Monte Carlo study of the universal area distribution of clusters in the honeycomb O(n) loop model*

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We investigate the area distribution of clusters (loops) in the honeycomb O(n) loop model by means of the worm algorithm with $n = 0.5, 1, 1.5$, and 2. At the critical point, the number of clusters, whose enclosed area is greater than A, is proportional to A^{-1} with a proportionality constant C. We confirm numerically that C is universal, and its value agrees well with the predictions based on the Coulomb gas method.

Keywords: worm algorithm, O(n) loop model, universality, Coulomb gas method

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1. Introduction

Among various statistic models, the q-state Potts model,[1–4] and the O(n) spin model[5,6] have played important roles in the theory of critical phenomena. Parameter q or n is initially a positive integer, but the Fortuin–Kasteleyn (FK)[7,8] representation and the loop representation respectively show how the models can be extended to arbitrary real or even complex values of q and n. In particular, for $q, n > 0$, the extended models have probabilistic interpretations as models of random geometric objects, i.e., clusters[9] and loops[10,11], respectively. In the present work, we focus on the latter model.

The O(n) model consists of n-component spins $\boldsymbol{s}_i = (s_i^1, s_i^2, \ldots, s_i^n)$ on a lattice, with isotropic, i.e., O(n) invariant, couplings. The Hamiltonian of the O(n) spin model is usually written as

$$\mathcal{H}/(k_{\rm B}T) = -J/(k_{\rm B}T)\sum_{\langle ij\rangle}\boldsymbol{s}_i\cdot\boldsymbol{s}_j, \tag{1}$$

where indices i and j represent lattice sites, J is the coupling constant, $k_{\rm B}$ is the Boltzmann constant, T is the temperature, and $\sum_{\langle ij\rangle}$ means the sum is taken over all nearest-neighbor pairs. For the special cases of $n = 0, 1, 2, 3$, this model corresponds to the self-avoiding walk, the Ising, the XY, and the Heisenberg models, respectively. In the case of $n \to \infty$, the model corresponds to the spherical model,[12] which is one of the few models of ferromagnetism that can be solved exactly in the presence of an external field. According to Eq. (1), the partition function of the model reads

$$Z_{\rm spin} = \int \prod_{\langle i,j\rangle} \exp\left(\frac{J}{k_{\rm B}T}\boldsymbol{s}_i\cdot\boldsymbol{s}_j\right)\prod_k {\rm d}\boldsymbol{s}_k. \tag{2}$$

In the high-temperature limit, the bond weight $w(\boldsymbol{s}_i\cdot\boldsymbol{s}_j)$ reduces in first order to $(1 + x\boldsymbol{s}_i\cdot\boldsymbol{s}_j)$,[13] with $x = J/(k_{\rm B}T)$. Thus the partition function takes the form

$$Z_{\rm spin} = \int \prod_{\langle i,j\rangle}(1 + x\boldsymbol{s}_i\cdot\boldsymbol{s}_j)\prod_k {\rm d}\boldsymbol{s}_k. \tag{3}$$

The bond weight still satisfies the O(n) symmetry implied by Eq. (1). According to the assumption of universality, the universality class of a phase transition is determined by only very few parameters, including the symmetry of the spin–spin interactions. It is thus reasonable to expect[10] that the reduced Hamiltonian that corresponds to Eq. (3), namely, $\mathcal{H} = -\sum_{\langle i,j\rangle}\ln(1 + x\boldsymbol{s}_i\cdot\boldsymbol{s}_j)$ with $x = J/(k_{\rm B}T)$ not necessarily small, still belongs to the O(n) universality class in two dimensions.

The O(n) model on lattices with coordination number of at most three, such as the honeycomb lattice, can be mapped into the O(n) loop model on the

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same lattice, with the partition sum[13]

$$Z_{\text{loop}} = \sum_G x^{N_\text{b}} n^{N_\text{l}} = n^{-N} \sum_G (nx)^{N_\text{b}} n^{N_\text{k}}, \qquad (4)$$

where the sum is over all possible configurations of graph, and each graph consists of non-intersecting loops, N_b is the number of total bonds, N_l is the number of loops, N_k is the number of clusters, N the number of total sites, x is the weight of a bond visited by a loop, and n is the loop weight. Using the Euler relation $N_\text{b} + N_\text{k} = N + N_\text{l}$, we can obtain the latter equation. Now, the loop weight n is no longer restricted to be an integer, thus can be continuous. The research on the O(n) model has a considerable history, in which a prominent place is occupied by the exact results[10,11] for the O(n) loop model and the fully packed O(n) loop model on the honeycomb lattice.[14] Those results include the critical points for $-2 \leq n \leq 2$, the temperature, and the magnetic exponents. Recently, two of us conducted a relatively comprehensive worm Monte Carlo study on the honeycomb O(n) loop model,[15] found some new exponents, and confirmed the existence of the 3-state Potts transition in the range of $n > 2$. Also in that work, we explored some exponents of the geometric property of the honeycomb O(n) loop model. In Ref. [16], Ding *et al.* adopted another local Monte Carlo algorithm other than the worm algorithm to explore the geometric property of the two-dimensional O(n) loop model. However, the area distribution of loops still needs further research.

