Critical Line of the O(N) Loop Model on the Square Lattice

Antônio Márcio P. Silva, Adriaan M. J. Schakel, and Giovani L. Vasconcelos

Laboratório de Física Teórica e Computacional, Departamento de Física,
Universidade Federal de Pernambuco, 50670-901, Recife-PE, Brazil

Abstract

An efficient algorithm is presented to simulate the $O(N)$ loop model on the square lattice for arbitrary values of $N > 0$. The scheme combines the worm algorithm with a new data structure to resolve both the problem of loop crossings and the necessity of counting the number of loops at each Monte Carlo update. With the use of this scheme, the line of critical points (and other properties) of the $O(N)$ model on the square lattice for $0 < N \leq 2$ have been determined.

PACS numbers: 05.10.Ln, 64.60.De, 64.60.Cn, 64.60.F-
The self-avoiding walk together with the Ising and XY models formulated on the square lattice are among the most studied models in statistical physics, with many applications in diverse fields. These spin systems belong to the class of $N$-vector models with $N = 0, 1,$ and $2$, respectively. Their analytic continuation to arbitrary $N$, with $-2 \leq N \leq 2$, was, until recently, almost exclusively studied on the honeycomb lattice instead. These models undergo a continuous phase transition between a disordered high-temperature phase and an ordered low-temperature phase. Studies for non-integer $N$ are facilitated by the high-temperature (HT) representation of the spin system where contributions to the partition function are represented by even graphs along the links of the underlying lattice. On a honeycomb lattice, even graphs cannot cross and thus automatically form mutually and self-avoiding polygons. This fact greatly simplifies the analysis and explains the “exorbitant amount of work” done on the honeycomb lattice [1]. In most of these studies it was tacitly assumed that the long-distance behavior found on the honeycomb lattice is universal and insensitive to the lattice structure. This turned out to be true for the long-distance behavior controlled by the $O(N)$ critical point with $-2 \leq N \leq 2$ found in Ref. [2]. But in the low-temperature phase, which also displays long-range spin-spin correlations with powerlike decay, the situation changes dramatically. By working on a square lattice, Jacobsen et. al. [3] argued that allowing for crossings gives rise to a completely different long-distance behavior from that found on a honeycomb lattice [2]. Although several numerical studies of $O(N)$ models for non-integer $N$ on the square lattice recently appeared in the literature, see, for example, [4, 5], a proper account of crossings has not yet been accomplished.

This task is hindered by two main obstacles. The first one is that each even HT graph must be decomposed into an unambiguous set of polygons or loops, with each loop carrying a degeneracy factor $N$ that arises because any of the $N$ spin components or colors can be routed through the loop. This problem was formally solved by Chayes et al. [1] by resolving each crossing of a HT graph into three routings, with unique instructions as how to connect the four legs, see Fig. 1. A given even graph configuration then breaks into a set of interlocking colorless loops that can be assigned unambiguous degeneracy factors. To the best of our knowledge, this scheme has never been employed in numerical studies.

The second obstacle is that at each update step the number of loops present on the entire lattice is required. Since this quantity is nonlocal, the use of a tracing algorithm would slow down simulations in the critical region as well as in the low-temperature phase to the extent of rendering them useless on larger lattices.
In this paper, we implement the scheme due to Chayes et al. [1] by adopting the worm algorithm [6] and overcome the tracking problem by coding loops into a new data structure, called a satellite list [7]. As an application, we determine the line of critical points of the O(N) model on the square lattice for arbitrary $0 < N < 2$.

Our starting point is the partition function [8]

$$Z_\square = \text{Tr} \prod_{(i,j)} (1 + K S_i \cdot S_j),$$

obtained by truncating the series expansion of the conventional Boltzmann factor, $\exp(K S_i \cdot S_j)$, at the first order in the coupling constant $K$. In Eq. (1), the $N$-component spin variable $S_i$ at each site $i$ is normalized, $|S_i| = 1$, the trace Tr stands for the (normalized) sum or integral over all possible spin configurations, and the product is restricted to nearest neighbor pairs. Notice that $K$ in Eq. (1) must satisfy the condition $|K| \leq 1$, if the weight of a spin configuration is to be non-negative. In the following, we take $K > 0$.

