation function

$$\langle s_{i_0} s_{j_0} \rangle = \sum_{\{s_i\}} s_{i_0} s_{j_0} e^{\beta \sum_b s_i s_j} / Z \equiv Z(i_0, j_0)/Z \quad . \tag{3}$$

Typical high-temperature graph configurations for a square lattice are depicted in Fig. 1. For the special case $j_0 = i_0$, this ensemble of loops plus an open chain trivially reduces to the pure loop gas.

For general lattice geometries the loop gas contains intersection points ("knots"). At least in two dimensions this can be avoided by choosing a honeycomb lattice with coordination number $z = 3$ which we will consider in the following. The honeycomb lattice is dual to the triangular (hexagonal) lattice [7], mapping high temperatures for the honeycomb onto low temperatures for the triangular lattice and *vice versa* via

$$K = \tanh \beta = e^{-2\tilde{\beta}} \tag{4}$$

and high-temperature loops on the honeycomb onto Peierls boundaries of spin clusters on the triangular lattice. The critical point for these lattices is known to be at $K_c = 1/\sqrt{3}$ or via duality $\tilde{\beta}_c = \frac{1}{4} \ln 3$.

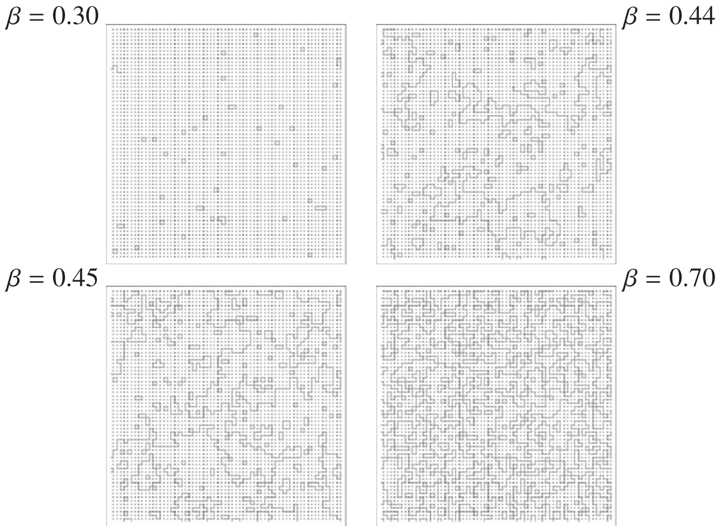

Figure 1: Typical high-temperature graph configurations on a 64×64 square lattice (where $\beta_c = 0.440\,686\ldots$) with periodic boundary conditions.

3. Worm update algorithm

In our simulations of the Ising model on the honeycomb lattice we focused on the $n_b = 0, 1$ loop-gas representation (2). The worm update then involves Metropolis flips of single bonds where the current value n_b of the bond variable is attempted to be replaced with $1 - n_b$. During the Monte Carlo simulation, chain endpoints move and, thus, accumulate information about open chain properties, such as their end-to-end distance. As there is a finite probability for an open chain to close and form a closed loop, or polygon, the algorithm automatically also acquires information about the loops. We adapted the original worm algorithm [3] as follows, see, e.g., Ref. [8] for a related adaptation.

For configurations containing, in addition to polygons, a single chain with end-to-end distance larger than one lattice spacing, the updating scheme proceeds by

1. randomly choosing either endpoint of the chain,
2. randomly choosing any of the links attached to the chosen endpoint,
3. updating the corresponding bond variable n_b with a single-hit Metropolis flip proposal $n_b \to n_b' = 1 - n_b$ with acceptance probability
$$P_{\mathrm{accept}} = \min\left(1, K^{1-2n_b}\right) \tag{5}$$
as can be inferred from the weight K^{N_b} in the partition function (2), assuming that $0 < K < 1$. The exponent $1 - 2n_b = \pm 1$ denotes the difference in the number of bonds contained in the proposed and the existing configurations. It follows that a proposal to *create* a bond is accepted with probability $P_{\mathrm{accept}} = K\,(< 1)$, whereas a proposal to *delete* one is always accepted.