Nearly a decade ago, Cardy and Ziff[17] gave predictions for the cluster area distributions in percolation, Ising, and Potts models. Here we illustrate this in the language of the honeycomb O(n) loop model. Let $N(A)$ denote the number of loops (per unit area) whose area is greater than or equal to A, we can write

$$N(A) \sim \frac{C}{A}, \ (a^2 \ll A \ll L^2), \qquad (5)$$

where a and L are the lattice spacing and the lattice size, respectively, and C depends on the choice of the area measure. The measure can be the area of the smallest disk covering the loop, the area enclosed by the loop, and so on. Note that besides the enclosed area A shown in Fig. 1, we can use any other macroscopic measure of the length scale of the loop. For each measure, there is a corresponding value of C, and this C should be universal. In their work, they calculated the exact value of C based on the Coulomb gas theory as

$$C = \frac{(g-1)}{4\pi g} \cot(\pi g), \qquad (6)$$

where g is the Coulomb gas coupling. They also did some numerical simulations to support this result by using the Potts model with $q = 1$ (percolation), 2 (Ising), 3, and 4. For the convenience of data analysis, they considered quantity $N(A, 2A)$, which is the number of loops whose enclosed area is greater than or equal to A and less than $2A$. According to Eq. (5), this quantity behaves as

$$N(A, 2A) = N(A) - N(2A) \sim \frac{C}{2A}, \qquad (7)$$

so $2AN(A, 2A) \sim C$. They fitted the data of the percolation and the Ising models according to the ansatz $2AN(A, 2A) = C + bA^{-0.875}$, and found that the results agree with the theoretical predictions for the Potts model. However, for the O(n) loop model, it is still unknown. This work aims to check whether the predictions hold in the honeycomb O(n) loop model by using the worm algorithm proposed in Ref. [15].

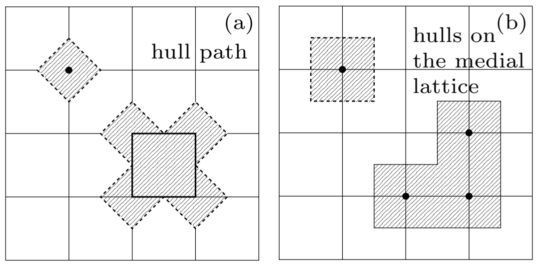


Fig. 1. Two typical measures of enclosed area adopted on square lattice.[17] Panel (a) uses the hulls of the clusters, and panel (b) presents a more natural measure for site percolation. If we set the lattice spacing as 1, the smallest enclosed areas for panels (a) and (b) are 1/2 and 1, respectively.

2. Worm algorithm

The worm algorithm for the high-temperature expansion graphs of the Ising model was first formulated by Prokof'ev and Svistunov.[18] The essence of the worm algorithm is to enlarge the configuration space by introducing two special points, u and v, and moving these two points through a biased random walk. The research of the dynamical behavior of the worm algorithm[19] shows that the worm algorithm for the Ising model hardly suffers from critical slowing down. In Ref. [15], we generalized this algorithm to non-integer n by introducing the connectivity checking procedure and coloring technics on the honeycomb lattice. Here we only apply the connectivity checking version algorithm.

For the loop model, let u and v be the two special vertices that when $u \neq v$, namely u and v are two different vertices, the degrees (numbers of incident bonds) of u and v are both odd. When they are on the same vertex $u = v$, the degree of either vertex is even (zero included). Now we adopt a notation (A, u, v) to denote the configuration of a worm state with A being the loop configuration and u and v being the two special vertices. Note that u and v can be on any vertex of the hydrogen peroxide lattice. The statistical weight for state (A, u, v) is given by Eq. (4). With the loop fugacity n existing in the partition sum, the proposed update includes 4 types as shown in Table 1.