In the HT representation of the model (1), a factor $K S_i \cdot S_j$ is represented by a bond drawn between the nearest neighbor sites $i$ and $j$ which is given a weight $K$. The advantage of the truncated model (1) compared to the conventional one is that links cannot be multiply occupied. Unlike crossings, this simplification is believed to be irrelevant both at the critical point and in the low-temperature phase. (For recent numerical support of this assumption, see [5].) Each site carries a weight $Q(k_i)$ that depends on the number of bonds $k_i$ attached to that site. Specifically, $Q(0) = 1$, $Q(2) = 1/N$, and $Q(4) = 1/N(N+2)$ for sites connecting 0, 2, or 4 bonds [1]. The partition function for $N > 0$ can then be written as a sum over configurations, $C$, consisting of arbitrary many colorless loops [1]:

$$Z_\square = \sum_C K^b \left( \frac{1}{N} \right)^{m_2} \left( \frac{1}{N(N+2)} \right)^{m_4} N^\ell.$$  

Here, $b$ denotes the total number of bonds, $K$ plays the role of a bond fugacity, $m_2$ is the number of lattice sites connecting two bonds, $m_4$ is the number of intersections (each with a unique routing
instruction), and ℓ is the number of loops in a given loop configuration. Finally, the degeneracy factor \( N \) appears as a loop fugacity in the HT representation. Whereas in the spin representation \( K \) must satisfy the bound \( K \leq 1 \), no such restriction is required in the HT representation and \( K \) can be continued to the region \( K > 1 \).

We simulate the model on a square lattice (with periodic boundary conditions) for arbitrary \( N > 0 \) by using the worm algorithm, a very efficient Monte Carlo scheme that is not hampered by critical slowing down. This scheme directly generates HT graphs through the motion of an endpoint of an open chain, or worm. When the head of the worm encounters a site that already connects two bonds, our algorithm randomly chooses one of the three possible routings, so that the resulting graphs are always unambiguous. At each time step, the worm attempts to either set or erase a bond, depending on whether the link under consideration was previously empty or not. As time proceeds, the worm constantly changes its shape and length until its head eventually returns to its tail to form a loop. After this, a new worm is attempted to be created by proposing to move both endpoints together to a randomly chosen site and the process continues for as long as necessary to accumulate sufficient statistics. Notice that although the head shifts smoothly through the lattice, taking steps of one lattice spacing at a time, the worm can change its shape and length abruptly, either by opening up and annexing an existing loop or by intersecting itself and thereby shedding a loop. The latter process is known in polymer physics as backbiting. The Metropolis update probabilities for setting or erasing a bond readily follow from detailed balance and will not be discussed here for want of space, save for noting that the existence of multiple routings at intersections complicates matters, for they can lead to different degeneracy factors.

Whereas only loop configurations contribute to the partition function \( Z \), configurations that include a worm with endpoints \( i_1 \) and \( i_2 \) contribute to the unnormalized two-point spin-spin correlation function \( Z_{i_1 i_2} \). This function is related to the normalized correlation function through \( \langle S_{i_1} \cdot S_{i_2} \rangle = Z_{i_1 i_2} / Z \). Because of the dot product appearing here, a worm, like a loop, carries a degeneracy factor \( N \). For the truncated model, each lattice site on a square lattice can connect only 0, 2, or 4 bonds, with the exception of the sites housing an endpoint of the worm which connect 1 or 3 bonds. In that case, the site \( i \) hosting an additional endpoint is assigned the weight \( Q(k_i + 1) \) for \( k_i = 1, 3 \), where the extra term “1” in the argument is to indicate explicitly the presence of an endpoint at that site. Since \( S_i \cdot S_i = 1 \), a site \( i \) housing both endpoints at the same time acts as if they are absent, and \( Z_{ii} = Z \). Note that our convention here differs from that used in Ref. [6]. The critical exponents can be determined directly from the HT graphs through the use of observables.
FIG. 2. A satellite list: two singly-linked lists (the two sidepieces) running through the satellites (dots) of each node (crosspiece).

known from percolation theory and the theory of self-avoiding random walks [9].

We have overcome the problem of keeping track of the number of loops at each Monte Carlo update by coding the worm (and the loops it generates) into a satellite list [7]. Such a list, which is a variation on the more familiar doubly-linked list, is a ladderlike data structure, see Fig. 2. A crosspiece in the ladder represents a node where the relevant information (in our case, an occupied link) is stored. Each node contains two satellites, represented by the endpoints of the corresponding crosspiece, and the sidepieces represent singly-linked lists connecting the respective satellites on the two sides of the ladder. In this way, nodes are linked indirectly through their satellites in such a way that the next node in the list depends on the current direction. The possibility to traverse the list in one direction and, by sidestepping to the complement satellite, also in the reverse direction is crucial for our purposes. As with all linked lists, memory allocation is dynamic so that efficient memory usage is guaranteed.

A backbite is computationally the most costly update. Because the worm breaks into two parts, a new satellite list must be created to accommodate either the detached loop or the remaining, shortened worm. While the cost of cutting a segment out of the old satellite list and pasting it into the new list is independent of the length of that segment, the bonds belonging to the new list must be relabeled to indicate that they are now part of a new list. Since the computational cost of relabeling increases linearly with the number of bonds, it is expedient to move the shortest segment into the new list. To identify this part, we simultaneously iterate through the list, starting at each of the two legs in front of the head of the worm until either the head or the tail is reached. After inserting the shortest segment into the new list and relabeling the bonds involved, we reconnect the loose ends at fixed cost, using the unique properties of a satellite list.