These updates are simple and straightforward as long as the chain remains open. Once, however, the chain has an end-to-end distance of just one lattice spacing, the existing configuration can be turned into a loop-gas configuration by a single bond flip. Such an update then connects the two different sectors of the model, namely the one with an open chain which samples the numerator $Z(i_0, j_0)$ of the correlation function (3), and the loop sector which samples the partition function Z. In their original work [3], Prokof'ev and Svistunov introduced conditional probabilities, parameterized by $0 < p_0 < 1$, for Monte Carlo moves between the two sectors. We in this work put this parameter to unity and thus always attempt to close such a chain by using the update scheme above with the Metropolis acceptance probability (5). If the update is accepted, and the open chain turns into a polygon, we proceed by randomly choosing one link among all links of the lattice as the new location for the worm. The bond variable on that link is then subjected to a Metropolis trial move with the acceptance probability (5).

To check the correctness of this implementation of the worm algorithm, we simulated the critical Ising loop-gas model on a small 5×5 square lattice with periodic boundary conditions, i.e., on a torus and measured the spin-spin correlation function. Comparing our Monte Carlo results with exact results, obtained by complete enumeration, we found perfect agreement within statistical error bars [6].

4. Simulation results

In this section we focus on estimators of physical observables which directly exploit the nature of the worm update algorithm and which can be naturally measured in this scheme. One important quantity is the loop-length distribution ℓ_n of polygons of n steps per unit volume. Close to the critical point K_c it takes asymptotically a form [4] similar to the cluster distribution near the percolation threshold known from percolation theory [9],

$$\ell_n \sim n^{-d/D-1} \mathrm{e}^{-\theta n}, \quad \theta \propto (K - K_c)^{1/\sigma} \quad , \tag{6}$$

where θ is the line tension (in suitable units) which vanishes close to K_c at a rate determined by the exponent σ, d denotes the dimension of space, and D is the fractal dimension of the loops at the critical point. A standard definition of the fractal dimension is through the asymptotic behavior of the average square radius of gyration, $\langle R_g^2 \rangle \sim n^{2/D}$, of loops or chains of n steps or of the square end-to-end distance, $\langle R_e^2 \rangle \sim n^{2/D}$, of open chains. For the two-dimensional Ising model it is known [10] that $D = 11/8$ and $\sigma = 1/\nu D = 8/11$ (Ref. [5]), where $\nu = 1$ is the standard correlation length critical exponent.

By compiling the histogram of loop lengths during long Monte Carlo runs at the critical point on the largest hexagonal lattice considered ($L = 352$) we obtained the results shown in the log-log plot of Fig. 2 (left). Loops at all scales are observed. The bump at the end of the distribution followed by a rapid falloff is typical for such distributions measured on a finite lattice with periodic boundary conditions. The straight line fitting the data shows the theoretically expected behavior (6) with $D = D_{\text{exact}} = 11/8$. The analogous distribution z_n of open chains of n steps with arbitrary end-to-end distance is shown in Fig. 2 (right). It can be shown [6] that the area under this distribution gives the magnetic susceptibility,

$$\sum_n z_n = \chi(K_c) \propto L^{\gamma/\nu} \quad . \tag{7}$$

The inset of Fig. 2 (right) shows a log-log plot of $L^2/\chi \propto L^{2-\gamma/\nu} = L^\eta$ as a function of L and the two-parameter straight-line fit yields $\eta = 0.2498(26)$ in very good agreement with the exact value $\eta = 1/4$.