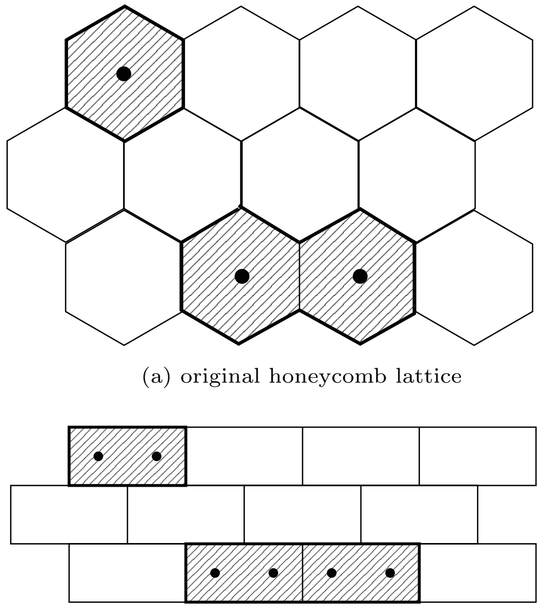
Table 1. Weight and probability for each type of update. Note that the probability is calculated according to the heat-bath prescription.

Type	ΔN_{b}	ΔN_{k}	Weight	Probability p
1	$+1$	0	nx	$nx/(1+nx)$
2	$+1$	-1	x	$x/(1+x)$
3	-1	0	$(nx)^{-1}$	$1/(1+nx)$
4	-1	$+1$	x^{-1}	$1/(1+x)$

The worm algorithm carries out a biased random walk for u and v according to the associated statistical weight, which can be formulated as follows. (i) If $u = v$, move $u = v$ to a randomly chosen vertex. (ii) Randomly chose u or v, say u, and randomly pick up one of the three neighboring edges, denote it as uu'. (iii) Propose to move u to u' and flip the edge state between u and u' as vacant$\leftrightarrow$occupied, i.e., if uu' is currently occupied, delete it, otherwise it is currently unoccupied, add it. (iv) Determine ΔN_{b} and ΔN_{k} and accept the update with the appropriate probability listed in Table 1. As we can see, the detailed balance is automatically satisfied because of the heat-bath prescription. Before discussing the induced subgraph algorithm, we give some remarks regarding the practical implementation of connectivity queries that determine ΔN_{k}. We illustrate this in the language of case $n > 1$ when we propose to occupy a bond which is previously vacant. Considering the case $n > 1$, $p = nx/(1+nx) > x/(1+x) = q$, then we draw a random number $r \in [0, 1]$. If $r < q$, occupy this bond, if $r > p$, do nothing. When $q < r < p$, we need to perform connectivity queries to determine ΔN_{k}. This trick really improves the efficiency of this algorithm. An analogous trick can be employed when $n < 1$ to delete a bond which is previously occupied.

3. Simulation and result

We simulate the O(n) loop model on an $L \times L$ honeycomb lattice with the periodic boundary conditions with $n = 0.5, 1, 1.5$, and 2 right at the critical point $x_{\mathrm{c}} = (\sqrt{2 + \sqrt{2-n}})^{-1}$.[10,11] For each n, we generate 5×10^6 independent samples on the lattice with $L = 900$. For the loop model, the loops enclose certain area by themselves, we decide to sample the number of loops whose enclosed area is greater than A. However, some modifications are made in the real implementation for the sake of convenience, see Fig. 2.



(a) original honeycomb lattice

(b) brick-lattice form of honeycomb lattice

Fig. 2. Panel (a) shows a typical loop configuration and the shaded enclosed area by loops on the honeycomb lattice. Panel (b) transforms a hexagon into two squares, thus the configuration corresponds to that in panel (a). In this loop configuration, we have $N(2) = 2$ and $N(6) = 1$.

With this area measure, we sample quantity $N(A, 2A)$ with $A = 2^i$, where $i = 2, 3, \ldots, 12$. However, because we use the periodic boundary conditions, there is a certain possibility that some loops wrap around the torus. The enclosed areas for such loops are undefined, we discard them because we are interested in the loops whose sizes are much smaller than the system size. For $n = 1$, we show the measured value of $2AN(A, 2A)$ in Fig. 3. As we can see from the figure, there is a disruption between $A = 512$ and $A = 1024$. We attribute this increase to the interference of loops with themselves due to the periodic boundary conditions, and thus ignore such data. Fitting the 5 data points from $A = 8$ to 128 as a function of $A^{-\theta}$, we find a good linear fit with $\theta = -0.875$, as shown in that figure. So we have

$$2AN(A,2A) = 0.01148(2) + 0.0117(3)A^{-0.875}. \quad (8)$$

The result $C = 0.01148(2)$ agrees with the prediction $C = 0.01149$. Likewise, according to ansatz $2AN(A,2A) = C + bA^{-0.875}$, we obtain that C for $n = 0.5$ and 1.5 are 0.00608(2) and 0.01686(3), respectively. Both results agree with the predictions (0.00607 and 0.01688).