Using the algorithm outlined above, we determine the line of critical points of the $O(N)$ loop model on the square lattice for $0 < N < 2$. To locate the critical point for a given $N$, we measure the probability $\Pi_L(K)$ that one or more loops wrap the lattice as a function of the bond fugacity $K$ on systems of different linear size $L$. This percolation observable, shown in the top row of Fig. 3.
FIG. 3. Top: Probability $\Pi_L$ that one or more loops wrap the lattice as a function of $K'$ for various lattices of linear size $L$ and for $N = 0.01, 1,$ and $1.8$ (from left to right). Bottom: Same data as above, but now plotted as a function of $(K' - K'_c)/L^{1/\nu}$ with the estimated values for $K'_c$ and the exactly known values for $\nu$.

For $N = 0.01, 1, 1.8$, has no scaling dimension so that, when plotted as a function of $K$ or of the rescaled bond fugacity $K' \equiv K/N$, the curves obtained for different $L$ should cross at exactly one point. Being $L$-independent, this crossing point marks the value of $K$ for which wrapping loops first appear on the infinite lattice. This percolation threshold of HT loops coincides with the onset of long-range spin-spin correlations $K_c$. Figure 3 shows that the crossing point can be accurately identified for the Ising model $(N = 1)$, but this task becomes increasingly more difficult as $N$ approaches either 0 or 2, where the crossing points move towards the plateaus at the beginning and at the end of the curves, respectively.

To determine $K_c$ more precisely, we use a second property of $\Pi_L$, namely, that it is a function only of the ratio of the two relevant length scales in the problem: the linear lattice size $L$ and the correlation length $\xi$. The latter diverges as $\xi \sim |K - K_c|^{-\nu}$, for $K \to K_c$, where $\nu$ is the correlation length exponent. When replotted as a function of $(K - K_c)L^{1/\nu}$, the data should consequently collapse onto a single curve. Since $\nu$ is exactly known for all $-2 \leq N \leq 2$, we estimate the location of the threshold by keeping $\nu$ fixed and varying $K_c$ until the best data collapse is achieved. As an illustration, we plot in the bottom row of Fig. 3 the best collapse achieved for the data shown in the top row of the figure. The quality of collapse is excellent for all values of $N$ we investigated in the range $0 < N \lesssim 1.8$. Table I summarizes our estimates obtained
in this way. The error bars represent the range in which the quality of collapse, assessed by visual inspection, remains more or less the same. This simple method turns out to be very sensitive and yields surprisingly precise results [10]. For \( N \gtrsim 1.8 \), the quality diminishes, with the limiting case, \( N \to 2 \), where \( 1/\nu \to 0 \), showing no collapse at all.

To investigate this issue, we consider in detail the limiting case \( N = 2 \), corresponding to the XY model. Besides logarithmic corrections to scaling, the XY critical point is special also because the correlation length diverges exponentially instead of powerlike as happens for \( N < 2 \) [11]. These two complicating factors make it notoriously difficult to determine \( K_c \) for \( N = 2 \) and usually require Monte Carlo simulations on lattices of sizes much larger than those used for \( N < 2 \) to achieve comparable precisions. One way to circumvent this problem [12] is by analyzing the size-dependence of the helicity modulus \( \Upsilon \), which exhibits a universal jump at the critical point that is unique to this the BKT phase transition [13]. In the HT representation, the helicity modulus is determined by the average squared winding number of loop configurations, \( \langle w^2 \rangle \), where \( w \) is the number of times the loops wrap the lattice (in any of the two directions) for a given loop configuration [14]. As shown in Fig. 4, this observable has the expected behavior, namely, it is finite in the low-temperature phase and rapidly falls to zero when \( 1/K \) increases.

The quantity \( \langle w^2 \rangle \) features in the Kosterlitz renormalization group equations [11] through the combination

\[
x \equiv 2 - \frac{\pi}{2} \langle w^2 \rangle.
\]  

For the infinite system, one has \( \lim_{K \to K_c^+} \langle w^2 \rangle = 4/\pi \), so that \( x \) vanishes at the critical point in the thermodynamic limit. On a finite lattice, \( x \) remains finite at the critical point and its size

| \( N \) | \( K'_c \)   | \( N \) | \( K'_c \)   | \( N \) | \( K'_c \)   |
|-----|------|-----|------|-----|------|
| 0.01 | 0.37930(5) | 0.7  | 0.4014(2) | 1.4  | 0.4374(2) |
| 0.1  | 0.38178(3) | 0.8  | 0.4053(1) | 1.5  | 0.4450(2) |
| 0.2  | 0.38464(4) | 0.9  | 0.4096(2) | 1.6  | 0.4539(2) |
| 0.3  | 0.3877(4)  | 1.0  | 0.4141(1) | 1.7  | 0.4647(2) |
| 0.4  | 0.3908(3)  | 1.1  | 0.4192(1) | 1.8  | 0.4785(2) |
| 0.5  | 0.3941(1)  | 1.2  | 0.4246(2) | 2.0  | 0.520(4)  |
| 0.6  | 0.3977(2)  | 1.3  | 0.4307(1) |      |      |