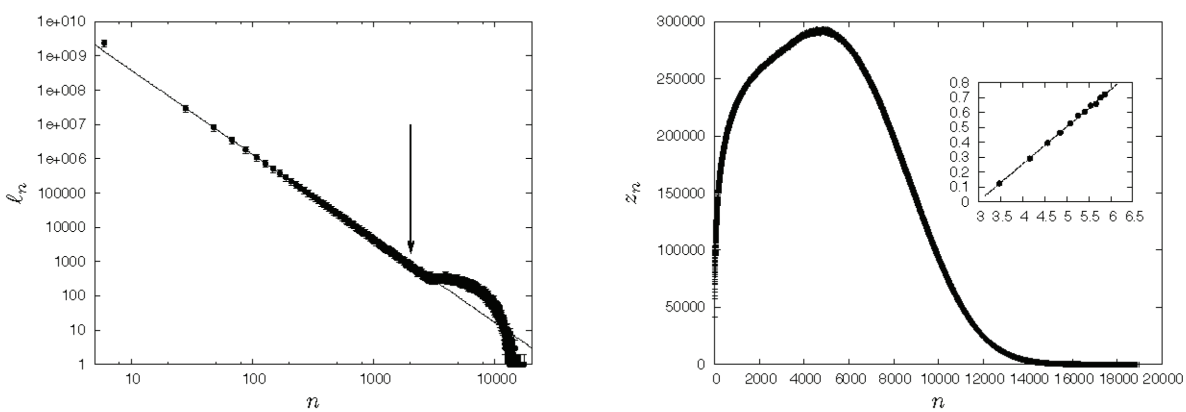

Figure 2: *Left:* Log-log plot of the loop distribution ℓ_n as a function of the loop length n on a honeycomb lattice of size $L = 352$ at the critical point. The arrow indicates the minimal length $n_0 \approx 2000$ where loops start winding around the lattice. The straight line proportional to $n^{-2/D-1}$ with $D = 11/8$ shows the theoretically expected behavior (6). *Right:* Distribution z_n of open chains as a function of chain length n. The log-log plot in the inset shows $L^2/\chi \propto L^\eta$ with $\chi = \sum_n z_n$ versus L and a linear fit yielding $\eta = 0.2498(26) \approx 1/4$.

In order to independently estimate the characteristic fractal dimension D, we also determined for each loop and open chain the square radius of gyration $\langle R_g^2 \rangle \sim n^{2/D}$ as well as for open chains the average square end-to-end distance $\langle R_e^2 \rangle \sim n^{2/D}$, see Fig. 3 (left). By performing fits of the asymptotic scaling ansatz including the leading correction-to-scaling term, $\langle R_{g,e}^2 \rangle = an^{2/D}(1 + b/n)$, to the open chain data, we obtained for the $L = 352$ lattice $D = 1.3789(55)$ from $\langle R_e^2 \rangle$ and $D = 1.3755(31)$ from $\langle R_g^2 \rangle$, in very good agreement with the theoretical prediction $D_{\text{exact}} = 11/8 = 1.375$. Interestingly, by paying attention to the topology of the lattice induced by the periodic boundary conditions, that is by monitoring the average length $\langle n_w \rangle \propto L^D$ of loops winding the honeycomb lattice of linear extent L and performing a linear two-parameter fit in the log-log representation of Fig. 3 (right), the accuracy in estimating the fractal dimension D can be significantly improved by one order of magnitude: $D = 1.37504(32)$. A more detailed discussion of winding properties is given in Ref. [6].

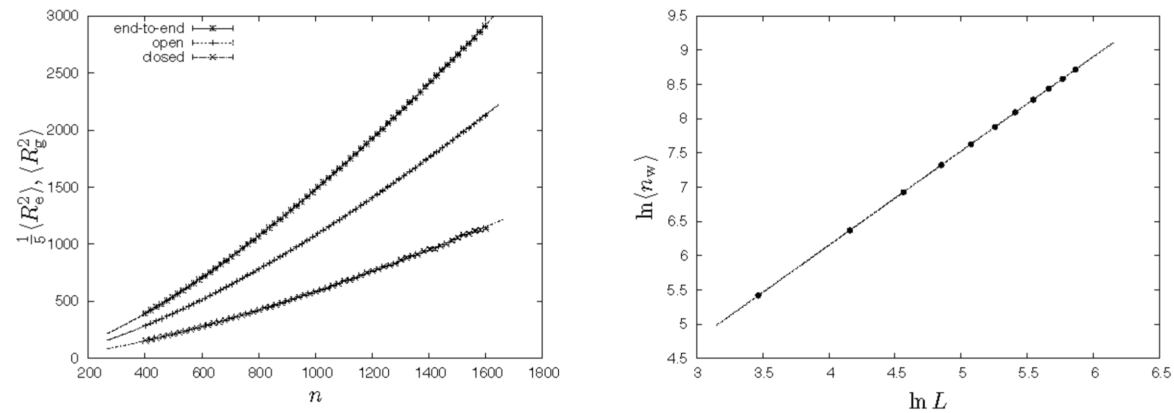

Figure 3: *Left:* Average square end-to-end distance $\langle R_e^2 \rangle$ of open chains, as well as the average square radius of gyration $\langle R_g^2 \rangle$ of open and closed chains as a function of their length n at the critical point on a honeycomb lattice of linear size $L = 352$. *Right:* Log-log plot of the average length $\langle n_w \rangle \propto L^D$ of loops winding the honeycomb lattice of linear extent L. The straight line shows a linear fit with $D = 1.37504(32) \approx 1.000029 D_{\text{exact}}$.

5. Conclusions

The worm algorithm is a perfect tool for studying the loop-gas approach to fluctuating spins or fields on a lattice. Quantities that are directly accessible in this formulation can be estimated with very high precision. On the other hand, one should keep in mind that coming from the high-temperature representation, some standard quantities such as the magnetization are difficult (or even impossible) to obtain.

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