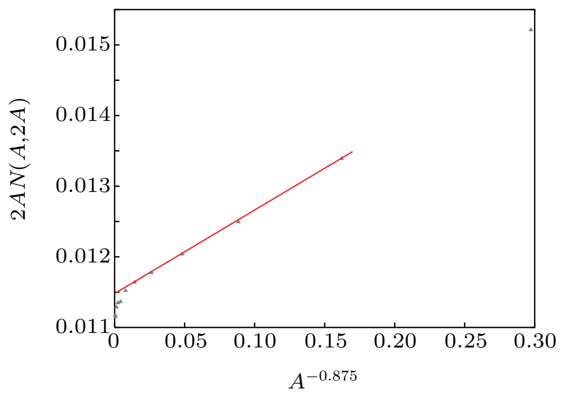


Fig. 3. (colour online) Plot of $2AN(A,2A)$ versus $A^{-0.875}$ for O(1) loop model on a honeycomb lattice.

It is a little complicated for the case of $n = 2$. For the critical Potts model with $q = 4$, which corresponds to the O(n) model in the dense phase, the model is expected to be logarithmic in character. In Ref. [17], the authors calculated the large finite-size corrections analytically

$$N(A) \sim \frac{C}{A}\left(1 - \frac{2a}{(\ln A)^2} + \mathrm{O}((\ln A)^{-3})\right), \quad (9)$$

which implies

$$2AN(A,2A) = C + \mathrm{O}((\ln A)^{-2}).$$

However, for the O(2) model right at the critical line, this logarithmic correction is absent. We try to fit the data and fail to obtain a good fitting result according to the simple ansatz. So we plot $2AN(A,2A)$ as a function of $(\ln A)^{-2}$, see Fig. 4(a), the intercept yields $C = 0.0257$. In Ref. [17], they found a rather good linear behavior with an abcissa of $A^{-0.5}$. From the plot of $2AN(A,2A)$ as a function of $A^{-0.5}$ shown in Fig. 4(b), we can see that the intercept is around 0.0253. In both cases, C is comparable to the predicted value $1/4\pi^2 = 0.0253$. We conjecture that the inaccurate result in this case is due to that with the decreasing critical temperature, the loops are getting dense, so the finite size effect becomes bigger. In this case, a bigger lattice size reduces such an effect.

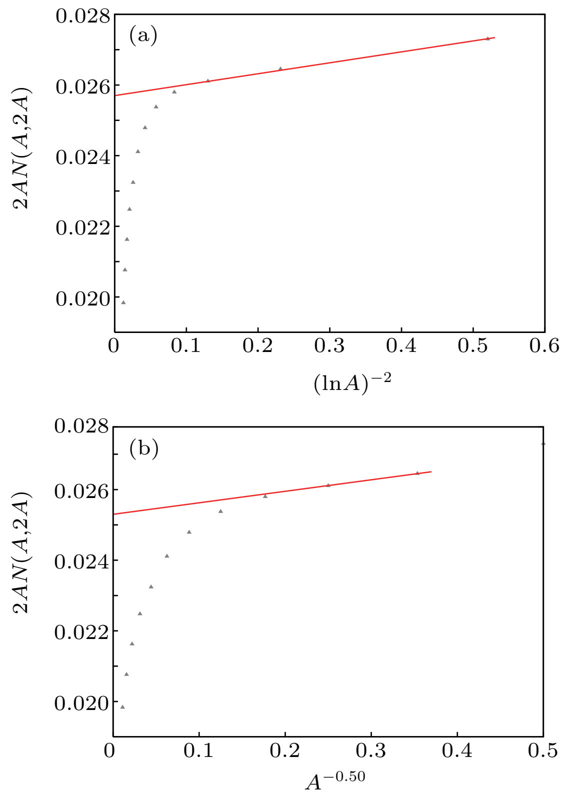


Fig. 4. (colour online) The $2AN(A,2A)$ versus (a) $(\ln A)^{-2}$ and (b) $A^{-0.5}$.

4. Conclusion

In this work, we investigate the area distribution of clusters (loops) of the honeycomb O(n) loop model by means of the worm algorithm. We confirm numerically that in Eq. (5), C is universal and its value agrees well with the predictions based on the Coulomb gas method. However, the intrinsic pattern governing the behavior of the area distribution of clusters (loops) is still unknown, including the finite size effect. This hampers the accurate determination of C and the further exploration to the densely packed O(n) loop model, which corresponds to the critical q-state Potts model. We leave this for future work.

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