**TABLE I.** Estimates of \( K'_c \) for various values of \( N \).
FIG. 4. The (scaled) helicity modulus $\langle w^2 \rangle$ as a function of $1/K$ for various $L$. The horizontal line denotes the value $\langle w^2 \rangle = 4/\pi$.

FIG. 5. The negative of the inverse of the renormalization group variable $x$, defined in Eq. (3), as a function of lattice size $L$ for $K = 1.030, 1.040, 1.050, 1.060$ (from top to bottom). The curve in the inset is the best fit to the data at $K = 1.040$.

dependence is known [12] to be given by

$$\lim_{K \to K_c^+} x = -\frac{1}{\ln(L/L_0)}, \quad (4)$$

where $L_0$ is a characteristic length of the order of the lattice spacing. Relation (4) can be used to estimate the critical point of the infinite lattice as follows [12]. First one measures $x$ on lattices of different sizes for different values of $K$ and then fits the size-dependence (4) to the data for each $K$, using $L_0$ as the only free parameter, see Fig. 5. The value of $K$ that produces the best fit is taken as estimate of the critical point of the infinite lattice. We in this way arrive at the estimate $K_c = 1.040(7)$ and $L_0 = 0.88(5)$, for which $\chi^2/\text{DOF} = 0.25$, see inset of Fig. 5.

In conclusion, taking full account of crossing, we have simulated the $O(N)$ loop model on the
square lattice with the worm algorithm. By representing the worm and the loops it generates by satellite lists, we have succeeded to monitor the number of loops present on the lattice, a non-local quantity, throughout the simulations in a very efficient way. This enabled us to determine the critical point (and other properties) of the $O(N)$ model on the square lattice for arbitrary $0 < N \leq 2$. We presently investigate the behavior of the model in the low-temperature phase for $0 < N \leq 2$ and that for $N > 2$, where no transition associated with the appearance of loops wrapping the infinite lattice is expected. The algorithm presented here is by no means restricted to the square lattice, and can be used to simulate the $O(N)$ model for arbitrary $N > 0$ on any (higher-dimensional) lattice.

The work of A.M.J.S. was financially supported by CAPES, Brazil through a visiting professor scholarship. That author would like to thank Wolfhard Janke for helpful discussions. A.M.P.S and G.L.V. acknowledge financial support from CNPq and FACEPE (Brazilian agencies).

[1] L. Chayes, L. P. Pryadko, and K. Shtengel, Nucl. Phys. B 570, 590 (2000).
[2] B. Nienhuis, Phys. Rev. Lett. 49, 1062 (1982).
[3] J. L. Jacobsen, N. Read, and H Saleur, Phys. Rev. Lett. 90, 090601 (2003).
[4] Y. Deng, T. M. Garoni, W. Guo, H. W. J. Blöte, and A. D. Sokal, Phys. Rev. Lett. 98, 120601 (2007).
[5] W. Guo and H. W. J. Blöte, Phys. Rev. E 83, 021115 (2011).
[6] N. Prokof’ev and B. Svistunov, Phys. Rev. Lett. 87, 160601 (2001).
[7] C. Osterman and C. Rego, The Satellite List and New Data Structures for Symmetric Traveling Salesman Problems; preprint HCES-06-03, University of Mississippi; C. Osterman, C. Rego, and D. Gamboa in: Adaptive and Natural Computing Algorithms, edited by B. Ribeiro et al. (Springer, Vienna, 2005), p. 542.
[8] E. Domany, D. Mukamel, B. Nienhuis, and A. Schwimmer, Nucl. Phys. B 190, 279 (1981).
[9] W. Janke, T. Neuhaus, and A. M. J. Schakel, Nucl. Phys. B [FS] 829, 573 (2010).
[10] F. Winter, W. Janke, and A. M. J. Schakel, Phys. Rev. E 77, 061108 (2008).
[11] J. M. Kosterlitz, J. Phys. C 7, 1046 (1974).
[12] H. Weber and P. Minnhagen, Phys. Rev. B 37, 5986 (1988).
[13] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. 39, 1201 (1977).
[14] D. M. Ceperley and E. L. Pollock, Phys. Rev. Lett. 56, 351 (1986).